Interior point methods and simulated annealing for nonsymmetric conic optimization

Badenbroek, Riley

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Interior Point Methods and Simulated Annealing for Nonsymmetric Conic Optimization

RILEY BADENBROEK

TILBURG UNIVERSITY

Interior Point Methods and Simulated Annealing for Nonsymmetric Conic Optimization

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan Tilburg University op gezag van de rector magnificus, prof. dr. W.B.H.J. van de Donk, in het openbaar te verdedigen ten overstaan van een door het college voor promoties aangewezen commissie in de Aula van de Universiteit op

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PROMOTIECOMMISSIE:

PROMOTOR:	prof. dr. Etienne de Klerk
COPROMOTOR:	dr. Nikolaus Schweizer
OVERIGE LEDEN:	prof. dr. Emile Aarts prof. dr. Nikhil Bansal prof. dr. Mirjam Dür dr. François Glineur prof. dr. Monique Laurent dr. Juan Vera Lizcano

Interior Point Methods and Simulated Annealing for Nonsymmetric Conic Optimization

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Riley Badenbroek
Tilburg, December 2020

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Notation

Sets

$\mathcal{L}(U;V)$	the bounded linear operators from U to V
$\mathcal{L}(U_1,...,U_m;V)$	the bounded multilinear operators from $U_1 \times \cdots \times U_m$ to V
$\mathbb{R}^n$	the n-dimensional vectors of reals
$\mathbb{R}_+$	the nonnegative reals
$\mathbb{N}$	the natural numbers
$\mathbb{Z}$	the integer numbers
$\mathbb{S}^d$	the $d \times d$ real symmetric matrices
$\mathcal{CO}^d$	the copositive matrices $\{A \in \mathbb{S}^d : x^\top A x \geq 0 \ \ \forall x \geq 0\}$
$\mathcal{CP}^d$	the completely positive matrices $\{A \in \mathbb{S}^d : A = BB^\top, B \geq 0\}$
$\mathcal{S}$	a convex body
$\mathcal{K}$	a proper cone
$\mathcal{K}^\circ$	polar cone $\{s \in \mathbb{R}^n : \langle x, s\rangle \leq 0 \ \ \forall x \in \mathcal{K}\}$ of $\mathcal{K}$
$\mathfrak{B}(z,r)$	open ball $\{y : \|y-z\| < r\}$ with radius $r > 0$
$\mathfrak{B}_x(z,r)$	open ball $\{y : \|y-z\|_x < r\}$ with radius $r > 0$
$\mathfrak{B}_x^*(z,r)$	open ball $\{y : \|y-z\|_x^* < r\}$ with radius $r > 0$
$[0,1]^n$	the hypercube $\{x \in \mathbb{R}^n : 0 \leq x_i \leq 1 \ \ \forall i \in \{1,...,n\}\}$

Functions

f	a convex functional
g	gradient of f
H	Hessian of f
T	third derivative of f

f^*	conjugate $f^*(x) \coloneqq \sup_\theta\{\langle\theta, x\rangle - f(\theta) : \theta \in \operatorname{dom} f\}$ of f
g^*	gradient of f^*
H^*	Hessian of f^*
T^*	third derivative of f^*
$\operatorname{dom} f$	effective domain $\{\theta : f(\theta) \in \mathbb{R}\}$ of f
$g_x(y)$	gradient with respect to $\langle\cdot,\cdot\rangle_x$; equals $H(x)^{-1}g(y)$
$H_x(y)$	Hessian with respect to $\langle\cdot,\cdot\rangle_x$; equals $H(x)^{-1}H(y)$
$g_x^*(y)$	conjugate gradient with respect to $\langle\cdot,\cdot\rangle_x^*$; equals $H^*(x)^{-1}g^*(y)$
$H_x^*(y)$	conjugate Hessian with respect to $\langle\cdot,\cdot\rangle_x^*$; equals $H^*(x)^{-1}H^*(y)$

Inner Products and Norms

$\langle\cdot,\cdot\rangle_A$	inner product induced by A
$\|\cdot\|_A$	norm induced by A
$\langle\cdot,\cdot\rangle_x$	inner product induced by $H(x)$
$\langle\cdot,\cdot\rangle_x^*$	inner product induced by $H^*(x)$
$\langle\cdot,\cdot\rangle_x^{-1}$	inner product induced by $H(x)^{-1}$
$\|\cdot\|_x$	norm induced by $H(x)$
$\|\cdot\|_x^*$	norm induced by $H^*(x)$
$\|\cdot\|_x^{-1}$	norm induced by $H(x)^{-1}$
$\|A\|$	operator norm $\max\{\|Ax\| : \|x\| \le 1\}$ of the linear operator A

Linear Algebra

I	identity operator c.q. identity matrix
e	all-ones vector
$A^\top$	adjoint of the operator A with respect to $\langle\cdot,\cdot\rangle$
$A \succeq B$	Löwner ordering $\langle x, Ax\rangle \ge \langle x, Bx\rangle$ for all x
$\lambda_{\min}(A)$	smallest eigenvalue of A
$\lambda_{\max}(A)$	largest eigenvalue of A
v^k	$\begin{bmatrix} v_1^k & \cdots & v_n^k \end{bmatrix}^\top$ for $v \in \mathbb{R}^n$ and $k \in \mathbb{Z}$

$\operatorname{vec}(A)$	vector $\begin{bmatrix} A_{11} & A_{12} & A_{22} & A_{13} & A_{23} & \cdots & A_{dd} \end{bmatrix}^\top$ containing the upper triangular elements of $A \in \mathbb{S}^d$
mat	inverse of vec

Interior Point Theory

ϑ_f	complexity parameter of f
ϑ_{f^*}	complexity parameter of f^*
$z(\eta)$	minimizer of $x \mapsto \eta\langle c, x\rangle + f^*(x)$
$\tilde{x}$	shadow iterate $g^*(s) \in \mathcal{K}$
$\tilde{s}$	shadow iterate $g(x) \in \mathcal{K}^\circ$
μ	complementarity gap $-\langle x, s\rangle/\vartheta_f$
μ'	extended complementarity gap $-(\langle x, s\rangle + \tau\kappa)/(\vartheta_f + 1)$
$\tilde{\mu}$	shadow complementarity gap $-\langle \tilde{x}, \tilde{s}\rangle/\vartheta_f$
$\tilde{\mu}'$	extended shadow complementarity gap $-[\langle \tilde{x}, \tilde{s}\rangle + 1/(\tau\kappa)]/(\vartheta_f + 1)$
$O^*(\cdot)$	asymptotic complexity that disregards polylogarithmic factors

Measure and Probability Theory

$x(\theta)$	mean of the Boltzmann distribution with parameter θ
$\Sigma(\theta)$	covariance of the Boltzmann distribution with parameter θ
$\theta(x)$	parameter of the Boltzmann distribution whose mean is x
$\mathbb{P}\{\cdot\}$	probability measure
$\mathbb{E}[\cdot]$	expectation operator
$\mathbb{E}_\varphi[\phi(X)]$	expectation of $\phi(X)$, where X follows distribution φ
$\mathbb{E}_\theta[\phi(X)]$	expectation of $\phi(X)$, where X follows a Boltzmann distribution with parameter $\theta \in \mathbb{R}^n$
$\mathcal{N}(0, \Sigma)$	normal distribution with mean 0 and covariance matrix Σ
$\mathcal{B}^n$	Borel σ-algebra on $\mathbb{R}^n$
$\mathcal{B}[0,1]$	Borel σ-algebra on $[0,1]$
$\mathbb{1}_U(x)$	indicator function: 1 if $x \in U$, 0 otherwise

1

Introduction

Mathematical optimization is about making a best possible choice. A problem may have many feasible solutions, and we are interested in finding the best of these solutions. To be precise, we will try to minimize a certain objective function over a certain feasible set. How hard this is to do depends on the properties of the objective function and the feasible set. For instance, a linear objective function and a feasible set defined by linear inequalities yield a so-called *linear program*, which was the first problem type to receive much research interest. More generally, *convex programming* concerns the minimization of a convex objective function over a convex feasible set.

In this thesis, we analyze several classes of algorithms for convex programming, emphasizing both computational complexity and practical performance. Our focus is on interior point methods, simulated annealing algorithms, and analytic center cutting plane methods. This chapter provides a bird's-eye view of these algorithms.

1.1 Interior Point Methods

Linear programming became popular after Dantzig developed the simplex method in 1947, as he recalls in his account [31]. He recognized that it suffices to consider only the vertices of the feasible set: if one keeps moving from a vertex to an adjacent vertex with a better objective value, one eventually reaches an optimal solution. Armed with this method, researchers could find an optimal solution to large scale problems in – usually – very reasonable time. For this reason, the simplex method is still one of the most-used approaches for solving linear programming problems today. The method does have a major drawback though: on some instances, it takes a very long time to find an optimal solution. Researchers therefore tried to find algorithms that work in polynomial time on all instances.

The first polynomial-time algorithm for linear programming was given by Khachiyan [61] in 1979, who introduced an ellipsoid method for this problem. While this result was theoretically very important, it only outperformed the simplex method on specifically constructed families of instances.

A more competitive alternative was presented in 1984, when Karmarkar [59] introduced another polynomial-time algorithm to solve linear programming problems. Where the simplex method would travel between the vertices of the feasible set, Karmarkar's new algorithm would traverse the interior of the feasible set. This interior point method boasted performance that could rival the simplex method. But the ideas Karmarkar developed also gave rise to theoretical offspring: researchers such as Nesterov and Nemirovskii [85] recognized that an interior-point approach can be used to minimize a convex objective function over a convex set, a problem referred to as *convex programming*.

Let us illustrate the main idea behind (short-step) interior point methods with a simple example; a more formal introduction to this topic can be found in the textbook by Renegar [95]. Suppose we want to solve the convex programming problem

$$\min_{x \in \mathbb{R}^2} \{x_1 : x_1^2 + x_2^2 \leq 1\}. \tag{1.1}$$

This requires a so-called *barrier* function for the feasible set $\{x \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 1\}$. Informally, a barrier is a function that has the interior of the feasible set as its domain, tends to infinity as we approach the boundary of the feasible set, and is

in some well-defined sense smooth. For the Euclidean ball, the function $x \mapsto -\log(1-x_1^2-x_2^2)$ suffices. The minimizer $(0,0)$ of this function can be approximated with unconstrained minimization techniques such as Newton's method. We then add a positive multiple of the objective to the barrier – for the sake of simplicity, say we consider $x \mapsto x_1 - \log(1-x_1^2-x_2^2)$. If this addition does not change the function too much, the minimizer of the function also does not shift too much. Starting from our approximation of the previous minimizer $(0,0)$, we can then again use unconstrained minimization techniques to approximate the minimizer of the new function $x \mapsto x_1 - \log(1-x_1^2-x_2^2)$. The weight on the objective is then increased, and this scheme is repeated a number of times. All the minimizers thus approximated lie on the curve

$$\left\{z(\eta) : \eta > 0,\ \ z(\eta) \text{ is the minimizer of } x \mapsto \eta x_1 - \log(1-x_1^2-x_2^2)\right\},$$

which is called the *central path*. See Figure 1.1 for an illustration.

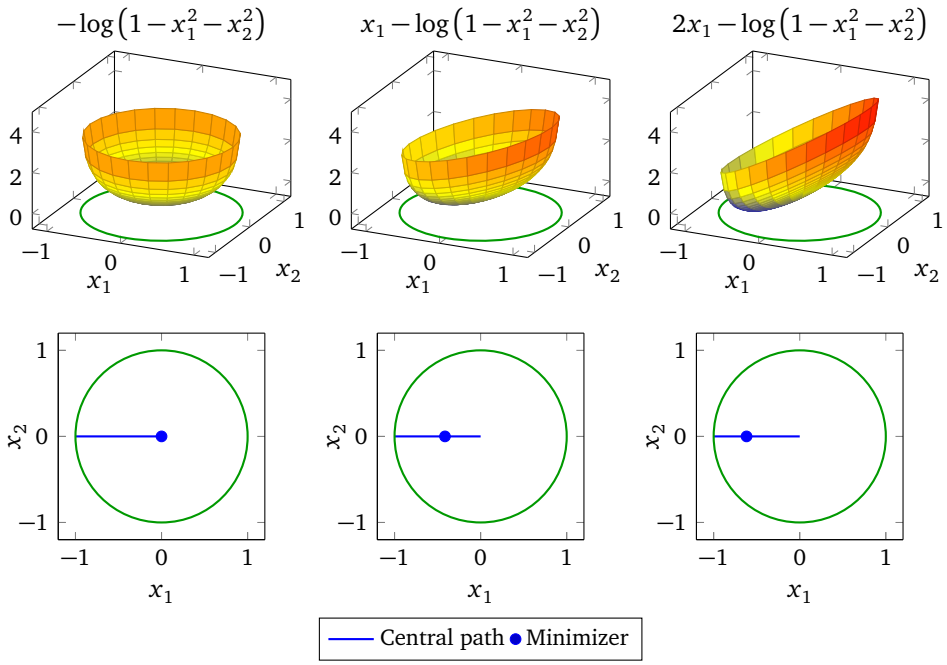

Figure 1.1: Three iterations of an interior point method to solve problem (1.1)

Intuitively, increasing the weight on the objective function means the minimizer shifts towards an optimal solution of (1.1). Indeed, it can be shown that following the central path to a point near its end is sufficient to generate a near-optimal solution to (1.1).

Whether a convex programming problem can be solved by interior point methods is therefore mainly determined by the availability of a barrier for the feasible set. In principle, such a barrier exists for every convex set that does not contain lines, as Nesterov and Nemirovskii [85] showed, but only certain sets have one that we know in closed form. These sets include the nonnegative orthant $\mathbb{R}^n_+$ that is so instrumental in linear programming, for which we can use the function $x \mapsto -\sum_{i=1}^n \log x_i$. As a generalization, one can use the function $X \mapsto -\log\det X$ as a barrier for the set of symmetric positive semidefinite matrices. And similar to what we saw above, $(t,x) \mapsto -\log(t^2 - \|x\|^2)$ serves as a barrier for the second order cone $\{(t,x) \in \mathbb{R}^{n+1} : \|x\| \leq t\}$.

These three cones are all *symmetric*, meaning that they are closed, convex, self-dual with respect to the Euclidean c.q. trace inner product, and have a transitive automorphism group; see Jordan et al. [55] for a complete characterization of symmetric cones. For these cones, Nesterov and Todd [87, 88] introduced what became known as the Nesterov-Todd directions, which lead to successful implementations in e.g. SeDuMi [104] and MOSEK [78].

This thesis is mainly concerned with feasible sets that cannot be described by symmetric cones. Two examples are the exponential cone

$$\left\{x \in \mathbb{R}^3 : x_1 \geq x_2 e^{x_3/x_2}, x_2 > 0\right\} \cup \left\{x \in \mathbb{R}^3 : x_1 \geq 0, x_2 = 0, x_3 \leq 0\right\},$$

and, for any $t \in (0,1)$, the three-dimensional power cone

$$\left\{x \in \mathbb{R}^3 : x_1^t x_2^{1-t} \geq |x_3|\right\}.$$

The lack of symmetry in these cones means that solvers cannot use the Nesterov-Todd directions. The search for alternatives (see Chapter 10 for references) yielded the method described by Dahl and Andersen [30], which is also implemented in the commercial solver MOSEK 9 [78]. Dahl and Andersen developed their algorithm to work well in practice, and did not provide a running time analysis. In Chapter 10, we provide a theoretical foundation for their algorithm.

But this algorithm does not cover all convex programing problems. There are convex sets for which no efficiently computable barrier exists, unless P = NP. One of those sets is the copositive cone, which consists of the symmetric matrices X such that $y^\top X y \geq 0$ for all $y \geq 0$; see Motzkin [79] for the origins of copositivity. To use an interior point method to solve copositive programming problems, we will use a barrier whose derivatives we can approximate.

1.2 Hit-and-Run Sampling and Simulated Annealing

We do have a *membership oracle* for the copositive cone: we can test for any given matrix whether it is copositive (see Section 8.2), even though Murty and Kabadi [81] showed this problem is co-NP-complete. With such an oracle, we can use a Markov chain Monte Carlo method to generate samples from a probability distribution over the feasible set. In this thesis, we will use *hit-and-run sampling*, originally introduced by Smith [102] for the uniform distribution in 1984, and later generalized to absolutely continuous distributions by e.g. Bélisle et al. [11]. In short, this method picks a random line through the current iterate and intersects this line with the feasible set (if we only have a membership oracle, this intersection can be approximated by the bisection method). The next iterate is then drawn from the target distribution restricted to the chord. This is effectively a one-dimensional sampling problem, which is usually much easier than high-dimensional sampling. An illustration is given in Figure 1.2.

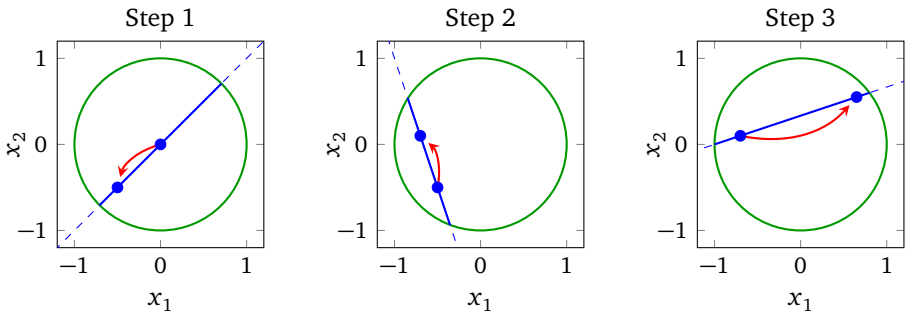

Figure 1.2: Three steps of hit-and-run sampling applied to the uniform distribution over $\{x \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 1\}$

Sampling can be geared towards optimization in a number of ways. One of the more classical approaches is to use *simulated annealing*, which was first proposed by Kirkpatrick et al. [63] for combinatorial optimization, and later applied to convex programming by Kalai and Vempala [56]. In real-world annealing, a piece of metal is heated for a certain time, then slowly cooled to make it more workable. The simulated version of this process involves a family of distributions known as Boltzmann distributions. For the problem (1.1) and some temperature $T > 0$, simulated annealing looks at probability distributions whose density (with respect to the Lebesgue measure) is proportional to $(x_1, x_2) \mapsto \exp(-x_1/T)$ on the feasible set. The idea is to generate a sample from such a distribution, and then use that sample to generate a new sample from a distribution with a lower temperature. This is repeated until the temperature is sufficiently low, at which point most of the distribution's probability mass is concentrated near an optimal solution. The means of the considered distributions lie on the *heat path*, which is defined as

$$\left\{ \frac{\int_{\mathfrak{B}(0,1)} x e^{-\langle c,x\rangle/T} \, \mathrm{d}x}{\int_{\mathfrak{B}(0,1)} e^{-\langle c,x\rangle/T} \, \mathrm{d}x} : T > 0 \right\},$$

where $\mathfrak{B}(0,1) = \{x \in \mathbb{R}^2 : x_1^2 + x_2^2 \leq 1\}$ is the unit ball in $\mathbb{R}^2$. See Figure 1.3 for an illustration.

If one compares Figures 1.1 and 1.3, it seems the interior point method and the simulated annealing algorithm that we sketched follow the same path. Indeed, Abernethy and Hazan [1] showed that the heat path and the central path coincide for an interior point method that uses the *entropic barrier* by Bubeck and Eldan [21].

The entropic barrier is interesting because its derivatives have a stochastic interpretation. For instance, the Hessian of the entropic barrier at some x is the inverted covariance matrix of the Boltzmann distribution whose mean is x. This stochastic interpretation allows us to approximate the barrier's derivatives through sampling. With a sampling method such as hit-and-run, all we need is a membership oracle to approximate the gradient and Hessian of the entropic barrier, with which we can solve (1.1). This will be shown in Chapter 6 with the tools developed in Chapters 2 to 5.

Because of the close relation between interior point methods and simulated

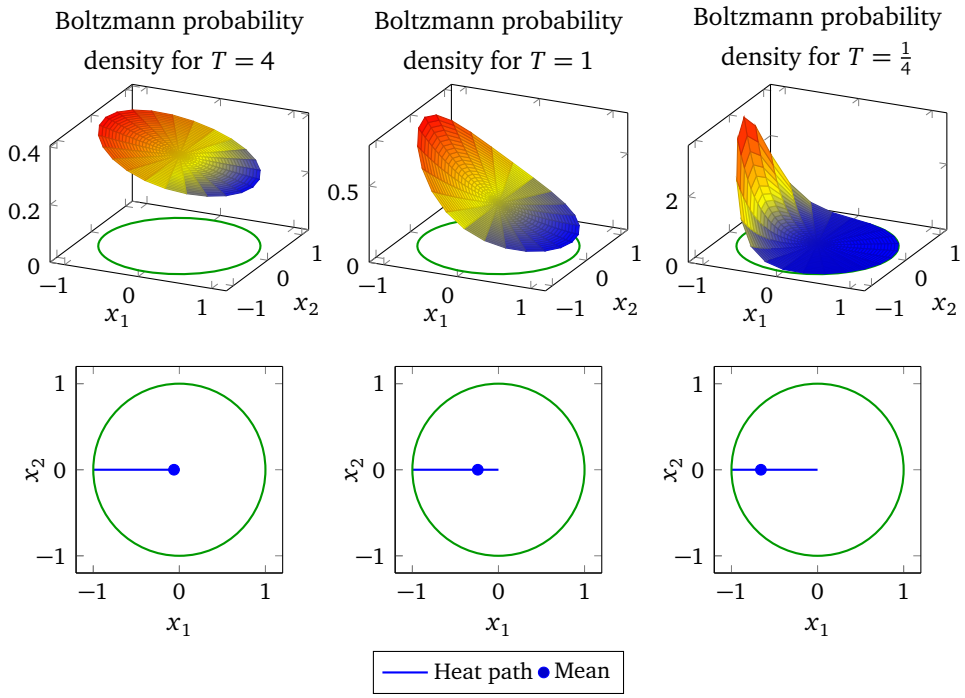

Figure 1.3: Three stages of simulated annealing to solve problem (1.1)

annealing that Abernethy and Hazan [1] established, we can also critically analyze Kalai and Vempala's algorithm [56] with these same tools. This is the topic of Chapter 7.

Both of these methods – the interior point method from Chapter 6 and the simulated annealing algorithm by Kalai and Vempala [56] – can be used for optimization over the copositive cone. The number of oracle calls made by these methods is, as we will show, asymptotically bounded by a polynomial, even though the calls themselves correspond to an NP-hard problem. However, we will see that this number of oracle calls is still so large that these methods are not competitive with e.g. the ellipsoid method. We therefore also investigate an alternative that is significantly faster in practice, even if it lacks an analysis of its computational complexity.

1.3 Analytic Center Cutting Plane Methods

The minimizer of a barrier is known as its *analytic center*. The name already suggests that an analytic center is somehow a central point in the barrier's domain. This fact is used by a specific class of cutting plane algorithms known as *analytic center cutting plane methods*, due to Goffin and Vial [43]. In general, cutting plane algorithms maintain some outer approximation of the set of optimal solutions. They take a query point from inside this outer approximation – in the case of analytic center cutting plane methods, this is the approximation's analytic center. If the query point lies in the feasible set, any optimal solution has an objective value that is at least as good as the query point's, and this information can be used to shrink the outer approximation. Alternatively, if the query point can be separated from the feasible set, this also allows us to shrink the approximation. An example is shown in Figure 1.4.

Analytic center cutting plane methods turn out to perform quite well in practice; see Goffin and Vial [44, Section 6] and the references therein. We therefore propose such a method to solve copositive programming problems in Chapter 8. In Chapter 9, we compare this method to the alternatives we touched upon above, and find that it indeed performs relatively well. The main drawback is that we do not analyze the running time of our method: in designing an algorithm that performs well in practice, we make some design choices that would be difficult to analyze rigorously. These include taking deep cuts (which means that we often have to start approximating an analytic center from outside the barrier's domain) and pruning the least relevant constraints. Nevertheless, the empirical evidence should convince even a skeptical reader that out of the approaches we discuss, this one is the most promising in practice.

1.4 Thesis Outline

We recall the fundamentals of interior point theory in Chapter 2. This is largely a collection of results from the textbook by Renegar [95], although we add some details to his proofs. We use a different definition of a function's conjugate, but this has no consequences other than sign changes.

The entropic barrier of Bubeck and Eldan [21] is formally introduced in Chap-

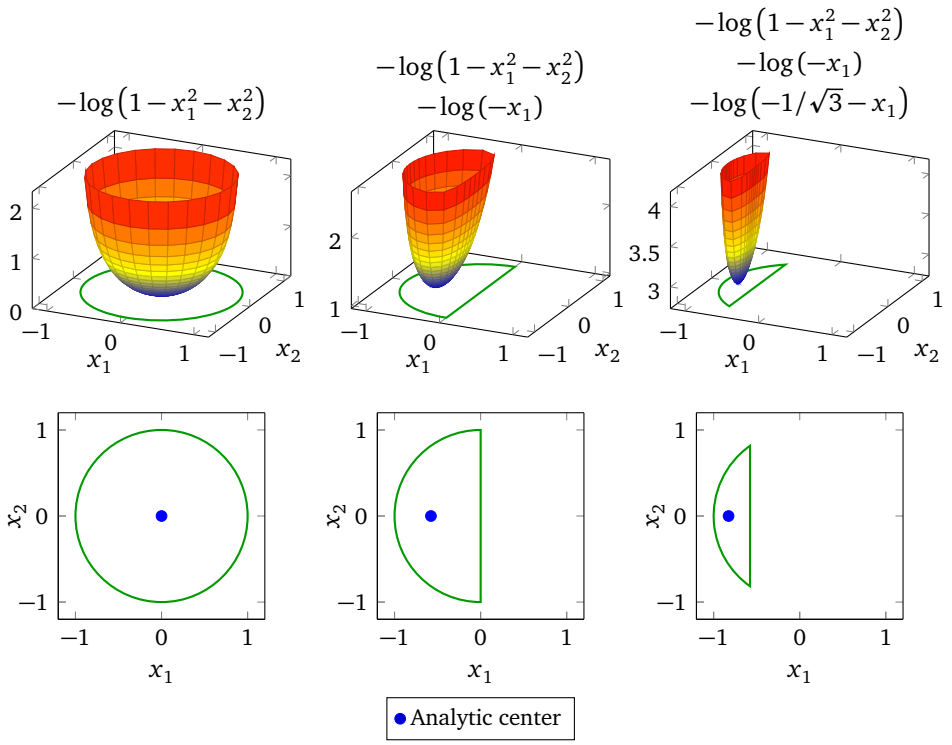

Figure 1.4: Three iterations of an analytic center cutting plane method to solve problem (1.1)

ter 3, along with its most important properties. We then propose and analyze a short-step interior point method that uses this barrier, under the assumption that its derivatives can be computed exactly. The iteration complexity of this method turns out to be the same as that of short-step methods in the literature, e.g. Renegar [95]. The difficulty in using the entropic barrier therefore lies in using its approximate derivatives.

To approximate these derivatives, we will use hit-and-run sampling (see Smith [102], Bélisle et al. [11]). Building on work by Lovász and Vempala [71], it will be shown in Chapter 4 that one can generate samples that approximately follow a Boltzmann distribution, provided one has some information from a Boltzmann distribution close to it.

These samples are used in Chapter 5 to approximate the mean and covariance of a Boltzmann distribution. We carefully analyze the quality of such approximations when the samples are not exactly from the correct distribution, and not exactly independent, as is the case when using hit-and-run sampling. This analysis is conceptually similar to earlier work by Kannan et al. [58].

It is then possible to analyze a sampling-based short-step interior point method in Chapter 6. The main assumption on the feasible set is that it admits a membership oracle, such that this method is widely applicable.

As an alternative to interior point methods, we consider the simulated annealing algorithm by Kalai and Vempala [56] in Chapter 7. With the tools developed in Chapters 4 and 5, we can rigorously analyze this algorithm. Moreover, we propose some modifications to improve its practical performance.

In Chapter 8, we develop a method aimed solely at practical performance. This analytic center cutting plane method (see Goffin and Vial [43]) was designed to solve copositive programming problems, and does not come with a formal complexity guarantee.

The proposed methods will be compared against each other and the ellipsoid method in Chapter 9. The analytic center cutting plane method from Chapter 8 seems to be the most appealing in practice, and also seems to scale reasonably well.

Chapter 10 moves the scope to somewhat more structured problems: optimization problems over proper cones that admit a barrier with readily computable derivatives. The cones in question do not even have to be self-dual, though. An algorithm that works well in practice on these problems was presented by Dahl and Andersen [30], and we provide some theoretical foundation for this algorithm. In particular, we prove polynomial time convergence of a method that uses their scaling matrix, search direction, and neighborhood.

1.5 Contributions to the Literature

This thesis is based on the following articles:

[7] R. Badenbroek and J. Dahl. An algorithm for nonsymmetric conic optimization inspired by mosek. *arXiv preprint arXiv:2003.01546*, 2020

[8] R. Badenbroek and E. de Klerk. Complexity analysis of a sampling-based interior point method for convex optimization. *arXiv preprint arXiv:1811.07677*, 2018

[9] R. Badenbroek and E. de Klerk. Simulated annealing with hit-and-run for convex optimization: rigorous complexity analysis and practical perspectives for copositive programming. *arXiv preprint arXiv:1907.02368*, 2019

[10] R. Badenbroek and E. de Klerk. An analytic center cutting plane method to determine complete positivity of a matrix. *arXiv preprint arXiv:2006.05319*, 2020

These articles are used in the chapters of this thesis as follows:

Chapter 2	Background material
Chapter 3	Background material
Chapter 4	Based on [8, Sections 2.3 and 4]
Chapter 5	Based on [8, Sections 2.4 and 5]
Chapter 6	Improves on [8, Section 6]
Chapter 7	Based on [9, Sections 1.1, 4, 5.3, and 5.4] and [10, Section 1]
Chapter 8	[10, Sections 1 and 2] and [7, Section 1]
Chapter 9	Based on [9, Sections 5.1 and 5.2] and [10, Section 3]
Chapter 10	Based on [7], excluding the proofs from [7, Sections 4, 5, and 6]
Appendix A	Background material
Appendix B	[8, Section 3.1]
Appendix C	Based on the proofs from [7, Sections 4, 5, and 6]

2

Properties of Self-Concordant Barriers

In this chapter, we collect the foundations of the interior point method theory in the notation that will be used throughout the thesis. After defining the gradient and Hessian, we will discuss self-concordant barriers in Section 2.1. Next, we consider the conjugate function and its properties in Section 2.2, and show that conjugation preserves self-concordance in Section 2.3. Finally, in Section 2.4 we consider an important situation where conjugation also preserves the barrier property: when the domain of the barrier is a cone.

The results in this chapter are mostly standard tools from the field of interior point methods. Aside from rephrasing them in our notation, we add some details to the proofs from Renegar [95].

2.1 Derivatives and Self-Concordant Barriers

We start with some preliminary definitions, which follow the notation from Renegar [95]. We fix a reference inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{R}^n$, which induces a norm $\| \cdot \|$ and a norm topology. For two linear operators A and B, we write $A \succeq B$ whenever

$\langle x, Ax\rangle \geq \langle x, Bx\rangle$ for all $x \in \mathbb{R}^n$. Any self-adjoint, positive definite linear operator A induces a new inner product $\langle \cdot, \cdot \rangle_A$ by $\langle x, y\rangle_A := \langle x, Ay\rangle$. The norm induced by $\langle \cdot, \cdot \rangle_A$ will be denoted by $\| \cdot \|_A$. For any norm $\| \cdot \|$ on $\mathbb{R}^n$, the *operator norm* $\|A\|$ for a linear operator A is given by $\max\{\|Ax\| : \|x\| \leq 1\}$.

A *functional* is a function that maps into $\mathbb{R}$. The gradient and Hessian of some functional f will depend on the reference inner product.

Definition 2.1 ([95, page 6])**.** Let f be a functional such that $\operatorname{dom} f$ is an open subset of $\mathbb{R}^n$. Then, f is *differentiable* at $\theta \in \operatorname{dom} f$ if there exists a vector $g(\theta) \in \mathbb{R}^n$ such that

$$\lim_{\|\Delta\theta\| \to 0} \frac{f(\theta + \Delta\theta) - f(\theta) - \langle g(\theta), \Delta\theta\rangle}{\|\Delta\theta\|} = 0.$$

The vector $g(\theta)$ is called the *gradient* of f at θ with respect to $\langle \cdot, \cdot \rangle$.

Definition 2.2 ([95, page 9])**.** Let f be a functional such that $\operatorname{dom} f$ is an open subset of $\mathbb{R}^n$. Then, f is *twice differentiable* if it is continuously differentiable at $\theta \in \operatorname{dom} f$ and there exists a bounded linear operator $H(\theta) : \mathbb{R}^n \to \mathbb{R}^n$ such that

$$\lim_{\|\Delta\theta\| \to 0} \frac{\|g(\theta + \Delta\theta) - g(\theta) - H(\theta)\Delta\theta\|}{\|\Delta\theta\|} = 0.$$

The linear operator $H(\theta)$ is called the *Hessian* of f at θ with respect to $\langle \cdot, \cdot \rangle$.

We denote the gradient and Hessian with respect to some other inner product $\langle \cdot, \cdot \rangle_A$ by g_A and H_A respectively, where A is a positive definite self-adjoint linear operator. It can be shown that $g_A(\theta) = A^{-1} g(\theta)$ and $H_A(\theta) = A^{-1} H(\theta)$, provided that the value of f does not depend on the chosen inner product (see e.g. Theorems 1.2.1 and 1.3.1 in Renegar [95]). For brevity, define the local inner product $\langle \cdot, \cdot \rangle_\theta := \langle \cdot, \cdot \rangle_{H(\theta)}$ and the local norm $\| \cdot \|_\theta := \| \cdot \|_{H(\theta)}$ for any $\theta \in \mathbb{R}^n$ and let g_θ and H_θ be the gradient and Hessian of f with respect to the local inner product $\langle \cdot, \cdot \rangle_\theta$.

The class of self-concordant functions plays an important role in the theory of interior point methods. The change in the Hessians of these functions when taking a small step is bounded by the size of the step (as measured in the local norm). We use the definition by Renegar [95].

Definition 2.3 ([95, page 23])**.** Let f be a twice continuously differentiable, strictly convex functional such that $\operatorname{dom} f$ is an open and convex subset of $\mathbb{R}^n$.

Then, f is *self-concordant* if, for all $\theta_0 \in \operatorname{dom} f$ and $\theta_1 \in \mathbb{R}^n$ such that $\|\theta_1 - \theta_0\|_{\theta_0} < 1$, the following two properties hold:

(i) $\theta_1 \in \operatorname{dom} f$.

(ii) For all nonzero $v \in \mathbb{R}^n$, we have

$$1 - \|\theta_1 - \theta_0\|_{\theta_0} \leq \frac{\|v\|_{\theta_1}}{\|v\|_{\theta_0}} \leq \frac{1}{1 - \|\theta_1 - \theta_0\|_{\theta_0}}, \tag{2.1}$$

or equivalently,

$$(1 - \|\theta_1 - \theta_0\|_{\theta_0})^2 H(\theta_0) \preceq H(\theta_1) \preceq \frac{1}{(1 - \|\theta_1 - \theta_0\|_{\theta_0})^2} H(\theta_0). \tag{2.2}$$

It can be seen that the sum of a self-concordant functional and a linear functional on $\mathbb{R}^n$ must also be self-concordant, since the self-concordance of a functional is entirely determined by its Hessians.

One may expect that if the change in the Hessians of some function is bounded, something similar can be said about the inverse Hessians. An application of the following result from Horn and Johnson [53] shows that this is the case. Horn and Johnson's original proof concerns positive definite matrices, so we include a proof to show that their statement also holds in the setting of linear operators.

Lemma 2.4 ([53, Corollary 7.7.4(a)])**.** *Let A, B be positive definite, self-adjoint linear operators from $\mathbb{R}^n$ to $\mathbb{R}^n$. Then, $A \succeq B$ if and only if $B^{-1} \succeq A^{-1}$.*

Proof. If $S : \mathbb{R}^n \to \mathbb{R}^n$ is some invertible linear operator, then $\langle x, (A-B)x \rangle \geq 0$ for all $x \in \mathbb{R}^n$ if and only if $\langle Sy, (A-B)Sy \rangle \geq 0$ for all $y \in \mathbb{R}^n$. Hence,

$$A \succeq B \quad \text{if and only if} \quad S^\top A S \succeq S^\top B S, \tag{2.3}$$

where $S^\top$ is the adjoint of S. Applying (2.3) with $S = A^{-1/2}$ shows that $A \succeq B$ is equivalent to $I \succeq A^{-1/2} B A^{-1/2}$, that is, all eigenvalues of $A^{-1/2} B A^{-1/2}$ are at most 1. The vector v is an eigenvector for $A^{-1/2} B A^{-1/2}$ with eigenvalue λ if and only if $B^{1/2} A^{-1/2} v$ is an eigenvector for $B^{1/2} A^{-1} B^{1/2}$ with eigenvalue λ. Hence, all eigenvalues of $B^{1/2} A^{-1} B^{1/2}$ are also at most 1, meaning $I \succeq B^{1/2} A^{-1} B^{1/2}$. Another application of (2.3) with $S = B^{-1/2}$ completes the proof. □

This lemma shows that (2.2) is equivalent to

$$(1-\|\theta_1-\theta_0\|_{\theta_0})^2 H(\theta_1)^{-1} \preceq H(\theta_0)^{-1} \preceq \frac{1}{(1-\|\theta_1-\theta_0\|_{\theta_0})^2} H(\theta_1)^{-1}, \tag{2.4}$$

and therefore (2.1) is equivalent to

$$1-\|\theta_1-\theta_0\|_{\theta_0} \leq \frac{\|\nu\|_{\theta_0}^{-1}}{\|\nu\|_{\theta_1}^{-1}} \leq \frac{1}{1-\|\theta_1-\theta_0\|_{\theta_0}}, \tag{2.5}$$

where $\|\cdot\|_\theta^{-1}$ is the norm induced by $H(\theta)^{-1}$ for any $\theta \in \mathbb{R}^n$.

It should be noted that our definition of self-concordance is not the original one by Nesterov and Nemirovskii [85]. Their definition assumes the function f is three times differentiable, which we define first. To do so, we will use $\mathcal{L}(U;V)$ to denote the space of linear operators from the vector space U to the vector space V. The third derivative is a Fréchet derivative, just like the gradient and Hessian from Definitions 2.1 and 2.2. We refer the reader to Appendix A for details.

Definition 2.5 ((A.4) in Appendix A.4)**.** Let f be a functional such that $\operatorname{dom} f$ is an open subset of $\mathbb{R}^n$. Then, f is *three times differentiable* if it is twice continuously differentiable at $\theta \in \operatorname{dom} f$ and there exists a bounded linear operator $T(\theta) : \mathbb{R}^n \to \mathcal{L}(\mathbb{R}^n;\mathbb{R}^n)$ such that

$$\lim_{\|\Delta\theta\|\to 0} \frac{\|H(\theta+\Delta\theta)-H(\theta)-T(\theta)\Delta\theta\|}{\|\Delta\theta\|} = 0,$$

where the norm in the numerator is the operator norm on $\mathcal{L}(\mathbb{R}^n;\mathbb{R}^n)$. The linear operator $T(\theta)$ is called the *third derivative* of f at θ with respect to $\langle\cdot,\cdot\rangle$.

We are now ready to show that Definition 2.3 is equivalent to the definition of self-concordance by Nesterov and Nemirovskii [85], provided that f is three times continuously differentiable. This was originally shown by Renegar [95], but we provide some details on the proof in the appendix.

Theorem 2.6 ([95, Theorem 2.5.3])**.** *Let f be a three times continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open subset of $\mathbb{R}^n$. Then, f is self-concordant if and only if the following two properties hold:*

(i) For any sequence $\{\theta_k\} \subset \operatorname{dom} f$ *that converges to a point on the boundary of* $\operatorname{dom} f$*, we have* $f(\theta_k) \to \infty$.

(ii) For any $\theta \in \operatorname{dom} f$ *and* $\Delta\theta \in \mathbb{R}^n$*, the function* $\phi(t) := f(\theta + t\Delta\theta)$ *satisfies* $\phi'''(t) \leq 2\phi''(t)^{3/2}$ *for all* $t \in \operatorname{dom}\phi$.

Proof. See Appendix A. □

We end this section with another important concept from the theory of interior point methods: the complexity parameter. Some self-concordant functionals have such a parameter, and it often appears in the complexity analysis of interior point methods that rely on these functionals. We again use the definition by Renegar [95].

Definition 2.7 ([95, page 35])**.** A functional f is a *(self-concordant) barrier* if it is self-concordant and

$$\vartheta_f := \sup_{\theta \in \operatorname{dom} f} \|g_\theta(\theta)\|_\theta^2,$$

is finite. The value ϑ_f is called the *complexity parameter* of the barrier f.

The barrier property of f is often applied directly, that is, to upper bound $\|g_\theta(\theta)\|_\theta$ for some $\theta \in \operatorname{dom} f$, or through the following result.

Theorem 2.8 ([95, Theorem 2.3.3])**.** *Let* f *be a self-concordant barrier. Then, for any* $\theta_0, \theta_1 \in \operatorname{dom} f$*,*

$$\langle g(\theta_0), \theta_1 - \theta_0 \rangle < \vartheta_f.$$

2.2 The Conjugate and its Derivatives

A function $f : \mathbb{R}^n \to \mathbb{R}$ has a dual of sorts, called the conjugate function. It is invaluable for defining the entropic barrier (see Chapter 3) as well as primal-dual interior point methods. For the sake of consistency, we phrase the definition and properties of the conjugate in terms of $\mathbb{R}^n$, but these statements can easily be generalized to arbitrary Hilbert spaces.

Definition 2.9. Let f be a functional such that $\operatorname{dom} f$ is an open subset of $\mathbb{R}^n$. Then, the *conjugate* of f is defined by

$$f^*(x) \coloneqq \sup_{\theta \in \operatorname{dom} f} \{\langle \theta, x \rangle - f(\theta)\}.$$

In the remainder of this section, we establish some basic properties of the conjugate: its domain, gradient, and Hessian. In Section 2.3, we look at self-concordance of the conjugate.

Before we determine the domain of the conjugate function, let us fix some notation that we will use in the analysis. Denote the open ball with radius r around $\theta_0 \in \mathbb{R}^n$, as measured in the reference norm $\|\cdot\|$, by $\mathfrak{B}(\theta_0, r)$. Moreover, let $\mathfrak{B}_\theta(\theta_0, r)$ be the open ball with radius r around θ_0, as measured in the local norm $\|\cdot\|_\theta$. Finally, let $\langle \cdot, \cdot \rangle_\theta^{-1}$ be the inner product induced by $H(\theta)^{-1}$, and $\|\cdot\|_\theta^{-1}$ the corresponding norm.

Our proof follows that of Renegar [95], although he uses a different definition of the conjugate.

Proposition 2.10 ([95, Proposition 3.3.3])**.** *Let f be a twice continuously differentiable, strictly convex functional such that $\operatorname{dom} f$ is an open and convex subset of $\mathbb{R}^n$. Then, the gradient map $g : \operatorname{dom} f \to \mathbb{R}^n$ is injective. If f is self-concordant, then*

$$\operatorname{dom} f^* = \{g(\theta) : \theta \in \operatorname{dom} f\}, \tag{2.6}$$

and $\operatorname{dom} f^*$ is open.

Proof. Suppose $\theta_1, \theta_2 \in \operatorname{dom} f$ satisfy $g(\theta_1) = g(\theta_2) = x$. Then they both maximize the strictly concave function

$$\theta \mapsto \langle \theta, x \rangle - f(\theta), \tag{2.7}$$

and hence $\theta_1 = \theta_2$, proving that g is injective. Moreover, because (2.7) has a maximizer θ_1, we have $x = g(\theta_1) \in \operatorname{dom} f^*$. In other words,

$$\{g(\theta) : \theta \in \operatorname{dom} f\} \subseteq \operatorname{dom} f^*. \tag{2.8}$$

Next suppose $x \in \operatorname{dom} f^*$. Then $f^*(x)$ is finite, and therefore (2.7) is bounded above. If f is self-concordant, Theorem 2.2.8 in Renegar [95] shows (2.7) has

a maximizer $\theta \in \operatorname{dom} f$. This maximizer must satisfy $g(\theta) = x$, and we may therefore conclude that

$$\operatorname{dom} f^* \subseteq \{g(\theta) : \theta \in \operatorname{dom} f\}.$$

Combined with (2.8), we find (2.6).

Finally, we show that $\operatorname{dom} f^*$ is open if f is self-concordant via the suggestion in Renegar's proof. Let $\theta \in \operatorname{dom} f$ and consequently, $g(\theta) \in \operatorname{dom} f^*$. Let $\Delta x \in \mathbb{R}^n$ be a vector satisfying

$$\|\Delta x\|_\theta^{-1} < \tfrac{1}{4}. \tag{2.9}$$

(In particular, all Δx in $\mathfrak{B}(0, \frac{1}{4}\lambda_{\min}(H(\theta)^{1/2}))$ satisfy (2.9), where $\lambda_{\min}(H(\theta)^{1/2})$ is the smallest eigenvalue of $H(\theta)^{1/2}$, which by assumption is positive.) Define $v = H(\theta)^{-1}\Delta x$, and observe that

$$\|v\|_\theta = \sqrt{\langle v, H(\theta)v\rangle} = \sqrt{\langle H(\theta)^{-1}\Delta x, \Delta x\rangle} = \|\Delta x\|_\theta^{-1} < \tfrac{1}{4}.$$

Noting that $\frac{3t^2}{(1-t)^3} \leq 9t^2$ for $t \in [0, \frac{1}{4}]$, Proposition 2.2.10 in Renegar [95] shows that if $\|v\|_\theta \leq \frac{1}{4}$, then there exists a vector $u \in \mathfrak{B}_\theta(v, 9\|v\|_\theta^2)$ such that $\theta + u \in \operatorname{dom} f$ and

$$g(\theta + u) = g(\theta) + \Delta x.$$

Consequently, $g(\theta) + \Delta x \in \operatorname{dom} f^*$, which shows $\operatorname{dom} f^*$ is open. □

Having established the domain of the conjugate f^*, our next goal is describing the gradient g^* and Hessian H^* of f^*. Before we can do that, we cite a general version of the inverse function theorem from Lang [66].

Theorem 2.11 ([66, Chapter I, Theorem 5.2])**.** *Let V, W be normed vector spaces, and let $V' \subseteq V$ be an open subset of V. Let $\phi : V' \to W$ be a k times continuously differentiable mapping, where $k \geq 1$. If at some point $\theta \in V'$, the Fréchet derivative $D\phi(\theta)$ is an invertible linear operator, then ϕ has a k times continuously differentiable local inverse $\phi^{-1} : W' \to V$ in a neighborhood W' around $\phi(\theta)$, i.e.*

$$\phi(\phi^{-1}(x)) = x \qquad \forall x \in W'.$$

We now establish relationships between the derivatives of f and f^*. Such relationships can be found for convex functionals under some mild conditions (see

Rockafellar [96, Corollary 23.5.1] and Crouzeix [29]), but we restrict ourselves to self-concordant functionals to keep the proof concise. We again follow the proof from Renegar [95], but provide some details on the application of Theorem 2.11.

Theorem 2.12 ([95, Theorem 3.3.4])**.** *Let f be a self-concordant functional. Then, f^* is twice continuously differentiable. If moreover $\theta \in \operatorname{dom} f$ and x satisfy $x = g(\theta)$, then*

$$g^*(x) = \theta \quad \text{and} \quad H^*(x) = [H(\theta)]^{-1}.$$

Proof. Proposition 2.10 shows that $g : \operatorname{dom} f \to \operatorname{dom} f^*$ is invertible. The first differential of g at $\theta \in \operatorname{dom} f$ is the Hessian $H(\theta)$. Since it was assumed that $H(\theta)$ is positive definite for all $\theta \in \operatorname{dom} f$, we see that $H(\theta)$ is invertible. Hence, Theorem 2.11 shows that, for any $\theta \in \operatorname{dom} f$, g has a continuously differentiable inverse g^{-1} around $g(\theta)$. It is shown in Proposition 2.10 that $\operatorname{dom} f^* = \{g(\theta) : \theta \in \operatorname{dom} g\}$, and hence for any $x \in \operatorname{dom} f^*$, the mapping $x \mapsto g^{-1}(x)$ is continuously differentiable.

Let us define $\theta(x) := g^{-1}(x)$ for all $x \in \operatorname{dom} f^*$. Since $g(\theta(x)) = x$, we have

$$f^*(x) = \langle \theta(x), x \rangle - f(\theta(x)), \tag{2.10}$$

for all $x \in \operatorname{dom} f^*$. We know that $x \mapsto \theta(x)$ is continuously differentiable, and therefore f^* is as well. To determine its derivative, we first differentiate $f_1^*(x) := \langle \theta(x), x \rangle$. Denote the Fréchet derivative of $\theta(x)$ by $D\theta(x)$, and the adjoint of $D\theta(x)$ by $(D\theta(x))^\top$. We then claim that the derivative of f_1^* is $g_1^*(x) = \theta(x) + (D\theta(x))^\top x$. To see this, note that

$$\begin{aligned}
&\lim_{\|\Delta x\| \downarrow 0} \tfrac{1}{\|\Delta x\|} |f_1^*(x + \Delta x) - f_1^*(x) - \langle g_1^*(x), \Delta x \rangle| \\
&= \lim_{\|\Delta x\| \downarrow 0} \tfrac{1}{\|\Delta x\|} |\langle \theta(x + \Delta x), x + \Delta x \rangle - \langle \theta(x), x \rangle - \langle \theta(x) + (D\theta(x))^\top x, \Delta x \rangle| \\
&= \lim_{\|\Delta x\| \downarrow 0} \tfrac{1}{\|\Delta x\|} |\langle \theta(x + \Delta x) - \theta(x), x + \Delta x \rangle - \langle x, D\theta(x)\Delta x \rangle| \\
&= \lim_{\|\Delta x\| \downarrow 0} \tfrac{1}{\|\Delta x\|} |\langle \theta(x + \Delta x) - \theta(x) - D\theta(x)\Delta x, x \rangle| = 0.
\end{aligned} \tag{2.11}$$

Second, the derivative of $f_2^*(x) := f(\theta(x))$ is given by the chain rule (see Theorem A.2) as the linear operator $g_2^*(x) = g(\theta(x)) \circ D\theta(x)$. Applying this operator to Δx gives

$$g_2^*(x)[\Delta x] = \langle g(\theta(x)), D\theta(x)\Delta x \rangle = \langle (D\theta(x))^\top g(\theta(x)), \Delta x \rangle,$$

so in vector form, we have $g_2^*(x) = (D\theta(x))^\top g(\theta(x)) = (D\theta(x))^\top x$. Combining this fact with (2.11) gives the derivative of (2.10) as

$$g^*(x) = \theta(x) + (D\theta(x))^\top x - (D\theta(x))^\top x = \theta(x).$$

Recall that $x \mapsto \theta(x)$ is continuously differentiable, so g^* is continuously differentiable. This shows that f^* is twice continuously differentiable. Differentiating the identity $g(\theta(x)) = x$ with respect to x using the chain rule (see e.g. Theorem A.2) gives $H(\theta(x))D\theta(x) = I$, showing

$$H^*(x) = D\theta(x) = H(\theta(x))^{-1}. \qquad \square$$

2.3 Self-Concordance of the Conjugate

Now that we have some information about the gradient and the Hessian of the conjugate, we can show that f^* is self-concordant if and only if f itself is self-concordant.

Before we do so, we extend our notation once more. Let $\langle\cdot,\cdot\rangle_x^*$ and $\|\cdot\|_x^*$ be the local inner product and local norm induced by $H^*(x)$, where $x \in \operatorname{dom} f$. Moreover, let $\mathfrak{B}_x^*(y,r)$ be the open ball with radius r around a fixed $y \in \operatorname{dom} f$, as measured in the local norm $\|\cdot\|_x^*$.

Theorem 2.13 ([95, Theorem 3.3.1])**.** *Let f be a twice continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open and convex subset of $\mathbb{R}^n$. Then, f is self-concordant if and only if f^* is self-concordant.*

Proof. The proof of the "only if" implication is the same as in Renegar [95], but again we provide some additional details. Pick any $\theta \in \operatorname{dom} f$ and $x \in \operatorname{dom} f^*$ such that $g(\theta) = x$. By Theorem 2.12, we then have for all $y, z \in \mathbb{R}^n$,

$$\langle y,z\rangle_x^* = \langle y, H^*(x)z\rangle = \langle y, H(\theta)^{-1}z\rangle = \langle H(\theta)^{-1}y, H(\theta)^{-1}z\rangle_\theta, \tag{2.12}$$

and consequently,

$$\|y\|_x^* = \|H(\theta)^{-1}y\|_\theta = \|y\|_\theta^{-1}. \tag{2.13}$$

Assume f is self-concordant. By Theorem 2.5.2 in Renegar [95], if we show that

$$\mathfrak{B}_x^*(x, \tfrac{1}{4}) \subseteq \operatorname{dom} f^*, \tag{2.14}$$

and

$$\limsup_{\|\Delta x\|\downarrow 0} \frac{\|I - H_x^*(x+\Delta x)\|_x^*}{\|\Delta x\|_x^*} \leq 2, \tag{2.15}$$

where $H_x^*(x+\Delta x) := H^*(x)^{-1}H^*(x+\Delta x)$, then f^* is self-concordant.

Towards proving (2.14), let $\Delta x \in \mathfrak{B}_x^*(0, \frac{1}{4})$. Then by (2.13), Δx satisfies (2.9). By the same argument as in the proof of Proposition 2.10, there exists a

$$u \in \mathfrak{B}_\theta(H(\theta)^{-1}\Delta x, 9\|H(\theta)^{-1}\Delta x\|_\theta^2), \tag{2.16}$$

such that $\theta + u \in \operatorname{dom} f$ and $g(\theta+u) = g(\theta) + \Delta x$. Since $g(\theta+u)$ must lie in $\operatorname{dom} f^*$ and $g(\theta) = x$, we have that (2.14) holds. Moreover, (2.16) and (2.13) demonstrate that

$$\|u\|_\theta \leq \|H(\theta)^{-1}\Delta x\|_\theta + 9\|H(\theta)^{-1}\Delta x\|_\theta^2 = \|\Delta x\|_x^* + 9(\|\Delta x\|_x^*)^2. \tag{2.17}$$

To prove (2.15), note that since $H(\theta)$ has full rank, and by application of (2.12) and (2.13),

$$\begin{aligned}
\|I - H_x^*(x+\Delta x)\|_x^* &= \max_{w\in\mathbb{R}^n} \frac{|\langle H(\theta)w, [I - H_x^*(x+\Delta x)]H(\theta)w\rangle_x^*|}{(\|H(\theta)w\|_x^*)^2} \\
&= \max_{w\in\mathbb{R}^n} \frac{|\langle w, H(\theta)^{-1}[I - H_x^*(x+\Delta x)]H(\theta)w\rangle_\theta|}{\|w\|_\theta^2} \\
&= \|I - H(\theta)^{-1}H_x^*(x+\Delta x)H(\theta)\|_\theta.
\end{aligned}$$

Using the expressions from Theorem 2.12 gives

$$\begin{aligned}
\|I - H_x^*(x+\Delta x)\|_x^* &= \|I - H(\theta)^{-1}H^*(x)^{-1}H^*(x+\Delta x)H(\theta)\|_\theta \\
&= \|I - H(\theta)^{-1}H(\theta)H(\theta+u)^{-1}H(\theta)\|_\theta \\
&= \|I - H_\theta(\theta+u)^{-1}\|_\theta.
\end{aligned} \tag{2.18}$$

Since f is self-concordant, Theorem 2.2.1 in Renegar [95] and (2.17) show

$$\|I - H_\theta(\theta+u)^{-1}\|_\theta \leq \frac{1}{(1-\|u\|_\theta)^2} - 1 \leq \frac{1}{(1-\|\Delta x\|_x^* + 9(\|\Delta x\|_x^*)^2)^2} - 1.$$

Combined with (2.18), we thus find

$$\limsup_{\|\Delta x\|\downarrow 0} \frac{\|I - H_x^*(x+\Delta x)\|_x^*}{\|\Delta x\|_x^*} \leq \limsup_{t\downarrow 0} \left(\frac{1}{t(1-t+9t^2)^2} - \frac{1}{t} \right) = 2,$$

where the equality follows from l'Hôpital's rule. This establishes (2.15) and thus f^* is self-concordant.

To prove the reverse implication, it suffices to note that $(f^*)^* = f$ by the Fenchel-Moreau theorem (f is proper, lower semi-continuous and convex). □

2.4 Conjugates of Barriers over Cones

Theorem 2.13 shows that a function is self-concordant if and only if its conjugate is self-concordant too. The reader may wonder if such a relation also holds for the barrier property. In general, the answer is no. The entropic barrier – to be introduced in Chapter 3 – is one example where f is not a barrier, but f^* is. There is however an important case where f being a barrier implies f^* being a barrier: when f is logarithmically homogeneous. Let us first define this property as in Renegar [95], and then show the claim.

Definition 2.14 ([95, page 42])**.** Let $\mathcal{K} \subseteq \mathbb{R}^n$ be a *proper cone*, i.e. a cone that is convex, closed, pointed, and full-dimensional. Then, a self-concordant barrier $f : \operatorname{int}\mathcal{K} \to \mathbb{R}$ is *logarithmically homogeneous* if for all $\theta \in \operatorname{int}\mathcal{K}$ and $t > 0$,

$$f(t\theta) = f(\theta) - \vartheta_f \log t. \tag{2.19}$$

We will often abbreviate 'logarithmically homogeneous self-concordant barrier' to '*LHSCB*'.

By computing the first and second derivative of both sides of (2.19) with respect to θ (see Theorem A.2 for the chain rule for Fréchet derivatives), we see that a LHSCB f satisfies

$$g(t\theta) = \tfrac{1}{t} g(\theta) \tag{2.20}$$

$$H(t\theta) = \tfrac{1}{t^2} H(\theta), \tag{2.21}$$

for all $\theta \in \operatorname{dom} f$ and $t > 0$. Taking the derivative of (2.20) with respect to t shows $H(t\theta)\theta = -\frac{1}{t^2} g(\theta)$, implying for $t = 1$ that

$$\theta = -g_\theta(\theta). \tag{2.22}$$

We will now show that a LHSCB f has a conjugate that is also a LHSCB. Additionally, we will show that the complexity parameter of f^*, defined as

$$\vartheta_{f^*} := \sup_{x \in \operatorname{dom} f^*} (\|g_x^*(x)\|_x^*)^2,$$

is equal to ϑ_f. We again largely follow the proof by Renegar [95], but providing a different argument that the interior of the polar cone is contained in $\{g(\theta) : \theta \in \operatorname{dom} f\}$, and that f^* is logarithmically homogeneous.

Theorem 2.15 ([95, Theorem 3.3.1])**.** *Let f be a LHSCB with $\operatorname{dom} f = \operatorname{int} \mathcal{K}$, where $\mathcal{K} \subseteq \mathbb{R}^n$ is a proper cone. Then f^* is a LHSCB with domain $\operatorname{int}(\mathcal{K}^\circ)$, where $\mathcal{K}^\circ := \{x \in \mathbb{R}^n : \langle \theta, x \rangle \leq 0 \ \ \forall \theta \in \mathcal{K}\}$. Moreover, $\vartheta_{f^*} = \vartheta_f$.*

Proof. We first show that $\operatorname{dom} f^* = \operatorname{int}(\mathcal{K}^\circ)$. By Proposition 2.10, it suffices to show that $\{g(\theta) : \theta \in \operatorname{dom} f\} = \operatorname{int}(\mathcal{K}^\circ)$.

Pick any $\theta_0, \theta_1 \in \operatorname{int} \mathcal{K}$. By Theorem 2.8, we have

$$\langle g(\theta_0), t\theta_1 - \theta_0 \rangle < \vartheta_f,$$

for any $t > 0$. Letting t tend to infinity, we see that $\langle g(\theta_0), \theta_1 \rangle \leq 0$, showing $g(\theta_0) \in \mathcal{K}^\circ$. Since $\{g(\theta) : \theta \in \operatorname{dom} f\}$ is open by Proposition 2.10, we have $\{g(\theta) : \theta \in \operatorname{dom} f\} \subseteq \operatorname{int}(\mathcal{K}^\circ)$.

Conversely, pick an $x \in \operatorname{int}(\mathcal{K}^\circ)$. We will argue that there exists a $\theta \in \operatorname{dom} f$ such that $g(\theta) = x$, that is, the function $\phi(\theta) := f(\theta) - \langle \theta, x \rangle$ has a minimizer. Since $x \in \operatorname{int}(\mathcal{K}^\circ)$, it satisfies $\langle \theta, x \rangle < 0$ for all $\theta \in \mathcal{K}$, meaning there exists an $\alpha > 0$ such that

$$-\langle \theta, x \rangle \geq \alpha \qquad \text{for all } \theta \in \mathcal{K} \text{ with } \|\theta\| = 1.$$

For all $\theta \in \operatorname{int} \mathcal{K}$ with $\|\theta\| = 1$ and $t > 0$, we therefore have by logarithmic homogeneity

$$\phi(t\theta) = f(t\theta) - \langle t\theta, x \rangle = f(\theta) - \vartheta_f \log t - t\langle \theta, x \rangle \geq \phi(\theta) - \vartheta_f \log t + \alpha(t-1).$$

In other words, there exists some $t^* > 1$ such that for all $t \geq t^*$, we have $\phi(t\theta) \geq \phi(\theta)$. We thus see that

$$\inf_\theta \{\phi(\theta) : \theta \in \operatorname{int} \mathcal{K}\} = \inf_\theta \{\phi(\theta) : \theta \in \operatorname{int} \mathcal{K}, \|\theta\| \leq t^*\}. \tag{2.23}$$

As a consequence of Theorem 2.6(i), there exists a closed inner approximation $\mathcal{K}'$ of $\operatorname{int}\mathcal{K}$ such that the values of ϕ on $\operatorname{int}(\mathcal{K}) \setminus \mathcal{K}'$ are irrelevant for minimization. Consequently,

$$\inf_\theta\{\phi(\theta) : \theta \in \operatorname{int}\mathcal{K}, \|\theta\| \le t^*\} = \inf_\theta\{\phi(\theta) : \theta \in \mathcal{K}', \|\theta\| \le t^*\},$$

which has a minimizer by Weierstrass' Theorem. Combined with (2.23), we see that ϕ has a minimizer on $\operatorname{int}\mathcal{K}$, showing that $\operatorname{int}(\mathcal{K}^\circ) \subseteq \{g(\theta) : \theta \in \operatorname{dom} f\}$.

To show that f^* is a self-concordant barrier with complexity parameter ϑ_f, note that by Theorem 2.12 and (2.22),

$$\vartheta_{f^*} = \sup_{x\in\operatorname{dom} f^*} (\|g_x^*(x)\|_x^*)^2 = \sup_{\theta\in\operatorname{dom} f} \|\theta\|_\theta^2 = \sup_{\theta\in\operatorname{dom} f} \|g_\theta(\theta)\|_\theta^2 = \vartheta_f.$$

Finally, logarithmic homogeneity of f^* follows from the fact that for any $x \in \operatorname{dom} f^*$ and $t > 0$,

$$\begin{aligned} f^*(tx) &= \sup_{\theta\in\operatorname{dom} f} \{\langle\theta, tx\rangle - f(\theta) + [f(t\theta) - f(t\theta)]\} \\ &= \sup_{\theta\in\operatorname{dom} f} \left\{\langle t\theta, x\rangle - f(t\theta) - \vartheta_f \log t\right\} \\ &= f^*(x) - \vartheta_f \log t = f^*(x) - \vartheta_{f^*} \log t. \end{aligned}$$

□

3

A Simple Interior Point Method Using the Entropic Barrier

In this chapter, we focus on a particular self-concordant barrier: the entropic barrier, as proposed by Bubeck and Eldan [21]. This barrier can be defined on any convex body, and its gradients and Hessians may be approximated through sampling. As we will see in later chapters, it is possible to generate sufficiently good samples using a technique called hit-and-run sampling, which only requires a membership oracle for the feasible set. Hence, the entropic barrier can be used for interior point methods on very general sets.

Before we continue, let us define this entropic barrier.

Definition 3.1. Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body. The *log-partition function* $f : \mathbb{R}^n \to \mathbb{R}$ associated with $\mathcal{S}$ is defined as

$$f(\theta) \coloneqq \log \int_{\mathcal{S}} e^{\langle \theta, x \rangle} \, \mathrm{d}x.$$

Its conjugate f^* is called the *entropic barrier*.

The derivatives of the log-partition function and the entropic barrier have an interpretation in terms of so-called Boltzmann distributions over the convex body $\mathcal{S}$. Let us define these distributions first, and then discuss their relevance to the log-partition function and the entropic barrier.

Definition 3.2. Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $\theta \in \mathbb{R}^n$. Then, the *Boltzmann distribution with parameter* θ is the probability distribution supported on $\mathcal{S}$ having density with respect to the Lebesgue measure proportional to $x \mapsto e^{\langle \theta, x \rangle}$.

As we will prove below, the gradient $g : \mathbb{R}^n \to \operatorname{int} \mathcal{S}$ of the log-partition function f assigns to each $\theta \in \mathbb{R}^n$ the mean of the Boltzmann distribution with parameter θ. On the other hand, the gradient $g^* : \operatorname{int} \mathcal{S} \to \mathbb{R}^n$ of the entropic barrier f^* maps a point $x \in \operatorname{int} \mathcal{S}$ to the $\theta \in \mathbb{R}^n$ such that the mean of the Boltzmann distribution with the parameter θ is x. This interpretation can offer a bit of intuition why f^* is a barrier for $\mathcal{S}$: as one lets $x \in \operatorname{int} \mathcal{S}$ approach the boundary of $\mathcal{S}$, the Boltzmann distribution that has mean x will have to concentrate more and more probability mass near the boundary of $\mathcal{S}$. This will cause the norm of the parameter of the Boltzmann distribution, i.e. the norm of $g^*(x)$, to tend to infinity.

The name of the entropic barrier derives from the fact that, at some $x \in \operatorname{int} \mathcal{S}$, the entropic barrier equals the negative entropy of the Boltzmann distribution whose mean is x, as was shown by e.g. Wainwright and Jordan [109, Theorem 3.4(a)]. The negative entropy of a probability density $\phi : \mathcal{S} \to \mathbb{R}_+$ is $\int_{\mathcal{S}} \phi(y) \log \phi(y) \, \mathrm{d}y$, but we will not use this concept – we mention it only for etymological reasons.

We provide an overview of the most important properties of the entropic barrier in Section 3.1. In Section 3.2, we consider the complexity parameter of this barrier for the Euclidean unit ball, which suggests there are convex bodies where this parameter is smaller than the number of variables. Section 3.3 proposes an interior point method tailored to the entropic barrier. We analyze this method in Section 3.4 under the idealistic assumption that we can compute the barrier's gradients and Hessians exactly. The next chapters will deal with the more realistic case that we have to use sampling to approximate these derivatives.

The analysis of a simplified method serves two purposes. First, it demonstrates that using the entropic barrier in itself does not significantly increase the

algorithm's number of iterations. Instead, the number of oracle calls in later chapters is largely determined by the complexity of the sampling routines. Moreover, this analysis lays some of the foundations for the more realistic discussion in later chapters.

The properties of the entropic barrier are already known, although we derive the derivatives of the log-partition function more formally than in the existing literature. The proposed interior point method is new, even though it is closely related to an algorithm by De Klerk et al. [35]. The analysis of our method has also not appeared before, but it is largely traditional.

3.1 Properties of the Entropic Barrier

Before we summarize the most important properties of the entropic barrier, let us introduce a piece of notation. If ϕ is a measurable function whose domain is the convex body $\mathcal{S}$, we define for any $\theta \in \mathbb{R}^n$

$$\mathbb{E}_\theta[\phi(X)] := \frac{\int_{\mathcal{S}} \phi(x) e^{\langle \theta, x \rangle} \, \mathrm{d}x}{\int_{\mathcal{S}} e^{\langle \theta, x \rangle} \, \mathrm{d}x}.$$

In other words, $\mathbb{E}_\theta[\phi(X)]$ is the expected value of ϕ applied to a random variable X following a Boltzmann distribution with parameter θ. Note that we suppress the dependence on $\mathcal{S}$; this should cause no confusion, as no other convex bodies will be introduced.

The following properties were originally shown by Klartag [64] and Bubeck and Eldan [21]. However, we derive the derivatives of the log-partition function more formally. Recall that the first, second, and third Fréchet derivatives of f at θ are denoted by $g(\theta)$, $H(\theta)$, and $T(\theta)$, respectively. Recall moreover that g^* denotes the gradient of f^*.

Proposition 3.3 ([64, Lemma 3.1], [21, Theorem 1])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let f and f^* be its associated log-partition function and entropic barrier, respectively. Then,*

(i) $g(\theta)[w] = \langle \mathbb{E}_\theta[X], w \rangle$ *for all* $w \in \mathbb{R}^n$*, or in vector notation,* $g(\theta) = \mathbb{E}_\theta[X]$*, for all* $\theta \in \mathbb{R}^n$.

(ii) $H(\theta)[v,w] = \mathbb{E}_\theta[\langle X-\mathbb{E}_\theta[X],v\rangle\langle X-\mathbb{E}_\theta[X],w\rangle]$ *for all* $v,w\in\mathbb{R}^n$ *and* $\theta\in\mathbb{R}^n$.

(iii) $T(\theta)[u,v,w] = \mathbb{E}_\theta[\langle X-\mathbb{E}_\theta[X],u\rangle\langle X-\mathbb{E}_\theta[X],v\rangle\langle X-\mathbb{E}_\theta[X],w\rangle]$ *for all* $u,v,w\in\mathbb{R}^n$ *and* $\theta\in\mathbb{R}^n$.

(iv) f *is self-concordant with* $\operatorname{dom} f = \mathbb{R}^n$.

(v) f^* *is self-concordant with* $\operatorname{dom} f^* = \operatorname{int}\mathcal{S}$.

(vi) The function g *is a bijection from* $\mathbb{R}^n$ *to* $\operatorname{int}\mathcal{S}$*, and* g^* *is its inverse.*

Proof. (i): Let $\tilde{f}(\theta) \coloneqq \exp(f(\theta)) = \int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x$ such that $f(\theta) = \log(\tilde{f}(\theta))$. By the chain rule (see Theorem A.2), we have for all $\theta, w\in\mathbb{R}^n$,

$$g(\theta)[w] = \frac{1}{\tilde{f}(\theta)}\tilde{g}(\theta)[w] = \frac{\tilde{g}(\theta)[w]}{\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x},$$

where $\tilde{g}(\theta)$ is the gradient of $\tilde{f}$ at θ. It therefore remains to show that $\tilde{g}(\theta)[w] = \int_{\mathcal{S}}\langle w,x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x$. Indeed,

$$\begin{aligned}
0 &\le \lim_{\|w\|\downarrow 0} \frac{|\tilde{f}(\theta+w)-\tilde{f}(\theta)-\int_{\mathcal{S}}\langle w,x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x|}{\|w\|}\\
&= \lim_{\|w\|\downarrow 0} \frac{\left|\int_{\mathcal{S}}\left(e^{\langle w,x\rangle}-1-\langle w,x\rangle\right)e^{\langle\theta,x\rangle}\,\mathrm{d}x\right|}{\|w\|}\\
&\le \int_{\mathcal{S}} \lim_{\|w\|\downarrow 0} \frac{\left|e^{\langle w,x\rangle}-1-\langle w,x\rangle\right|}{\|w\|} e^{\langle\theta,x\rangle}\,\mathrm{d}x = 0,
\end{aligned}$$

where the second inequality is due to the dominated convergence theorem and the upper bound is equal to zero because $e^t - 1 - t = o(t^2)$.

(ii): Using the quotient rule from Theorem A.4, we find for all $\theta, v\in\mathbb{R}^n$

$$H(\theta)[v] = \frac{1}{\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x}\tilde{H}(\theta)[v] - \frac{1}{\left(\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x\right)^2}\tilde{g}(\theta)[v]\tilde{g}(\theta),$$

where $\tilde{H}(\theta)$ is the Hessian of $\tilde{f}$ at θ. We claim that, for any $w\in\mathbb{R}^n$, $\tilde{H}(\theta)[v,w] =$

$\int_{\mathcal{S}} \langle v,x\rangle\langle w,x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x$, since

$$\begin{aligned}
0 &\leq \lim_{\|v\|\downarrow 0} \max_{w:\|w\|=1} \frac{\left|\tilde{g}(\theta+v)[w]-\tilde{g}(\theta)[w]-\int_{\mathcal{S}}\langle v,x\rangle\langle w,x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x\right|}{\|v\|} \\
&= \lim_{\|v\|\downarrow 0} \max_{w:\|w\|=1} \frac{\left|\int_{\mathcal{S}}\left(e^{\langle v,x\rangle}-1-\langle v,x\rangle\right)\langle w,x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x\right|}{\|v\|} \\
&\leq \int_{\mathcal{S}} \lim_{\|v\|\downarrow 0} \frac{\left|e^{\langle v,x\rangle}-1-\langle v,x\rangle\right|}{\|v\|}\|x\|e^{\langle\theta,x\rangle}\,\mathrm{d}x = 0,
\end{aligned}$$

where we now also use the Cauchy-Schwarz inequality and the boundedness of $\mathcal{S}$ to apply the dominated convergence theorem. In conclusion,

$$\begin{aligned}
H(\theta)[v,w] &= \frac{1}{\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x}\tilde{H}(\theta)[v,w]-\frac{1}{\left(\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x\right)^2}\tilde{g}(\theta)[v]\tilde{g}(\theta)[w] \\
&= \mathbb{E}_\theta[\langle X,v\rangle\langle X,w\rangle]-\mathbb{E}_\theta[\langle X,v\rangle]\mathbb{E}_\theta[\langle X,w\rangle] \\
&= \mathbb{E}_\theta[\langle X-\mathbb{E}_\theta[X],v\rangle\langle X-\mathbb{E}_\theta[X],w\rangle].
\end{aligned}$$

(iii): Can be shown in a way similar to (ii).

(iv): We check the conditions of Theorem 2.6 for f. First, by definition the domain of f is $\mathbb{R}^n$, which has no boundary. The first condition therefore holds vacuously. Second, it follows from Bubeck and Eldan [21, Lemma 2] that for any $\theta,u\in\mathbb{R}^n$,

$$\mathbb{E}_\theta[\langle X-\mathbb{E}_\theta[X],u\rangle^3] \leq 2\left(\mathbb{E}_\theta[\langle X-\mathbb{E}_\theta[X],u\rangle]\right)^{3/2}.$$

By (ii) and (iii), this statement is equivalent to $T(\theta)[u,u,u]\leq 2(H(\theta)[u,u])^{3/2}$ for all $\theta,u\in\mathbb{R}^n$. Hence, Lemma A.8 shows that the second condition of Theorem 2.6 also holds, proving that f is self-concordant.

(v): It was shown by Klartag [64, Lemma 3.1] that $\{g(\theta):\theta\in\mathbb{R}^n\}=\operatorname{int}\mathcal{S}$. Since f is self-concordant, Proposition 2.10 proves that $\operatorname{dom} f^*=\operatorname{int}\mathcal{S}$, and Theorem 2.13 proves f^* is self-concordant.

(vi): By Proposition 2.10, g is injective. The bijection is established through Klartag's result [64, Lemma 3.1] that $\{g(\theta):\theta\in\mathbb{R}^n\}=\operatorname{int}\mathcal{S}$. Theorem 2.12 shows g^* is the inverse of g. □

The results (i) and (ii) above show that the derivatives of the log-partition function f have a stochastic interpretation. The gradient $g(\theta)$ corresponds to the

expected value of a Boltzmann distribution with parameter θ, and $H(\theta)$ is the covariance operator of the same distribution. For this reason, we will use where appropriate the notation

$$x(\theta) \coloneqq g(\theta) \quad \text{and} \quad \Sigma(\theta) \coloneqq H(\theta), \quad \text{where } f(\theta) = \log \int_{\mathcal{S}} e^{\langle \theta, x \rangle} \, \mathrm{d}x.$$

By Proposition 3.3(vi), g^* and g are each other's inverses. Hence, if f is the log-partition function, g^* assigns to each $x \in \operatorname{int} \mathcal{S}$ the $\theta \in \mathbb{R}^n$ such that $g(\theta) = x$. We therefore also introduce the notation

$$\theta(x) \coloneqq g^*(x), \quad \text{where } f(\theta) = \log \int_{\mathcal{S}} e^{\langle \theta, x \rangle} \, \mathrm{d}x.$$

A summary of the notation and properties of the log-partition function and its conjugate is presented in Table 3.1.

	Log-partition function f	Entropic barrier f^*
Function	$f(\theta) = \log \int_{\mathcal{S}} e^{\langle \theta, x \rangle} \, \mathrm{d}x$	$f^*(x) = \sup_{\theta \in \mathbb{R}^n} \{\langle \theta, x \rangle - f(\theta)\}$
Gradient	$g(\theta) = \mathbb{E}_\theta[X] = x(\theta)$	$g^*(x) = \theta(x)$ such that $g(\theta(x)) = x$
Hessian	$H(\theta) = \Sigma(\theta)$	$H^*(x) = H(g^*(x))^{-1} = \Sigma(\theta(x))^{-1}$
Domain	$\theta \in \mathbb{R}^n$	$x \in \operatorname{int} \mathcal{S}$

Table 3.1: Overview of the properties of the log-partition function and its conjugate, the entropic barrier

So far we have seen that the entropic barrier is a self-concordant functional with domain $\operatorname{int} \mathcal{S}$. As its name suggests though, the entropic barrier is moreover a barrier in the sense of Definition 2.7, as shown by Bubeck and Eldan [21].

Theorem 3.4 ([21, Theorem 1])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let f^* be its associated entropic barrier. Then, f^* is a self-concordant barrier on $\mathcal{S}$ with complexity parameter*

$$\vartheta_{f^*} \leq \left(1 + 100\sqrt{\log(n)/n}\right) n,$$

for $n \geq 80$.

The proof of this theorem depends on the fact that by Proposition 3.3(vi) and Theorem 2.12,

$$\begin{aligned}\vartheta_{f^*} &= \sup_{x\in\operatorname{dom} f^*} (\|g_x^*(x)\|_x^*)^2 \\ &= \sup_{x\in\operatorname{int}\mathcal{S}} \langle g^*(x), H^*(x)^{-1} g^*(x)\rangle \\ &= \sup_{\theta\in\mathbb{R}^n} \langle g^*(g(\theta)), H^*(g(\theta))^{-1} g^*(g(\theta))\rangle \\ &= \sup_{\theta\in\mathbb{R}^n} \langle \theta, \Sigma(\theta)\theta\rangle = \sup_{\theta\in\mathbb{R}^n} \|\theta\|_\theta^2,\end{aligned} \tag{3.1}$$

such that the bound on ϑ_{f^*} can be established through a careful analysis of the variance along the direction θ of the Boltzmann distribution with parameter θ. For instance, it can be shown that if $\mathcal{S}$ is the hypercube $[0,1]^n$ in $\mathbb{R}^n$, the complexity parameter satisfies $\vartheta_{f^*} = n$. For general domains $\mathcal{S}$, such an analysis goes somewhat outside the scope of this thesis, so we refer the reader to Bubeck and Eldan [21]. They use technical log-concavity arguments to show that $\langle\theta, \Sigma(\theta)\theta\rangle$ can be upper bounded by the variance of a certain normal random variable. The constants in Theorem 3.4 are not fundamental to their proof.

It is worth noting that ϑ_{f^*} will only be used as an upper bound. If the value of ϑ_{f^*} is unknown, it is therefore allowed to replace ϑ_{f^*} by its upper bound from Theorem 3.4.

The entropic barrier has some interesting applications. For instance, we use it to derive a non-trivial lower bound on the spectrum of $\Sigma(\theta)$ for any $\theta \in \mathbb{R}^n$ in Appendix B.

3.2 The Complexity Parameter of the Entropic Barrier for the Unit Ball

Although we did not prove Theorem 3.4 for general convex bodies, we will consider (3.1) for the special case where $\operatorname{int}\mathcal{S} = \mathfrak{B}(0,1)$, the unit ball in $\mathbb{R}^n$, and $\langle\cdot,\cdot\rangle$ is the Euclidean inner product. This choice is interesting because numerical evidence presented below suggests that $\vartheta_{f^*} = \frac{1}{2}(n+1)$. For $n > 1$, this is, to our knowledge, the only set where it is suspected that $\vartheta_{f^*} < n$, i.e. where the bound

in Theorem 3.4 is significantly off. (Note that $\vartheta_{f^*} = \frac{1}{2}(n+1)$ would still be significantly worse than the complexity parameter 1 of the logarithmic barrier for the unit ball.) It follows from (3.1) that

$$\vartheta_{f^*} = \sup_{\theta\in\mathbb{R}^n} \mathbb{E}_\theta[\langle X - \mathbb{E}_\theta[X], \theta\rangle^2] = \sup_{\theta\in\mathbb{R}^n} \left\{\mathbb{E}_\theta[\langle X, \theta\rangle^2] - \langle \mathbb{E}_\theta[X], \theta\rangle^2\right\}.$$

For every $\theta \in \mathbb{R}^n$, there exists a rotation matrix Q with $|\det Q| = 1$ such that $\langle \theta, Qy\rangle = \|\theta\| y_1$ for all $y \in \mathbb{R}^n$. Using the fact that the volume of an $(n-1)$-dimensional ball with radius r is r^{n-1} times some factor depending only on n, we see that

$$\begin{aligned}\langle \mathbb{E}_\theta[X], \theta\rangle &= \frac{\int_{\mathfrak{B}(0,1)} \langle \theta, x\rangle e^{\langle\theta,x\rangle}\,\mathrm{d}x}{\int_{\mathfrak{B}(0,1)} e^{\langle\theta,x\rangle}\,\mathrm{d}x} \\ &= \frac{\int_{\mathfrak{B}(0,1)} \|\theta\| y_1 e^{\|\theta\| y_1}\,\mathrm{d}y}{\int_{\mathfrak{B}(0,1)} e^{\|\theta\| y_1}\,\mathrm{d}y} = \frac{\int_{-1}^1 \|\theta\| y_1 \left(\sqrt{1-y_1^2}\right)^{n-1} e^{\|\theta\| y_1}\,\mathrm{d}y_1}{\int_{-1}^1 \left(\sqrt{1-y_1^2}\right)^{n-1} e^{\|\theta\| y_1}\,\mathrm{d}y_1}.\end{aligned}$$

The final expression cannot be computed in closed form, but it can be approximated numerically for fixed n and $\|\theta\|$. Similarly,

$$\begin{aligned}\mathbb{E}_\theta[\langle X, \theta\rangle^2] &= \frac{\int_{\mathfrak{B}(0,1)} \langle \theta, x\rangle^2 e^{\langle\theta,x\rangle}\,\mathrm{d}x}{\int_{B_n} e^{\langle\theta,x\rangle}\,\mathrm{d}x} \\ &= \frac{\int_{\mathfrak{B}(0,1)} \|\theta\|^2 y_1^2 e^{\|\theta\| y_1}\,\mathrm{d}y}{\int_{\mathfrak{B}(0,1)} e^{\|\theta\| y_1}\,\mathrm{d}y} = \frac{\int_{-1}^1 \|\theta\|^2 y_1^2 \left(\sqrt{1-y_1^2}\right)^{n-1} e^{\|\theta\| y_1}\,\mathrm{d}y_1}{\int_{-1}^1 \left(\sqrt{1-y_1^2}\right)^{n-1} e^{\|\theta\| y_1}\,\mathrm{d}y_1}.\end{aligned}$$

Numerical approximation of $\mathbb{E}_\theta[\langle X, \theta\rangle^2] - \langle \mathbb{E}_\theta[X], \theta\rangle^2]$ for different values of n and $\|\theta\|$ using Matlab's `integral` function yields Figure 3.1, which suggests that $\vartheta_{f^*} = \frac{1}{2}(n+1)$.

3.3 Statement of a Simple Interior Point Method

With the main properties of the entropic barrier established, let us show that this barrier could be used to solve convex optimization problems. To be precise, we will consider the problem

$$\min_{x\in\mathcal{S}} \langle c, x\rangle, \tag{3.2}$$

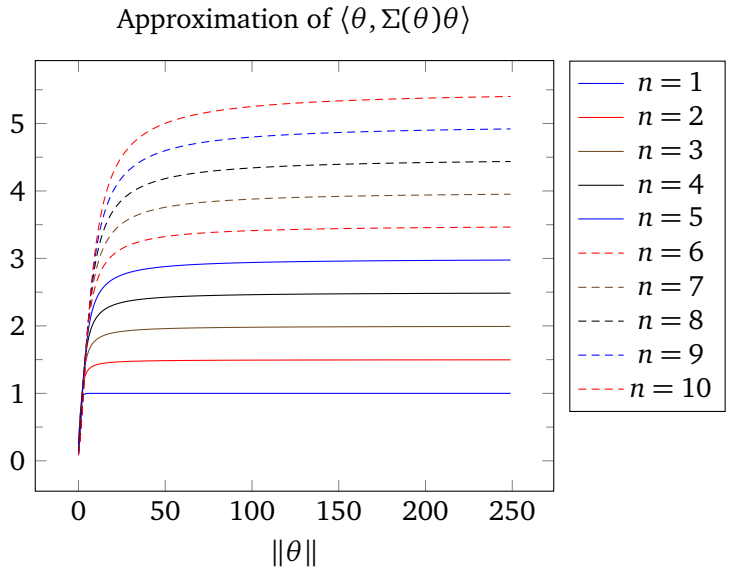

Figure 3.1: Numerical approximation of $\langle \theta, \Sigma(\theta)\theta \rangle$ for the Euclidean unit ball $\mathfrak{B}(0,1)$ in $\mathbb{R}^n$

where $\mathcal{S} \subset \mathbb{R}^n$ is a convex body, and $c \in \mathbb{R}^n$. There are a number of self-concordant barriers that we could define over $\mathcal{S}$, such as the entropic barrier or the universal barrier from Nesterov and Nemirovskii [85]. The main problem is that the derivatives of these barriers can usually not be computed in closed form. The derivatives of the universal barrier at $x \in \mathcal{S}$ could be approximated through sampling from the polar set $\{v \in \mathbb{R}^n : \langle v, y - x \rangle \leq 1 \, \forall y \in \mathcal{S}\}$. However, the derivatives of the entropic barrier can be approximated through sampling directly from $\mathcal{S}$, which is more attractive if we only have a membership oracle for $\mathcal{S}$. In this chapter, we will assume for simplicity's sake that we can compute the gradients and Hessians of the entropic barrier exactly.

One might argue that under this assumption, one could simply cite the analysis from any short-step interior point method (such as Section 2.4.2 in Renegar [95]). To make our analysis more realistic, we will not use the standard Newton step. The reason we would be interested in this change is the following: short-step

interior point methods start with an approximate minimizer to

$$f_\eta^*(x) := \eta\langle c, x\rangle + f^*(x),$$

for some $\eta > 0$, then increase η by a fixed factor to η_+, and take a (usually Newton) step to find an approximate minimizer to $f_{\eta_+}^*$, and so on. In case of the entropic barrier, the Newton step at $x \in \operatorname{dom} f^*$ to minimize f_η^* would be

$$-H^*(x)^{-1}[\eta c + g^*(x)] = -\Sigma(\theta(x))[\eta c + \theta(x)]. \tag{3.3}$$

In reality, we usually do not know $\theta(x)$, so it will have to be approximated. Likewise, $\Sigma(\theta)$ is generally unknown for any $\theta \in \mathbb{R}^n$, and will therefore also have to be approximated. Both these approximations introduce errors, and the composition of these errors in $\Sigma(\theta(x))$ is inconvenient to analyze. Abernethy and Hazan [1, Appendix D] therefore propose to use the Hessian at

$$z(\eta) := \operatorname*{arg\,min}_{x \in \operatorname{dom} f^*} f_\eta^*(x) = \operatorname*{arg\,min}_{x \in \operatorname{dom} f^*} \{\eta\langle c, x\rangle + f^*(x)\},$$

the minimizer of f_η^*. Since this minimizer satisfies $0 = \eta c + g^*(z(\eta))$, Theorem 2.12 shows

$$z(\eta) = g(-\eta c) = x(-\eta c). \tag{3.4}$$

Then, the following step could be used instead of (3.3):

$$\begin{aligned} -H^*(z(\eta))^{-1}[\eta c + g^*(x)] &= -H(-\eta c)[\eta c + g^*(x)] \\ &= -\Sigma(-\eta c)[\eta c + \theta(x)]. \end{aligned} \tag{3.5}$$

In this case, the parameter of the Boltzmann distribution for which we need to approximate the covariance is known exactly.

In the remainder of this chapter, we will show that the step (3.5) can be used in a short-step method that converges in polynomial time. However, we will not (necessarily) take the full step (3.5). Instead, we will scale the step (3.5) by a damping parameter $\gamma \in [\frac{4}{5}, 1]$ to

$$-\gamma H^*(z(\eta))^{-1}[\eta c + g^*(x)] = -\gamma\Sigma(-\eta c)[\eta c + \theta(x)], \tag{3.6}$$

and prove that the method still works. The reason is again due to the particular properties of the entropic barrier. Because in reality we cannot compute the

gradient or Hessian of the entropic barrier exactly, they will only be known up to some error. De Klerk et al. [35] analyze the performance of the step (3.6) for a particular γ when the Hessian and gradient contain errors. Our purpose is to analyze the step (3.6) if it is known exactly. This will bridge the gap between [35] and a classical short-step method that would use (3.3). As we will see, using (3.6) instead of (3.3) does not make solving the problem (3.2) significantly harder.

The short-step interior point method we will analyze is given in Algorithm 3.1. Note that we assume to know a starting point near the analytic curve $\{z(\eta) : \eta > 0\}$, which is known as the *central path*. Given any point in the interior of $\mathcal{S}$, such a starting point can be computed using a short-step method similar to Algorithm 3.1, see Renegar [95, pages 47-48].

Algorithm 3.1 A simple short-step algorithm using the entropic barrier f^*

Input: entropic barrier f^* over a convex body $\mathcal{S} \subset \mathbb{R}^n$;
objective $c \in \mathbb{R}^n$;
optimality tolerance $\varepsilon > 0$;
$\eta_0 > 0$ and $x_0 \in \operatorname{int}\mathcal{S}$ such that $\|x_0 - z(\eta_0)\|^*_{z(\eta_0)} \leq \frac{1}{6}$.

Output: $x_k \in \mathcal{S}$ such that $\langle c, x_k\rangle \leq \min_{x\in\mathcal{S}}\langle c, x\rangle + \varepsilon$.

1: $k \leftarrow 0$
2: **while** $\frac{7}{6}\vartheta_{f^*}/\eta_k > \varepsilon$ **do**
3: $\quad\eta_{k+1} \leftarrow \eta_0(1 + 1/(16\sqrt{\vartheta_{f^*}}))^{k+1}$
4: $\quad$Pick a $\gamma_k \in [\frac{4}{5}, 1]$
5: $\quad x_{k+1} \leftarrow x_k - \gamma_k H^*(z(\eta_{k+1}))^{-1}[\eta_{k+1}c + g^*(x_k)]$
6: $\quad k \leftarrow k + 1$
7: **return** x_k

3.4 Analysis of a Simple Interior Point Method

One of the starting conditions for Algorithm 3.1 is $\|x_0 - z(\eta_0)\|^*_{z(\eta_0)} \leq \frac{1}{6}$. The bulk of our argument will be dedicated to proving $\|x_k - z(\eta_k)\|^*_{z(\eta_k)} \leq \frac{1}{6}$ for all iterations k. It will then follow that for sufficiently high k, the point x_k is near-optimal.

The following lemma, based on Renegar [95], will be central to the analysis of the distance to the central path.

Lemma 3.5 (Based on [95, Theorem 2.2.1]). *Let f^* be a self-concordant functional. Then, for all $z \in \operatorname{dom} f^*$, $y \in \mathfrak{B}_z(z,1)$ and $\gamma \in (0,1]$,*

$$\left\|I - \gamma H_z^*(y)\right\|_z^* \leq \frac{1}{\gamma(1-\|y-z\|_z^*)^2} - 1.$$

Proof. Let $\lambda_1 \leq \cdots \leq \lambda_n$ denote the eigenvalues of $H_z^*(y)$ (with respect to $\langle\cdot,\cdot\rangle_z^*$). Since the eigenvalues of $I - \gamma H_z^*(y)$ are $1-\gamma\lambda_i$, where $i \in \{1,...,n\}$, we have

$$\begin{aligned}\left\|I - \gamma H_z^*(y)\right\|_z^* &= \max\{\gamma\lambda_n - 1, 1 - \gamma\lambda_1\} \\ &\leq \max\{\gamma\lambda_n - 1, \tfrac{1}{\gamma\lambda_1} - 1\} \\ &= \max\{\gamma\|H_z^*(y)\|_z^* - 1, \tfrac{1}{\gamma}\|H_z^*(y)^{-1}\|_z^* - 1\}.\end{aligned}$$

The inequality follows from the fact that if $1-\gamma\lambda_1 \geq \gamma\lambda_n - 1$, then we must have $2\gamma\lambda_1 \leq \gamma(\lambda_1+\lambda_n) \leq 2$, and hence $\gamma\lambda_1 \leq 1$. The result now follows from Equation (2.1) in Renegar [95]. □

We can now analyze the progress made to the next minimizer $z(\eta_{k+1})$ of $f_{\eta_{k+1}}^*$ by the step in Line 5 in Algorithm 3.1.

Lemma 3.6 (Based on [95, Theorems 1.6.2 and 2.2.3]). *Let f^* be a self-concordant functional with minimizer z, and let $x \in \mathfrak{B}_z(z,1)$. Define $x_+ = x - \gamma H^*(z)^{-1} g^*(x)$ for some $\gamma \in (0,1]$. Then,*

$$\|x_+ - z\|_z^* \leq \|x-z\|_z^* \left[\frac{1}{\gamma(1-\|x-z\|_z^*)} - 1\right].$$

Proof. Since $g^*(z) = 0 = g_z^*(z)$,

$$\|x_+ - z\|_z^* = \|x - z - \gamma g_z^*(x)\|_z^* = \|x - z - \gamma[g_z^*(x) - g_z^*(z)]\|_z^*.$$

Using $H_z^*(z) = I$, it follows from the fundamental theorem of calculus (see e.g. Theorem 1.5.6 in Renegar [95]) that

$$\begin{aligned}\|x_+ - z\|_z^* &= \left\| x - z - \gamma \int_0^1 H_z^*(z + t(x-z))[x-z]\,\mathrm{d}t \right\|_z^* \\ &= \left\| \int_0^1 \left[I - \gamma H_z^*(z + t(x-z))\right][x-z]\,\mathrm{d}t \right\|_z^* \\ &\leq \|x-z\|_z^* \int_0^1 \left\|I - \gamma H_z^*(z + t(x-z))\right\|_z^* \mathrm{d}t.\end{aligned}$$

We then invoke Lemma 3.5 to show that

$$\|x_+ - z\|_z^* \leq \|x - z\|_z^* \int_0^1 \left[\frac{1}{\gamma(1 - t\|x - z\|_z^*)^2} - 1 \right] \mathrm{d}t,$$

which completes the proof. □

Observe that if $\gamma = 1$ and $\|x - z\|_z^* < \frac{1}{2}$, then $\|x_+ - z\|_z^* < \|x - z\|_z^*$, meaning that we get closer to the minimizer in the z-norm by taking the step from x to x_+.

We see that the step in Line 5 in Algorithm 3.1 can be used to approximate the minimizer $z(\eta_{k+1})$ of $f_{\eta_{k+1}}^*$, provided we start close enough to $z(\eta_{k+1})$. Since our running assumption is that we have an x_k close to $z(\eta_k)$, it suffices to bound the distance between $z(\eta_{k+1})$ and $z(\eta_k)$. The next result provides a way to relate the distance between $z(\eta_{k+1})$ and $z(\eta_k)$ to the distance between $-\eta_{k+1}c$ and $-\eta_k c$ (which we know about, since we control the difference between η_{k+1} and η_k). We first state the result in general terms, and then derive a corollary about the minimizers.

Proposition 3.7. *Let f be a self-concordant functional, and let $x, y \in \operatorname{dom} f^*$. If $\|y - x\|_x^* < 1$,*

$$\|g^*(y) - g^*(x)\|_{g^*(x)} \leq \frac{\|y - x\|_x^*}{1 - \|y - x\|_x^*}. \tag{3.7}$$

Similarly, if $\|g^*(y) - g^*(x)\|_{g^*(x)} < 1$,

$$\|y - x\|_x^* \leq \frac{\|g^*(y) - g^*(x)\|_{g^*(x)}}{1 - \|g^*(y) - g^*(x)\|_{g^*(x)}}. \tag{3.8}$$

Proof. Assuming $\|y - x\|_x^* < 1$, we will show (3.7). By Theorem 2.12,

$$\|g^*(y) - g^*(x)\|_{g^*(x)} = \|g^*(y) - g^*(x)\|_{H^*(x)^{-1}} = \|g_x^*(y) - g_x^*(x)\|_x^*.$$

Since f is self-concordant, f^* is also self-concordant by Theorem 2.13. We can therefore invoke the fundamental theorem of calculus (see e.g. Theorem 1.5.6 in

Renegar [95]) and Theorem 2.2.1 from Renegar [95] to show

$$\begin{aligned}\|g^*(y)-g^*(x)\|_{g^*(x)} &= \|g_x^*(y)-g_x^*(x)\|_x^* \\ &= \left\| \int_0^1 H_x^*(x+t[y-x])[y-x]\,\mathrm{d}t \right\|_x^* \\ &\le \|y-x\|_x^* \int_0^1 \left\|H_x^*(x+t[y-x])\right\|_x^* \mathrm{d}t \\ &\le \|y-x\|_x^* \int_0^1 \frac{1}{(1-t\|y-x\|_x^*)^2}\,\mathrm{d}t = \frac{\|y-x\|_x^*}{1-\|y-x\|_x^*},\end{aligned}$$

which proves (3.7). The relation (3.8) can be derived in the same manner by interchanging x and $g^*(x)$, y and $g^*(y)$, and f and f^*. □

As a consequence, the following can now be said about the distance between $z(\eta_{k+1})$ and $z(\eta_k)$.

Corollary 3.8. *Let f^* be a self-concordant barrier, and fix $c \in \mathbb{R}^n$. Let $\eta > 0$ and $\eta_+ = (1+\beta/\sqrt{\vartheta_{f^*}})\eta$ for some $\beta \in [0,1)$. Assume $z(\eta)$ and $z(\eta_+)$ are well defined. Then,*

$$\|z(\eta_+)-z(\eta)\|_{z(\eta)}^* \le \frac{\beta}{1-\beta}.$$

Proof. By (3.4) and Theorem 2.12, we have $g^*(z(\eta)) = -\eta c$ and $g^*(z(\eta_+)) = -\eta_+ c$. Hence, by (3.8),

$$\|z(\eta_+)-z(\eta)\|_{z(\eta)}^* \le \frac{\|g^*(z(\eta_+))-g^*(z(\eta))\|_{g^*(z(\eta))}}{1-\|g^*(z(\eta_+))-g^*(z(\eta))\|_{g^*(z(\eta))}} = \frac{\|(\eta_+-\eta)c\|_{-\eta c}}{1-\|(\eta_+-\eta)c\|_{-\eta c}}.$$

By our choice of η_+ and (3.1),

$$\|(\eta_+-\eta)c\|_{-\eta c} = \frac{\eta_+-\eta}{\eta}\|-\eta c\|_{-\eta c} = \frac{\beta}{\sqrt{\vartheta_{f^*}}}\|-\eta c\|_{-\eta c} \le \frac{\beta}{\sqrt{\vartheta_{f^*}}}\sqrt{\vartheta_{f^*}} = \beta, \quad (3.9)$$

which completes the proof. □

Let us combine Lemma 3.6 and Corollary 3.8 to show that the distance to the central path remains below $\frac{1}{6}$ after taking the step in Line 5 of Algorithm 3.1.

Lemma 3.9. *Let f^* be a self-concordant barrier, and fix $c \in \mathbb{R}^n$. Let $\eta > 0$ and $\eta_+ = (1+\beta/\sqrt{\vartheta_{f^*}})\eta$ for $\beta = \frac{1}{16}$. Assume $z(\eta)$ and $z(\eta_+)$ are well defined. Let $x \in \operatorname{dom} f^*$ such that $\|x - z(\eta)\|^*_{z(\eta)} \le \delta = \frac{1}{6}$, and define*

$$x_+ := x - \gamma H^*(z(\eta_+))^{-1}[\eta_+ c + g^*(x)],$$

where $\gamma \in [\frac{4}{5}, 1]$. Then,

$$\|x_+ - z(\eta_+)\|^*_{z(\eta_+)} \le \delta.$$

Proof. Since $\beta < \frac{1}{2}$, Corollary 3.8 shows $\|z(\eta) - z(\eta_+)\|^*_{z(\eta)} < 1$. Application of self-concordance (2.1) thus shows

$$\begin{aligned}
\|x - z(\eta_+)\|^*_{z(\eta_+)} &\le \frac{\|x - z(\eta_+)\|^*_{z(\eta)}}{1 - \|z(\eta) - z(\eta_+)\|^*_{z(\eta)}} \\
&\le \frac{\|x - z(\eta)\|^*_{z(\eta)} + \|z(\eta) - z(\eta_+)\|^*_{z(\eta)}}{1 - \|z(\eta) - z(\eta_+)\|^*_{z(\eta)}} \\
&\le \frac{\delta + \beta/(1-\beta)}{1 - \beta/(1-\beta)} = \tfrac{1}{4}.
\end{aligned}$$

Therefore, Lemma 3.6 shows

$$\begin{aligned}
\|x_+ - z(\eta_+)\|^*_{z(\eta_+)} &\le \|x - z(\eta_+)\|^*_{z(\eta_+)} \left[\frac{1}{\gamma(1 - \|x - z(\eta_+)\|^*_{z(\eta_+)})} - 1 \right] \\
&\le \tfrac{1}{4} \left[\frac{1}{\gamma(1 - \frac{1}{4})} - 1 \right] \le \tfrac{1}{6} = \delta,
\end{aligned}$$

where the final inequality holds for all $\gamma \ge \frac{4}{5}$. □

Algorithm 3.1 thus stays close to the central path. The main thing left to show is that following the central path eventually yields a near-optimal solution. As the following result from Renegar [95] demonstrates, this will be the case for sufficiently large values of η.

Lemma 3.10 ([95, pages 44-45])**.** *Let f^* be a self-concordant barrier, and fix $c \in \mathbb{R}^n$. Let $\eta > 0$, and assume $z(\eta)$ is well defined. Let $x \in \operatorname{dom} f^*$ such that $\|x - z(\eta)\|^*_{z(\eta)} \le \delta$ for some $\delta \ge 0$. Then,*

$$\langle c, x \rangle \le \operatorname{val} + \frac{(1+\delta)\vartheta_{f^*}}{\eta},$$

where $\text{val} := \min_{x\in\mathcal{S}}\langle c, x\rangle$.

Proof. We have $g^*(z(\eta)) = -\eta c$, and therefore Theorem 2.8 shows that for all $y \in \operatorname{dom} f^*$,

$$\langle c, z(\eta)\rangle - \langle c, y\rangle = \frac{\langle g^*(z(\eta)), y - z(\eta)\rangle}{\eta} < \frac{\vartheta_{f^*}}{\eta}.$$

Consequently,

$$\langle c, z(\eta)\rangle \le \text{val} + \vartheta_{f^*}/\eta. \tag{3.10}$$

For a point $x \in \operatorname{dom} f^*$ such that $\|x - z(\eta)\|^*_{z(\eta)} \le \delta$, we therefore have by Cauchy-Schwarz,

$$\begin{aligned}\langle c, x\rangle &\le \langle c, z(\eta)\rangle + \langle H^*(z(\eta))^{-1}c, x - z(\eta)\rangle^*_{z(\eta)} \\ &\le \text{val} + \frac{\vartheta_{f^*}}{\eta} + \delta\|H^*(z(\eta))^{-1}c\|^*_{z(\eta)}.\end{aligned} \tag{3.11}$$

To bound $\|H^*(z(\eta))^{-1}c\|^*_{z(\eta)}$, note that for any $v \in \mathbb{R}^n$ and $0 \le t < 1/\|v\|^*_{z(\eta)}$, it holds that $z(\eta) - tv \in \operatorname{dom} f^*$. Hence, $\text{val} \le \langle c, z(\eta)\rangle - \langle c, v\rangle/\|v\|^*_{z(\eta)}$. For $v = H^*(z(\eta))^{-1}c$, this inequality shows

$$\langle c, z(\eta)\rangle - \text{val} \ge \frac{\langle c, v\rangle}{\|v\|^*_{z(\eta)}} = \frac{\langle c, H^*(z(\eta))^{-1}c\rangle}{\sqrt{\langle c, H^*(z(\eta))^{-1}c\rangle}} = \|H^*(z(\eta))^{-1}c\|^*_{z(\eta)}.$$

Combined with (3.11) and (3.10), the above shows that for all $x \in \operatorname{dom} f^*$ such that $\|x - z(\eta)\|^*_{z(\eta)} \le \delta$,

$$\langle c, x\rangle \le \text{val} + \frac{\vartheta_{f^*}}{\eta} + \delta(\langle c, z(\eta)\rangle - \text{val}) \le \text{val} + \frac{(1+\delta)\vartheta_{f^*}}{\eta}.$$ □

We end this section by proving that $O(\sqrt{\vartheta_{f^*}}\log(\vartheta_{f^*}/\varepsilon))$ steps suffice for Algorithm 3.1 to reach an ε-optimal solution. The analysis largely follows Renegar [95].

Proposition 3.11 ([95, pages 45-47])**.** *After*

$$k \le 17\sqrt{\vartheta_{f^*}}\log\left(\frac{7\vartheta_{f^*}}{6\varepsilon\eta_0}\right) + 1 = O\left(\sqrt{\vartheta_{f^*}}\log\left(\frac{\vartheta_{f^*}}{\varepsilon\eta_0}\right)\right) \tag{3.12}$$

iterations, Algorithm 3.1 will return a solution $x_k \in \mathcal{S}$ *with* $\langle c, x_k\rangle \le \text{val} + \varepsilon$*, where* $\text{val} := \min_{x\in\mathcal{S}}\langle c, x\rangle$.

Proof. Repeated application of Lemma 3.9 shows that $\|x_k - z(\eta_k)\|^*_{z(\eta_k)} \leq \frac{1}{6}$ for all iterations k of Algorithm 3.1. By Lemma 3.10, the proof will be completed by showing that the number of iterations k before $\frac{7}{6}\vartheta_{f^*}/\eta_k \leq \varepsilon$ satisfies (3.12). In other words, we are looking for the smallest solution k to

$$\frac{7\vartheta_{f^*}}{6\varepsilon} \leq \eta_0 \left(1 + \frac{1}{16\sqrt{\vartheta_{f^*}}}\right)^k.$$

The smallest k that satisfies this inequality is

$$k = \left\lceil \frac{\log\left(\frac{7\vartheta_{f^*}}{6\varepsilon\eta_0}\right)}{\log\left(1 + \frac{1}{16\sqrt{\vartheta_{f^*}}}\right)} \right\rceil \leq 17\sqrt{\vartheta_{f^*}} \log\left(\frac{7\vartheta_{f^*}}{6\varepsilon\eta_0}\right) + 1,$$

where the inequality uses $\vartheta_{f^*} \geq 1$. □

Let us briefly summarize this chapter. Due to the properties of the entropic barrier outlined in Section 3.1, we argued in Section 3.3 that a short-step method using this barrier and the standard Newton step would be inconvenient to analyze. Instead, we proposed Algorithm 3.1, where the main difference with a textbook short-step method is the step in Line 5. However, as we saw above, the worst-case complexity for Algorithm 3.1 is the same as for traditional short-step methods, see e.g. Renegar [95, page 47]. In this sense, the entropic barrier does not yet present any difficulties that lead to a worse complexity for a short-step method.

Of course, there is one problem we sidestepped in this chapter: we generally do not have access to the derivatives of the entropic barrier, and they will have to be approximated by sampling. This is the topic of the next few chapters. In Chapter 4, we will introduce the sampling technique of our choice: hit-and-run sampling. Chapter 5 shows how this sampling technique can be used to approximate the mean and covariance matrix of a Boltzmann distribution to a desired accuracy. These tools are used in Chapter 6 to analyze a short-step method using the entropic barrier where the derivatives are approximated using hit-and-run sampling.

4

Hit-and-Run Sampling

As we saw in the last chapter, the gradient and Hessian of the entropic barrier have a stochastic interpretation. If we want to use this barrier in practice, we will need to find a way to (approximately) compute its gradient and Hessian. Since these derivatives are not known in closed form for general domains $\mathcal{S}$, the most promising approach is sampling. We therefore want to generate samples from some Boltzmann distribution over a convex body $\mathcal{S}$ with a given parameter $\theta \in \mathbb{R}^n$.

In this chapter, we explore how this can be done with a technique called hit-and-run sampling, to be defined in Section 4.1. In order to analyze this procedure, we collect some background material from probability and measure theory in Section 4.2. The chapter concludes in Section 4.3 with an analysis of the *mixing time* for hit-and-run applied to the Boltzmann distribution. In other words, we will investigate how many hit-and-run steps are necessary to find a point that approximately follows the desired Boltzmann distribution.

The chapter largely follows Sections 2.3 and 4 from Badenbroek and De Klerk [8]. Lemma 4.10 and Corollary 4.13 replace [8, Lemmas 4.4 and 4.6], leading to

a simpler statement of Theorem 4.14.

4.1 Hit-and-Run and its Implementation

The procedure we will use to generate samples is called *hit-and-run* sampling. This random walk was introduced for the uniform distribution by Smith [102] and later generalized to absolutely continuous distributions (see for example Bélisle et al. [11]). It was shown by Lovász [70] that, after preprocessing, hit-and-run sampling can generate an approximately uniformly distributed point from $O^*(n^3)$ membership oracle calls, where O^* suppresses polylogarithmic terms in the problem parameters. Lovász and Vempala [72] later showed that hit-and-run sampling can also be used to generate a point that approximately follows a Boltzmann distribution, while using $O^*(n^3)$ oracle calls after preprocessing. The mixing time for hit-and-run sampling is attractive compared to alternatives such as the ball walk, as argued in the survey by Vempala [107]. We will use the version of hit-and-run sampling in Algorithm 4.1, based on Lovász and Vempala [71].

This procedure samples a random direction D_i from a normal distribution $\mathcal{N}(0, \Sigma)$ with mean 0 and covariance matrix Σ (we will see some good choices of Σ later). The next iterate X_i is then sampled from the desired distribution restricted to the line through X_{i-1} in the direction D_i, intersected with $\mathcal{S}$. Effectively, this reduces a high-dimensional sampling problem to a sequence of one-dimensional sampling problems.

We continue with some comments on the implementation of Algorithm 4.1. If $\mathcal{S}$ is a set which is easy to work with, such as a polyhedron, Line 5 may be implemented in closed form. For general sets for which only a membership oracle is known, one can use the bisection method to efficiently approximate the end points of the line segment. If we are using hit-and-run sampling to solve an optimization problem over $\mathcal{S}$, the tolerance in this approximation could be a fraction of the optimality tolerance. Thus, the number of calls to the membership oracle by Algorithm 4.1 would be $O^*(\ell)$. After compensating the optimality tolerance for the inaccuracy in the end points of the line segments, we are (in the worst case) in the setting where we can compute the end point of the line segments exactly. To prevent such trivial complications, we will assume that the end points of the

Algorithm 4.1 The hit-and-run sampling procedure

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$;
function $\phi : \mathcal{S} \to \mathbb{R}_+$ proportional to the probability density with respect to the Lebesgue measure of the distribution to sample from (i.e. the target distribution);
covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$;
starting point $x \in \mathcal{S}$;
number of hit-and-run steps ℓ.

Output: X_ℓ following a distribution close to the distribution induced by ϕ.

1: $X_0 \leftarrow x$
2: Sample directions $D_1, ..., D_\ell$ i.i.d. from a $\mathcal{N}(0, \Sigma)$-distribution
3: Sample $P_1, ..., P_\ell$ i.i.d. from a uniform distribution over $[0, 1]$, independent from $D_1, ..., D_\ell$
4: **for** $i \in \{1, ..., \ell\}$ **do**
5: Determine end points Y_i and Z_i of the line segment $\mathcal{S} \cap \{X_{i-1} + tD_i : t \in \mathbb{R}\}$
6: Find $s \in [0, 1]$ such that $\int_0^s \phi(Y_i + t(Z_i - Y_i))\,\mathrm{d}t = P_i \int_0^1 \phi(Y_i + t(Z_i - Y_i))\,\mathrm{d}t$
7: $X_i \leftarrow Y_i + s(Z_i - Y_i)$
8: **return** X_ℓ

line segments can be computed exactly, and that Algorithm 4.1 always uses $O^*(\ell)$ oracle calls.

For the sake of completeness, let us illustrate how Line 6 in Algorithm 4.1 could be implemented if the target distribution were a Boltzmann distribution over $\mathcal{S}$ with parameter $\theta \in \mathbb{R}^n$. In other words, we are looking for the $s \in [0, 1]$ such that

$$\int_0^s e^{\langle \theta, Y_i + t(Z_i - Y_i) \rangle}\,\mathrm{d}t = P_i \int_0^1 e^{\langle \theta, Y_i + t(Z_i - Y_i) \rangle}\,\mathrm{d}t.$$

This condition can equivalently be written as

$$\frac{e^{\langle \theta, Y_i + s(Z_i - Y_i) \rangle} - e^{\langle \theta, Y_i \rangle}}{\langle \theta, Z_i - Y_i \rangle} = P_i \frac{e^{\langle \theta, Z_i \rangle} - e^{\langle \theta, Y_i \rangle}}{\langle \theta, Z_i - Y_i \rangle},$$

which has solution

$$s = \frac{\log\left((1 - P_i)e^{\langle \theta, Y_i \rangle} + P_i e^{\langle \theta, Z_i \rangle}\right) - \langle \theta, Y_i \rangle}{\langle \theta, Z_i - Y_i \rangle}.$$

4.2 Divergence of Probability Distributions and Log-Concavity

To analyze the mixing time of hit-and-run applied to a Boltzmann distribution, we need some more theory. We want to define Radon-Nikodym derivatives, a generalization of probability density functions. Such a derivative is guaranteed to exist under two conditions: absolute continuity and σ-finiteness. We first define absolute continuity.

Definition 4.1. Let $(\mathcal{S}, \mathcal{F})$ be a measurable space, and let φ and ψ be measures on this space. Then, φ is *absolutely continuous* with respect to ψ if $\psi(A) = 0$ implies $\varphi(A) = 0$ for all $A \in \mathcal{F}$. We write this property as $\varphi \ll \psi$.

Next, we call a positive measure φ on the measurable space $(\mathcal{S}, \mathcal{F})$ *σ-finite* if $\mathcal{S}$ can be covered by countably many measurable sets with finite measure. In particular, if $\varphi(\mathcal{S})$ is finite, it is σ-finite by definition.

With these two concepts defined, we can state the Radon-Nikodym theorem, which provides conditions under which the Radon-Nikodym derivatives exist. Although it was originally proven on general measurable spaces by Nikodym [91, Theorem IV], we cite the version from Billingsley [15].

Theorem 4.2 ([15, Theorem 32.2])**.** *Let $(\mathcal{S}, \mathcal{F})$ be a measurable space, and let φ and ψ be positive, σ-finite measures on $(\mathcal{S}, \mathcal{F})$ such that $\varphi \ll \psi$. Then, there exists a measurable function $\phi : \mathcal{S} \to \mathbb{R}_+$ such that for all $A \in \mathcal{F}$,*

$$\varphi(A) = \int_A \phi \, \mathrm{d}\psi.$$

Such a function ϕ is called a Radon-Nikodym derivative *of φ with respect to ψ, and is denoted by $\mathrm{d}\varphi / \mathrm{d}\psi$ or $\frac{\mathrm{d}\varphi}{\mathrm{d}\psi}$.*

Note that if one lets $\mathcal{S} \subseteq \mathbb{R}^n$ and ψ be the Lebesgue measure in the theorem above, then the Radon-Nikodym derivative of a probability measure φ is simply the familiar probability density function.

One reason for introducing the Radon-Nikodym derivative is that it is used in our first measure of divergence between probability distributions: the L_2-norm.

Definition 4.3. Let $(\mathcal{S}, \mathcal{F})$ be a measurable space. Let φ and ψ be two probability distributions over this space, such that $\varphi \ll \psi$. Then, the *L_2-norm* of φ with respect to ψ is

$$\|\varphi/\psi\| := \int_{\mathcal{S}} \frac{\mathrm{d}\varphi}{\mathrm{d}\psi}\,\mathrm{d}\varphi = \int_{\mathcal{S}} \left(\frac{\mathrm{d}\varphi}{\mathrm{d}\psi}\right)^2 \mathrm{d}\psi.$$

To provide some more insight into this definition, we remark that if $\mathcal{S} \subseteq \mathbb{R}^n$, and φ and ψ have probability densities ϕ_φ and ϕ_ψ, respectively, with respect to the Lebesgue measure, it can be shown that

$$\|\varphi/\psi\| = \int_{\mathcal{S}} \frac{\phi_\varphi(x)}{\phi_\psi(x)} \phi_\varphi(x)\,\mathrm{d}x.$$

The second way in which we will measure distance between probability distributions is by total variation distance.

Definition 4.4. Let $(\mathcal{S}, \mathcal{F})$ be a measurable space. For two probability distributions φ and ψ over this space, their *total variation distance* is

$$\|\varphi - \psi\|_{\mathrm{TV}} := \sup_{A \in \mathcal{F}} |\varphi(A) - \psi(A)|.$$

A useful property of the total variation distance is that it allows coupling of random variables, as the following lemma from Levin et al. [68] asserts.

Lemma 4.5 (e.g. [68, Proposition 4.7])**.** *Let X be a random variable on $\mathcal{S}$ with distribution φ, and let ψ be a different probability distribution on $\mathcal{S}$. If $\|\varphi - \psi\|_{\mathrm{TV}} = p$, we can construct another random variable Y on $\mathcal{S}$ distributed according to ψ such that $\mathbb{P}\{X = Y\} = 1 - p$.*

Another reason to introduce Radon-Nikodym derivatives is that they admit a convenient interpretation of log-concave measures. We will use the definition from Saumard and Wellner [98], which defines such measures on $(\mathbb{R}^n, \mathcal{B}^n)$, where $\mathcal{B}^n$ is the Borel σ-algebra.

Definition 4.6 ([98, Definitions 2.1 and 2.4, Theorem 2.7])**.** A positive measure φ on $(\mathbb{R}^n, \mathcal{B}^n)$ is *log-concave* if for all $A, B \in \mathcal{B}^n$ and $t \in (0, 1)$,

$$\varphi(tA + (1-t)B) \geq \varphi(A)^t \varphi(B)^{1-t}, \tag{4.1}$$

where $tA + (1-t)B \coloneqq \{tx + (1-t)y : x \in A, y \in B\}$. Moreover, a function $\phi : \mathbb{R}^n \to \mathbb{R}_+$ is *log-concave* if for all $x, y \in \mathbb{R}^n$ and $t \in (0,1)$,

$$\phi(tx + (1-t)y) \geq \phi(x)^t \phi(y)^{1-t}.$$

(In other words, if the function ϕ is strictly positive, then it is log-concave if and only if $x \mapsto \log(\phi(x))$ is concave.)

The definition (4.1) of a log-concave probability distribution does not immediately offer a lot of intuition. It is thus convenient to note that log-concave probability distributions have a log-concave probability density function, and vice versa. Formally, a probability measure on $(\mathbb{R}^n, \mathcal{B}^n)$ with full-dimensional support is log-concave if and only if it admits a log-concave Radon-Nikodym derivative with respect to the Lebesgue measure (see Saumard and Wellner [98, Theorem 2.7]). In particular, any Boltzmann distribution over a convex body is log-concave. As a matter of fact, Boltzmann distributions lie at the boundary of all log-concave distributions, since the logarithm of their densities is linear.

A considerable body of literature surrounds log-concave probability distributions, a small part of which we will use. For instance, as we will see later, the tails of log-concave distributions contain relatively little probability mass. Another property is that the level sets of log-concave probability density functions are convex (see e.g. Section 3.5 in Boyd and Vandenberghe [19]). Let us define these sets for general probability density functions.

Definition 4.7. Let $\phi : \mathbb{R}^n \to \mathbb{R}_+$ be a probability density function supported on $\mathcal{S} \subseteq \mathbb{R}^n$. Then, the *level set* of (the distribution with density) ϕ with probability $p \in (0,1)$ is $\{x \in \mathcal{S} : \phi(x) \geq t_p\}$, where t_p is chosen such that the integral of ϕ over this set equals p.

4.3 Mixing Time

With these preliminaries established, we can start our analysis of the mixing time of hit-and-run. To approximate the derivatives of the entropic barrier, we should be able to generate samples from a Boltzmann distribution with parameter $\theta_1 \in \mathbb{R}^n$. Because we are interested in a short-step interior point method, we may

assume that we already have reasonable approximations of $\Sigma(\theta_0)$ for some θ_0 close to θ_1 (this section will use the notation summarized in Table 3.1 on page 32.). Our goal for this section is to find a walk length ℓ such that after ℓ steps, the hit-and-run sample approximately follows the Boltzmann distribution with parameter θ_1.

The following theorem from Lovász and Vempala [71] is the starting point of our analysis. We use $\mathbb{E}_\psi[\phi(X)]$ to refer to the expectation of $\phi(X)$, where X follows the distribution ψ.

Theorem 4.8 ([71, Theorem 1.1])**.** *Let ψ be a log-concave probability distribution supported on a convex body $\mathcal{S} \subseteq \mathbb{R}^n$, and let $p > 0$. Consider a hit-and-run random walk as in Algorithm 4.1 with respect to the target distribution ψ from a random starting point with distribution φ supported on $\mathcal{S}$. Assume that the following holds:*

(i) the level set of ψ with probability $\frac{1}{8}$ contains a ball of radius υ with respect to $\|\cdot\|$;

(ii) $\frac{\mathrm{d}\varphi}{\mathrm{d}\psi}(x) \leq \bar{M}$ for all $x \in \mathcal{S} \setminus A$ for some set $A \subseteq \mathcal{S}$ with $\varphi(A) \leq p$;

(iii) $\mathbb{E}_\psi[\|X - \mathbb{E}_\psi[X]\|^2] \leq \Upsilon^2$.

Let φ^ℓ be the distribution of the current hit-and-run point after ℓ steps of hit-and-run sampling applied to ψ, where the directions are chosen from a $\mathcal{N}(0, I)$-distribution. Then, after

$$\ell = \left\lceil 10^{30} \frac{n^2\Upsilon^2}{\upsilon^2} \log^2\left(\frac{2\bar{M}n\Upsilon}{\upsilon p}\right) \log^3\left(\frac{2\bar{M}}{p}\right) \right\rceil,$$

hit-and-run steps, we have $\|\varphi^\ell - \psi\|_{\mathrm{TV}} \leq p$.

Suppose that rather than (ii), we know $\|\varphi/\psi\| \leq M$, i.e. $\int_{\mathcal{S}} \frac{\mathrm{d}\varphi}{\mathrm{d}\psi}(x)\,\mathrm{d}\varphi(x) \leq M$. If $A = \{x \in \mathcal{S} : \frac{\mathrm{d}\varphi}{\mathrm{d}\psi}(x) > M/p\}$, then

$$M \geq \int_A \frac{\mathrm{d}\varphi}{\mathrm{d}\psi}(x)\,\mathrm{d}\varphi(x) \geq \frac{M}{p}\varphi(A),$$

and thus we have $\varphi(A) \leq p$. (This construction was also applied by Lovász and Vempala [72, page 10].) We can therefore set $\bar{M} = M/p$ in the theorem. If one additionally applies a transformation $x \mapsto \Sigma^{-1/2}x$ to $\mathcal{S}$ for some invertible matrix Σ before Theorem 4.8 is applied, we arrive at the following corollary.

Corollary 4.9 ([8, Corollary 4.2])**.** *Let ψ be a log-concave probability distribution supported on a convex body $\mathcal{S} \subseteq \mathbb{R}^n$, and let $p > 0$. Consider a hit-and-run random walk as in Algorithm 4.1 with respect to the target distribution ψ from a random starting point with distribution φ supported on $\mathcal{S}$. Assume that the following holds for some invertible matrix Σ:*

(i) the level set of ψ with probability $\frac{1}{8}$ contains a ball of radius υ with respect to $\|\cdot\|_{\Sigma^{-1}}$;

(ii) $\|\varphi/\psi\| \leq M$;

(iii) $\mathbb{E}_\psi\left[\|X - \mathbb{E}_\psi[X]\|_{\Sigma^{-1}}^2\right] \leq \Upsilon^2$.

Let φ^ℓ be the distribution of the hit-and-run point after ℓ steps of hit-and-run sampling applied to ψ, where the directions are drawn from a $\mathcal{N}(0,\Sigma)$-distribution. Then, after

$$\ell = \left\lceil 10^{30} \frac{n^2\Upsilon^2}{\upsilon^2} \log^2\left(\frac{2Mn\Upsilon}{\upsilon p^2}\right) \log^3\left(\frac{2M}{p^2}\right) \right\rceil, \tag{4.2}$$

hit-and-run steps, we have $\|\varphi^\ell - \psi\|_{\mathrm{TV}} \leq p$.

In the remainder of this section, we aim to show that the conditions of Corollary 4.9 are satisfied if φ and ψ are Boltzmann distributions with parameters θ_0 and θ_1, respectively, such that $\|\theta_1 - \theta_0\|_{\theta_0}$ is sufficiently small. Note that Kalai and Vempala [56] only show these conditions to be satisfied if θ_0 and θ_1 are collinear. In studying interior point methods, we are also interested in (small) deviations from the central path, so it is important to know that the mixing conditions can be shown to hold for these cases. We remind the reader that it was shown in Proposition 3.3(iv) that the log-partition function is self-concordant, a fact that will be used frequently below. In fact, one might say that this self-concordance alone implies the conditions of Corollary 4.9 holding for Boltzmann distributions.

We begin with Condition (i) from Corollary 4.9. It is different from [8, Lemma 4.4] in that it does not use the $\|\cdot\|_{x(\theta)}^*$-norm. This will simplify the statement of Theorem 4.14.

Lemma 4.10. *Let f be the log-partition function associated with a convex body $\mathcal{S} \subset \mathbb{R}^n$. Let $q \in (0,1)$ and $\theta_0, \theta_1 \in \mathbb{R}^n$ such that $\|\theta_1 - \theta_0\|_{\theta_0} < 1$. Let $\phi : \mathbb{R}^n \to \mathbb{R}$*

be the density of the Boltzmann distribution with parameter θ_1 over $\mathcal{S}$. Let L be the level set of ϕ with probability q. Then, L contains a closed $\|\cdot\|_{\Sigma(\theta_0)^{-1}}$-ball with radius

$$\frac{q}{e}\big(1-\|\theta_1-\theta_0\|_{\theta_0}\big).$$

Proof. It follows from Lemma 5.13 in Lovász and Vempala [74] that L contains a $\|\cdot\|_{\Sigma(\theta_1)^{-1}}$-ball with radius q/e. In other words, there exists some $z \in L$ such that for all $y \in \mathbb{R}^n$ with $\|y-z\|_{\theta_1}^{-1} \le q/e$ it holds that $y \in L$. Thus, for all $y \in \mathbb{R}^n$ with $\|y-z\|_{\theta_0}^{-1} \le (1-\|\theta_1-\theta_0\|_{\theta_0})q/e$, (2.5) shows

$$\|y-z\|_{\theta_1}^{-1} \le \frac{\|y-z\|_{\theta_0}^{-1}}{1-\|\theta_1-\theta_0\|_{\theta_0}} \le \frac{q}{e},$$

which proves that all such y lie in L. □

Next, we prove upper and lower bounds on the L_2 norm of two Boltzmann distributions. This corresponds to Condition (ii) in Corollary 4.9.

Lemma 4.11 ([8, Lemma 4.5])**.** *Let f be the log-partition function associated with a convex body $\mathcal{S} \subset \mathbb{R}^n$. Let φ_0 and φ_1 be Boltzmann distributions supported on $\mathcal{S}$ with parameters θ_0 and θ_1 respectively. Then, if $\|\theta_1-\theta_0\|_{\theta_0} < 1$,*

$$\|\varphi_0/\varphi_1\| \le \frac{\exp(-2\|\theta_1-\theta_0\|_{\theta_0})}{(1-\|\theta_1-\theta_0\|_{\theta_0})^2}.$$

Proof. For ease of notation, let $\theta := \theta_0$ and $u := \theta_1-\theta_0$. By definition,

$$\begin{aligned}\|\varphi_0/\varphi_1\| = \mathbb{E}_{\theta_0}\left[\frac{\mathrm{d}\varphi_0}{\mathrm{d}\varphi_1}(X)\right] &= \int_{\mathcal{S}} \frac{e^{\langle 2\theta,x\rangle}}{e^{\langle\theta+u,x\rangle}}\,\mathrm{d}x \frac{\int_{\mathcal{S}} e^{\langle\theta+u,x\rangle}\,\mathrm{d}x}{\left(\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x\right)^2} \\ &= \frac{\int_{\mathcal{S}} e^{\langle\theta-u,x\rangle}\,\mathrm{d}x}{\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x} \frac{\int_{\mathcal{S}} e^{\langle\theta+u,x\rangle}\,\mathrm{d}x}{\int_{\mathcal{S}} e^{\langle\theta,x\rangle}\,\mathrm{d}x}. \end{aligned} \tag{4.3}$$

The key observation is that the natural logarithm of (4.3) equals

$$\begin{aligned}
&f(\theta+u)-f(\theta)+f(\theta-u)-f(\theta)\\
&=\int_0^1 \langle g(\theta+tu),u\rangle\,\mathrm{d}t-\int_0^1 \langle g(\theta-tu),u\rangle\,\mathrm{d}t\\
&=\int_0^1 \left\langle g(\theta)+\int_0^1 H(\theta+stu)(tu)\,\mathrm{d}s,u\right\rangle \mathrm{d}t\\
&\quad-\int_0^1 \left\langle g(\theta)+\int_0^1 H(\theta-stu)(-tu)\,\mathrm{d}s,u\right\rangle \mathrm{d}t\\
&=\int_0^1 t\int_0^1 \langle H(\theta+stu)u,u\rangle\,\mathrm{d}s\,\mathrm{d}t+\int_0^1 t\int_0^1 \langle H(\theta-stu)u,u\rangle\,\mathrm{d}s\,\mathrm{d}t, \qquad (4.4)
\end{aligned}$$

where we used the fundamental theorem of calculus twice. By the second inequality in (2.1),

$$\langle H(\theta+stu)u,u\rangle=\|u\|^2_{\theta+stu}\le\frac{\|u\|^2_\theta}{(1-st\|u\|_\theta)^2},$$

and the same upper bound holds for $\langle H(\theta-stu)u,u\rangle$. Then, (4.4) can be bounded above by

$$2\int_0^1 t\int_0^1 \frac{\|u\|^2_\theta}{(1-st\|u\|_\theta)^2}\,\mathrm{d}s\,\mathrm{d}t=-2[\|u\|_\theta+\ln(1-\|u\|_\theta)],$$

which is nonnegative for $0\le\|u\|_\theta<1$. Since (4.4) is the natural logarithm of (4.3),

$$\|\varphi_0/\varphi_1\|\le\exp(-2[\|u\|_\theta+\ln(1-\|u\|_\theta)])=\frac{\exp(-2\|u\|_\theta)}{(1-\|u\|_\theta)^2}.$$ □

The bound in this lemma are more general than the ones used in Kalai and Vempala [56, Lemma 4.4]. They consider the case where $\theta_1=(1+t)\theta_0$ for some $t\in(-1,1)$. By using the log-concavity of the Boltzmann distribution, they show

$$\|\varphi_0/\varphi_1\|\le\frac{1}{(1+t)^n(1-t)^n}, \qquad (4.5)$$

where φ_0 and φ_1 are Boltzmann distributions with parameters θ_0 and θ_1, respectively. This bound may outperform Lemma 4.11, but that comes at the cost of generality.

Finally, we show that Condition (iii) in Corollary 4.9 holds. The first step is computing the expression $\mathbb{E}[\|X-\mathbb{E}[X]\|_{\Sigma^{-1}}^2]$ for random variables X with covariance Σ. (We state this result separately because we will refer to it later.)

Lemma 4.12. *Let X be a random variable in $\mathbb{R}^n$ with covariance operator Σ, i.e. $\Sigma[v,w]=\mathbb{E}[\langle X-\mathbb{E}[X],v\rangle\langle X-\mathbb{E}[X],w\rangle]$ for all $v,w\in\mathbb{R}^n$. Then,*

$$\mathbb{E}\left[\|X-\mathbb{E}[X]\|_{\Sigma^{-1}}^2\right]=n.$$

Proof. Since Σ is a positive definite linear operator, it has a spectral decomposition given by an orthonormal basis $v_1,\dots,v_n\in\mathbb{R}^n$ and positive reals $\lambda_1,\dots,\lambda_n$ such that

$$\Sigma w=\sum_{i=1}^n\lambda_i\langle v_i,w\rangle v_i \quad\text{and}\quad \Sigma^{-1}w=\sum_{i=1}^n\frac{1}{\lambda_i}\langle v_i,w\rangle v_i$$

for all $w\in\mathbb{R}^n$. Consequently,

$$\begin{aligned}\mathbb{E}\left[\|X-\mathbb{E}[X]\|_{\Sigma^{-1}}^2\right]&=\mathbb{E}\left[\langle X-\mathbb{E}[X],\Sigma^{-1}[X-\mathbb{E}[X]]\rangle\right]\\&=\sum_{i=1}^n\frac{1}{\lambda_i}\mathbb{E}\left[\langle X-\mathbb{E}[X],v_i\rangle^2\right]=\sum_{i=1}^n\frac{1}{\lambda_i}\Sigma[v_i,v_i].\end{aligned}$$

The proof is completed by noting that $\Sigma[v_i,v_i]=\lambda_i$ for all i. □

Condition (iii) in Corollary 4.9 can now be satisfied by an application of self-concordance. The following is more general than [8, Lemma 4.6], since it does not assume the reference inner product is Euclidean.

Corollary 4.13. *Let f be the log-partition function associated with a convex body $\mathcal{S}\subset\mathbb{R}^n$. For all $\theta_0,\theta_1\in\mathbb{R}^n$ such that $\|\theta_0-\theta_1\|_{\theta_0}<1$,*

$$\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|_{\Sigma(\theta_0)^{-1}}^2\right]\le\frac{n}{(1-\|\theta_0-\theta_1\|_{\theta_0})^2}.$$

Proof. By (2.4), $\Sigma(\theta_0)^{-1}\preceq(1-\|\theta_0-\theta_1\|_{\theta_0})^{-2}\Sigma(\theta_1)^{-1}$, showing

$$\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|_{\Sigma(\theta_0)^{-1}}^2\right]\le\frac{1}{(1-\|\theta_0-\theta_1\|_{\theta_0})^2}\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|_{\Sigma(\theta_1)^{-1}}^2\right].$$

The claim thus follows from Lemma 4.12. □

It is interesting to compare the upper bound in Corollary 4.13 with the one Kalai and Vempala [56] arrive at through a near-isotropy argument. It is shown by [56, Lemmas 4.2 and 4.3] that

$$\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|^2_{\Sigma(\theta_0)^{-1}}\right] \le 16n\|\varphi_1/\varphi_0\| \max_{v\in\mathbb{R}^n} \frac{\mathbb{E}_{\theta_0}\left[\langle v, X-\mathbb{E}_{\theta_0}[X]\rangle^2_{\Sigma(\theta_0)^{-1}}\right]}{\|v\|^2_{\Sigma(\theta_0)^{-1}}}, \tag{4.6}$$

where μ_0 and μ_1 are Boltzmann distributions with parameters θ_0 and θ_1, respectively. Observe that for all $v \in \mathbb{R}^n$,

$$\frac{\mathbb{E}_{\theta_0}\left[\langle \Sigma(\theta_0)^{-1}v, X-\mathbb{E}_{\theta_0}[X]\rangle^2\right]}{\|v\|^2_{\Sigma(\theta_0)^{-1}}} = \frac{\langle \Sigma(\theta_0)^{-1}v, \Sigma(\theta_0)\Sigma(\theta_0)^{-1}v\rangle}{\|v\|^2_{\Sigma(\theta_0)^{-1}}} = 1,$$

and therefore the right hand side of (4.6) is just $16n\|\varphi_1/\varphi_0\|$. If we upper bound this norm by Lemma 4.11, we find

$$\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|^2_{\Sigma(\theta_0)^{-1}}\right] \le \frac{16n\exp(-2\|\theta_1-\theta_0\|_{\theta_1})}{(1-\|\theta_1-\theta_0\|_{\theta_1})^2}. \tag{4.7}$$

By the second inequality in (2.1), we have

$$\frac{n}{(1-\|\theta_0-\theta_1\|_{\theta_0})^2} \le \frac{n}{\left(1-\frac{\|\theta_0-\theta_1\|_{\theta_1}}{1-\|\theta_0-\theta_1\|_{\theta_1}}\right)^2} \le \frac{16n\exp(-2\|\theta_1-\theta_0\|_{\theta_1})}{(1-\|\theta_1-\theta_0\|_{\theta_1})^2},$$

where the second inequality holds for $\|\theta_1-\theta_0\|_{\theta_1} \le 0.438$. In this case, the bound in Corollary 4.13 is stronger than (4.7). Alternatively, if $\theta_0 = (1+t)\theta_1$ for some $t \in (-1,1)$, (4.5) shows that (4.6) can be bounded by

$$\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|^2_{\Sigma(\theta_0)^{-1}}\right] \le \frac{16n}{(1+t)^n(1-t)^n}. \tag{4.8}$$

Since (3.1) shows $\|\theta_1-\theta_0\|_{\theta_0} = t\|\theta_0\|_{\theta_0} \le t\sqrt{\vartheta}$, the upper bound from Corollary 4.13 is better than (4.8) as long as $t\sqrt{\vartheta} < 1$.

Let us now summarize the results from this section. Since Lemma 4.10 and Corollary 4.13 differ from the results in [8], the following theorem is also different from [8, Theorem 4.7].

Theorem 4.14. *Let f be the log-partition function associated with a convex body $\mathcal{S} \subset \mathbb{R}^n$. Suppose $\theta_0, \theta_1 \in \mathbb{R}^n$ satisfy $\Delta\theta := \|\theta_0 - \theta_1\|_{\theta_0} < 1$. Pick $\epsilon \geq 0$ and $p > 0$, and suppose we have an invertible matrix $\widehat{\Sigma}(\theta_0)$ such that*

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(\theta_0)^{-1} \preceq \Sigma(\theta_0)^{-1} \preceq (1+\epsilon)\widehat{\Sigma}(\theta_0)^{-1}. \tag{4.9}$$

Consider a hit-and-run random walk as in Algorithm 4.1 applied to the Boltzmann distribution φ_1 with parameter θ_1 from a random starting point drawn from a Boltzmann distribution φ_0 with parameter θ_0. Let φ^ℓ be the distribution of the hit-and-run point after ℓ steps of hit-and-run sampling applied to φ_1, where the directions are drawn from a $\mathcal{N}(0, \widehat{\Sigma}(\theta_0))$-distribution. Then, after

$$\ell = \left\lceil 10^{30} \frac{64e^2 n^3 (1+\epsilon)^2}{(1-\Delta\theta)^4} \log^2\left(\frac{16n\sqrt{n}\sqrt{1+\epsilon}e^{1-2\Delta\theta}}{p^2(1-\Delta\theta)^4}\right) \log^3\left(\frac{2e^{-2\Delta\theta}}{p^2(1-\Delta\theta)^2}\right)\right\rceil \tag{4.10}$$

hit-and-run steps, we have $\|\varphi^\ell - \varphi_1\|_{\mathrm{TV}} \leq p$.

Proof. We will apply Corollary 4.9 with respect to $\widehat{\Sigma}(\theta_0)$. To do this, we use Lemmas 4.10 and 4.11 and Corollary 4.13 to find values of υ, M, and Υ such that the conditions of Corollary 4.9 are satisfied.

By Lemma 4.10, the level set of ψ with probability $\frac{1}{8}$ contains a $\|\cdot\|_{\Sigma(\theta_0)^{-1}}$-ball with radius $\frac{1}{8e}(1 - \|\theta_0 - \theta_1\|_{\theta_0})$. Denote the center of this ball by $z \in \mathcal{S}$. Then, for all $y \in \mathcal{S}$ with $\|y - z\|_{\widehat{\Sigma}(\theta_0)^{-1}} \leq \frac{1}{8e\sqrt{1+\epsilon}}(1 - \|\theta_0 - \theta_1\|_{\theta_0})$, it can be seen from (4.9) that

$$\|y - z\|_{\Sigma(\theta_0)^{-1}} \leq \sqrt{1+\epsilon}\|y - z\|_{\widehat{\Sigma}(\theta_0)^{-1}} \leq \frac{1}{8e}(1 - \|\theta_0 - \theta_1\|_{\theta_0}),$$

and thus y lies in the level set. Therefore, the level set of ψ with probability $\frac{1}{8}$ contains a $\|\cdot\|_{\widehat{\Sigma}(\theta_0)^{-1}}$-ball with radius

$$\frac{1 - \|\theta_0 - \theta_1\|_{\theta_0}}{8e\sqrt{1+\epsilon}} =: \upsilon.$$

Moreover, by Lemma 4.11,

$$\|\varphi_0/\varphi_1\| \leq \frac{\exp(-2\|\theta_1 - \theta_0\|_{\theta_0})}{(1 - \|\theta_1 - \theta_0\|_{\theta_0})^2} =: M.$$

Finally, (4.9) and Corollary 4.13 show

$$\begin{aligned}\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|^2_{\widehat{\Sigma}(\theta_0)^{-1}}\right] &\leq (1+\epsilon)\mathbb{E}_{\theta_1}\left[\|X-\mathbb{E}_{\theta_1}[X]\|^2_{\Sigma(\theta_0)^{-1}}\right]\\ &\leq \frac{n(1+\epsilon)}{(1-\|\theta_0-\theta_1\|_{\theta_0})^2} =: \Upsilon^2.\end{aligned}$$

With the values of υ, M, and Υ defined above, Corollary 4.9 proves the result. □

5

Approximation Quality with Hit-and-Run

Last chapter's main result, Theorem 4.14, showed that hit-and-run sampling could be used to generate samples from distributions close to a desired Boltzmann distribution. This is a step in the right direction: remember that our goal is to approximate the gradients and Hessians of the entropic barrier, which have an interpretation in terms of the mean and covariance of certain Boltzmann distributions. In this chapter, we will investigate how many hit-and-run samples and steps are needed to approximate the mean and covariance of a Boltzmann distribution.

There are however two complicating factors. First, the hit-and-run samples do not follow the target distribution, but rather a probability distribution close to it. (This is already apparent from Theorem 4.14.) Second, it is not hard to imagine that the distribution of the end point of a hit-and-run random walk depends on its starting point. Hence, two hit-and-run random walks sharing a starting point will not be independent. We can therefore only generate samples that do not follow the target distribution and are not independent. For these reasons, a careful analysis is needed.

We start in Section 5.1 by quantifying the dependence between different hit-

and-run samples. Combined with Theorem 4.14, we then have the tools to analyze how well the mean of a number of hit-and-run samples approximates the mean of the target distribution. This is the topic of Section 5.2. An analysis with a similar goal for the covariance will follow in Section 5.3.

This chapter is based on Sections 2.4 and 5 from Badenbroek and De Klerk [8]. The major contribution of this chapter is the generalization of those results to arbitrary inner products, not simply the Euclidean one. Moreover, we include formal proofs of Lemma 5.7 and Corollary 5.8, which were lacking in the literature.

5.1 Near-Independence for Random Walks

The end point of a random walk such as hit-and-run depends on the starting point of the walk, but as the walk length increases, this dependence starts to vanish. We will use the notion of near-independence to quantify this, as in e.g. Lovász and Vempala [73].

Definition 5.1 ([73, Section 3.2])**.** Let $p > 0$. Two random variables X and Y taking values in measurable space $(\mathcal{S}, \mathcal{F})$ are *near-independent* or *p-independent* if for all $A, B \in \mathcal{F}$,

$$|\mathbb{P}\{X \in A \wedge Y \in B\} - \mathbb{P}\{X \in A\}\mathbb{P}\{Y \in B\}| \leq p.$$

Before we can analyze the near-independence of starting and end points of a random walk, we need the formal machinery of Markov kernels (see for instance Heidergott and Hordijk [50]). Intuitively, a Markov kernel assigns to any point in $\mathcal{S}$ a probability distribution over $\mathcal{S}$. Its analogue for discrete space Markov chains is a transition probability matrix.

Definition 5.2 ([50, Definition 1])**.** Let $(\mathcal{S}, \mathcal{F})$ be a measurable space, and let $\mathcal{B}[0,1]$ be the Borel σ-algebra over $[0,1]$. A *Markov kernel* is a map $Q : \mathcal{S} \times \mathcal{F} \to [0,1]$ with the properties

(i) For every $x \in \mathcal{S}$, the map $B \mapsto Q(x, B)$ for $B \in \mathcal{F}$ is a probability measure on $(\mathcal{S}, \mathcal{F})$;

(ii) For every $B \in \mathcal{F}$, the map $x \mapsto Q(x, B)$ for $x \in \mathcal{S}$ is $(\mathcal{F}, \mathcal{B}[0,1])$-measurable.

Since $Q(x, \cdot)$ is a measure for any fixed $x \in \mathcal{S}$, we can integrate a function ϕ over $\mathcal{S}$ with respect to this measure. This integral will be denoted by $\int_{\mathcal{S}} \phi(y) Q(x, \mathrm{d}y)$. We emphasize again that for any $x \in \mathcal{S}$, this expression is just a Lebesgue integral.

Suppose the Markov kernel Q corresponds to one step of a random walk, i.e. after one step from $x \in \mathcal{S}$, the probability of ending up in $B \in \mathcal{F}$ is $Q(x, B)$. The probability that after $m \geq 2$ steps a random walk starting at $x \in \mathcal{S}$ ends up in $B \in \mathcal{F}$ is then given by

$$Q^m(x, B) := \int_{\mathcal{S}} Q(y, B) Q^{m-1}(x, \mathrm{d}y),$$

where $Q^1 := Q$. Another interpretation of $Q^m(x, B)$ is the probability of a random walk ending in B, conditional on the random starting point X of the walk taking value x. If moreover the starting point of the random walk is not fixed, but follows a probability distribution φ, then the end point of the random walk after m steps follows distribution φQ^m, defined by

$$(\varphi Q^m)(B) := \int_{\mathcal{S}} Q^m(x, B) \, \mathrm{d}\varphi(x),$$

for all $B \in \mathcal{F}$.

The following lemma connects total variation distance to near-independence. It will ensure that if the distribution of the end point Y of a random walk approaches some fixed desired distribution ψ, then the start point X of this random walk and Y are near-independent. The conditions of this lemma may appear to be somewhat mysterious. The reason we chose them is that they coincide with the hit-and-run mixing conditions from Corollary 4.9. Thus, the upcoming lemma can be used to show that – under certain conditions – a hit-and-run sample is near-independent from its starting point.

A similar relation was established by Lovász and Vempala [73], but we will use a version that does not assume Y follows the desired distribution ψ.

Lemma 5.3 ([73, Lemma 4.3(a)]). *Fix a probability distribution ψ over a set $\mathcal{S}$, and let Q be a Markov kernel on $\mathcal{S}$. Let $\ell : \mathbb{R}_+ \to \mathbb{N}$ be a function such that for any*

$\bar{M} \geq 0$, $\bar{p} > 0$ and any distribution $\bar{\varphi}$ satisfying $\bar{\varphi} \ll \psi$ and $\|\bar{\varphi}/\psi\| \leq \bar{M}$, it holds that

$$\|\bar{\varphi}Q^{\ell(\bar{M}/\bar{p}^2)} - \psi\|_{\mathrm{TV}} \leq \bar{p}.$$

Let $M \geq 0, p > 0$, and let φ be a distribution such that $\varphi \ll \psi$ and $\|\varphi/\psi\| \leq M$. If X is a random variable with distribution φ, and Y is a random variable with distribution conditional on $X = x$ given by $Q^{\ell(M/p^2)}(x, \cdot)$ for any $x \in \mathcal{S}$, then X and Y are $3p$-independent.

Proof. Let A and B be measurable subsets of $\mathcal{S}$. As noted in Lovász and Vempala [73, relation (4)], one has the elementary relation

$$\begin{aligned}&|\mathbb{P}\{Y \in B \wedge X \in A\} - \mathbb{P}\{Y \in B\}\mathbb{P}\{X \in A\}| \\ &= |\mathbb{P}\{Y \in B \wedge X \notin A\} - \mathbb{P}\{Y \in B\}\mathbb{P}\{X \notin A\}|.\end{aligned}$$

We may therefore assume $\mathbb{P}\{X \in A\} = \varphi(A) \geq \frac{1}{2}$.

The marginal distribution of Y satisfies

$$\mathbb{P}\{Y \in B\} = \int_{\mathcal{S}} Q^{\ell(M/p^2)}(x, B)\,\mathrm{d}\varphi(x) = \varphi Q^{\ell(M/p^2)}(B). \tag{5.1}$$

Consider the restriction φ_A of φ to A, scaled to be a probability measure. Then,

$$\begin{aligned}\mathbb{P}\{Y \in B | X \in A\} &= \frac{\mathbb{P}\{Y \in B \wedge X \in A\}}{\mathbb{P}\{X \in A\}} \\ &= \frac{\int_A Q^{\ell(M/p^2)}(x, B)\,\mathrm{d}\varphi(x)}{\varphi(A)} \\ &= \int_{\mathcal{S}} Q^{\ell(M/p^2)}(x, B)\,\mathrm{d}\varphi_A(x) \\ &= \varphi_A Q^{\ell(M/p^2)}(B).\end{aligned} \tag{5.2}$$

Since $\varphi(A) \geq \frac{1}{2}$, we have $\frac{\mathrm{d}\varphi_A}{\mathrm{d}\varphi}(x) \leq 2$ for φ-almost all $x \in \mathcal{S}$. Then,

$$\|\varphi_A/\psi\| = \int_{\mathcal{S}} \left(\frac{\mathrm{d}\varphi_A}{\mathrm{d}\psi}\right)^2 \mathrm{d}\psi = \int_{\mathcal{S}} \left(\frac{\mathrm{d}\varphi_A}{\mathrm{d}\varphi}\right)^2 \left(\frac{\mathrm{d}\varphi}{\mathrm{d}\psi}\right)^2 \mathrm{d}\psi \leq 4\|\varphi/\psi\| \leq 4M.$$

Therefore, $\|\varphi_A Q^{\ell(M/p^2)} - \psi\|_{\mathrm{TV}} = \|\varphi_A Q^{\ell(4M/(2p)^2)} - \psi\|_{\mathrm{TV}} \leq 2p$ by assumption. Since $\|\varphi/\psi\| \leq M$, we also have $\|\varphi Q^{\ell(M/p^2)} - \psi\|_{\mathrm{TV}} \leq p$ by assumption. Hence,

by combining (5.1) and (5.2) with the triangle inequality and Definition 4.4, it follows that

$$\begin{aligned}
&|\mathbb{P}\{Y \in B | X \in A\} - \mathbb{P}\{Y \in B\}| \\
&= \left| \varphi_A Q^{\ell(M/p^2)}(B) - \varphi Q^{\ell(M/p^2)}(B) \right| \\
&\leq \left| \varphi_A Q^{\ell(M/p^2)}(B) - \psi(B) \right| + \left| \psi(B) - \varphi Q^{\ell(M/p^2)}(B) \right| \\
&\leq \|\varphi_A Q^{\ell(M/p^2)} - \psi\|_{\mathrm{TV}} + \|\varphi Q^{\ell(M/p^2)} - \psi\|_{\mathrm{TV}} \\
&\leq 2p + p = 3p.
\end{aligned}$$

Multiplying both sides of the outermost inequality by $\mathbb{P}\{X \in A\}$ shows

$$|\mathbb{P}\{Y \in B \wedge X \in A\} - \mathbb{P}\{Y \in B\}\mathbb{P}\{X \in A\}| \leq 3p\mathbb{P}\{X \in A\} \leq 3p,$$

which completes the proof. □

Having shown that the start and end point of a random walk are near-independent, we continue by proving the near-independence of the result of two independent random walks with the same random starting point. Note that the randomness of the common starting point is the issue here: if the starting point were fixed, the end points of the two random walks would be independent.

This analysis is important if we are going to generate many hit-and-run samples to approximate the derivatives of the entropic barrier. The reader may wonder why; there are more practically appealing alternatives, such as starting a random walk from the end point of the previous random walk. However, Kalai and Vempala [56] use a common starting point, and we aim to analyze their algorithm in Chapter 7. As we will see, this choice only leads to a deterioration of the near-independence by a constant factor, which will not influence the computational complexity of algorithms based on hit-and-run sampling in this thesis.

Lemma 5.4 ([8, Lemma 2.17])**.** *Let Y_1 and Y_2 be random variables that are both p-independent of a random variable X, all supported on a set $\mathcal{S}$. Assume that Y_1 and Y_2 are conditionally independent given X and that for all measurable events $\{Y_1 \in A\}$ and $\{Y_2 \in B\}$, the following sets are measurable:*

$$\{x \in \mathcal{S} : \mathbb{P}\{Y_1 \in A | X = x\} \geq \mathbb{P}\{Y_1 \in A\}\},$$
$$\{x \in \mathcal{S} : \mathbb{P}\{Y_2 \in B | X = x\} \geq \mathbb{P}\{Y_2 \in B\}\}.$$

Then, Y_1 and Y_2 are $2p$-independent.

Proof. Denote the probability distribution of X by φ. We want to bound the following term.

$$\begin{aligned}
&|\mathbb{P}\{Y_1 \in A \wedge Y_2 \in B\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{Y_2 \in B\}| \\
&= \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A \wedge Y_2 \in B|X\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{Y_2 \in B\})\, \mathrm{d}\varphi \right| \\
&= \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\}\mathbb{P}\{Y_2 \in B|X\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{Y_2 \in B\})\, \mathrm{d}\varphi \right|, \qquad (5.3)
\end{aligned}$$

where the last equality holds by the conditional independence of Y_1 and Y_2. We will use the identity $ab-cd = (a-c)(b-d)+(a-c)d+(b-d)c$, where $a, b, c, d \in \mathbb{R}$. Selecting $a = \mathbb{P}\{Y_1 \in A|X = x\}$, $b = \mathbb{P}\{Y_2 \in B|X = x\}$, $c = \mathbb{P}\{Y_1 \in A\}$, and $d = \mathbb{P}\{Y_2 \in B\}$ allows us to expand (5.3) in an obvious manner. The triangle inequality then gives

$$\begin{aligned}
&|\mathbb{P}\{Y_1 \in A \wedge Y_2 \in B\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{Y_2 \in B\}| \\
&\leq \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\})(\mathbb{P}\{Y_2 \in B|X\} - \mathbb{P}\{Y_2 \in B\})\, \mathrm{d}\varphi \right| \qquad (5.4) \\
&\quad + \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\})\mathbb{P}\{Y_2 \in B\}\, \mathrm{d}\varphi \right| \qquad (5.5) \\
&\quad + \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_2 \in B|X\} - \mathbb{P}\{Y_2 \in B\})\mathbb{P}\{Y_1 \in A\}\, \mathrm{d}\varphi \right|. \qquad (5.6)
\end{aligned}$$

We will upper bound each of these terms.

For (5.4), we can use Hölder's inequality as follows.

$$\begin{aligned}
&\left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\})(\mathbb{P}\{Y_2 \in B|X\} - \mathbb{P}\{Y_2 \in B\})\, \mathrm{d}\varphi \right| \\
&\leq \sqrt{\int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\})^2\, \mathrm{d}\varphi \int_{\mathcal{S}} (\mathbb{P}\{Y_2 \in B|X\} - \mathbb{P}\{Y_2 \in B\})^2\, \mathrm{d}\varphi}. \qquad (5.7)
\end{aligned}$$

Define

$$C := \{x \in \mathcal{S} : \mathbb{P}\{Y_1 \in A|X = x\} \geq \mathbb{P}\{Y_1 \in A\}\}.$$

Since both $\mathbb{P}\{Y_1 \in A|X = x\}$ and $\mathbb{P}\{Y_1 \in A\}$ lie in $[0,1]$ for all $x \in \mathcal{S}$, the square of their difference can be upper bounded by their absolute difference. Therefore,

$$\begin{aligned}
&\int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\})^2 \,\mathrm{d}\varphi \\
&\leq \int_{\mathcal{S}} |\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\}| \,\mathrm{d}\varphi \\
&= \int_{C} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\}) \,\mathrm{d}\varphi + \int_{\mathcal{S}\setminus C} (\mathbb{P}\{Y_1 \in A\} - \mathbb{P}\{Y_1 \in A|X\}) \,\mathrm{d}\varphi \\
&= \mathbb{P}\{Y_1 \in A \wedge X \in C\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{X \in C\} \\
&\quad + \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{X \notin C\} - \mathbb{P}\{Y_1 \in A \wedge X \notin C\} \leq 2p,
\end{aligned}$$

since X and Y_1 are p-independent. Because the same holds for $\mathbb{P}\{Y_2 \in B|X = x\}$ and $\mathbb{P}\{Y_2 \in B\}$ for all $x \in \mathcal{S}$, (5.7) is upper bounded by $2p$.

For (5.5), observe that

$$\begin{aligned}
&\left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\}) \mathbb{P}\{Y_2 \in B\} \,\mathrm{d}\varphi \right| \\
&= \mathbb{P}\{Y_2 \in B\} \left| \int_{\mathcal{S}} (\mathbb{P}\{Y_1 \in A|X\} - \mathbb{P}\{Y_1 \in A\}) \,\mathrm{d}\varphi \right| \\
&= \mathbb{P}\{Y_2 \in B\} \, |\mathbb{P}\{Y_1 \in A\} - \mathbb{P}\{Y_1 \in A\}| = 0.
\end{aligned}$$

The same clearly holds for (5.6). Hence,

$$|\mathbb{P}\{Y_1 \in A \wedge Y_2 \in B\} - \mathbb{P}\{Y_1 \in A\}\mathbb{P}\{Y_2 \in B\}| \leq 2p. \qquad \square$$

The measurability condition in this result holds for sufficiently detailed σ-algebras, and we will quietly assume it holds in the remainder of this thesis.

Recall that Lemma 5.3 can be used to show that a hit-and-run sample is near-independent from its starting point. By applying Lemma 5.4, the next result shows that two hit-and-run samples with a common starting point are also near-independent.

Theorem 5.5 ([8, Lemma 4.3])**.** *Let ψ be a log-concave probability distribution supported on a convex body $\mathcal{S} \subseteq \mathbb{R}^n$, and let $p > 0$. Suppose the conditions of Corollary 4.9 are satisfied for some Σ, υ, M, and Υ. Let X be a random variable*

with distribution φ supported on $\mathcal{S}$. Consider two hit-and-run random walks as in Algorithm 4.1, applied to ψ, both starting from the realization of X, where all D_i and P_i in one random walk are independent of all D_i and P_i in the other random walk. Let the number of steps ℓ of both walks be given by (4.2)*, and call the resulting end points Y_1 and Y_2. Then, Y_1 and Y_2 are $6p$-independent.*

Proof. Let Q be the Markov kernel of a hit-and-run step, where directions are chosen from $\mathcal{N}(0, \Sigma)$, and the iterates are drawn from ψ restricted to appropriate line segments, as defined in Algorithm 4.1. Note that the only dependence of (4.2) on M and p is through the fraction M/p^2. Thus, the conditions in Lemma 5.3 are satisfied. It follows that X and Y_1 are $3p$-independent, and X and Y_2 are $3p$-independent. Since the D_i and P_i in the random walks are independent, Y_1 and Y_2 are conditionally independent given X. Therefore, Lemma 5.4 shows the result. □

Since Theorem 4.14 was essentially an application of Corollary 4.9 to Boltzmann distributions, Theorem 5.5 also applies to this setting. For ease of reference, we state this result below.

Corollary 5.6 ([8, Lemma 4.8])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $p > 0$. Let $\theta_0, \theta_1 \in \mathbb{R}^n$ such that the conditions of Theorem 4.14 are satisfied for some ϵ and $\widehat{\Sigma}(\theta_0)$. Let X be a random variable following a Boltzmann distribution supported on $\mathcal{S}$ with parameter θ_0. Consider two hit-and-run random walks as in Algorithm 4.1, applied to the Boltzmann distribution with parameter θ_1, both starting from the realization of X, where all D_i and P_i in one random walk are independent of all D_i and P_i in the other random walk. Let the number of steps ℓ of both walks be given by* (4.10)*, and call the resulting end points Y_1 and Y_2. Then, Y_1 and Y_2 are $6p$-independent.*

5.2 Quality of Mean Approximation

Now that we know that two hit-and-run samples with the same starting point are near-independent, we can start to analyze how well the mean of a number of hit-and-run samples approximates the mean of the target Boltzmann distribution. This analysis requires us to consider the expectation of the inner product of two

near-independent random variables. As a stepping stone, we first consider one-dimensional random variables.

It is well known that the expectation of the product of two *independent* random variables is the product of their expectations. The next lemma shows that this almost holds for near-independent random variables. Kannan et al. [58] first stated this result, but their proof contains errors. (In general $\mathbb{E}[X] \neq \int_{-a}^{a} \mathbb{P}\{X > x\}\,\mathrm{d}x$ and $\mathbb{E}[XY] \neq \int_{-a}^{a}\int_{-b}^{b} \mathbb{P}\{X > x, Y > y\}\,\mathrm{d}x\,\mathrm{d}y$.)

Lemma 5.7 (Based on [58, Lemma 2.7])**.** *Let X and Y be p-independent random variables in $\mathbb{R}$ such that $|X| \leq a$ and $|Y| \leq b$ almost surely. Then,*

$$|\mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]| \leq 4pab.$$

Proof. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be the probability space on which X and Y are defined. Define

$$X^+(\omega) := \max\{0, X(\omega)\} \quad \text{and} \quad X^-(\omega) := \max\{0, -X(\omega)\},$$

and similar for Y, for all $\omega \in \Omega$. We then have $X = X^+ - X^-$ and $Y = Y^+ - Y^-$, such that

$$X(\omega)Y(\omega) = X^+(\omega)Y^+(\omega) - X^-(\omega)Y^+(\omega) - X^+(\omega)Y^-(\omega) + X^-(\omega)Y^-(\omega), \quad (5.8)$$

for all $\omega \in \Omega$. Noting that

$$X^+(\omega) = \int_0^{X^+(\omega)} \mathrm{d}x = \int_0^{\infty} \mathbb{1}_{\{(\bar{\omega},\bar{x}):\bar{x} < X^+(\bar{\omega})\}}(\omega, x)\,\mathrm{d}x,$$

we can write the expectation of the first term on the right hand side of (5.8) as

$$\begin{aligned}\mathbb{E}[X^+Y^+] &= \int_\Omega X^+(\omega)Y^+(\omega)\,\mathrm{d}\mathbb{P}(\omega) \\ &= \int_\Omega \int_0^\infty \int_0^\infty \mathbb{1}_{\{(\bar{\omega},\bar{x},\bar{y}):\bar{x} < X^+(\bar{\omega}), \bar{y} < Y^+(\bar{\omega})\}}(\omega, x, y)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\mathbb{P}(\omega).\end{aligned}$$

Since the integrand is nonnegative, Tonelli's theorem shows we can change the

order of integration. Hence,

$$\begin{aligned}\mathbb{E}[X^+Y^+] &= \int_0^\infty \int_0^\infty \int_\Omega \mathbb{1}_{\{(\bar\omega,\bar x,\bar y):\bar x<X^+(\bar\omega),\bar y<Y^+(\bar\omega)\}}(\omega,x,y)\,\mathrm{d}\mathbb{P}(\omega)\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_0^\infty \int_0^\infty \mathbb{P}\{X^+>x, Y^+>y\}\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_0^b \int_0^a \mathbb{P}\{X>x, Y>y\}\,\mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

Following a similar approach, one can show that $\mathbb{E}[X^+] = \int_0^a \mathbb{P}\{X>x\}\,\mathrm{d}x$ and $\mathbb{E}[Y^+] = \int_0^b \mathbb{P}\{Y>y\}\,\mathrm{d}y$. By the near-independence property of X and Y, we therefore have

$$|\mathbb{E}[X^+Y^+] - \mathbb{E}[X^+]\mathbb{E}[Y^+]| \le pab.$$

The other terms in (5.8) can be handled similarly. In conclusion,

$$\begin{aligned}|\mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]| &= |\mathbb{E}[(X^+-X^-)(Y^+-Y^-)] - \mathbb{E}[X^+-X^-]\mathbb{E}[Y^+-Y^-]| \\ &\le 4pab.\end{aligned}$$

□

Now we can generalize this result to higher dimensions.

Corollary 5.8. *Let X and Y be p-independent random variables in $\mathbb{R}^n$ such that $\|X\| \le a$ and $\|Y\| \le b$ almost surely. Let $e_1, \ldots, e_n$ be an orthonormal basis for $\mathbb{R}^n$ with respect to $\langle\cdot,\cdot\rangle$, and assume $x \mapsto \langle x, e_k\rangle$ is measurable for all $k \in \{1,\ldots,n\}$. Then,*

$$|\mathbb{E}[\langle X, Y\rangle] - \langle \mathbb{E}[X], \mathbb{E}[Y]\rangle| \le 4npab.$$

Proof. We have $X = \sum_{k=1}^n \langle X, e_k\rangle e_k$ and $Y = \sum_{k=1}^n \langle Y, e_k\rangle e_k$, such that

$$\mathbb{E}[\langle X, Y\rangle] = \sum_{k=1}^n \mathbb{E}[\langle X, e_k\rangle\langle Y, e_k\rangle] \quad \text{and} \quad \langle \mathbb{E}[X], \mathbb{E}[Y]\rangle = \sum_{k=1}^n \mathbb{E}[\langle X, e_k\rangle]\mathbb{E}[\langle Y, e_k\rangle].$$

By Lemma 3.5 in Lovász and Vempala [73], $\langle X, e_k\rangle$ and $\langle Y, e_k\rangle$ are p-independent for all k. Almost surely, $|\langle X, e_k\rangle| \le \|X\| \le a$ and $|\langle X, e_k\rangle| \le \|Y\| \le b$ by the Cauchy-Schwarz inequality. Applying Lemma 5.7 thus shows

$$\begin{aligned}|\mathbb{E}[\langle X, Y\rangle] - \langle \mathbb{E}[X], \mathbb{E}[Y]\rangle| &\le \sum_{k=1}^n |\mathbb{E}[\langle X, e_k\rangle\langle Y, e_k\rangle] - \mathbb{E}[\langle X, e_k\rangle]\mathbb{E}[\langle Y, e_k\rangle]| \\ &\le 4npab.\end{aligned}$$

□

As with Lemma 5.4, the measurability condition in this result holds for sufficiently detailed σ-algebras. We will quietly assume it holds in the remainder of this thesis.

As a final tool for our analysis of the mean estimate, we remark that for random variables Y and Z taking values in a set $\mathcal{S}$ and a function ϕ on $\mathcal{S}$,

$$\begin{aligned}\mathbb{E}[\phi(Y)] &= \mathbb{E}[\phi(Z)] + \mathbb{E}[\phi(Y) - \phi(Z)] \\ &= \mathbb{E}[\phi(Z)] + \mathbb{E}[\phi(Y) - \phi(Z) | Y \neq Z]\mathbb{P}\{Y \neq Z\}.\end{aligned} \tag{5.9}$$

We are ready to analyze the quality of the mean estimate. The general approach is the same as in [8, Theorem 5.1], except that we use a general inner product here. Moreover, the differences between Theorem 4.14 and [8, Theorem 4.7] also lead to a slightly simpler statement of the mixing conditions. We remind the reader of the notation summarized in Table 3.1 on page 32.

Theorem 5.9. *Let f be the log-partition function associated with a convex body $\mathcal{S} \subset \mathbb{R}^n$. Assume $\mathcal{S}$ is contained in a ball with radius $R > 0$. Suppose $\theta_0, \theta_1 \in \mathbb{R}^n$ satisfy $\Delta\theta := \|\theta_0 - \theta_1\|_{\theta_0} < 1$. Let $\rho > 0$, $\epsilon \geq 0$, and $q \in (0, 1]$, and suppose we have an invertible matrix $\widehat{\Sigma}(\theta_0)$ such that*

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(\theta_0)^{-1} \preceq \Sigma(\theta_0)^{-1} \preceq (1+\epsilon)\widehat{\Sigma}(\theta_0)^{-1}.$$

Pick

$$N \geq \frac{2n}{q\rho^2} \quad \text{and} \quad p \leq \frac{q \min\{1, \rho^2\} \min\{1, \lambda_{\min}(\Sigma(\theta_1))\}}{204n \max\{1, R^2\}}. \tag{5.10}$$

Let X be a random starting point drawn from a Boltzmann distribution with parameter θ_0. Let $Y^1, \ldots, Y^N$ be the end points of N hit-and-run random walks applied to the Boltzmann distribution with parameter θ_1 having starting point X, where the directions are drawn from a $\mathcal{N}(0, \widehat{\Sigma}(\theta_0))$-distribution, and each walk has length ℓ given by (4.10). *(Note that ℓ depends on ϵ, n, p, and $\Delta\theta$.) Then, the empirical mean $\widehat{x}(\theta_1) := \frac{1}{N}\sum_{j=1}^N Y^j$ satisfies*

$$\mathbb{P}\left\{\|\widehat{x}(\theta_1) - x(\theta_1)\|_{\Sigma(\theta_1)^{-1}} \leq \rho\right\} \geq 1 - q. \tag{5.11}$$

Proof. Theorem 4.14 ensures that the distributions of the samples $Y^1, \ldots, Y^N$ all have a total variation distance to the Boltzmann distribution with parameter θ_1 of

at most p. By Corollary 5.6, the samples are pairwise $6p$-independent. It therefore remains to be shown that N pairwise $6p$-independent samples with total variation distance to the Boltzmann distribution with parameter θ_1 of at most p are enough to guarantee (5.11).

We start by investigating an expression resembling the variance of $\widehat{x}(\theta_1)$ in the norm induced by $\Sigma(\theta_1)^{-1}$:

$$\begin{aligned}
&\mathbb{E}\Big[\|\widehat{x}(\theta_1)-x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}}\Big] \\
&= \mathbb{E}\left[\left\langle \frac{1}{N}\sum_{j=1}^{N}\big(Y^j-x(\theta_1)\big), \frac{1}{N}\sum_{j=1}^{N}\big(Y^j-x(\theta_1)\big)\right\rangle_{\Sigma(\theta_1)^{-1}}\right] \\
&= \frac{1}{N^2}\sum_{j=1}^{N}\mathbb{E}\Big[\big\|Y^j-x(\theta_1)\big\|^2_{\Sigma(\theta_1)^{-1}}\Big] \qquad (5.12)\\
&\quad + \frac{1}{N^2}\sum_{j=1}^{N}\sum_{k\neq j}\mathbb{E}\Big[\big\langle Y^j-x(\theta_1), Y^k-x(\theta_1)\big\rangle_{\Sigma(\theta_1)^{-1}}\Big] \qquad (5.13)
\end{aligned}$$

To bound (5.12), note Lemma 4.5 guarantees that for each Y^j there exists a Z^j following the Boltzmann distribution with parameter θ_1 such that $\mathbb{P}\{Y^j \neq Z^j\} \leq p$. Using (5.9), we have for all $j \in \{1,\ldots,N\}$,

$$\begin{aligned}
&\mathbb{E}\Big[\big\|Y^j-x(\theta_1)\big\|^2_{\Sigma(\theta_1)^{-1}}\Big] \\
&\leq \mathbb{E}\Big[\big\|Z^j-x(\theta_1)\big\|^2_{\Sigma(\theta_1)^{-1}}\Big] + p\left(\max_{y\in\mathcal{S}}\|y-x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}} - 0\right) \\
&\leq n + p(2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1}) = n + \frac{4pR^2}{\lambda_{\min}(\Sigma(\theta_1))}, \qquad (5.14)
\end{aligned}$$

where the final inequality also uses Lemma 4.12.

To bound (5.13), note that since Y^j and Y^k are $6p$-independent for all $j \neq k$, so are $Y^j - x(\theta_1)$ and $Y^k - x(\theta_1)$. Moreover, $\|Y^j - x(\theta_1)\|_{\Sigma(\theta_1)^{-1}} \leq 2R\sqrt{\lambda_{\max}(\Sigma(\theta_1)^{-1})}$ for all j. By Corollary 5.8, we therefore have for all $j \neq k$,

$$\begin{aligned}
&\mathbb{E}\Big[\big\langle Y^j-x(\theta_1), Y^k-x(\theta_1)\big\rangle_{\Sigma(\theta_1)^{-1}}\Big] \\
&\leq \big\langle \mathbb{E}\big[Y^j-x(\theta_1)\big], \mathbb{E}\big[Y^k-x(\theta_1)\big]\big\rangle_{\Sigma(\theta_1)^{-1}} + 4n(6p)(2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1}) \\
&= \big\langle \mathbb{E}\big[Y^j-x(\theta_1)\big], \mathbb{E}\big[Y^k-x(\theta_1)\big]\big\rangle_{\Sigma(\theta_1)^{-1}} + \frac{96npR^2}{\lambda_{\min}(\Sigma(\theta_1))}. \qquad (5.15)
\end{aligned}$$

Using Lemma 4.5 and (5.9) in the same manner as before, we get for all j,

$$\begin{aligned}
&\left\|\mathbb{E}\left[Y^j - x(\theta_1)\right]\right\|_{\Sigma(\theta_1)^{-1}} \\
&\leq \left\|\mathbb{E}\left[Z^j - x(\theta_1)\right]\right\|_{\Sigma(\theta_1)^{-1}} + p\left(\max_{y\in\mathcal{S}} \|y - x(\theta_1)\|_{\Sigma(\theta_1)^{-1}} - 0\right) \\
&\leq 0 + \frac{2pR}{\sqrt{\lambda_{\min}(\Sigma(\theta_1))}}.
\end{aligned}$$

Hence, (5.15) shows

$$\mathbb{E}\left[\left\langle Y^j - x(\theta_1), Y^k - x(\theta_1)\right\rangle_{\Sigma(\theta_1)^{-1}}\right] \leq \frac{4p^2R^2}{\lambda_{\min}(\Sigma(\theta_1))} + \frac{96npR^2}{\lambda_{\min}(\Sigma(\theta_1))}.$$

Combined with (5.12), (5.13), and (5.14), we thus find

$$\begin{aligned}
\mathbb{E}\left[\|\widehat{x}(\theta_1) - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}}\right] &\leq \frac{n}{N} + \frac{4pR^2}{N\,\lambda_{\min}(\Sigma(\theta_1))} + \frac{4p^2R^2}{\lambda_{\min}(\Sigma(\theta_1))} + \frac{96npR^2}{\lambda_{\min}(\Sigma(\theta_1))} \\
&\leq q\rho^2,
\end{aligned}$$

where the second inequality uses the values of N and ρ from (5.10). The proof is completed by applying Markov's inequality:

$$\mathbb{P}\left\{\|\widehat{x}(\theta_1) - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}} > \rho^2\right\} \leq \frac{\mathbb{E}\left[\|\widehat{x}(\theta_1) - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}}\right]}{\rho^2} \leq q. \qquad \square$$

This theorem requires a lower bound on $\lambda_{\min}(\Sigma(\theta_1))$, the smallest eigenvalue of $\Sigma(\theta_1)$. We refer the reader to Appendix B for such a bound.

5.3 Quality of Covariance Approximation

Above, we saw how well the mean of a number of hit-and-run samples approximates the mean of a Boltzmann distribution. The next step is performing a similar analysis for the covariance. If $Y^1, \ldots, Y^N$ are random variables, we define the associated empirical covariance as the linear operator $\widehat{\Sigma}$ satisfying

$$\widehat{\Sigma}v := \frac{1}{N}\sum_{j=1}^{N}\langle Y^j, v\rangle Y^j - \left(\frac{1}{N}\sum_{j=1}^{N}\langle Y^j, v\rangle\right)\left(\frac{1}{N}\sum_{j=1}^{N} Y^j\right), \tag{5.16}$$

for all $v \in \mathbb{R}^n$. (Note that for the Euclidean inner product, this is simply the empirical covariance matrix.)

Our analysis will require a bound on the fourth moment of a log-concave random variable with identity covariance.

Lemma 5.10 ([8, Theorem 5.3])**.** *Let X be a log-concave random variable on $\mathbb{R}^n$ with covariance operator Σ, i.e. $\Sigma[v,w] = \mathbb{E}[\langle X - \mathbb{E}[X], v\rangle \langle X - \mathbb{E}[X], w\rangle]$ for all $v, w \in \mathbb{R}^n$. Assume $x \mapsto \|x\|_{\Sigma^{-1}}$ is measurable. Then,*

$$\mathbb{E}\left[\|X - \mathbb{E}[X]\|_{\Sigma^{-1}}^4\right] \le 65n^2.$$

Proof. Let $Y := \frac{1}{\sqrt{n}}\|X - \mathbb{E}[X]\|_{\Sigma^{-1}}$, and note that its distribution is log-concave by the measurability assumption and the log-concavity definition (4.1). Then, Lemma 4.12 shows $\mathbb{E}[Y^2] = \frac{1}{n}\mathbb{E}[\|X - \mathbb{E}[X]\|_{\Sigma^{-1}}^2] = 1$. Therefore, Lemma 5.7 in Lovász and Vempala [74] shows that for all $t > 1$,

$$\mathbb{P}\{Y > t\} \le e^{1-t}. \tag{5.17}$$

(See also Lemma 3.3 in Lovász and Vempala [73].) Hence,

$$\mathbb{E}\left[\|X - \mathbb{E}[X]\|_{\Sigma^{-1}}^4\right] = n^2\mathbb{E}[Y^4] = n^2 \int_0^\infty \mathbb{P}\{Y^4 > s\}\,\mathrm{d}s.$$

By a change of variables $s = t^4$ and (5.17), we get

$$\begin{aligned}\mathbb{E}\left[\|X - \mathbb{E}[X]\|_{\Sigma^{-1}}^4\right] &= n^2 \int_0^\infty \mathbb{P}\{Y^4 > t^4\} 4t^3\,\mathrm{d}t \\ &\le n^2 \int_0^1 4t^3\,\mathrm{d}t + n^2 \int_1^\infty 4t^3 e^{1-t}\,\mathrm{d}t = 65n^2. \qquad \square\end{aligned}$$

For some $\theta \in \mathbb{R}^n$ and $\xi > 0$, the next theorem analyzes when the empirical covariance $\widehat{\Sigma}$ approximates $\Sigma(\theta)$ in the sense that $\frac{1}{1+\xi}\widehat{\Sigma} \preceq \Sigma(\theta) \preceq (1+\xi)\widehat{\Sigma}$. It is worth noting that by Lemma 2.4,

$$\frac{1}{1+\xi}\widehat{\Sigma} \preceq \Sigma(\theta) \preceq (1+\xi)\widehat{\Sigma} \quad \text{if and only if} \quad \frac{1}{1+\xi}\widehat{\Sigma}^{-1} \preceq \Sigma(\theta)^{-1} \preceq (1+\xi)\widehat{\Sigma}^{-1}.$$

In other words, the next theorem also guarantees that the inverse of $\widehat{\Sigma}$ is a good approximation of the inverse of $\Sigma(\theta)$.

The major differences between this theorem and [8, Theorem 5.3] are the fact this theorem holds for general inner products and has a slightly different result (5.19). This difference also leads to different constants in (5.18), though the overall complexity does not change. Finally, the differences between Theorem 4.14 and [8, Theorem 4.7] lead to a slightly simpler statement of the mixing conditions.

Theorem 5.11. *Let f be the log-partition function associated with a convex body $\mathcal{S} \subset \mathbb{R}^n$. Assume $\mathcal{S}$ is contained in a ball with radius $R > 0$, and that $x \mapsto \langle x, v\rangle\langle x, w\rangle$ is a measurable function on $\mathcal{S}$ for any $v, w \in \mathbb{R}^n$. Suppose $\theta_0, \theta_1 \in \mathbb{R}^n$ satisfy $\Delta\theta := \|\theta_0 - \theta_1\|_{\theta_0} < 1$. Let $\epsilon \geq 0$ and $\xi, q \in (0, 1]$, and suppose we have an invertible matrix $\widehat{\Sigma}(\theta_0)$ such that*

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(\theta_0)^{-1} \preceq \Sigma(\theta_0)^{-1} \preceq (1+\epsilon)\widehat{\Sigma}(\theta_0)^{-1}.$$

Pick

$$N \geq \frac{475n^2}{q\xi^2} \quad \textit{and} \quad p \leq \frac{q\xi^2 \min\{1, \lambda_{\min}(\Sigma(\theta_1))^2\}}{48450n^2 \max\{1, R^4\}}. \tag{5.18}$$

Let X be a random starting point drawn from a Boltzmann distribution with parameter θ_0. Let $Y^1, \ldots, Y^N$ be the end points of N hit-and-run random walks applied to the Boltzmann distribution with parameter θ_1 having starting point X, where the directions are drawn from a $\mathcal{N}(0, \widehat{\Sigma}(\theta_0))$-distribution, and each walk has length ℓ given by (4.10)*. (Note that ℓ depends on ϵ, n, p, and $\Delta\theta$.) Then, the empirical mean $\widehat{\Sigma} \approx \Sigma(\theta_1)$ as defined in* (5.16) *satisfies*

$$\mathbb{P}\left\{\frac{1}{1+\xi}\widehat{\Sigma} \preceq \Sigma(\theta_1) \preceq (1+\xi)\widehat{\Sigma}\right\} \geq 1 - q. \tag{5.19}$$

Proof. By the argument also used in the proof of Theorem 5.9, $Y^1, \ldots, Y^N$ are pairwise $6p$-independent samples, each with a distribution that has total variation distance to the Boltzmann distribution with parameter θ_1 of at most p. As before, define $\widehat{x}(\theta_1) := \frac{1}{N}\sum_{j=1}^{N} Y^j$.

The remainder of this proof follows an approach similar to Theorem 5.11 from Kannan et al. [58], although their result only applies to the uniform distribution and the Euclidean inner product. We want to prove that with probability at least

$1-q$,

$$\frac{1}{1+\xi} \leq \frac{\langle v, \widehat{\Sigma} v\rangle}{\|v\|_{\theta_1}^2} \leq 1+\xi \qquad \forall v \in \mathbb{R}^n. \tag{5.20}$$

It is elementary to show $\langle v, \widehat{\Sigma} v\rangle = \frac{1}{N}\sum_{j=1}^N \langle Y^j - x(\theta_1), v\rangle^2 - \langle \widehat{x}(\theta_1) - x(\theta_1), v\rangle^2$, so (5.20) is equivalent to the condition that for all $v \in \mathbb{R}^n$,

$$\frac{1}{1+\xi} + \frac{\langle \widehat{x}(\theta_1) - x(\theta_1), v\rangle^2}{\|v\|_{\theta_1}^2} \leq \frac{\sum_{j=1}^N \langle Y^j - x(\theta_1), v\rangle^2}{N\|v\|_{\theta_1}^2} \leq 1+\xi+\frac{\langle \widehat{x}(\theta_1) - x(\theta_1), v\rangle^2}{\|v\|_{\theta_1}^2}. \tag{5.21}$$

To ease notation, let P be the linear operator such that

$$Pv \coloneqq \frac{1}{N}\sum_{j=1}^N \langle Y^j - x(\theta_1), v\rangle (Y^j - x(\theta_1)) \qquad \forall v \in \mathbb{R}^n. \tag{5.22}$$

Noting that the left hand side of (5.21) can be upper bounded using Theorem 5.9, and the right hand side can be lower bounded by $1+\xi$, the condition (5.21) boils down to showing $\langle v, Pv\rangle / \|v\|_{\theta_1}^2 \approx 1$ for all $v \in \mathbb{R}^n$. Equivalently, we would like to show that $\langle v, (\Sigma(\theta_1)^{-1}P - I)v\rangle_{\theta_1} / \|v\|_{\theta_1}^2 \approx 0$ for all v. If $\Sigma(\theta_1)^{-1}P$ has eigenvalues $\lambda_1, \ldots, \lambda_n$ with respect to $\langle \cdot, \cdot \rangle_{\theta_1}$, we are thus interested in showing that $\lambda_1, \ldots, \lambda_n \approx 1$. One way to accomplish this is by noting

$$\begin{aligned} \max_{v \in \mathbb{R}^n} \frac{|\langle v, (\Sigma(\theta_1)^{-1}P - I)v\rangle_{\theta_1}|}{\|v\|_{\theta_1}^2} &= \max_i |\lambda_i - 1| \\ &= \sqrt{\max_i \{(\lambda_i - 1)^2\}} \\ &\leq \sqrt{\sum_{i=1}^n (\lambda_i - 1)^2}, \end{aligned} \tag{5.23}$$

so it suffices to bound the trace of $(\Sigma(\theta_1)^{-1}P - I)^2$ from above with high probability. To apply Markov's inequality, we will thus look for an upper bound on

$$\mathbb{E}\left[\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\Sigma(\theta_1)^{-1}P\right)\right] - 2\mathbb{E}\left[\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\right)\right] + n. \tag{5.24}$$

Let us start with the second term in (5.24), since it is the easiest to bound. If $v_1, \ldots, v_n$ are the orthonormal eigenvectors corresponding to the eigenvalues

$\lambda_1, ..., \lambda_n$ of $\Sigma(\theta_1)^{-1}P$ with respect to $\langle \cdot, \cdot \rangle_{\theta_1}$, we have

$$\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\right) = \sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} \langle v_i, \Sigma(\theta_1)^{-1} P v_i \rangle_{\theta_1} = \sum_{i=1}^{n} \langle v_i, P v_i \rangle.$$

Using the definition (5.22) of P,

$$\begin{aligned}
\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\right) &= \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{N} \langle Y^j - x(\theta_1), v_i \rangle^2 \\
&= \frac{1}{N} \sum_{j=1}^{N} \left\langle Y^j - x(\theta_1), \sum_{i=1}^{n} \langle \Sigma(\theta_1)^{-1}[Y^j - x(\theta_1)], v_i \rangle_{\theta_1} v_i \right\rangle \\
&= \frac{1}{N} \sum_{j=1}^{N} \|Y^j - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}},
\end{aligned}$$

where we used the fact that the second line contains a decomposition of the vector $\Sigma(\theta_1)^{-1}[Y^j - x(\theta_1)]$ in the basis $v_1, ..., v_n$ with respect to $\langle \cdot, \cdot \rangle_{\theta_1}$. To bound the expectation of this term, note that by Lemma 4.5, there exists for each Y^j a Z^j following the Boltzmann distribution with parameter θ_1 such that $\mathbb{P}\{Y^j \neq Z^j\} \leq p$. It then follows from (5.9) and Lemma 4.12 that

$$\begin{aligned}
\mathbb{E}\left[\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\right)\right] &\geq \mathbb{E}\left[\frac{1}{N} \sum_{j=1}^{N} \|Z^j - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}}\right] - p \max_{y \in \mathcal{S}} \|y - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}} \\
&\geq n - p(2R)^2 \lambda_{\max}(\Sigma(\theta_1)^{-1}),
\end{aligned} \tag{5.25}$$

where the final inequality uses the assumption that $\mathcal{S}$ is contained in a ball with radius R.

We continue by upper bounding the first term in (5.24). We have, by definition of the trace,

$$\operatorname{tr}\left(\Sigma(\theta_1)^{-1} P \Sigma(\theta_1)^{-1} P\right) = \sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n} \|\Sigma(\theta_1)^{-1} P v_i\|^2_{\theta_1}.$$

Again using the definition (5.22) of P,

$$\begin{aligned}
&\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\Sigma(\theta_1)^{-1}P\right)\\
&=\sum_{i=1}^{n}\left\|\frac{1}{N}\sum_{j=1}^{N}\langle Y^j-x(\theta_1),v_i\rangle\Sigma(\theta_1)^{-1}[Y^j-x(\theta_1)]\right\|_{\theta_1}^2\\
&=\frac{1}{N^2}\sum_{i=1}^{n}\sum_{j=1}^{N}\sum_{k=1}^{N}\langle Y^j-x(\theta_1),v_i\rangle\langle Y^k-x(\theta_1),v_i\rangle\langle Y^j-x(\theta_1),Y^k-x(\theta_1)\rangle_{\theta_1}^{-1}.
\end{aligned}$$

We can get rid of the outer summation by noting that it decomposes the vector $\Sigma(\theta_1)^{-1}[Y^k-x(\theta_1)]$ in the basis $v_1,\ldots,v_n$ with respect to $\langle\cdot,\cdot\rangle_{\theta_1}$:

$$\begin{aligned}
&\sum_{i=1}^{n}\langle Y^j-x(\theta_1),v_i\rangle\langle Y^k-x(\theta_1),v_i\rangle\\
&=\left\langle Y^j-x(\theta_1),\sum_{i=1}^{n}\langle Y^k-x(\theta_1),v_i\rangle v_i\right\rangle\\
&=\left\langle Y^j-x(\theta_1),\sum_{i=1}^{n}\langle\Sigma(\theta_1)^{-1}[Y^k-x(\theta_1)],v_i\rangle_{\theta_1}v_i\right\rangle\\
&=\langle Y^j-x(\theta_1),Y^k-x(\theta_1)\rangle_{\theta_1}^{-1}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\Sigma(\theta_1)^{-1}P\right)\\
&=\frac{1}{N^2}\sum_{j=1}^{N}\sum_{k=1}^{N}\langle Y^j-x(\theta_1),Y^k-x(\theta_1)\rangle_{\Sigma(\theta_1)^{-1}}^2\\
&=\frac{1}{N^2}\sum_{j=1}^{N}\|Y^j-x(\theta_1)\|_{\Sigma(\theta_1)^{-1}}^4 \qquad (5.26)\\
&\quad+\frac{1}{N^2}\sum_{j=1}^{N}\sum_{k\neq j}\left(\sum_{i=1}^{n}\langle Y^j-x(\theta_1),v_i\rangle\langle Y^k-x(\theta_1),v_i\rangle\right)^2. \qquad (5.27)
\end{aligned}$$

To upper bound the expectation of (5.26), we use (5.9) and Lemma 5.10 as

follows:

$$\begin{aligned}
&\mathbb{E}\left[\frac{1}{N^2}\sum_{j=1}^{N}\|Y^j - x(\theta_1)\|^4_{\Sigma(\theta_1)^{-1}}\right] \\
&\leq \frac{1}{N^2}\sum_{j=1}^{N}\mathbb{E}\Big[\|Z^j - x(\theta_1)\|^4_{\Sigma(\theta_1)^{-1}}\Big] + \frac{p}{N}\max_{y\in\mathcal{S}}\|y - x(\theta_1)\|^4_{\Sigma(\theta_1)^{-1}} \\
&\leq \frac{65n^2}{N} + \frac{p(2R)^4\,\lambda_{\max}(\Sigma(\theta_1)^{-1})^2}{N}. \qquad (5.28)
\end{aligned}$$

To upper bound the expectation of (5.27), we use Lemma 5.7 to find that, for any $j \neq k$,

$$\begin{aligned}
&\mathbb{E}\left[\left(\sum_{i=1}^{n}\langle Y^j - x(\theta_1), v_i\rangle\langle Y^k - x(\theta_1), v_i\rangle\right)^2\right] \\
&= \sum_{i=1}^{n}\sum_{l=1}^{n}\mathbb{E}\big[\langle Y^j - x(\theta_1), v_i\rangle\langle Y^j - x(\theta_1), v_l\rangle\langle Y^k - x(\theta_1), v_i\rangle\langle Y^k - x(\theta_1), v_l\rangle\big] \\
&\leq \sum_{i=1}^{n}\sum_{l=1}^{n}\mathbb{E}\big[\langle Y^j - x(\theta_1), v_i\rangle\langle Y^j - x(\theta_1), v_l\rangle\big]\mathbb{E}\big[\langle Y^k - x(\theta_1), v_i\rangle\langle Y^k - x(\theta_1), v_l\rangle\big] \\
&\quad + \sum_{i=1}^{n}\sum_{l=1}^{n}4(6p)\left(\max_{y\in\mathcal{S}}|\langle y - x(\theta_1), v_i\rangle\langle y - x(\theta_1), v_l\rangle|\right)^2.
\end{aligned}$$

By (5.9) and the triangle inequality,

$$\begin{aligned}
&\Big|\mathbb{E}\big[\langle Y^j - x(\theta_1), v_i\rangle\langle Y^j - x(\theta_1), v_l\rangle\big] - \mathbb{E}\big[\langle Z^j - x(\theta_1), v_i\rangle\langle Z^j - x(\theta_1), v_l\rangle\big]\Big| \\
&\leq p\left|\max_{y,z\in\mathcal{S}}\{\langle y - x(\theta_1), v_i\rangle\langle y - x(\theta_1), v_l\rangle - \langle z - x(\theta_1), v_i\rangle\langle z - x(\theta_1), v_l\rangle\}\right| \\
&\leq p\max_{y,z\in\mathcal{S}}\{|\langle y - x(\theta_1), v_i\rangle\langle y - x(\theta_1), v_l\rangle| + |\langle z - x(\theta_1), v_i\rangle\langle z - x(\theta_1), v_l\rangle|\} \\
&\leq 2p\max_{y\in\mathcal{S}}\|y - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}} \leq 2p(2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1}).
\end{aligned}$$

It was shown in Proposition 3.3(ii) that $\mathbb{E}[\langle Z^j - x(\theta_1), v_i\rangle\langle Z^j - x(\theta_1), v_l\rangle] = \Sigma(\theta_1)[v_i, v_l]$. Because v_i and v_l are orthonormal with respect to $\langle\cdot,\cdot\rangle_{\theta_1}$, we have

that $\mathbb{E}[\langle Z^j - x(\theta_1), v_i\rangle\langle Z^j - x(\theta_1), v_l\rangle]$ is one if $i = l$ and zero otherwise. We conclude that

$$\begin{aligned}
&\mathbb{E}\left[\left(\sum_{i=1}^{n}\langle Y^j - x(\theta_1), v_i\rangle\langle Y^k - x(\theta_1), v_i\rangle\right)^2\right] \\
&\leq n\left(1 + 2p(2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1})\right)^2 + n(n-1)\left(2p(2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1})\right)^2 \\
&\quad + 4n^2(6p)\left((2R)^2\,\lambda_{\max}(\Sigma(\theta_1)^{-1})\right)^2.
\end{aligned}$$

Combining this bound on the expectation of (5.27) with the bound (5.28) on the expectation of (5.26) yields

$$\begin{aligned}
&\mathbb{E}\left[\operatorname{tr}\left(\Sigma(\theta_1)^{-1}P\Sigma(\theta_1)^{-1}P\right)\right] \\
&\leq \frac{65n^2}{N} + \frac{p(2R)^4}{N\,\lambda_{\min}(\Sigma(\theta_1))^2} + \frac{N(N-1)}{N^2}\left[n\left(1 + \frac{2p(2R)^2}{\lambda_{\min}(\Sigma(\theta_1))}\right)^2\right. \\
&\quad \left. + n(n-1)\left(\frac{2p(2R)^2}{\lambda_{\min}(\Sigma(\theta_1))}\right)^2 + 4n^2(6p)\left(\frac{(2R)^2}{\lambda_{\min}(\Sigma(\theta_1))}\right)^2\right] \\
&\leq n + 0.1451q\xi^2,
\end{aligned}$$

for the values of N and p from (5.18). (The constant 0.1451 above is exact.) Together with (5.25), this yields an upper bound on (5.24) of

$$\mathbb{E}\left[\operatorname{tr}\left((\Sigma(\theta_1)^{-1}P - I)^2\right)\right] \leq 0.1451q\xi^2 + 2p\frac{(2R)^2}{\lambda_{\min}(\Sigma(\theta_1))} \leq 0.1453q\xi^2.$$

By (5.23) and Markov's inequality, we therefore have

$$\mathbb{P}\left\{\max_{w\in\mathbb{R}^n}\frac{|\langle w, (P - \Sigma(\theta_1))w\rangle|}{\|w\|_{\theta_1}^2} > \tfrac{7}{18}\xi\right\} \leq \left(\frac{18}{7\xi}\right)^2 0.1453q\xi^2 \leq 0.9608q.$$

Applying Theorem 5.9 for $\rho = \frac{1}{3}\xi$ shows that for the values of N and p in (5.18),

$$\mathbb{P}\left\{\|\widehat{x}(\theta_1) - x(\theta_1)\|_{\Sigma(\theta_1)^{-1}} > \tfrac{1}{3}\xi\right\} \leq \frac{2q\xi^2}{475\rho^2} = \frac{18}{475}q \leq 0.0379q.$$

Since $0.9608q + 0.0379q \leq q$,

$$\mathbb{P}\left\{\max_{w\in\mathbb{R}^n}\frac{|\langle w, (P - \Sigma(\theta_1))w\rangle|}{\|w\|_{\theta_1}^2} \leq \tfrac{7}{18}\xi \wedge \|\widehat{x}(\theta_1) - x(\theta_1)\|_{\Sigma(\theta_1)^{-1}} \leq \tfrac{1}{3}\xi\right\} \geq 1 - q.$$

It remains to prove that in this high-probability event, (5.21) holds. To show the left inequality in (5.21), we first remark that for all $\xi \in (0,1]$, $\frac{1}{1+\xi} + \frac{1}{9}\xi^2 \leq 1 - \frac{7}{18}\xi$. Then, we have for all $v \in \mathbb{R}^n$,

$$\begin{aligned}
\frac{1}{1+\xi} + \frac{\langle \widehat{x}(\theta_1) - x(\theta_1), v\rangle^2}{\|v\|_{\theta_1}^2} &\leq \frac{1}{1+\xi} + \|\widehat{x}(\theta_1) - x(\theta_1)\|^2_{\Sigma(\theta_1)^{-1}} \\
&\leq \frac{1}{1+\xi} + \tfrac{1}{9}\xi^2 \leq 1 - \tfrac{7}{18}\xi \\
&\leq \frac{\langle v, \Sigma(\theta_1) v\rangle}{\|v\|_{\theta_1}^2} - \max_{w \in \mathbb{R}^n} \frac{|\langle w, (P - \Sigma(\theta_1))w\rangle|}{\|w\|_{\theta_1}^2} \\
&\leq \frac{\langle v, Pv\rangle}{\|v\|_{\theta_1}^2} = \frac{\sum_{j=1}^N \langle Y^j - x(\theta_1), v\rangle^2}{N\|v\|_{\theta_1}^2}.
\end{aligned}$$

Finally, the right inequality in (5.21) follows from

$$\begin{aligned}
\frac{\sum_{j=1}^N \langle Y^j - x(\theta_1), v\rangle^2}{N\|v\|_{\theta_1}^2} &\leq \frac{\langle v, \Sigma(\theta_1) v\rangle}{\|v\|_{\theta_1}^2} + \max_{w \in \mathbb{R}^n} \frac{|\langle w, (P - \Sigma(\theta_1))w\rangle|}{\|w\|_{\theta_1}^2} \\
&\leq 1 + \tfrac{7}{18}\xi \leq 1 + \xi + \frac{\langle \widehat{x}(\theta_1) - x(\theta_1), v\rangle^2}{\|v\|_{\theta_1}^2}. \qquad \square
\end{aligned}$$

As before, the measurability condition in this theorem is satisfied for detailed σ-algebras, and we will assume it holds in the remainder of this thesis.

The tools we developed in this chapter are useful if one wants to analyze sampling-based optimization algorithms. In the next chapters, we will look at two of those. Chapter 6 proposes an interior point method that uses hit-and-run sampling to approximate the derivatives of the entropic barrier. After that, we rigorously analyze Kalai and Vempala's simulated annealing algorithm [56] in Chapter 7.

6

Interior Point Method Using Hit-and-Run Sampling and the Entropic Barrier

We have seen how we can use hit-and-run sampling to approximate the mean and covariance of a Boltzmann distribution to a desired accuracy. The reason for our interest in these objects was that they relate to the derivatives of the entropic barrier. In Chapter 3, we assumed that we could compute these derivatives exactly. This was of course unrealistic, so we relax that assumption in this chapter. As such, we will need the results from Chapter 5 to guarantee that our approximations of the barrier's derivatives are sufficiently accurate.

In Section 6.1, we propose an algorithm to approximate the gradient of the entropic barrier at a given point. This algorithm only uses hit-and-run sampling, and can therefore be implemented on any convex body for which a membership oracle is known. With this method, we state a short-step interior point method that only uses hit-and-run sampling in Section 6.2. As we will see, its asymptotic complexity will be the same as that of Kalai and Vempala's algorithm from Chapter 7. We sketch the relationship between the algorithms in this chapter and those

in the preceding chapters in Figure 6.1.

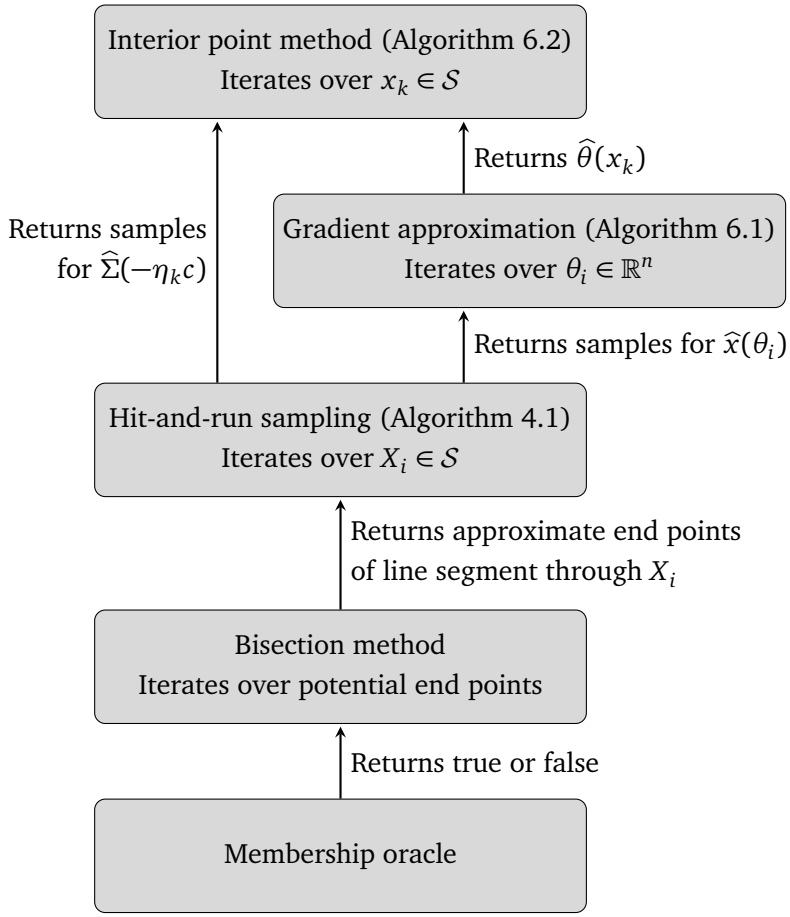

Figure 6.1: Sketch of the dependencies of the algorithms in Chapter 6

This chapter improves Section 6 from Badenbroek and De Klerk [8]. In Line 6 of Algorithm 6.2 below, we included a test that was not present in [8]. This test allows us to use constants for various parameters that depended on the problem dimension in [8]. As a result, here we get a significantly better asymptotic complexity for our short-step method than in [8]. Moreover, the results below apply to arbitrary inner products.

Let us first recall the setting from Section 3.3. The problem we consider is

(3.2), that is,

$$\min_{x\in\mathcal{S}}\langle c, x\rangle, \tag{6.1}$$

where $\mathcal{S}\subset\mathbb{R}^n$ is a convex body, and $c\in\mathbb{R}^n$. Let f and f^* be the log-partition function and the entropic barrier associated with $\mathcal{S}$, respectively. (See Table 3.1 on page 32 for a summary of the notation involving these functions.) For any $\eta>0$, define

$$f_\eta^*(x) := \eta\langle c, x\rangle + f^*(x), \tag{6.2}$$

and denote its minimizer by $z(\eta)$, that is, $g^*(z(\eta)) = -\eta c$. We also saw that $H^*(z(\eta)) = \Sigma(-\eta c)^{-1}$. We want to use the step (3.6), which was

$$-\gamma H^*(z(\eta))^{-1}[\eta c + g^*(x)] = -\gamma\Sigma(-\eta c)[\eta c + \theta(x)], \tag{6.3}$$

for some $\gamma\in[0,1]$ to approximate the minimizer of f_η^*.

6.1 Gradient Approximation

We cannot compute $\Sigma(-\eta c)$ and $\theta(x)$ directly, so we will use sampling-based approximations. The approximation of $\Sigma(-\eta c)$ in (6.3) is conceptually straightforward: we generate a number of hit-and-run samples from the Boltzmann distribution with parameter $-\eta c$ and compute the empirical covariance. How to approximate $\theta(x)$ for some $x\in\operatorname{int}\mathcal{S}$ may be less apparent.

We will use the suggestion from Abernethy and Hazan [1, Appendix D], which involves minimizing a certain functional. For our target $x\in\operatorname{int}\mathcal{S}$, we introduce the functional

$$\phi(\theta) := f(\theta) - \langle\theta, x\rangle. \tag{6.4}$$

Note that the minimizer of ϕ is $\theta(x)$ and that the Hessian of ϕ is equal to the Hessian of f. Hence, we are interested in approximating the minimizer of a convex function ϕ. This will be done with respect to the inner product induced by $\Sigma(-\eta c)$ because we need an approximation $\widehat{\theta}(x)$ of $\theta(x)$ such that $\|\widehat{\theta}(x)-\theta(x)\|_{-\eta c}$ is small, in order to analyze (6.3). The gradient of ϕ at $\theta\in\mathbb{R}^n$ with respect to $\langle\cdot,\cdot\rangle_{-\eta c}$ is $\Sigma(-\eta c)^{-1}[x(\theta)-x]$, which we can approximate if we have good enough estimates of $\Sigma(-\eta c)^{-1}$ and $x(\theta)$. With this approximate gradient, we can apply the results from De Klerk et al. [35] to approximate the minimizer $\theta(x)$ of ϕ.

The following lemma combines some results from [35]. It shows that even with the mean and covariance approximations from Chapter 5, we can make progress to the minimizer $\theta(x)$ of (6.4) for a given $x \in \mathcal{S}$. The parameter $\bar{\theta}$ is introduced below to fix an inner product. In the next section, we will set $\bar{\theta} = -\eta c$ for some $\eta > 0$.

Lemma 6.1. *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let f be its associated log-partition function. Let $\theta_0, \bar{\theta} \in \mathbb{R}^n$ and $x \in \mathcal{S}$. Let $\delta < 1$ such that $\|\theta_0 - \bar{\theta}\|_{\bar{\theta}}, \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \leq \delta$. Let $\epsilon \geq 0$, and assume we have an approximation $\widehat{\Sigma}(\bar{\theta})$ of $\Sigma(\bar{\theta})$ such that*

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(\bar{\theta}) \preceq \Sigma(\bar{\theta}) \preceq (1+\epsilon)\widehat{\Sigma}(\bar{\theta}). \tag{6.5}$$

Moreover, let $\rho \geq 0$, and suppose we have an approximation $\widehat{x}(\theta)$ of $x(\theta)$ for which it is known that $\|\widehat{x}(\theta_0) - x(\theta_0)\|_{\Sigma(\theta_0)^{-1}} \leq \rho$. Assume $\alpha \in \mathbb{R}$ satisfies

$$\frac{\rho\sqrt{1+\epsilon}}{(1-\delta)\|x(\theta_0) - x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}}} \leq \alpha \leq \frac{2(1-\delta)^4}{(1+\epsilon)^2 + (1-\delta)^4}. \tag{6.6}$$

Let $\theta_1 \coloneqq \theta_0 - \gamma\widehat{\Sigma}(\bar{\theta})^{-1}[\widehat{x}(\theta_0) - x]$, where

$$\gamma = \frac{2(1-\delta)^2(1+\epsilon)}{(1-\alpha)[(1+\epsilon)^2 + (1-\delta)^4]} - \frac{\alpha(1+\epsilon)}{(1-\alpha)(1-\delta)^2}.$$

Then,

$$\|\theta_1 - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} \leq \left(\frac{(1+\epsilon)^2 - (1-\delta)^4}{(1+\epsilon)^2 + (1-\delta)^4} + \alpha\right)\|\theta_0 - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})}.$$

Proof. Let ϕ be as in (6.4). Note that the minimizer of ϕ is $\theta(x)$ and that the Hessian of ϕ is equal to the Hessian of f. It follows from (6.5) and Lemma 2.4 that the approximation $\widehat{\Sigma}(\bar{\theta})^{-1}[\widehat{x}(\theta_0) - x]$ for the gradient of ϕ at θ_0 with respect to the inner product induced by $\widehat{\Sigma}(\bar{\theta})$ satisfies

$$\begin{aligned}\left\|\widehat{\Sigma}(\bar{\theta})^{-1}[\widehat{x}(\theta_0) - x] - \widehat{\Sigma}(\bar{\theta})^{-1}[x(\theta_0) - x]\right\|_{\widehat{\Sigma}(\bar{\theta})} &= \|\widehat{x}(\theta_0) - x(\theta_0)\|_{\widehat{\Sigma}(\bar{\theta})^{-1}} \\ &\leq \sqrt{1+\epsilon}\|\widehat{x}(\theta_0) - x(\theta_0)\|_{\Sigma(\bar{\theta})^{-1}} \\ &\leq \frac{\sqrt{1+\epsilon}}{1-\delta}\|\widehat{x}(\theta_0) - x(\theta_0)\|_{\Sigma(\theta_0)^{-1}},\end{aligned}$$

where the final inequality used $\|\theta_0 - \bar{\theta}\|_{\bar{\theta}} \leq \delta$ and (2.5). Since by assumption $\|\widehat{x}(\theta_0) - x(\theta_0)\|_{\Sigma(\theta_0)^{-1}} \leq \rho$,

$$\left\|\widehat{\Sigma}(\bar{\theta})^{-1}[\widehat{x}(\theta_0) - x] - \widehat{\Sigma}(\bar{\theta})^{-1}[x(\theta_0) - x]\right\|_{\widehat{\Sigma}(\bar{\theta})} \leq \alpha \|x(\theta_0) - x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}}.$$

Hence, α is a relative bound on the error in the approximation of the gradient.

By the assumption that $\|\theta_0 - \bar{\theta}\|_{\bar{\theta}}, \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \leq \delta$, it holds for both $\theta \in \{\theta_0, \theta(x)\}$ that

$$\langle v, \widehat{\Sigma}(\bar{\theta})^{-1}\Sigma(\theta)v\rangle_{\widehat{\Sigma}(\bar{\theta})} = \|v\|_{\theta}^2 \leq \frac{\|v\|_{\bar{\theta}}^2}{(1 - \|\theta - \bar{\theta}\|_{\bar{\theta}})^2} \leq \frac{1+\epsilon}{(1-\delta)^2}\langle v, Iv\rangle_{\widehat{\Sigma}(\bar{\theta})},$$

that is, the eigenvalues of the Hessian of ϕ at θ with respect to the inner product induced by $\widehat{\Sigma}(\bar{\theta})$ are bounded above by $(1+\epsilon)/(1-\delta)^2$. Similarly, we can derive the lower bound $(1-\delta)^2/(1+\epsilon)$ on this spectrum.

As noted in the proof of Theorem 5.4 in De Klerk et al. [35], the result on convergence to the minimizer from Theorem 5.3 in [35] only requires bounds on the Hessians of ϕ at θ_0 and the minimizer $\theta(x)$, and not necessarily at θ_1. The claim thus follows from Theorem 5.3 in [35]. □

At a first glance, the presence of $\|x(\theta_0) - x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}}$ in (6.6) may seem troublesome. If this norm were very small, it would be hard to satisfy the inequality (6.6). Fortunately, we do not have to proceed with our approximate gradient descent algorithm when this norm is small: if $x(\theta_0) \approx x$, then θ_0 is a good approximation of $\theta(x)$.

This idea is formalized in Algorithm 6.1. The algorithm requires, among others, a target $x \in \mathcal{S}$ and an initial guess $\theta_0 \in \mathbb{R}^n$, and tries to find a θ_i near θ_0 such that $\|\theta_i - \theta(x)\|_{\bar{\theta}}$ is smaller than some bound κ with high probability. The approach is to minimize (6.4) by approximating its gradient with hit-and-run sampling. Note that we fix various constants – this will be convenient when we refer to Algorithm 6.1 later.

The following theorem provides conditions under which Algorithm 6.1 returns a θ_i such that $\|\theta_i - \theta(x)\|_{\bar{\theta}} \leq \kappa$ with probability at least $1 - q$ for a small value of $q \in (0, 1]$. The core of the proof is a repeated application of Lemma 6.1. This result is loosely based on [8, Theorem 6.1], but here we provide more elegant bounds.

Algorithm 6.1 Approximation routine for $\theta(x)$

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$ contained in a ball with radius $R \geq 1$;
log-partition function f and entropic barrier f^* associated with $\mathcal{S}$;
target $x \in \operatorname{int}\mathcal{S}$, starting point $\theta_0 \in \mathbb{R}^n$, and reference point $\bar{\theta} \in \mathbb{R}^n$;
real K such that $\|\theta_0 - \theta(x)\|_{\bar{\theta}} \leq K = \frac{1}{8}$ and tolerance $\kappa = \frac{1}{100}$;
approximation $\widehat{\Sigma}(\bar{\theta})$ of $\Sigma(\bar{\theta})$ satisfying (6.5) for $\epsilon = \frac{1}{100}$;
real $\delta = \frac{1}{4}$ such that $(1+\epsilon)K + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \leq \delta$;
sample $\overline{X}$ from the Boltzmann distribution with parameter $\bar{\theta}$;
number of iterations m; damping parameter γ;
number of samples N; number of hit-and-run steps ℓ.

Output: θ_i such that $\|\theta_i - \theta(x)\|_{\bar{\theta}} \leq \kappa$ with high probability.

1: **for** $i \in \{0, \ldots, m-1\}$ **do**
2: Generate $Y_1, \ldots, Y_N$ by applying hit-and-run sampling to the Boltzmann distribution with parameter θ_i, starting the walk from $\overline{X}$, taking ℓ steps, drawing directions from $\mathcal{N}(0, \widehat{\Sigma}(\bar{\theta}))$-distribution
3: Compute sample mean: $\widehat{x}(\theta_i) \leftarrow \frac{1}{N}\sum_{j=1}^{N} Y_j$
4: **if** $\|\widehat{x}(\theta_i) - x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}} \leq \frac{5}{12}\kappa(1-\delta)^2/\sqrt{1+\epsilon}$ **then**
5: **return** θ_i
6: **else**
7: $\theta_{i+1} \leftarrow \theta_i - \gamma\widehat{\Sigma}(\bar{\theta})^{-1}[\widehat{x}(\theta_i) - x]$
8: **return** θ_m

Theorem 6.2. *Consider the setting of Algorithm 6.1. Let $q \in (0,1]$, and*

$$m = \left\lceil \frac{\log(\kappa/[K(1+\epsilon)])}{\log\left(\frac{(1+\epsilon)^2-(1-\delta)^4}{(1+\epsilon)^2+(1-\delta)^4} + \frac{1+\epsilon}{5(1-\delta)^2}\right)} \right\rceil, \tag{6.7}$$

$$N = \left\lceil \frac{288nm}{q(1-\delta)^2\kappa^2} \right\rceil, \tag{6.8}$$

$$p = \frac{q(1-\delta)^4\kappa^2}{29376nR^2}\left(\frac{1}{16}\right)\left(\frac{1}{\max\{1, 4R\|\bar{\theta}\|\}}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)), \tag{6.9}$$

and let ℓ be as in (4.10). *(Note that ℓ depends on ϵ, n, p, and $\Delta\theta := \delta$.) Finally,*

set

$$\gamma = \frac{10(1-\delta)^4(1+\epsilon)}{[5(1-\delta)^2-(1+\epsilon)][(1+\epsilon)^2+(1-\delta)^4]} - \frac{(1+\epsilon)^2}{(1-\delta)^2[5(1-\delta)^2-(1+\epsilon)]}.$$

With these inputs, Algorithm 6.1 returns a θ_i with

$$\mathbb{P}\left\{\|\theta_i - \theta(x)\|_{\bar{\theta}} \leq \kappa\right\} \geq 1-q.$$

Proof. We will apply Lemma 6.1 to every iteration i of Algorithm 6.1 until termination.

The first condition we will investigate is $\|\theta_i - \bar{\theta}\|_{\bar{\theta}} \leq \delta$. This holds for $i = 0$, since

$$\begin{aligned}\|\theta_0 - \bar{\theta}\|_{\bar{\theta}} &\leq \|\theta_0 - \theta(x)\|_{\bar{\theta}} + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq K + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq \delta.\end{aligned}$$

The remainder of this proof will show that $\|\theta_{i+1} - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} \leq \|\theta_i - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})}$ for all i, meaning that we make progress to the minimizer. Using this inequality repeatedly, we will see that for all i,

$$\begin{aligned}\|\theta_{i+1} - \bar{\theta}\|_{\bar{\theta}} &\leq \|\theta_{i+1} - \theta(x)\|_{\bar{\theta}} + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq \sqrt{1+\epsilon}\|\theta_{i+1} - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq \sqrt{1+\epsilon}\|\theta_0 - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq (1+\epsilon)\|\theta_0 - \theta(x)\|_{\bar{\theta}} + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \\ &\leq (1+\epsilon)K + \|\theta(x) - \bar{\theta}\|_{\bar{\theta}} \leq \delta. \end{aligned} \tag{6.10}$$

To find an approximation $\widehat{x}(\theta_i)$ of $x(\theta_i)$ such that $\|\widehat{x}(\theta_i) - x(\theta_i)\|_{\Sigma(\theta_i)^{-1}} \leq \rho$ (with high probability), we can use Theorem 5.9. Since we already have $\|\theta_i - \bar{\theta}\|_{\bar{\theta}} \leq \delta = \Delta\theta$, it remains to state a lower bound on $\lambda_{\min}(\Sigma(\theta_i))$. It follows from (2.2) that $\Sigma(\theta_i) \succeq (1 - \|\theta_i - \bar{\theta}\|_{\bar{\theta}})^2\Sigma(\bar{\theta}) \succeq (1-\delta)^2\Sigma(\bar{\theta})$, so

$$\lambda_{\min}(\Sigma(\theta_i)) = \min_{v:\|v\|=1} \langle v, \Sigma(\theta_i)v\rangle \geq (1-\delta)^2\,\lambda_{\min}(\Sigma(\bar{\theta})).$$

Hence, an application of Theorem B.3 shows

$$\lambda_{\min}(\Sigma(\theta_i)) \geq \tfrac{1}{16}(1-\delta)^2\left(\frac{1}{\max\{1, 4R\|\bar{\theta}\|\}}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)).$$

We then apply Theorem 5.9 to see that $\mathbb{P}\{\|\widehat{x}(\theta_i)-x(\theta_i)\|_{\Sigma(\theta_i)^{-1}} \le \rho\} \ge 1-q/m$, where $\rho = \frac{1}{12}(1-\delta)\kappa$. Below, we assume that

$$\|\widehat{x}(\theta_i)-x(\theta_i)\|_{\Sigma(\theta_i)^{-1}} \le \tfrac{1}{12}(1-\delta)\kappa \qquad \forall i \in \{0,\dots,m-1\}, \tag{6.11}$$

and show that this leads to a successful termination of the algorithm. Thus, the success probability of Algorithm 6.1 will be at least $1-q$.

Algorithm 6.1 distinguishes the following two cases in Lines 4 and 6:

(a) $\|\widehat{x}(\theta_i)-x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}} \le \frac{5}{12}\kappa(1-\delta)^2/\sqrt{1+\epsilon}$;

(b) $\|\widehat{x}(\theta_i)-x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}} > \frac{5}{12}\kappa(1-\delta)^2/\sqrt{1+\epsilon}$.

Let us first show that the algorithm's termination in Case (a) is successful. Applying the first inequality in (2.1), (6.10), and Proposition 3.7, it can be seen that

$$\|\theta_i-\theta(x)\|_{\bar{\theta}} \le \frac{\|\theta_i-\theta(x)\|_{\theta_i}}{1-\|\theta_i-\bar{\theta}\|_{\bar{\theta}}} \le \frac{\|\theta_i-\theta(x)\|_{\theta_i}}{1-\delta} \le \frac{\|x(\theta_i)-x\|^*_{x(\theta_i)}}{(1-\delta)\Big(1-\|x(\theta_i)-x\|^*_{x(\theta_i)}\Big)}.$$

By the triangle inequality, the assumption (6.11), self-concordance, and (6.10),

$$\begin{aligned}
\|x(\theta_i)-x\|^*_{x(\theta_i)} &\le \|x(\theta_i)-\widehat{x}(\theta_i)\|_{\Sigma(\theta_i)^{-1}} + \|\widehat{x}(\theta_i)-x\|_{\Sigma(\theta_i)^{-1}} \\
&\le \tfrac{1}{12}(1-\delta)\kappa + \frac{\|\widehat{x}(\theta_i)-x\|_{\Sigma(\bar{\theta})^{-1}}}{1-\|\theta_i-\bar{\theta}\|_{\bar{\theta}}} \\
&\le \tfrac{1}{12}(1-\delta)\kappa + \frac{\sqrt{1+\epsilon}\|\widehat{x}(\theta_i)-x\|_{\widehat{\Sigma}(\bar{\theta})^{-1}}}{1-\delta} \\
&\le \tfrac{1}{12}(1-\delta)\kappa + \tfrac{5}{12}(1-\delta)\kappa = \tfrac{1}{2}(1-\delta)\kappa,
\end{aligned}$$

where the final inequality uses Case (a). Hence, in Case (a), we have

$$\|\theta_i-\theta(x)\|_{\bar{\theta}} \le \frac{\frac{1}{2}(1-\delta)\kappa}{(1-\delta)[1-\frac{1}{2}(1-\delta)\kappa]} < \frac{\frac{1}{2}(1-\delta)\kappa}{(1-\delta)[1-\frac{1}{2}]} = \kappa,$$

so indeed Algorithm 6.1 terminates successfully.

Next, we will show that in Case (b), we make a certain amount of progress towards $\theta(x)$ by executing Line 7 in Algorithm 6.1. In Case (b), we can satisfy (6.6) by picking

$$\alpha = \frac{1+\epsilon}{5(1-\delta)^2}.$$

Lemma 6.1 therefore shows that for all i,

$$\|\theta_{i+1} - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} \leq \left(\frac{(1+\epsilon)^2 - (1-\delta)^4}{(1+\epsilon)^2 + (1-\delta)^4} + \frac{1+\epsilon}{5(1-\delta)^2} \right) \|\theta_i - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})}.$$

With m as in (6.7), we therefore get

$$\begin{aligned} \|\theta_m - \theta(x)\|_{\bar{\theta}} &\leq \sqrt{1+\epsilon} \|\theta_m - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} \\ &\leq \sqrt{1+\epsilon} \frac{\kappa}{(1+\epsilon)K} \|\theta_0 - \theta(x)\|_{\widehat{\Sigma}(\bar{\theta})} \\ &\leq (1+\epsilon) \frac{\kappa}{(1+\epsilon)K} \|\theta_0 - \theta(x)\|_{\bar{\theta}} \leq \kappa, \end{aligned}$$

so after m iterations in Case (b), Algorithm 6.1 also terminates successfully. □

We conclude this section with a few words on the complexity of Algorithm 6.1 for the configuration in Theorem 6.2. The number of oracle calls is determined by the number of hit-and-run steps, which is $O^*(mN\ell)$. Note that the expression (6.7) for m depends only on constants, so $m = O(1)$. It follows from (6.8) that $N = O(n/q)$. Finally, the complexity of the walk length (4.10) is

$$\ell = O\left(\frac{n^3}{(1-\Delta\theta)^4} \log^2 \left(\frac{n\sqrt{n} e^{1-2\Delta\theta}}{p^2(1-\Delta\theta)^4} \right) \log^3 \left(\frac{e^{-2\Delta\theta}}{p^2(1-\Delta\theta)^2} \right) \right), \tag{6.12}$$

which, for fixed $\Delta\theta$ and the value of p from (6.9), yields

$$\ell = O^*\left(n^3 \left(\sqrt{\vartheta_{f^*}} \right)^5 \log^5 \left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^2\}} \right) \right).$$

In conclusion, the number of oracle calls by Algorithm 6.1 for the configuration in Theorem 6.2 is

$$O^*(mN\ell) = O^*\left(\frac{n^4 \vartheta_{f^*}^{2.5}}{q} \log^5 \left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^2\}} \right) \right). \tag{6.13}$$

If $\langle \cdot, \cdot \rangle$ were the Euclidean inner product, the value of p in (6.9) could be made more explicit by replacing $\lambda_{\min}(\Sigma(0))$ with its lower bound from Lemma B.2. Then, the number of oracle calls by Algorithm 6.1 for the configuration in Theorem 6.2 would be $O^*(n^4 \vartheta_{f^*}^{2.5}/q) = O^*(n^{6.5}/q)$ by Theorem 3.4.

6.2 Analysis of a Short-Step Method Using Hit-and-Run Sampling

Let us now specify the main short-step interior point method in detail. It will depend on a parameter $\delta^* = \frac{1}{10}$ and a maximum failure probability q^*. The reader should keep in mind that the parameters with an asterisk pertain to the method using the entropic barrier f^*, while the parameters $\delta = \frac{1}{4}$ and q used earlier in this chapter concern a method using f. With this notation, we hope to distinguish parameters that have similar functions in different algorithms, and that have different values.

Our short-step method is initialized with an $x_0 \in \mathcal{S}$ and $\eta_0 > 0$ such that $\|x_0 - z(\eta_0)\|^*_{z(\eta_0)} \leq \delta^*$. Moreover, we assume to have an approximation $\widehat{\Sigma}(-\eta_0 c)$ of $\Sigma(-\eta_0 c)$ such that

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(-\eta_0 c) \preceq \Sigma(-\eta_0 c) \preceq (1+\epsilon)\widehat{\Sigma}(-\eta_0 c), \tag{6.14}$$

for some $\epsilon > 0$. Finally, we also need a sample X_0 from the Boltzmann distribution with parameter $-\eta_0 c$.

In every iteration k, we can start several hit-and-run random walks from a sample X_{k-1} from the Boltzmann distribution with parameter $-\eta_{k-1}c$. With these hit-and-run samples, we can create an approximation $\widehat{\Sigma}(-\eta_k c)$ of $\Sigma(-\eta_k c)$, where $\eta_k > \eta_{k-1}$. Using a result from Chapter 5, we can then show that with high probability

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(-\eta_k c) \preceq \Sigma(-\eta_k c) \preceq (1+\epsilon)\widehat{\Sigma}(-\eta_k c). \tag{6.15}$$

We also generate X_k, and use it in a call to Algorithm 6.1 to approximate the gradient $\eta_k c + \theta(x_{k-1})$ of $f^*_{\eta_k}$ at x_{k-1}. This approximation $\eta_k c + \widehat{\theta}(x_{k-1})$ is such that $\|\widehat{\theta}(x_{k-1}) - \theta(x_{k-1})\|_{-\eta_k c}$ is small. With these two ingredients, we can take a step of the type (6.3) to $x_k = x_{k-1} - \gamma\widehat{\Sigma}(-\eta_k c)[\eta_k c + \widehat{\theta}(x_{k-1})]$ for some $\gamma \in [0,1]$.

Let us first show that this step is close to (6.3) in a well defined sense. To simplify the notation, we drop the function arguments and subscripts in the lemma below. The reasoning is essentially the same as in De Klerk et al. [35], but they use slightly different assumptions.

Lemma 6.3 (Based on [35, Theorem 7.6 and Corollary 7.7]). *Let $\eta \in \mathbb{R}$, and $c, \theta, \widehat{\theta} \in \mathbb{R}^n$. Let $\widehat{\Sigma}$ and Σ be self-adjoint linear operators such that*

$$\frac{1}{1+\epsilon}\widehat{\Sigma} \preceq \Sigma \preceq (1+\epsilon)\widehat{\Sigma},$$

for some $\epsilon \geq 0$. Then,

$$\|\widehat{\Sigma}[\eta c + \widehat{\theta}] - \Sigma[\eta c + \theta]\|_{\Sigma^{-1}} \leq (1+\epsilon)\|\widehat{\theta} - \theta\|_{\Sigma} + \sqrt{2\epsilon(1+\epsilon)}\|\eta c + \theta\|_{\Sigma}.$$

Proof. By the triangle inequality,

$$\|\widehat{\Sigma}[\eta c + \widehat{\theta}] - \Sigma[\eta c + \theta]\|_{\Sigma^{-1}} \leq \|\widehat{\Sigma}[\eta c + \widehat{\theta} - (\eta c + \theta)]\|_{\Sigma^{-1}} + \|(\widehat{\Sigma} - \Sigma)[\eta c + \theta]\|_{\Sigma^{-1}}. \tag{6.16}$$

The first norm on the right hand side of (6.16) equals $\|\widehat{\Sigma}[\widehat{\theta} - \theta]\|_{\Sigma^{-1}}$, which can be bounded by

$$\|\widehat{\Sigma}[\widehat{\theta} - \theta]\|_{\Sigma^{-1}} \leq \sqrt{1+\epsilon}\|\widehat{\Sigma}[\widehat{\theta} - \theta]\|_{\widehat{\Sigma}^{-1}} = \sqrt{1+\epsilon}\|\widehat{\theta} - \theta\|_{\widehat{\Sigma}} \leq (1+\epsilon)\|\widehat{\theta} - \theta\|_{\Sigma},$$

where the first inequality uses Lemma 2.4. The second norm on the right hand side of (6.16) can be bounded by noting that its square satisfies

$$\begin{aligned}
\|(\widehat{\Sigma} - \Sigma)[\eta c + \theta]\|_{\Sigma^{-1}}^2 &= \|\widehat{\Sigma}[\eta c + \theta]\|_{\Sigma^{-1}}^2 - 2\|\eta c + \theta\|_{\widehat{\Sigma}}^2 + \|\eta c + \theta\|_{\Sigma}^2 \\
&\leq (1+\epsilon)\|\eta c + \theta\|_{\widehat{\Sigma}}^2 - 2\|\eta c + \theta\|_{\widehat{\Sigma}}^2 + (1+\epsilon)\|\eta c + \theta\|_{\widehat{\Sigma}}^2 \\
&= 2\epsilon\|\eta c + \theta\|_{\widehat{\Sigma}}^2 \\
&\leq 2\epsilon(1+\epsilon)\|\eta c + \theta\|_{\Sigma}^2,
\end{aligned}$$

where the first inequality also uses Lemma 2.4. □

We see that the distance between the approximation $\widehat{\Sigma}(-\eta_k c)[\eta_k c + \widehat{\theta}(x_{k-1})]$ and the true gradient $\Sigma(-\eta_k c)[\eta_k c + \theta(x_{k-1})]$ depends in part on $\|\widehat{\theta}(x_{k-1}) - \theta(x_{k-1})\|_{-\eta_k c}$, which can be made smaller than or equal to $\kappa = \frac{1}{100}$ with high probability by Theorem 6.2. The results from De Klerk et al. [35] however require this distance to be upper bounded by a multiple of $\|\Sigma(-\eta_k c)[\eta_k c + \theta(x_{k-1})]\|_{z(\eta_k)}^*$ = $\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}$. Therefore, the short-step method we propose below in Algorithm 6.2 tests if $\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}$ is sufficiently large before taking a step. Alternatively, if $\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}$ were very small, we would already have $x_{k-1} \approx z(\eta_k)$, so we do not need to take a step.

Algorithm 6.2 Short-step interior point method using hit-and-run sampling and the entropic barrier

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$ contained in a ball with radius $R \geq 1$;
log-partition function f and entropic barrier f^* associated with $\mathcal{S}$;
normalized (with respect to $\|\cdot\|$) objective $c \in \mathbb{R}^n$;
optimality tolerance $\varepsilon \in (0, 2R]$;
reals $\eta_0 > 0$ and $\delta^* = \frac{1}{10}$, and $x_0 \in \mathcal{S}$ such that $\|x_0 - z(\eta_0)\|^*_{z(\eta_0)} \leq \delta^*$;
approximation $\widehat{\Sigma}(-\eta_0 c)$ of $\Sigma(-\eta_0 c)$ satisfying (6.14) for $\epsilon = \frac{1}{100}$;
sample X_0 from the Boltzmann distribution with parameter $-\eta_0 c$;
growth parameter $\beta = \frac{1}{100}$;
number of iterations m; damping parameter γ;
number of samples N; number of hit-and-run steps ℓ.

Output: $x_m \in \mathcal{S}$ such that $\langle c, x_m \rangle - \min_{x \in \mathcal{S}} \langle c, x \rangle \leq \varepsilon$ with high probability.

1: **for** $k \in \{1, ..., m\}$ **do**
2: $\quad \eta_k \leftarrow \eta_0 (1 + \beta / \sqrt{\vartheta_{f^*}})^k$
3: $\quad$ Generate $Y_{1k}, ..., Y_{Nk}$ and X_k by applying hit-and-run sampling to the Boltzmann distribution with parameter $-\eta_k c$, starting the walk from X_{k-1}, taking ℓ steps, drawing directions from $\mathcal{N}(0, \widehat{\Sigma}(-\eta_{k-1} c))$-distribution
4: $\quad \widehat{\Sigma}(-\eta_k c) v \leftarrow \frac{1}{N} \sum_{j=1}^N \langle Y_{jk}, v \rangle Y_{jk} - \frac{1}{N} \sum_{j=1}^N \langle Y_{jk}, v \rangle \left(\frac{1}{N} \sum_{j=1}^N Y_{jk} \right) \quad \forall v \in \mathbb{R}^n$
5: $\quad$ Generate $\widehat{\theta}(x_{k-1})$ through Algorithm 6.1 with the settings in Theorem 6.2 and $q = \frac{1}{2} q^*/m$, $\bar{\theta} = -\eta_k c$, $\theta_0 = -\eta_{k-1} c$, $\overline{X} = X_k$
6: $\quad$ **if** $\|\eta_k c + \widehat{\theta}(x_{k-1})\|_{\widehat{\Sigma}(-\eta_k c)} \leq \frac{1}{30}$ **then**
7: $\quad\quad x_k \leftarrow x_{k-1}$
8: $\quad$ **else**
9: $\quad\quad x_k \leftarrow x_{k-1} - \gamma \widehat{\Sigma}(-\eta_k c)[\eta_k c + \widehat{\theta}(x_{k-1})]$
10: **return** x_m

The test in Line 6 of Algorithm 6.2 was not present in [8]. There, we always executed Line 9, so $\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}$ had to be bounded away from zero. This complicated the algorithm's analysis, because various parameters had to be dependent on the problem dimension. Not only is Algorithm 6.2 easier to analyze, but the asymptotic number of oracle calls is also better. The following theorem provides parameters for which Algorithm 6.2 terminates successfully with high

probability.

Theorem 6.4. *Consider the setting of Algorithm 6.2. Let $q^* \in (0,1]$, and*

$$m = \left\lceil \frac{\log\left((1+\delta^*)\vartheta_{f^*}/(\varepsilon\eta_0)\right)}{\log\left(1+\beta/\sqrt{\vartheta_{f^*}}\right)} \right\rceil, \tag{6.17}$$

$$N = \left\lceil \frac{969n^2m}{q^*\epsilon^2} \right\rceil, \tag{6.18}$$

$$p = \frac{q^*\epsilon^2}{98838n^2mR^4}\left(\frac{1}{256}\right)\left(\frac{\varepsilon}{4R(1+\delta^*)(1+\beta)\vartheta_{f^*}}\right)^{8\sqrt{\vartheta_{f^*}}} \min\{1, \lambda_{\min}(\Sigma(0))^2\}, \tag{6.19}$$

and let ℓ be as in (4.10)*. (Note that ℓ depends on ϵ, n, p, and $\Delta\theta = \beta$.) Finally, set*

$$\gamma = \frac{2(\frac{871}{980})^2}{0.4219[1+(\frac{871}{980})^4]} - \frac{0.5781}{0.4219(\frac{871}{980})^2} \approx 0.5712.$$

With these inputs, Algorithm 6.2 returns a solution x_m with

$$\mathbb{P}\left\{\langle c, x_m\rangle - \min_{x\in\mathcal{S}}\langle c, x\rangle \le \varepsilon\right\} \ge 1 - q^*.$$

Proof. Our goal is to prove that, with high probability, $\|x_k - z(\eta_k)\|^*_{z(\eta_k)} \le \delta^*$ in each iteration $k \in \{1, \ldots, m\}$. The result will then follow from Lemma 3.10 if we note that

$$\eta_m = \eta_0\left(1 + \frac{\beta}{\sqrt{\vartheta_{f^*}}}\right)^m \ge \frac{(1+\delta^*)\vartheta_{f^*}}{\varepsilon}.$$

To show that $\|x_k - z(\eta_k)\|^*_{z(\eta_k)} \le \delta^*$ for all k, it will be convenient to assume that all approximations $\widehat{\Sigma}(-\eta_k c)$ satisfy (6.15), and that all calls to Algorithm 6.1 are successful. We first show that this happens with high probability in iteration k, provided we have a $\widehat{\Sigma}(-\eta_{k-1}c)$ satisfying (6.15) and an x_{k-1} such that $\|x_{k-1} - z(\eta_{k-1})\|^*_{z(\eta_{k-1})} \le \delta^*$.

We consider the conditions of Theorem 5.11 to assert that $\widehat{\Sigma}(-\eta_k c)$ satisfies (6.15) with high probability. Observe first of all that

$$\|-\eta_k c + \eta_{k-1}c\|_{-\eta_{k-1}c} \le \beta, \tag{6.20}$$

by (3.9). Noting that for any k,

$$\eta_k \le \eta_m = \eta_0\left(1+\frac{\beta}{\sqrt{\vartheta_{f^*}}}\right)^m \le \frac{(1+\delta^*)\vartheta_{f^*}}{\varepsilon}\left(1+\frac{\beta}{\sqrt{\vartheta_{f^*}}}\right) \le \frac{(1+\delta^*)(1+\beta)\vartheta_{f^*}}{\varepsilon},$$

we have by Theorem B.3 and the assumption that $\|c\| = 1$,

$$\begin{aligned}\lambda_{\min}(\Sigma(-\eta_k c)) &\ge \tfrac{1}{16}\left(\frac{1}{\max\{1, 4R\|-\eta_k c\|\}}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0))\\ &\ge \tfrac{1}{16}\left(\frac{\varepsilon}{4R(1+\delta^*)(1+\beta)\vartheta_{f^*}}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)).\end{aligned}$$

Hence, Theorem 5.11 shows that

$$\mathbb{P}\left\{\frac{1}{1+\epsilon}\widehat{\Sigma}(-\eta_k c) \preceq \Sigma(-\eta_k c) \preceq (1+\epsilon)\widehat{\Sigma}(-\eta_k c)\right\} \ge 1 - \frac{25q^*}{51m}.$$

Moreover, X_k is equal to a random variable following the Boltzmann distribution with parameter $-\eta_k c$ with probability at least $1-p \ge 1-\frac{1}{102}q^*/m$ by Theorem 4.14.

Moving on to Line 5 in Algorithm 6.2, we will verify the conditions for Theorem 6.2. To see that $\|-\eta_{k-1}c-\theta(x_{k-1})\|_{-\eta_k c} \le K$, note that by the self-concordance of f, (6.20) and Proposition 3.7,

$$\begin{aligned}\|-\eta_{k-1}c-\theta(x_{k-1})\|_{-\eta_k c} &\le \frac{\|-\eta_{k-1}c-\theta(x_{k-1})\|_{-\eta_{k-1}c}}{1-\|-\eta_k c+\eta_{k-1}c\|_{-\eta_{k-1}c}}\\ &\le \left(\frac{1}{1-\beta}\right)\frac{\|z(\eta_{k-1})-x_{k-1}\|^*_{z(\eta_{k-1})}}{1-\|z(\eta_{k-1})-x_{k-1}\|^*_{z(\eta_{k-1})}}\\ &\le \frac{\delta^*}{(1-\beta)(1-\delta^*)} = \tfrac{100}{891}\\ &\le K = \tfrac{1}{8}.\end{aligned}$$

Moreover, we should have $(1+\epsilon)K + \|-\eta_k c-\theta(x_{k-1})\|_{-\eta_k c} \le \delta$. To this end, note that

$$\begin{aligned}\|-\eta_k c-\theta(x_{k-1})\|_{-\eta_k c} &\le \|-\eta_{k-1}c-\theta(x_{k-1})\|_{-\eta_k c} + \|-\eta_k c+\eta_{k-1}c\|_{-\eta_k c}\\ &\le \tfrac{100}{891} + \frac{\|-\eta_k c+\eta_{k-1}c\|_{-\eta_{k-1}c}}{1-\|-\eta_k c+\eta_{k-1}c\|_{-\eta_{k-1}c}}\\ &\le \tfrac{100}{891} + \frac{\beta}{1-\beta} = \tfrac{109}{891}.\end{aligned}$$

Then $(1+\epsilon)K + \|-\eta_k c - \theta(x_{k-1})\|_{-\eta_k c} \le 0.2486 \le \delta = \frac{1}{4}$. The success probability of each call to Algorithm 6.1 is therefore at least $1-q = 1-\frac{1}{2}q^*/m$ by Theorem 6.2.

Below, we assume that

$$\|\widehat{\theta}(x_{k-1}) - \theta(x_{k-1})\|_{-\eta_k c} \le \kappa := \tfrac{1}{100} \qquad \forall k \in \{1, ..., m\}, \tag{6.21}$$

and

$$\frac{1}{1+\epsilon}\widehat{\Sigma}(-\eta_k c) \preceq \Sigma(-\eta_k c) \preceq (1+\epsilon)\widehat{\Sigma}(-\eta_k c) \qquad \forall k \in \{1, ..., m\}. \tag{6.22}$$

and show that this leads to a successful termination of the algorithm. Thus, the success probability of Algorithm 6.2 will be at least $1-q^*$.

Algorithm 6.2 distinguishes the following two cases in Lines 6 and 8:

(a) $\|\eta_k c + \widehat{\theta}(x_{k-1})\|_{\widehat{\Sigma}(-\eta_k c)} \le \frac{1}{30}$;

(b) $\|\eta_k c + \widehat{\theta}(x_{k-1})\|_{\widehat{\Sigma}(-\eta_k c)} > \frac{1}{30}$.

Let us first show that in Case (a), we have $\|x_{k-1} - z(\eta_k)\|^*_{z(\eta_k)} \le \delta^*$, in which case we could take $x_k = x_{k-1}$. By Proposition 3.7, and the fact that $\theta(z(\eta_k)) = -\eta_k c$,

$$\|x_{k-1} - z(\eta_k)\|^*_{z(\eta_k)} \le \frac{\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}}{1 - \|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}}.$$

By the triangle inequality and assumptions (6.21) and (6.22), we have in Case (a),

$$\begin{aligned}
\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c} &\le \|\eta_k c + \widehat{\theta}(x_{k-1})\|_{-\eta_k c} + \|\widehat{\theta}(x_{k-1}) - \theta(x_{k-1})\|_{-\eta_k c} \\
&\le \sqrt{1+\epsilon}\|\eta_k c + \widehat{\theta}(x_{k-1})\|_{\widehat{\Sigma}(-\eta_k c)} + \kappa \\
&\le \tfrac{1}{30}\sqrt{1+\epsilon} + \kappa = \tfrac{1}{30}\sqrt{1.01} + \tfrac{1}{100} \\
&\le \tfrac{1}{2}\delta^* = \tfrac{1}{20}.
\end{aligned}$$

Because $\delta^* = \frac{1}{10}$, we therefore have

$$\|x_{k-1} - z(\eta_k)\|^*_{z(\eta_k)} \le \frac{\frac{1}{2}\delta^*}{1 - \frac{1}{2}\delta^*} = \frac{\frac{1}{2}\delta^*}{\frac{19}{20}} < \delta^*.$$

Now, let us suppose we are in Case (b), such that we take the step in Line 9. To prove that after this step, we again have $\|x_k - z(\eta_k)\|^*_{z(\eta_k)} \le \delta^*$, we should first

bound the initial distance $\|x_{k-1}-z(\eta_k)\|^*_{z(\eta_k)}$. By the self-concordance of f^* and Corollary 3.8,

$$\|x_{k-1}-z(\eta_k)\|^*_{z(\eta_k)} \leq \frac{\|x_{k-1}-z(\eta_k)\|^*_{z(\eta_{k-1})}}{1-\|z(\eta_{k-1})-z(\eta_k)\|^*_{z(\eta_{k-1})}} \leq \frac{\|x_{k-1}-z(\eta_k)\|^*_{z(\eta_{k-1})}}{1-\beta/(1-\beta)}.$$

Using Corollary 3.8 once more, along with the induction hypothesis that $\|x_{k-1}-z(\eta_{k-1})\|^*_{z(\eta_{k-1})} \leq \delta^*$ yields

$$\begin{aligned}\|x_{k-1}-z(\eta_k)\|^*_{z(\eta_k)} &\leq \frac{\|x_{k-1}-z(\eta_{k-1})\|^*_{z(\eta_{k-1})}+\|z(\eta_{k-1})-z(\eta_k)\|^*_{z(\eta_{k-1})}}{1-\beta/(1-\beta)} \\ &\leq \frac{\delta^*+\beta/(1-\beta)}{1-\beta/(1-\beta)} = \tfrac{109}{980}. \end{aligned} \tag{6.23}$$

To invoke the results from De Klerk et al. [35], we need an upper bound on the relative error in our estimate $\widehat{\Sigma}(-\eta_k c)[\eta_k c+\widehat{\theta}(x_{k-1})]$ of the gradient of $f^*_{\eta_k}$ with respect to $\langle\cdot,\cdot\rangle^*_{z(\eta_k)}$ at x_{k-1}. Using the assumption (6.22), it follows from Lemma 6.3 that

$$\begin{aligned}&\|\widehat{\Sigma}(-\eta_k c)[\eta_k c+\widehat{\theta}(x_{k-1})]-\Sigma(-\eta_k c)[\eta_k c+\theta(x_{k-1})]\|^*_{z(\eta_k)} \\ &\leq (1+\epsilon)\kappa+\sqrt{2\epsilon(1+\epsilon)}\|\eta_k c+\theta(x_{k-1})\|_{-\eta_k c}\end{aligned}$$

In Case (b), we have

$$\begin{aligned}\tfrac{1}{30} &< \|\eta_k c+\widehat{\theta}(x_{k-1})\|_{\widehat{\Sigma}(-\eta_k c)} \\ &\leq \sqrt{1+\epsilon}\left(\|\eta_k c+\theta(x_{k-1})\|_{-\eta_k c}+\|\widehat{\theta}(x_{k-1})-\theta(x_{k-1})\|_{-\eta_k c}\right) \\ &\leq \sqrt{1+\epsilon}\left(\|\eta_k c+\theta(x_{k-1})\|_{-\eta_k c}+\kappa\right),\end{aligned}$$

that is,

$$\|\eta_k c+\theta(x_{k-1})\|_{-\eta_k c} > \frac{1}{30\sqrt{1+\epsilon}}-\kappa = \frac{1}{3\sqrt{101}}-\tfrac{1}{100}.$$

Consequently, we can express the bound on the relative error in the gradient es-

timate as

$$\begin{aligned}
&\|\widehat{\Sigma}(-\eta_k c)[\eta_k c + \widehat{\theta}(x_{k-1})] - \Sigma(-\eta_k c)[\eta_k c + \theta(x_{k-1})]\|^*_{z(\eta_k)} \\
&\leq \left(\frac{(1+\epsilon)\kappa}{\|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}} + \sqrt{2\epsilon(1+\epsilon)} \right) \|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c} \\
&\leq \left(\frac{(1+\epsilon)\kappa}{\frac{1}{3\sqrt{101}} - \frac{1}{100}} + \sqrt{2\epsilon(1+\epsilon)} \right) \|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c} \\
&\leq 0.5781 \|\eta_k c + \theta(x_{k-1})\|_{-\eta_k c}. \qquad (6.24)
\end{aligned}$$

As noted in the proof of Theorem 5.4 in De Klerk et al. [35], the result on convergence to the minimizer from Theorem 5.3 in [35] only requires bounds on the Hessians with respect to $\langle \cdot, \cdot \rangle^*_{z(\eta_k)}$ of $f^*_{\eta_k}$ at x_{k-1} and the minimizer $z(\eta_k)$, and not necessarily at x_k. Since $H^*_{z(\eta_k)}(z(\eta_k)) = I$, it remains to note that by (6.23), we have for all $v \in \mathbb{R}^n$,

$$\begin{aligned}
\langle v, H^*_{z(\eta_k)}(x_{k-1}) v \rangle^*_{z(\eta_k)} &= (\|v\|^*_{x_{k-1}})^2 \\
&\leq \left(\frac{\|v\|^*_{z(\eta_k)}}{1 - \|x_{k-1} - z(\eta_k)\|^*_{z(\eta_k)}} \right)^2 \leq \left(\tfrac{980}{871}\right)^2 (\|v\|^*_{z(\eta_k)})^2,
\end{aligned}$$

and similarly $\langle v, H^*_{z(\eta_k)}(x_{k-1}) v \geq \left(\frac{871}{980}\right)^2 (\|v\|^*_{z(\eta_k)})^2$. It thus follows from Theorem 5.3 in [35], (6.24), and (6.23) that

$$\begin{aligned}
\|x_k - z(\eta_k)\|^*_{z(\eta_k)} &\leq \left(\frac{1 - \left(\frac{871}{980}\right)^4}{1 + \left(\frac{871}{980}\right)^4} + 0.5781 \right) \|x_{k-1} - z(\eta_k)\|^*_{z(\eta_k)} \\
&\leq (0.8097)^{\frac{109}{980}} \\
&\leq \delta^* = \tfrac{1}{10}. \qquad \square
\end{aligned}$$

We end this chapter with a complexity analysis of Algorithm 6.2 with the configuration from Theorem 6.4. To find an asymptotic bound on the value of m in (6.17), note that for fixed $\beta > 0$,

$$\frac{1}{\log\left(1 + \beta / \sqrt{\vartheta_{f^*}}\right)} = O\left(\sqrt{\vartheta_{f^*}}\right),$$

such that $m = O^*(\sqrt{\vartheta_{f^*}})$. Then, the number of samples in (6.18) satisfies $N = O^*(n^2\sqrt{\vartheta_{f^*}}/q^*)$. The complexity of the walk length is given by (6.12), which for the value of p from (6.19) is

$$\ell = O^*\left(n^3\left(\sqrt{\vartheta_{f^*}}\right)^5 \log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^4\}}\right)\right).$$

In conclusion, the total number of oracle calls by Line 3 in Algorithm 6.2 with the configuration from Theorem 6.4 is

$$O^*(mN\ell) = O^*\left(\frac{n^5\vartheta_{f^*}^{3.5}}{q^*}\log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^4\}}\right)\right). \tag{6.25}$$

The other potential bottleneck is Line 5, which calls Algorithm 6.1 m times. By (6.13), the number of oracle calls in this line is

$$\begin{aligned} &O^*\left(\sqrt{\vartheta_{f^*}}\frac{n^4\vartheta_{f^*}^{2.5}}{q}\log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^2\}}\right)\right) \\ &= O^*\left(\frac{n^4\vartheta_{f^*}^{3.5}}{q^*}\log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^2\}}\right)\right) \end{aligned}$$

for $q = \frac{1}{2}q^*/m$. Since $\vartheta_{f^*} = O(n)$ by Theorem 3.4, the factor (6.25) dominates the number of oracle calls in Algorithm 6.2. We have thus shown the following.

Theorem 6.5. *Consider Algorithm 6.2 with the configuration from Theorem 6.4. The number of oracle calls by this algorithm is*

$$\begin{aligned} &O^*\left(\frac{n^5\vartheta_{f^*}^{3.5}}{q^*}\log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^4\}}\right)\right) \\ &= O^*\left(\frac{n^{8.5}}{q^*}\log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^4\}}\right)\right). \end{aligned}$$

If $\langle\cdot,\cdot\rangle$ were the Euclidean inner product, the value of p in (6.19) *could be made more explicit by replacing $\lambda_{\min}(\Sigma(0))$ with its lower bound from Lemma B.2. Then, the number of oracle calls would be*

$$O^*\left(\frac{n^5\vartheta_{f^*}^{3.5}}{q^*}\right) = O^*\left(\frac{n^{8.5}}{q^*}\right).$$

7

Simulated Annealing for Convex Optimization

The approximation quality tools from Chapter 5 have wider applications than just the interior point method from Chapter 6. In this chapter, we look at a different method: the simulated annealing algorithm by Kalai and Vempala [56]. This algorithm was recently connected to the field of interior point methods by Abernethy and Hazan [1]. They showed that the means of the Boltzmann distributions that the simulated annealing algorithm encounters lie on the central path of an interior point method using the entropic barrier, such as the one in Chapter 6. Exploiting this connection, they propose a new temperature schedule for the simulated annealing algorithm that depends on the entropic barrier's complexity parameter, not on the problem dimension.

Our purpose in this chapter is to analyze the complexity of Kalai and Vempala's algorithm using Abernethy and Hazan's temperature schedule. This exercise is relevant because, in their original paper, Kalai and Vempala only sketch a crucial proof (i.e. [56, Theorem 4.2]). Abernethy and Hazan's improved temperature

schedule leans on this analysis, and therefore also lacks a rigorous foundation. With the tools developed in previous chapters, we can give a formal analysis. Moreover, we propose some heuristic modifications to the algorithm, and verify that they improve the algorithm's numerical performance.

We introduce Kalai and Vempala's algorithm with Abernethy and Hazan's temperature scheme in Section 7.1. Section 7.2 shows that this algorithm returns a solution that is near-optimal with high probability. In Section 7.3 we analyze the algorithm's complexity, and compare it with Kalai and Vempala's original analysis [56]. Section 7.4 features a numerical experiment, based on which we propose some heuristic changes to the algorithm. We sketch the relationship between the algorithms in this chapter and those in the preceding chapters in Figure 7.1.

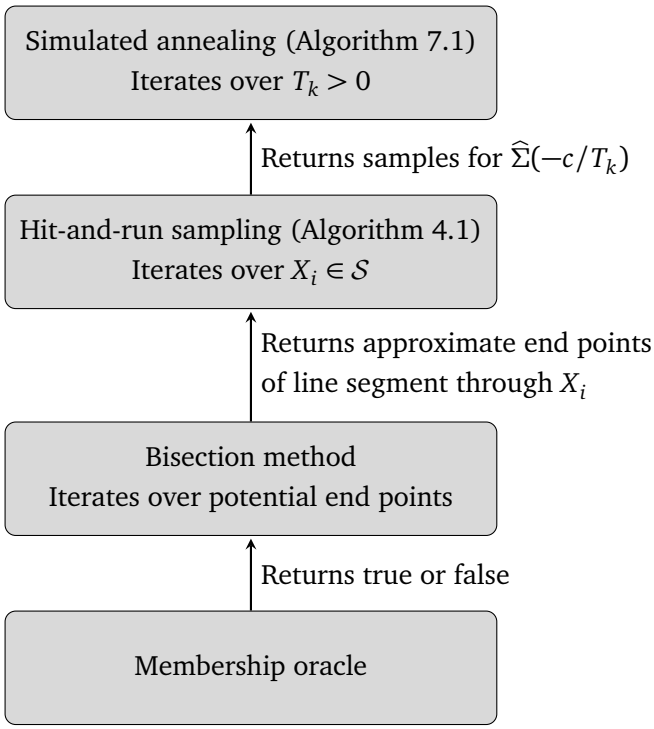

Figure 7.1: Sketch of the dependencies of the algorithms in Chapter 7

This chapter is based on Sections 1.1, 4, 5.3, and 5.4 from Badenbroek and De Klerk [9]. Background material on the completely positive cone (to be defined

in Section 7.4) was taken from the introduction of Badenbroek and De Klerk [10]. Aside from some minor differences due to changes in previous chapters, the main change in this chapter compared to [9] is that we perform the analysis with respect to arbitrary inner products. For the sake of concreteness, the convergence and complexity results will also be stated for the Euclidean inner product as corollaries.

The reader may wish to take note of the notation summarized in Table 3.1 on page 32.

7.1 Statement of a Simulated Annealing Algorithm

Kalai and Vempala's algorithm [56] aims to solve problem (3.2), that is,

$$\min_{x \in \mathcal{S}} \langle c, x \rangle, \tag{7.1}$$

where $c \in \mathbb{R}^n$ and $\mathcal{S} \subset \mathbb{R}^n$ is a convex body, through *simulated annealing*. Simulated annealing was originally introduced for combinatorial optimization problems by Kirkpatrick et al. [63]. The method is named after the annealing process from metallurgy where a metal is first heated for a while, and then slowly cooled to improve its physical properties. Simulated annealing borrows a temperature parameter from annealing, and decreases this temperature over the course of the process. The temperature signifies the randomness in the process in some sense. It was shown by Hajek [49] that simulated annealing on finite sets converges to the global optimum if one takes an exponentially long cooling schedule, even for non-convex problems. Furthermore, simulated annealing has good empirical performance as well and is often used as a heuristic in practice, see Kirkpatrick [62]. For a survey, we refer to Bertsimas et al. [14].

In each iteration k of Kalai and Vempala's algorithm [56], the temperature T_k is lowered. Then, hit-and-run samples are generated whose target distribution is the Boltzmann distribution with parameter $\theta_k = -c/T_k$. These random walks use an approximation $\widehat{\Sigma}(\theta_{k-1})$ of $\Sigma(\theta_{k-1})$ to generate search directions. With these samples, an approximation $\widehat{\Sigma}(\theta_k)$ of $\Sigma(\theta_k)$ is formed, which will then be used in the next iteration. As k grows sufficiently large, so does the norm of θ_k. The Boltzmann distributions with parameter θ_k will then concentrate more and more probability mass close to the set of optimal solutions to (7.1). For sufficiently

large k, any sample from such a Boltzmann distribution is near-optimal with high probability.

One thing that needs further clarification is how to decrease the temperature in each iteration. In their original paper, Kalai and Vempala [56] show that their algorithm returns a near-optimal solution with high probability for the temperature update

$$T_k = \left(1 - \frac{1}{\sqrt{n}}\right) T_{k-1}, \tag{7.2}$$

in $m = O^*(\sqrt{n})$ iterations. Abernethy and Hazan [1] propose the alternative temperature update

$$T_k = \left(1 - \frac{1}{4\sqrt{\vartheta_{f^*}}}\right) T_{k-1}, \tag{7.3}$$

where ϑ_{f^*} is the complexity parameter of the entropic barrier over the convex body $\mathcal{S}$. Abernethy and Hazan show that (7.3) leads to $m = O^*(\sqrt{\vartheta_{f^*}})$ iterations. By Theorem 3.4, we have $\vartheta_{f^*} \leq n + o(n)$ in general, but it is not currently known if $\vartheta_{f^*} < n$ for any convex bodies. (We presented numerical evidence in Figure 3.1 that suggests $\vartheta_{f^*} = \frac{1}{2}(n+1)$ for the Euclidean unit ball in $\mathbb{R}^n$, but did not prove this formally.) In particular, the temperature update (7.3) only improves on (7.2) if $\vartheta_{f^*} < \frac{1}{16}n$, which is not known to hold for any convex body. We therefore consider a variation on the temperature schedule (7.3) suggested by Abernethy and Hazan, namely

$$T_k = \left(1 - \frac{1}{\beta\sqrt{\vartheta_{f^*}}}\right) T_{k-1} \quad \text{for some} \quad \beta > 1 + \frac{1}{\sqrt{\vartheta_{f^*}}}, \tag{7.4}$$

which corresponds to (7.3) when $\beta = 4$, but gives larger temperature reductions when $\beta < 4$. We will refer to (7.4) as Abernethy-Hazan-type temperature updates. If $\vartheta_{f^*} < n$, this may result in a larger temperature decrease than the Kalai and Vempala [56] scheme (7.2), for a suitable choice of the parameter β.

The algorithm by Kalai and Vempala [56] that uses a temperature schedule of the type introduced by Abernethy and Hazan [1] is given in Algorithm 7.1.

One might wonder how to generate a good estimate $\widehat{\Sigma}(0)$ of the uniform covariance matrix $\Sigma(0)$ to start Algorithm 7.1. The "rounding the body" procedure from Lovász and Vempala [73] is suitable for this purpose. It is shown by Theorem

Algorithm 7.1 Algorithm by Kalai and Vempala [56] using temperature schedule of type introduced by Abernethy and Hazan [1]

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$ contained in a ball with radius $R \geq 1$;
log-partition function f and entropic barrier f^* associated with $\mathcal{S}$;
normalized (with respect to $\|\cdot\|$) objective $c \in \mathbb{R}^n$;
optimality tolerance $\varepsilon \in (0, 2R]$;
approximation $\widehat{\Sigma}(0)$ of $\Sigma(0)$ satisfying $\frac{1}{2}\widehat{\Sigma}(0)^{-1} \preceq \Sigma(0)^{-1} \preceq 2\widehat{\Sigma}(0)^{-1}$;
$x_0 \in \mathcal{S}$ drawn from the uniform distribution over $\mathcal{S}$;
number of iterations m; growth parameter $\beta > 1 + 1/\sqrt{\vartheta_{f^*}}$;
number of samples N; number of hit-and-run steps ℓ.

Output: $X_m \in \mathcal{S}$ such that $\langle c, X_m\rangle - \min_{x\in\mathcal{S}}\langle c, x\rangle \leq \varepsilon$ with high probability.

$X_0 \leftarrow x_0$
$\theta_0 \leftarrow 0$
$T_0 \leftarrow 2\beta R$
for $k \in \{1, ..., m\}$ **do**
  $T_k \leftarrow \left(1 - 1/(\beta\sqrt{\vartheta_{f^*}})\right) T_{k-1}$
  $\theta_k \leftarrow -c/T_k$
  Generate $Y_{1k}, ..., Y_{Nk}$ and X_k by applying hit-and-run sampling to the Boltzmann distribution with parameter θ_k, starting the walk from X_{k-1}, taking ℓ steps, drawing directions from a $\mathcal{N}(0, \widehat{\Sigma}(\theta_{k-1}))$-distribution
  $\widehat{\Sigma}(\theta_k)v \leftarrow \frac{1}{N}\sum_{j=1}^N \langle Y_{jk}, v\rangle Y_{jk} - \frac{1}{N}\sum_{j=1}^N \langle Y_{jk}, v\rangle \left(\frac{1}{N}\sum_{j=1}^N Y_{jk}\right) \qquad \forall v \in \mathbb{R}^n$
return X_m

5.3 in [73] that this procedure returns a $\widehat{\Sigma}(0)$ for which

$$\mathbb{P}\left\{\tfrac{1}{2}\widehat{\Sigma}(0) \preceq \Sigma(0) \preceq 2\widehat{\Sigma}(0)\right\} \geq 1 - \frac{1}{n}.$$

By Lemma 2.4, $\frac{1}{2}\widehat{\Sigma}(0) \preceq \Sigma(0) \preceq 2\widehat{\Sigma}(0)$ if and only if $\frac{1}{2}\widehat{\Sigma}(0)^{-1} \preceq \Sigma(0)^{-1} \preceq 2\widehat{\Sigma}(0)^{-1}$, so the starting condition for Algorithm 7.1 can be satisfied by the "rounding the body" procedure. The number of calls to the membership oracle for this procedure is $O^*(n^4)$. As we will see in Section 7.3, this number of oracle calls will be overshadowed by the oracle calls from Algorithm 7.1.

7.2 Proof of Convergence

Suppose we could show that hit-and-run sampling mixes with the target distribution in each iteration of Algorithm 7.1. Then, it would suffice to argue that the final iterate X_m is near-optimal with high probability. Keeping Markov's inequality in mind, this near-optimality can be shown if the expected objective value of a random variable following a low-temperature distribution is close to the optimal value. This is the topic of the next lemma. It was established by Kalai and Vempala [56] for linear functions, and extended from linear to convex functions by De Klerk and Laurent [32].

Lemma 7.1 ([32, Corollary 1])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body. For any convex functional $\phi : \mathbb{R}^n \to \mathbb{R}$ and temperature $T > 0$, we have*

$$\frac{\int_{\mathcal{S}} \phi(x) e^{-\phi(x)/T} \, \mathrm{d}x}{\int_{\mathcal{S}} e^{-\phi(x)/T} \, \mathrm{d}x} \leq nT + \min_{x \in \mathcal{S}} \phi(x).$$

The main step in the analysis of Algorithm 7.1 is thus to show that we maintain a good approximation $\widehat{\Sigma}(\theta_k)$ of $\Sigma(\theta_k)$ for all k, to guarantee that the hit-and-run sampling continues to work in all iterations. This analysis was done with respect to the Euclidean inner product in [9, Theorem 14], but here we do it for arbitrary inner products.

Theorem 7.2. *Consider the setting of Algorithm 7.1. Let $\Delta\theta = \sqrt{\vartheta_{f^*}}/(\beta\sqrt{\vartheta_{f^*}}-1)$, $q \in (0,1]$,*

$$m = \left\lceil \frac{\log(q\varepsilon/(4\beta nR))}{\log\left(1-1/(\beta\sqrt{\vartheta_{f^*}})\right)} \right\rceil, \tag{7.5}$$

$$N = \left\lceil \frac{969n^2m}{q} \right\rceil, \tag{7.6}$$

$$p = \frac{q}{98838mn^2R^4}\left(\frac{1}{256}\right)\left(\frac{q\varepsilon}{16nR}\right)^{8\sqrt{\vartheta_{f^*}}} \min\{1, \lambda_{\min}(\Sigma(0))^2\}, \tag{7.7}$$

and let ℓ be as in (4.10)*. (Note that ℓ depends on $\epsilon = 1$, n, p, and $\Delta\theta$.) With these inputs, Algorithm 7.1 returns a solution X_m with*

$$\mathbb{P}\left\{\langle c, X_m\rangle - \min_{x \in \mathcal{S}} \langle c, x\rangle \leq \varepsilon\right\} \geq 1-q.$$

Proof. Throughout all iterations k of Algorithm 7.1, we want to maintain the conditions that X_k is equal to a sample from the Boltzmann distribution with parameter θ_k, and

$$\tfrac{1}{2}\widehat{\Sigma}(\theta_k)^{-1} \preceq \Sigma(\theta_k)^{-1} \preceq 2\widehat{\Sigma}(\theta_k)^{-1}, \tag{7.8}$$

with a certain high probability. We assume that these conditions hold in iteration $k-1$, and we will show that they then also hold for iteration k with high probability.

First, let us show that the conditions of Theorem 4.14 are satisfied. For $k=1$, (B.1) in Appendix B shows

$$\|\theta_1-\theta_0\|_{\theta_0} = \frac{\|c\|_0}{T_1} \le \frac{2R}{T_1} = \frac{2R}{2\beta R\left(1-1/(\beta\sqrt{\vartheta_{f^*}})\right)} = \Delta\theta.$$

For all $k>1$, our choice of θ_k and (3.1) yield

$$\|\theta_k-\theta_{k-1}\|_{\theta_{k-1}} = \left(\frac{T_{k-1}}{T_k}-1\right)\|\theta_{k-1}\|_{\theta_{k-1}} \le \left(\frac{1}{1-1/(\beta\sqrt{\vartheta_{f^*}})}-1\right)\sqrt{\vartheta_{f^*}} = \Delta\theta.$$

Therefore, for any $k\in\{1,\dots,m\}$, Theorem 4.14 and Lemma 4.5 show that with probability at least $1-p$, X_k is equal to a random variable drawn from a Boltzmann distribution with parameter θ_k.

Next, we will apply Theorem 5.11 with $\xi=1$ to show $\widehat{\Sigma}(\theta_k)$ is a good approximation of $\Sigma(\theta_k)$. For that, we need a lower bound on $\lambda_{\min}(\Sigma(\theta_k))$, such as the one given by Theorem B.3:

$$\lambda_{\min}(\Sigma(\theta_k)) \ge \tfrac{1}{16}\left(\frac{1}{\max\{1,4R\|\theta_k\|\}}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)).$$

To upper bound $\|\theta_k\|$, note that

$$m \le \frac{\log(q\varepsilon/(2nR))}{\log\left(1-1/(\beta\sqrt{\vartheta_{f^*}})\right)}+1,$$

such that for all $k\le m$,

$$\|\theta_k\| \le \|\theta_m\| = \frac{\|c\|}{T_m} = \frac{1}{R(1-1/(\beta\sqrt{\vartheta_{f^*}}))^m} \le \frac{2n}{(1-1/(\beta\sqrt{\vartheta_{f^*}}))q\varepsilon}.$$

Since $\vartheta_{f^*} \geq 1$ for any self-concordant barrier f^* (see Nesterov and Nemirovskii [85]), it holds for any $\beta > 1 + 1/\sqrt{\vartheta_{f^*}} \geq 2/\sqrt{\vartheta_{f^*}}$ that

$$\frac{1}{1 - 1/(\beta\sqrt{\vartheta_{f^*}})} < \frac{1}{1 - \frac{1}{2}} = 2.$$

Hence, $\|\theta_k\| \leq 4n/(q\varepsilon)$ and

$$\lambda_{\min}(\Sigma(\theta_k)) \geq \tfrac{1}{16}\left(\frac{q\varepsilon}{16nR}\right)^{4\sqrt{\vartheta_{f^*}}} \lambda_{\min}(\Sigma(0)).$$

It follows that the chosen values for N and p satisfy

$$N \geq \frac{475n^2}{(\frac{25}{51}q/m)} \quad \text{and} \quad p \leq \frac{(\frac{25}{51}q/m)\min\{1, \lambda_{\min}(\Sigma(\theta_k))^2\}}{48450n^2 \max\{1, R^4\}},$$

such that Theorem 5.11 shows that (7.8) holds in iteration k with probability at least $1 - \frac{25}{51}q/m$.

By induction, X_m is equal to a random variable drawn from a Boltzmann distribution with parameter θ_m and (7.8) holds for $k = m$ with probability at least

$$1 - m\left(p + \frac{25q}{51m}\right) \geq 1 - m\left(\frac{q}{102m} + \frac{25q}{51m}\right) = 1 - \tfrac{1}{2}q,$$

by the union bound. In this event, Markov's inequality and Lemma 7.1 show

$$\mathbb{P}\left\{\langle c, X_m\rangle - \min_{x\in\mathcal{S}}\langle c, x\rangle > \varepsilon\right\} \leq \frac{\mathbb{E}[\langle c, X_m\rangle - \min_{x\in\mathcal{S}}\langle c, x\rangle]}{\varepsilon} \leq \frac{nT_m}{\varepsilon} \leq \tfrac{1}{2}q, \quad (7.9)$$

where the final inequality uses the chosen value of m as follows:

$$T_m = 2\beta R\left(1 - \frac{1}{\beta\sqrt{\vartheta_{f^*}}}\right)^m \leq 2\beta R\frac{q\varepsilon}{4\beta nR} = \frac{q\varepsilon}{2n}. \qquad \square$$

This result is still phrased in terms of an arbitrary inner product, and the value of p depends on this inner product. If we were to restrict ourselves to the Euclidean inner product, we could use the lower bound on $\lambda_{\min}(\Sigma(0))$ from Lemma B.2 to make the value of p more explicit. The following result is essentially [9, Theorem 14] with slightly different constants.

Corollary 7.3. *Consider the setting of Algorithm 7.1, and let $\langle\cdot,\cdot\rangle$ be the Euclidean inner product. Assume $\mathcal{S}$ contains a ball with radius $r > 0$. Let $q \in (0,1]$, $\Delta\theta = \sqrt{\vartheta_{f^*}}/(\beta\sqrt{\vartheta_{f^*}} - 1)$,*

$$m = \left\lceil \frac{\log(q\varepsilon/(4\beta nR))}{\log\left(1 - 1/(\beta\sqrt{\vartheta_{f^*}})\right)} \right\rceil,$$
$$N = \left\lceil \frac{969n^2m}{q} \right\rceil,$$
$$p = \frac{q}{98838mn^2R^4}\left(\frac{1}{256}\right)\left(\frac{q\varepsilon}{16nR}\right)^{8\sqrt{\vartheta_{f^*}}} \min\left\{1, \tfrac{1}{16}\left(\frac{r}{n+1}\right)^4\right\},$$

and let ℓ be as in (4.10). *(Note that ℓ depends on $\epsilon = 1$, n, p, and $\Delta\theta$.) With these inputs, Algorithm 7.1 returns a solution X_m with*

$$\mathbb{P}\left\{\langle c, X_m\rangle - \min_{x\in\mathcal{S}}\langle c, x\rangle \le \varepsilon\right\} \ge 1 - q.$$

7.3 Complexity Analysis and Discussion

We saw that for some combination of inputs, Algorithm 7.1 returns a solution which is near-optimal with high probability. Let us now consider the number of membership oracle calls required for this configuration. As we saw in Section 4.1, the number of oracle calls for one hit-and-run walk is $O^*(\ell)$. Hence, Algorithm 7.1 uses $O^*(mN\ell)$ oracle calls.

First, let us look at the number of iterations from (7.5). Since

$$\frac{-1}{\log\left(1 - 1/(\beta\sqrt{\vartheta_{f^*}})\right)} = O(\beta\sqrt{\vartheta_{f^*}}),$$

we have $m = O^*(\sqrt{\vartheta_{f^*}})$ for fixed β. Next, the number of samples from (7.6) satisfies $N = O^*(n^2m/q) = O^*(n^2\sqrt{\vartheta_{f^*}}/q)$.

Finally, we bound the number of hit-and-run steps used in Theorem 7.2. For the $\Delta\theta$ from Theorem 7.2 and the value of p from (7.7), (6.12) shows

$$\ell = O^*\left(n^3\left(\sqrt{\vartheta_{f^*}}\right)^5 \log^5\left(\frac{1}{\min\{1, \lambda_{\min}(\Sigma(0))^4\}}\right)\right).$$

In particular, Lemma B.2 shows that $\ell = O^*(n^3\vartheta_{f^*}^{2.5})$ for the Euclidean inner product.

Summarizing, the total number of oracle calls by Algorithm 7.1 is

$$\begin{aligned} O^*(mN\ell) &= O^*\left(\frac{n^5\vartheta_{f^*}^{3.5}}{q}\log^5\left(\frac{1}{\min\{1,\lambda_{\min}(\Sigma(0))^4\}}\right)\right) \\ &= O^*\left(\frac{n^{8.5}}{q}\log^5\left(\frac{1}{\min\{1,\lambda_{\min}(\Sigma(0))^4\}}\right)\right), \end{aligned}$$

where we used Theorem 3.4. For the Euclidean inner product in particular, the total number of oracle calls is $O^*(n^5\vartheta_{f^*}^{3.5}/q) = O^*(n^{8.5}/q)$.

Kalai and Vempala [56, Theorem 2.1] claim that the number of oracle calls made by their algorithm is $O^*(n^{4.5})$. The complexity $O^*(n^5\vartheta_{f^*}^{3.5}/q)$ shown above is worse because Kalai and Vempala use the following corollary to a theorem by Rudelson [97].

Theorem 7.4 ([56, Theorem A.1])**.** *Let ψ be a logconcave probability distribution over $\mathbb{R}^n$ with mean 0 and identity covariance, and let $\xi > 0, t > 1$. Then, there exists a number N with*

$$N = O\left(\frac{nt^2}{\xi^2}\log^2(n/\xi^2)\max\{t,\log n\}\right), \tag{7.10}$$

such that for N independent samples $X_1,\ldots,X_N$ from ψ we have

$$\mathbb{E}\left[\left\|\frac{1}{N}\sum_{j=1}^{N}X_jX_j^\top - I\right\|^t\right] \le \xi^t.$$

This theorem cannot be directly applied in the setting of Algorithm 7.1 for three reasons: the hit-and-run samples do not follow the target distribution ψ, the samples are not independent, and ψ does not have mean 0 and identity covariance. As we have seen in Theorem 4.14, the samples are drawn from a distribution that has total variation distance $p > 0$ to ψ. Moreover, the samples were shown to be $6p$-independent by Corollary 5.6. Finally, to apply Theorem 7.4 to a Boltzmann distribution with parameter $\theta \in \mathbb{R}^n$ over a convex body $\mathcal{S} \subset \mathbb{R}^n$, we should apply the transformation $y \mapsto \Sigma(\theta)^{-1/2}(y - x(\theta))$ to $\mathcal{S}$ to make the mean

0 and the covariance the identity. Consequently, the transformed body is not necessarily contained in a ball with radius R anymore; in the worst case, the radius of the new enclosing ball depends on the smallest eigenvalue of $\Sigma(\theta)$. Since we do not have a better bound on this eigenvalue than Theorem B.3 (or Corollary B.4 for the Euclidean inner product), the diameter of $\Sigma(\theta)^{-1/2}(\mathcal{S} - x(\theta))$ may be exponential in n. The suggestions by Kalai and Vempala to prove a statement similar to Theorem 7.4 in the hit-and-run setting require a bound on this diameter. If this bound grows exponentially in n, then p should decrease exponentially in n to compensate (see for instance Kannan et al. [58, Lemma 2.7 and the proof of Theorem 5.9]). Such a small p would contribute a polynomial factor of n to the final algorithm complexity.

While Kalai and Vempala claim that Theorem 7.4 can be extended to the hit-and-run setting without significantly changing (7.10), a formal proof is not given. In particular, it is not shown how the relaxation of the independence assumption can be aligned with Rudelson's proof, and how to bound the diameter of the transformed body $\Sigma(\theta)^{-1/2}(\mathcal{S} - x(\theta))$. Assuming these issues can be overcome, Kalai and Vempala show the following.

Theorem 7.5 ([56, Theorem 4.2])**.** *Let $t \geq 0$. With $N = O^*(t^3 n)$ samples per iteration in each of m iterations, the approximations $\widehat{\Sigma}(\theta_{k-1})$ of $\Sigma(\theta_{k-1})$ generated by Algorithm 7.1 satisfy*

$$\mathbb{P}\left\{\tfrac{1}{160}\widehat{\Sigma}(\theta_{k-1}) \preceq \Sigma(\theta_k) \preceq 160\widehat{\Sigma}(\theta_{k-1}) \qquad \forall k \in \{1, \ldots, m\}\right\} \geq 1 - \frac{m}{2^t}.$$

If $\frac{1}{160}\widehat{\Sigma}(\theta_{k-1}) \preceq \Sigma(\theta_k) \preceq 160\widehat{\Sigma}(\theta_{k-1})$ for all k, hit-and-run sampling mixes in all iterations. Kalai and Vempala are thus able to pick $t = O(\log(m/q))$, and can therefore claim $N = O^*(n)$. We find in Theorem 5.11 that $N = O(n^2/(q/m))$ samples are required, which is $O^*(n\sqrt{\vartheta_{f^*}}/q) = O^*(n^{1.5}/q)$ worse than Kalai and Vempala's result.

Moreover, by considering the diameter of $\Sigma(\theta)^{-1/2}(\mathcal{S} - x(\theta))$, we let p decrease quadratically in $\lambda_{\min}(\Sigma(\theta))$. Since the best lower bound on $\lambda_{\min}(\Sigma(\theta))$ we have is exponential in ϑ_{f^*}, we introduce a factor of $\vartheta_{f^*}^{2.5}$ in the algorithm complexity. If a lower bound on $\lambda_{\min}(\Sigma(\theta))$ were found that was not exponential in ϑ_{f^*}, then the algorithm complexity would improve by a factor $\vartheta_{f^*}^{2.5}$.

Together, these factors explain the gap of size $O^*(n^4/q)$ between our analysis and Kalai and Vempala's.

7.4 Heuristic Adaptation Based on Experimental Results

We see that Algorithm 7.1 and Algorithm 6.2 from Chapter 6 have the same asymptotic complexity. That being said, each iteration from Algorithm 7.1 poses less work than an iteration from Algorithm 6.2. After all, most of the computational effort in Algorithm 7.1 is spent on approximating a covariance operator, while Algorithm 6.2 also approximates a gradient. If we want to find an algorithm that performs well in practice, it thus makes sense to start with Algorithm 7.1.

Running Algorithm 7.1 as stated immediately raises a problem: the number of hit-and-run steps ℓ in (4.10) contains a factor 10^{30}. For practical problems, the ℓ in (4.10) is thus too large to take this many hit-and-run steps. We therefore need to investigate the number of steps ℓ and samples N that suffice to run Algorithm 7.1 successfully in practice.

To introduce our test problem, let $\mathbb{S}^d$ denote the space of real symmetric $d \times d$ matrices. Fix $\langle \cdot, \cdot \rangle$ to the Euclidean inner product on $\mathbb{R}^n$, and to the trace inner product on $\mathbb{S}^d$. We define the *completely positive cone* $\mathcal{CP}^d \subset \mathbb{S}^d$ as

$$\mathcal{CP}^d := \{BB^\top : B \geq 0, B \in \mathbb{R}^{d \times k} \text{ for some } k\}.$$

Many properties of this cone are summarized in the book by Berman and Shaked-Monderer [12].

Completely positive matrices play an important role in optimization. For instance, by a theorem of Motzkin and Straus [80] (see also De Klerk and Pasechnik [33]), the stability number of a graph can be formulated as an optimization problem with linear objective and linear constraints over the completely positive cone (or its dual cone). A seminal result by Burer [24] shows that – under mild assumptions – binary quadratic problems can also be reformulated as optimization problems over the completely positive cone. Other applications build on the work by Kemperman and Skibinsky [60], who found that $\mathcal{CP}^d$ equals

$$\left\{ \int xx^\top \, \mathrm{d}\varphi(x) : \varphi \text{ is a finite-valued nonnegative measure supported on } \mathbb{R}^d_+ \right\}.$$

This equality has spawned a large number of applications in distributionally robust optimization, e.g. Natarajan et al. [83] and Kong et al. [65] (see Li et al. [69] for a survey).

Unfortunately, testing if a matrix is completely positive is NP-hard, as Dickinson and Gijben [38] showed. Several approaches to this testing problem exist in the literature. Jarre and Schmallowsky [54] propose an augmented primal-dual method that provides a certificate if $X \in \mathcal{CP}^d$ by solving a sequence of second-order cone problems. However, their algorithm converges slowly if X is on the boundary of $\mathcal{CP}^d$, and the regularization they propose to solve this is computationally expensive.

An obvious way to verify that X is completely positive is to find a factorization $X = BB^\top$ where $B \geq 0$. Several authors have done this for specific matrix structures, see Dickinson and Dür [37], Bomze [16], and the references therein. For general matrices, factorization methods have been proposed by Nie [89], and Sponsel and Dür [103], but these methods do not perform well on bigger matrices. Groetzner and Dür [46] develop an alternating projection scheme that does scale well, but is not guaranteed to find a factorization for a given completely positive matrix. The method struggles in particular for matrices near the boundary of the completely positive cone. Another heuristic method based on projection is given by Elser [40]. Sikirić et al. [100] can find a rational factorization whenever it exists, although the running time is hard to predict.

To actually optimize over the completely positive cone is even harder. Bomze et al. [18] suggest a factorization heuristic with promising numerical performance. A more naive approach to solving completely positive optimization problems is to replace the cone $\mathcal{CP}^d$ with a tractable outer approximation, such as the cone of *doubly nonnegative* matrices (i.e. the symmetric positive semidefinite matrices with nonnegative elements). After optimizing over this outer approximation, one could then strengthen the approximation by the technique in Chapter 8 – an idea also mentioned in e.g. Sponsel and Dür [103] and Berman et al. [13].

We will, for some $C \in \mathbb{S}^d$, focus on the following relaxation to a completely positive optimization problem:

$$\inf_X \{\langle C, X\rangle : \|\operatorname{vec}(X)\| \leq 1, X \geq 0, X \succeq 0\}, \tag{7.11}$$

where $\operatorname{vec}(X)$ vectorizes $X = [X_{ij}] \in \mathbb{S}^d$ as

$$\operatorname{vec}(X) := \begin{bmatrix} X_{11} & X_{12} & X_{22} & X_{13} & X_{23} & \cdots & X_{dd} \end{bmatrix}^\top,$$

that is, $\operatorname{vec}(X)$ contains the upper triangular part of the matrix X. This simple problem can be seen as the relaxation of $\inf_X\{\langle C,X\rangle : \|\operatorname{vec}(X)\| \le 1, X \in \mathcal{CP}^d\}$, which tests if C is in the dual cone of $\mathcal{CP}^d$ or not. Since we place a nonnegativity constraint on every element of the matrix X, the Newton system in every interior point iteration is of size $O(d^2 \times d^2)$, which quickly leads to impractical computation times (see e.g. Burer [25]). Checking membership of the feasible set of (7.11) can however still be done in $O(d^3)$ operations.

Since $\mathbb{S}^d$ is isomorphic to $\mathbb{R}^{d(d+1)/2}$, we can also consider our optimization over $\mathbb{S}^d$ as an optimization over $\mathbb{R}^{d(d+1)/2}$. To do that, define $\operatorname{mat} : \mathbb{R}^{d(d+1)/2} \to \mathbb{S}^d$ to be the inverse of vec, and let $\operatorname{mat}^\top : \mathbb{S}^d \to \mathbb{R}^{d(d+1)/2}$ be the adjoint of mat. Problem (7.11) is then equivalent to

$$\operatorname{val} := \inf_x \left\{ \langle \operatorname{mat}^\top(C), x\rangle : \|x\| \le 1, x \ge 0, \operatorname{mat}(x) \succeq 0 \right\}. \tag{7.12}$$

We will run Algorithm 7.1 on the problem (7.12) for $d \in \{5, 10, 15, 20\}$. Let $n = \frac{1}{2}d(d+1)$. To generate an instance for the problem (7.12), we draw a random vector $c \in \mathbb{R}^n$ from the multivariate normal distribution $\mathcal{N}(0, I)$, and let $C = t \operatorname{mat}(c)$ where t is chosen such that $\|\operatorname{mat}^\top(C)\| = 1$. Because we do not know ϑ_{f^*} exactly, and Theorem 3.4 only yields an upper bound for $n \ge 80$, Line 5 in Algorithm 7.1 will be replaced by Kalai and Vempala's [56] original update $T_k \leftarrow (1 - 1/\sqrt{n})$. We set $\varepsilon = 10^{-3}$, $q = 10^{-1}$, $R = 1$, $\beta = 2$, and

$$m = \left\lceil \frac{\log(q\varepsilon/(8nR))}{\log\left(1 - 1/\sqrt{n}\right)} \right\rceil.$$

We let $X = dI + ee^\top \in \mathbb{S}^d$ and take $x = t \operatorname{vec}(X)$, where e is the all-ones vector, and t is chosen such that $\|x\| = \frac{1}{2}$. From this point, we first apply hit-and-run sampling with respect to the uniform distribution to generate an approximation $\widehat{\Sigma}(0)$ of $\Sigma(0)$. The mean of the samples this required will serve as x_0 in Algorithm 7.1.

The optimal value val of the problem in (7.12) can be computed with MOSEK 9 [78]. If X_m is the solution returned by Algorithm 7.1, we display the optimality gap $\langle \operatorname{mat}^\top(C), X_m\rangle - \operatorname{val}$ for different choices of N and ℓ in Figure 7.2. The values of N and ℓ are chosen such that the runtime of Algorithm 7.1 is still reasonable. Moreover, if we are going to draw hit-and-run directions from $\mathcal{N}(0, \widehat{\Sigma}(\theta_{k-1}))$, we need a Cholesky factorization of $\widehat{\Sigma}(\theta_{k-1})$. This requires the empirical covariance to be positive definite, which can only happen if $N \ge n$.

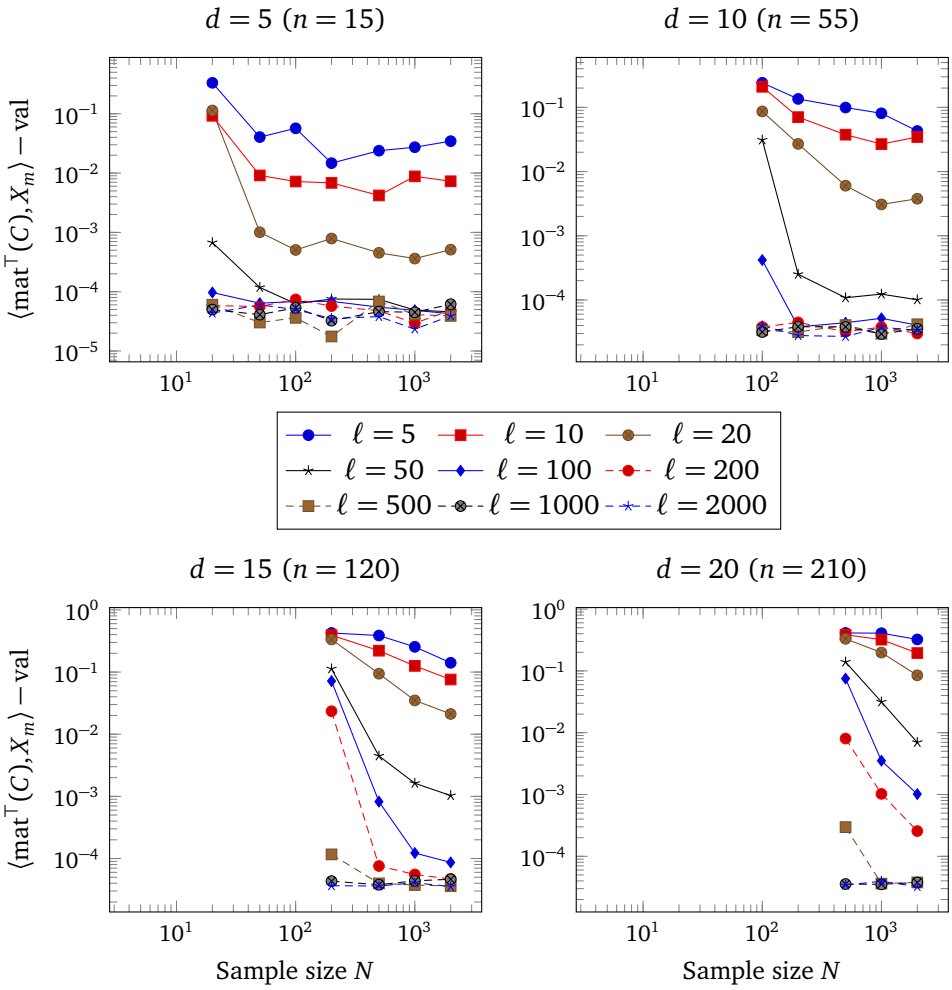

Figure 7.2: Effect of sample size N and walk length ℓ on the final gap of Algorithm 7.1

Figure 7.2 shows that

$$\ell = 4n \quad \text{and} \quad N = 6n \tag{7.13}$$

would be a decent heuristic choice in the context of Algorithm 7.1. With these values of ℓ and N, Algorithm 7.1 returns a near-optimal solution in our experiments.

To see if we can improve upon this performance by Algorithm 7.1, we propose the following modifications to Algorithm 7.1:

1. As a starting point for the first random walk in some iteration k, use the sample mean from iteration $k-1$. While this significantly changes the distribution of the starting point, it concentrates more probability mass around the mean of the Boltzmann distribution with parameter θ_{k-1}, such that the starting point of the random walk is likely already close to the mean of the Boltzmann distribution with parameter θ_k. In a similar vein, we return the mean of the samples in the final iteration, not just one sample. This will not change the expected objective value of the final result, and will therefore also not affect the probabilistic guarantee that we derived in (7.9) by Markov's inequality. However, using the mean does reduce the variance in the final solution.

2. Divide the number of samples that have to be drawn in some iteration k over $\mathcal{P}$ threads. Within each thread, start each random walk from the end point of the previous random walk. The idea here is that the random samples as a whole will then exhibit less dependence, thus improving the approximation quality of the empirical distribution. Note that each thread can be run in parallel, which we need in a method that would be faster than Algorithm 7.1: the sampling in Algorithm 7.1 can also be done in parallel, because each walk in a certain iteration has the same starting point.

These changes should improve the performance of the algorithm. For the sake of clarity, this modified version of Kalai and Vempala's algorithm is outlined in Algorithm 7.2.

With this modified algorithm, we repeat the experiment involving (7.12) using $\mathcal{P} = 8$ threads, and

$$m = \left\lceil \frac{\log\left(q\varepsilon/(4nR)\right)}{\log\left(1-1/\sqrt{n}\right)} \right\rceil \tag{7.14}$$

iterations. The results can be seen in Figure 7.3.

Figure 7.3 shows Algorithm 7.2 performs somewhat better than Algorithm 7.1. First, we see in Figure 7.3 that larger sample sizes will in the end lead to near-optimal solutions. This is more desirable than the behavior observed in Figure 7.2,

Algorithm 7.2 An adaptation of Algorithm 7.1 that changes the walks' starting points

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$ contained in a ball with radius $R \geq 1$;
normalized (with respect to $\|\cdot\|$) objective $c \in \mathbb{R}^n$;
number of samples N; number of hit-and-run steps ℓ;
number of iterations m; number of threads $\mathcal{P}$ that divides N (for simplicity);
starting point $x_0 \in \mathcal{S}$.

Output: $X_m \in \mathcal{S}$ such that $\langle c, X_m \rangle - \min_{x \in \mathcal{S}} \langle c, x \rangle$ is small with high probability.

for $i \in \{1, ..., \mathcal{P}\}$ **do**
  for $j \in \{1, ..., N/\mathcal{P}\}$ **do**
    Generate $Y_{(i-1)N/\mathcal{P}+j,0}$ by applying hit-and-run sampling to the uniform distribution over $\mathcal{S}$, starting the walk from x_0 if $j = 1$ and otherwise from $Y_{(i-1)N/\mathcal{P}+j-1,0}$, taking ℓ steps, drawing directions from a $\mathcal{N}(0, I)$-distribution
$X_0 \leftarrow \frac{1}{N} \sum_{j=1}^{N} Y_{j0}$
$T_0 \leftarrow 4R$
for $k \in \{1, ..., m\}$ **do**
  $T_k \leftarrow \left(1 - 1/\sqrt{n}\right) T_{k-1}$
  $\theta_k \leftarrow -c/T_k$
  for $i \in \{1, ..., \mathcal{P}\}$ **do**
    for $j \in \{1, ..., N/\mathcal{P}\}$ **do**
      Generate $Y_{(i-1)N/\mathcal{P}+j,k}$ by applying hit-and-run sampling to the Boltzmann distribution with parameter θ_k, starting the walk from X_{k-1} if $j = 1$ and otherwise from $Y_{(i-1)N/\mathcal{P}+j-1,k}$, taking ℓ steps, drawing directions from a $\mathcal{N}(0, \widehat{\Sigma}(\theta_{k-1}))$-distribution
  $X_k \leftarrow \frac{1}{N} \sum_{j=1}^{N} Y_{jk}$
  $\widehat{\Sigma}(\theta_k) v \leftarrow \frac{1}{N} \sum_{j=1}^{N} \langle Y_{jk}, v \rangle Y_{jk} - \langle X_k, v \rangle X_k \qquad \forall v \in \mathbb{R}^n$
return X_m

where increases in the sample size do not ensure convergence if the walk length ℓ is too small. We attribute this improvement to the walks no longer having a

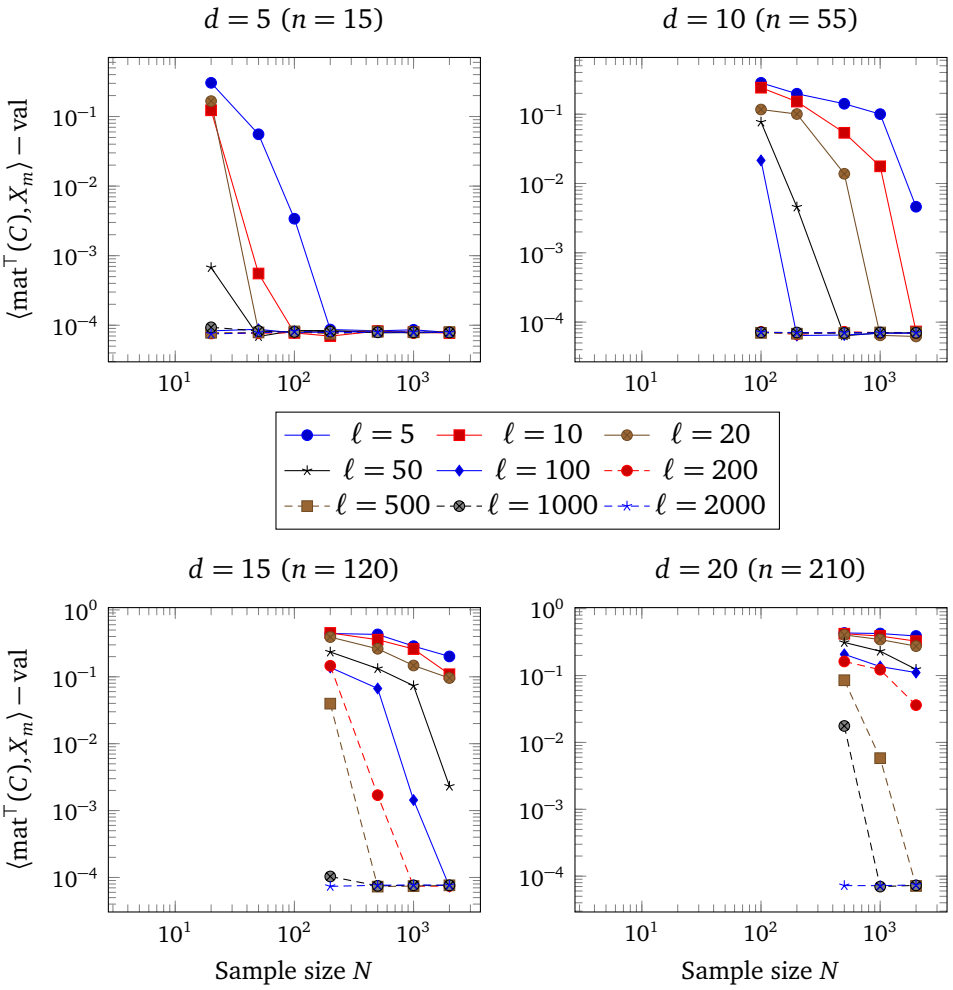

Figure 7.3: Effect of sample size N and walk length ℓ on the final gap of Algorithm 7.2

common starting point. For low walk lengths in particular, this change should lead to less dependence among the samples, and hence to a better approximation of the covariance.

What's more, the optimality gaps at termination of Algorithm 7.2 seem to be more tightly grouped around $10^{-4} = q\varepsilon$ than in Figure 7.2. (Note that $q\varepsilon$ is

exactly the size we would like the expected gap to have to guarantee that the gap is smaller than ε with probability $1-q$ by Markov's inequality.) This bahavior is likely caused by our returning the mean of our final collection of samples rather than one particular sample.

Despite these improvements, the number of hit-and-run steps and samples required to find a near-optimal solution did not change drastically compared to Figure 7.2. It seems (7.13) is still a good heuristic for the number of steps and samples.

There is one more modification that we will investigate. So far we have used hit-and-run sampling to approximate a distribution's covariance, only to then draw directions from a distribution with that same covariance. We could also draw directions directly from the centered samples from the previous iteration, eliminating the need to approximate some distribution's covariance. This idea is formalized in Algorithm 7.3.

Repeating the experiment that gave us Figure 7.3 now yields Figure 7.4. Note that we no longer require $N \geq n$, because we do not approximate a covariance matrix which should have full rank.

The results in Figure 7.4 are similar to Figure 7.3, except that Algorithm 7.3 can be run for more values of N. This additional flexibility does not lead to superior performance, though: for $N < n$, Algorithm 7.3 does not converge to a near-optimal solution. Since the performance of Algorithm 7.3 for $N \geq n$ appears similar to that of Algorithm 7.2, we propose to use Algorithm 7.2 with the values of N and ℓ from (7.13) in further experiments. In Chapter 9, this algorithm will be compared with alternative approaches to assess its competitiveness.

Algorithm 7.3 An adaptation of Algorithm 7.2 that changes the walks' directions

Input: convex body $\mathcal{S} \subset \mathbb{R}^n$ contained in a ball with radius $R \geq 1$;
normalized (with respect to $\|\cdot\|$) objective $c \in \mathbb{R}^n$;
number of samples N; number of hit-and-run steps ℓ;
number of iterations m; number of threads $\mathcal{P}$ that divides N (for simplicity);
starting point $x_0 \in \mathcal{S}$.

Output: $X_m \in \mathcal{S}$ such that $\langle c, X_m \rangle - \min_{x \in \mathcal{S}} \langle c, x \rangle$ is small with high probability.

for $i \in \{1, ..., \mathcal{P}\}$ **do**
  for $j \in \{1, ..., N/\mathcal{P}\}$ **do**
    Generate $Y_{(i-1)N/\mathcal{P}+j,0}$ by applying hit-and-run sampling to the uniform distribution over $\mathcal{S}$, starting the walk from x_0 if $j = 1$ and otherwise from $Y_{(i-1)N/\mathcal{P}+j-1,0}$, taking ℓ steps, drawing directions from a $\mathcal{N}(0, I)$-distribution
$X_0 \leftarrow \frac{1}{N} \sum_{j=1}^{N} Y_{j0}$
$T_0 \leftarrow 4R$
for $k \in \{1, ..., m\}$ **do**
  $T_k \leftarrow \left(1 - 1/\sqrt{n}\right) T_{k-1}$
  $\theta_k \leftarrow -c/T_k$
  for $i \in \{1, ..., \mathcal{P}\}$ **do**
    for $j \in \{1, ..., N/\mathcal{P}\}$ **do**
      Generate $Y_{(i-1)N/\mathcal{P}+j,k}$ by applying hit-and-run sampling to the Boltzmann distribution with parameter θ_k, starting the walk from X_{k-1} if $j = 1$ and otherwise from $Y_{(i-1)N/\mathcal{P}+j-1,k}$, taking ℓ steps, drawing directions uniformly from $\{Y_{1,k-1} - X_{k-1}, ..., Y_{N,k-1} - X_{k-1}\}$
  $X_k \leftarrow \frac{1}{N} \sum_{j=1}^{N} Y_{jk}$
return X_m

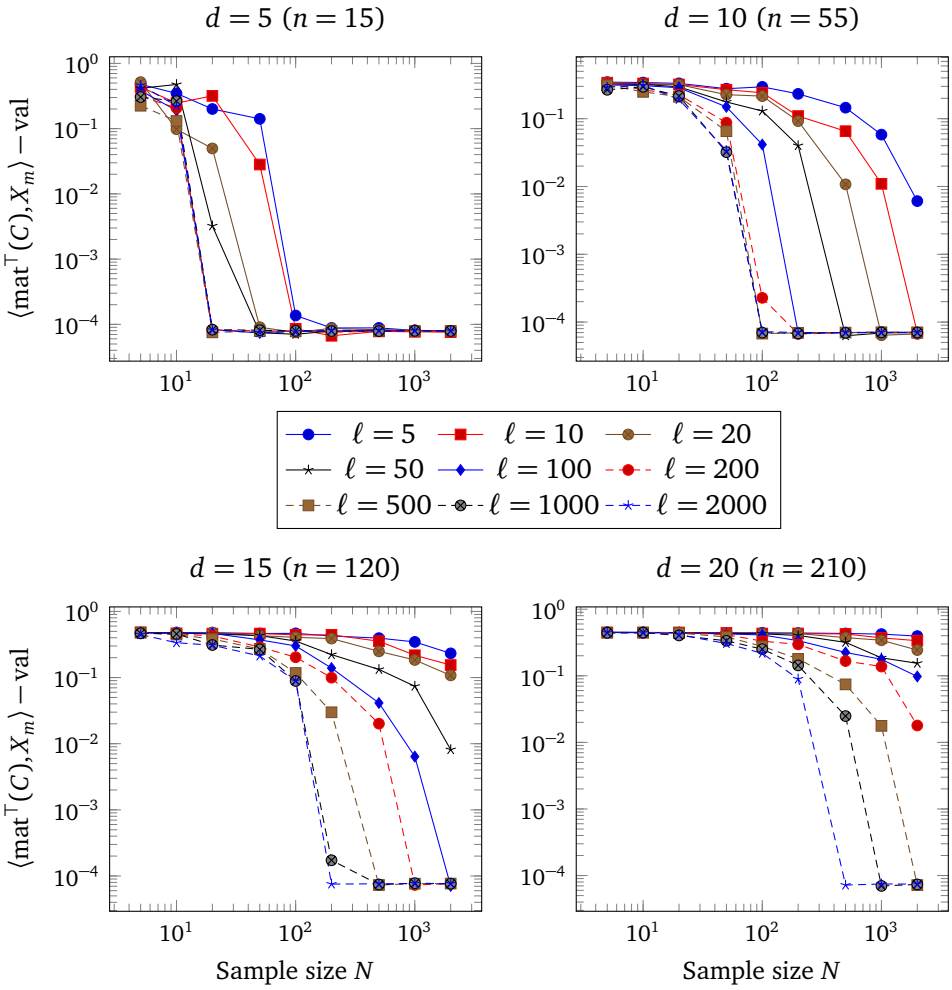

Figure 7.4: Effect of sample size N and walk length ℓ on the final gap of Algorithm 7.3

8

An Analytic Center Cutting Plane Method

In the previous two chapters, we have seen two sampling-based optimization algorithms. For the algorithm by Kalai and Vempala [56], we also proposed some changes to improve its numerical performance. In this chapter we introduce another algorithm that is aimed specifically at practical performance. The method we propose will be compared with an adaptation of Kalai and Vempala's algorithm and the ellipsoid method in Chapter 9.

This chapter is based on Sections 1 and 2 from Badenbroek and De Klerk [10], with only minor differences. Some information on symmetric cones is taken from the introduction of Badenbroek and Dahl [7].

8.1 Problem Statement and Solution Approach

Because we focus on practical computations, we only use the Euclidean inner product on $\mathbb{R}^n$ and the trace inner product on $\mathbb{S}^d$ in this chapter. The goal we have in mind is optimization over the *copositive cone* $\mathcal{COP}^d$, the dual of the completely

positive cone $\mathcal{CP}^d$. This cone is defined as

$$\mathcal{CO}^d := \left\{X \in \mathbb{S}^d : y^\top X y \geq 0 \text{ for all } y \in \mathbb{R}^d_+\right\}.$$

The application that we will focus on is separation from the completely positive cone. Separating a given doubly nonnegative matrix from the completely positive cone means that we can strengthen the relaxation (7.11) and reoptimize (this scheme is mentioned in e.g. Sponsel and Dür [103] and Berman et al. [13]). Burer and Dong [26] proposed a method to generate such a cut for 5×5 matrices. Sponsel and Dür [103] suggested an algorithm based on simplicial partition. Nevertheless, finding a cutting plane for the completely positive matrices is still listed as an open problem by Berman et al. [13].

Several approaches to copositive optimization exist in the literature. Bundfuss and Dür [22, 23] use polyhedral inner and outer approximations based on simplicial partitions that are refined in regions interesting to the optimization. Hierarchies of inner approximations of the copositive cone are proposed by Parrilo [92], De Klerk and Pasechnik [33] (see also Bomze and De Klerk [17]) and Peña et al. [93]. Yıldırım [113] proposes polyhedral outer approximations of the copositive cone, and analyzes the gap to the inner approximations by De Klerk and Pasechnik [33]. Lasserre [67] proposes a spectrahedral hierarchy of outer approximations of $\mathcal{CO}^d$. Perhaps most closely related to our work is the cutting-plane approach by Anstreicher et al. [4], although they do not implement their algorithms, and use a different separation oracle for the copositive cone.

Our approach is to use an *analytic center cutting plane method*. Analytic center cutting plane methods were first introduced by Goffin and Vial [43] (see [44] for a survey by the same authors, or Boyd et al. [20]). The advantage of analytic center cutting plane methods is that the number of iterations scales reasonably with the problem dimension. For instance, Goffin et al. [45] find that the number of iterations is $O^*(n^2/\varepsilon^2)$, where n is the number of variables and ε is the desired accuracy. In every iteration of our algorithm, the main computational effort is solving a mixed integer linear program (MILP) whose size does not change throughout the algorithm's run.

Analytic center cutting plane methods can be used to solve optimization problems of the form

$$\min_{x \in \mathcal{S}} c^\top x, \tag{8.1}$$

where $c \in \mathbb{R}^n$ and $\mathcal{S}$ is a convex body for which we know a separation oracle. In other words, given some point $x \in \mathbb{R}^n$, one should be able to determine if $x \in \mathcal{S}$ or not, and moreover, if $x \notin \mathcal{S}$, we must be able to generate a halfspace $\mathcal{H}$ such that $\mathcal{S} \subseteq \mathcal{H}$ but $x \notin \mathcal{H}$.

The idea behind analytic center cutting plane methods is to have a tractable outer approximation of the optimal set of (8.1). We will use one of the form

$$\mathcal{Q} = \left\{x \in \mathbb{R}^n : \|x\|^2 \leq R^2,\ \ a_i^\top x \leq b_i \,\forall i = 1, ..., M\right\}, \tag{8.2}$$

where $a_1^\top, ..., a_M^\top$ are the rows of a matrix A, b is a vector with elements $b_1, ..., b_M$, and $R > 0$. Assuming $\mathcal{Q}$ is non-empty, the self-concordant barrier

$$\Phi(x) := -\log(R^2 - \|x\|^2) - \sum_{i=1}^{M} \log(b_i - a_i^\top x) \tag{8.3}$$

has a unique minimizer called the *analytic center*, because its domain $\mathcal{Q}$ is bounded (see Corollary 2.3.6 in Renegar [95]). Of course, a more traditional outer approximation would be a polyhedron $\{x \in \mathbb{R}^n : Ax \leq b\}$ that is known to be bounded. We decided against this approach for reasons of numerical stability (more details in Section 8.5).

In every iteration k, one approximates the minimizer x_k of Φ. One of two things will happen. If x_k does not lie in $\mathcal{S}$, we use a separating hyperplane to remove x_k from $\mathcal{Q}$. If x_k lies in $\mathcal{S}$, x_k is feasible for (8.1). Hence any optimal solution must have an objective value that is at least as good as $c^\top x_k$. Any optimal solution will therefore lie in the halfspace $\{x \in \mathbb{R}^n : c^\top x \leq c^\top x_k\}$, and one may thus restrict the outer approximation to this halfspace.

The problem we will look at for some fixed $C \in \mathbb{S}^d$ is

$$\min_x \{\langle C, \mathrm{mat}(x)\rangle : \|x\|^2 \leq 1, \mathrm{mat}(x) \in \mathcal{CO}^d\}. \tag{8.4}$$

If $x \in \mathbb{R}^{d(d+1)/2}$ is an optimal solution to (8.4), then $C \in \mathcal{CP}^d$ if and only if $\langle C, \mathrm{mat}(x)\rangle \geq 0$. Note that the ball constraint in (8.4) is also present in the outer approximation (8.2), so it will suffice to generate linear inequalities to approximate the constraint $\mathrm{mat}(x) \in \mathcal{CO}^d$.

There are three remaining questions we have to answer before we can solve (8.4):

1. How will we generate separating hyperplanes for the constraint $\mathrm{mat}(x) \in \mathcal{CO}^d$?

2. How do we compute the analytic center of the outer approximation?

3. How can one prune constraints that do not have a large influence on the location of the analytic center?

These three questions will be answered in Sections 8.2, 8.3, and 8.4, respectively. Then, we state our algorithm in Section 8.5 and wrap up with some remarks concerning its complexity.

8.2 Membership of the Copositive Cone

It should be noted that determining if a matrix X lies in $\mathcal{CO}^d$ is co-NP-complete, see Murty and Kabadi [81]. The classical copositivity test is due to Gaddum [42], but his procedure requires performing a test for all principal minors of a matrix, which does not scale well to larger d. Nie et al. [90] have proposed an algorithm based on semidefinite programming that terminates in finite time, although the actual computation time is hard to predict. Anstreicher [5] shows that copositivity can be tested by solving an MILP, building on work by Dickinson [36]. See Hiriart-Urruty and Seeger [51] for a review of the properties of copositive matrices.

Our chosen method of testing if a matrix X is copositive is similar to Anstreicher's. Our method also solves an MILP, and also admits a $y \geq 0$ such that $y^\top X y < 0$ if X is not copositive. The main difference is that our method derives from Xia et al. [110] instead of Dickinson [36].

Note that $X \in \mathbb{S}^d$ is copositive if and only if

$$\min_y \{y^\top X y : e^\top y = 1, y \geq 0\}, \tag{8.5}$$

where e is the all-ones vector, is nonnegative. It was shown by Xia et al. [110] that the value of (8.5) is equal to the optimal value of the following mixed integer

linear program:

$$\left.\begin{aligned} \min_{y,w,\sigma,\nu} \; & -\sigma \\ \text{subject to } & Xy + \sigma e - \nu = 0 \\ & e^\top y = 1 \\ & 0 \le y_i \le w_i && \forall i \in \{1,...,d\} \\ & 0 \le \nu_i \le 2d(1-w_i)\max_{k,l}|X_{kl}| && \forall i \in \{1,...,d\} \\ & w_i \in \{0,1\} && \forall i \in \{1,...,d\}, \end{aligned}\right\} \tag{8.6}$$

and that any optimal y from (8.6) is also an optimal solution for (8.5). If the optimal value of (8.6) is nonnegative, then X is copositive. If the optimal value of (8.6) is negative, then an optimal solution $y \ge 0$ from (8.6) admits the halfspace $\mathcal{H} = \{X' \in \mathbb{S}^d : y^\top X' y \ge 0\}$ such that $\mathcal{COP}^d \subset \mathcal{H}$ but $X \notin \mathcal{H}$.

This test for matrix copositivity is attractive to use in practice. Gaddum's method [42] is already outperformed by the above method for very small matrices, and our method scales considerably better. The method by Nie et al. [90] can also become too slow for our purposes at moderate matrix dimensions. Anstreicher's recent method [5] also solves an MILP, which we expect to perform similarly to (8.6).

In theory, we can therefore determine if a matrix is copositive by solving one MILP. In practice however, a solver may return a solution $(\widehat{y}, \widehat{w}, \widehat{\sigma}, \widehat{\nu})$ to (8.6) where $\widehat{y}^\top \widehat{\nu} > 0$, violating the complementarity condition. This is caused by numerical tolerances allowing a solution with $\widehat{w} \notin \{0,1\}^d$, which mostly seems to occur if X has low rank (or is close to a low rank matrix). To find the optimal solution if this occurs, we fix w to the element-wise rounded value $\textsc{Round}(\widehat{w})$ of $\widehat{w}$. If the resulting problem is still feasible, we can compare its complementary solution with the solution to the model for $w \in \{0,1\}^d \setminus \{\textsc{Round}(\widehat{w})\}$. If the constraint $w = \textsc{Round}(\widehat{w})$ does make the problem infeasible, we know that any optimal solution will have $w \in \{0,1\}^d \setminus \{\textsc{Round}(\widehat{w})\}$. The details of this procedure are given in Algorithm 8.1, where $\text{val}(\mathcal{M})$ denotes the objective value of the optimal solution returned by the solver when solving the model $\mathcal{M}$.

Algorithm 8.1 Method for testing copositivity or finding deep cuts

Input: matrix $X \in \mathbb{S}^d$ which we want to test for copositivity.

Output: TRUE if X is copositive, otherwise a halfspace $\mathcal{H} \supset \mathcal{COP}^d$ with $X \notin \mathcal{H}$.

1: **function** TESTCOPOSITIVE(X)
2: Let $\mathcal{M}$ refer to the model (8.6) with input X
3: $(\widehat{y}, \widehat{w}, \widehat{\sigma}, \widehat{\nu}) \leftarrow$ SOLVEMODEL($\mathcal{M}$) ▷ See Line 8
4: **if** $\widehat{y}^\top X \widehat{y} \geq 0$ **then**
5: **return** TRUE
6: **else**
7: **return** $\{X' \in \mathbb{S}^d : \widehat{y}^\top X' \widehat{y} \geq 0\}$
8: **function** SOLVEMODEL($\mathcal{M}$, $u = +\infty$)
9: Let $(\widehat{y}, \widehat{w}, \widehat{\sigma}, \widehat{\nu})$ be the solution to the model $\mathcal{M}$ returned by the solver
10: **if** $\widehat{y}^\top \widehat{\nu} > 0$ and $\text{val}(\mathcal{M}) < u$ **then**
11: Let $\overline{\mathcal{M}}$ be the model $\mathcal{M}$ with the added constraint $w = \text{ROUND}(\widehat{w})$
12: Let $\mathcal{M}'$ be the model $\mathcal{M}$ with the added constraint $\sum_{i:\text{ROUND}(\widehat{w}_i)=0} w_i + \sum_{i:\text{ROUND}(\widehat{w}_i)=1}(1 - w_i) \geq 1$
13: **if** $\overline{\mathcal{M}}$ is feasible **then**
14: Compute the optimal solution to $\overline{\mathcal{M}}$
15: Also compute SOLVEMODEL($\mathcal{M}', \text{val}(\overline{\mathcal{M}})$) if $\mathcal{M}'$ is feasible
16: **return** the solution with the best objective value out of these two
17: **else**
18: **return** SOLVEMODEL($\mathcal{M}'$)
19: **else**
20: **return** the solution $(\widehat{y}, \widehat{w}, \widehat{\sigma}, \widehat{\nu})$

8.3 Approximating the Analytic Center

Now that we saw how to generate cuts for the copositive cone, we turn our attention to the second question: how to approximate the analytic center of our outer approximation. This was defined as the minimizer of the function Φ in (8.3). Since Φ can only be evaluated at x where $\|x\|^2 < R^2$ and $Ax < b$, we will use an infeasible-start Newton method to approximate its minimizer. Similar to Boyd et al. [20, Section 2], one can reformulate the problem of computing the analytic

center of $\mathcal{Q}$ as

$$\inf_{x,\pi,s}\left\{-\log(\pi)-\sum_{i=1}^{m}\log(s_i) : \pi \le R^2-\|x\|^2, s \le b-Ax\right\}, \tag{8.7}$$

which has Lagrangian

$$L(x,\pi,s,\lambda,\Lambda) := -\log(\pi)-\sum_{i=1}^{m}\log(s_i)+\lambda(\pi-R^2+\|x\|^2)+\Lambda^\top(s-b+Ax).$$

For some vector $v \in \mathbb{R}^n$ with all elements unequal to zero, and some integer $k \in \mathbb{Z}$, let $v^k := \begin{bmatrix} v_1^k & \cdots & v_n^k \end{bmatrix}^\top$. The gradient of the Lagrangian can then be written as

$$DL(x,\pi,s,\lambda,\Lambda) = \begin{bmatrix} 2\lambda x + A^\top\Lambda \\ -\pi^{-1}+\lambda \\ -s^{-1}+\Lambda \\ \pi - R^2 + \|x\|^2 \\ s-b+Ax \end{bmatrix}. \tag{8.8}$$

For the sake of completeness, let us show that it suffices to compute a stationary point of the Lagrangian.

Proposition 8.1 ([10, Proposition 1])**.** *Let $A \in \mathbb{R}^{M\times n}$ have rows $a_1^\top, \ldots, a_M^\top$, and let $b \in \mathbb{R}^M$, and $R > 0$. Let $\mathcal{Q}$ be as defined in* (8.2)*, and assume that it has nonempty interior. Then, z is the analytic center of $\mathcal{Q}$ if and only if there exist $\pi, s, \lambda, \Lambda > 0$ such that $DL(z,\pi,s,\lambda,\Lambda) = 0$.*

Proof. Because $\mathcal{Q}$ is bounded and has a nonempty interior, it has an analytic center (see e.g. Corollary 2.3.6 in Renegar [95]), and problem (8.7) has an optimal solution. The nonempty interior of $\mathcal{Q}$ also guarantees the existence of a Slater point of (8.7). Since (8.7) is convex, Slater's condition shows that a feasible solution (z,π,s) is optimal if and only if it satisfies the KKT conditions: there should exist λ, Λ such that

$$\begin{bmatrix} 2\lambda z + A^\top\Lambda \\ -\pi^{-1}+\lambda \\ -s^{-1}+\Lambda \end{bmatrix} = 0, \qquad \begin{matrix} \lambda(\pi - R^2 + \|z\|^2) = 0, \\ \Lambda^\top(s-b+Az) = 0, \end{matrix} \qquad \begin{matrix} \pi \le R^2 - \|z\|^2, \\ s \le b - Az, \\ \lambda, \Lambda \ge 0. \end{matrix}$$

Since $\lambda = \pi^{-1} > 0$ and $\Lambda = s^{-1} > 0$, the claim follows. □

Let us compute the Newton step $(\Delta x, \Delta\pi, \Delta s, \Delta\lambda, \Delta\Lambda)$ to approximate a stationary point of L. We find that

$$D^2L(x,\pi,s,\lambda,\Lambda) = \begin{bmatrix} 2\lambda I & 0 & 0 & 2x & A^\top \\ 0 & \pi^{-2} & 0 & 1 & 0 \\ 0 & 0 & \mathrm{Diag}(s^{-2}) & 0 & I \\ 2x^\top & 1 & 0 & 0 & 0 \\ A & 0 & I & 0 & 0 \end{bmatrix}. \tag{8.9}$$

Thus, using the expressions (8.8) and (8.9), we see that the Newton step is the solution to

$$0 = \begin{bmatrix} 2\lambda x + A^\top\Lambda \\ -\pi^{-1} + \lambda \\ -s^{-1} + \Lambda \\ \pi - R^2 + \|x\|^2 \\ s - b + Ax \end{bmatrix} + \begin{bmatrix} 2\lambda I & 0 & 0 & 2x & A^\top \\ 0 & \pi^{-2} & 0 & 1 & 0 \\ 0 & 0 & \mathrm{Diag}(s^{-2}) & 0 & I \\ 2x^\top & 1 & 0 & 0 & 0 \\ A & 0 & I & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\pi \\ \Delta s \\ \Delta\lambda \\ \Delta\Lambda \end{bmatrix}. \tag{8.10}$$

We could solve this system directly, but it is more efficient to note that the last conditions imply

$$\begin{cases} \Delta\lambda &= -\lambda + \pi^{-1} - \pi^{-2}\Delta\pi \\ \Delta\Lambda &= -\Lambda + s^{-1} - \mathrm{Diag}(s^{-2})\Delta s \\ \Delta\pi &= -\pi + R^2 - \|x\|^2 - 2x^\top\Delta x \\ \Delta s &= -s + b - Ax - A\Delta x \end{cases} \tag{8.11}$$

which means the entire Newton step can be expressed in terms of Δx. The first n equations of the Newton system (8.10) are thus

$$\begin{aligned} -2\lambda x - A^\top\Lambda &= 2\lambda\Delta x + 2x\Delta\lambda + A^\top\Delta\Lambda \\ &= 2\lambda\Delta x + 2x[\pi^{-1} - \lambda - \pi^{-2}\Delta\pi] + A^\top[s^{-1} - \Lambda - \mathrm{Diag}(s^{-2})\Delta s] \\ &= 2\lambda\Delta x + 2x[\pi^{-1} - \lambda - \pi^{-2}(-\pi + R^2 - \|x\|^2 - 2x^\top\Delta x)] \\ &\quad + A^\top[s^{-1} - \Lambda - \mathrm{Diag}(s^{-2})(-s + b - Ax - A\Delta x)], \end{aligned}$$

or equivalently,

$$\begin{aligned} &\left[2\lambda I + \frac{4}{\pi^2}xx^\top + A^\top\,\mathrm{Diag}(s^{-2})A\right]\Delta x \\ &= \frac{R^2 - \|x\|^2 - 2\pi}{\pi^2}2x + A^\top\,\mathrm{Diag}(s^{-2})(b - Ax - 2s). \end{aligned} \tag{8.12}$$

After solving this system for Δx, we can compute the other components of the Newton step through equations (8.11). Now that it is clear how one can compute the Newton step for problem (8.7), we propose Algorithm 8.2 to solve (8.7).

Algorithm 8.2 Infeasible start Newton method for (8.7)

Input: convex body $\mathcal{Q} = \{x \in \mathbb{R}^n : \|x\|^2 \leq R^2, Ax \leq b\}$, where $A \in \mathbb{R}^{M\times n}$ and $b \in \mathbb{R}^M$;
starting point $x_0 \in \mathbb{R}^n$;
maximum number of iterations $m = 50$;
gradient norm tolerance $\rho = 10^{-8}$.

Output: Approximation x_k of the analytic center of $\mathcal{Q}$.

1: $k \leftarrow 1$
2: $\pi_0 \leftarrow \begin{cases} R^2 - \|x_0\|^2 & \text{if } R^2 - \|x_0\|^2 > 0 \\ 1 & \text{otherwise} \end{cases}$
3: $(s_0)_i \leftarrow \begin{cases} b_i - a_i^\top x_0 & \text{if } b_i - a_i^\top x_0 > 0 \\ 1 & \text{otherwise} \end{cases}$ for all $i \in \{1, ..., M\}$
4: $\lambda_0 \leftarrow 1$
5: $\Lambda_0 \leftarrow 0$
6: **while** $k \leq m$ **do**
7: Compute Δx_k from (8.12)
8: Compute $(\Delta\pi_k, \Delta s_k, \Delta\lambda_k, \Delta\Lambda_k)$ from (8.11)
9: $t_k \leftarrow \min\{1, 0.9 \sup\{t \geq 0 : \pi_k + t\Delta\pi_k \geq 0, s_k + t\Delta s_k \geq 0, \lambda_k + t\Delta\lambda_k \geq 0\}\}$
10: $\phi_k(t) := \|DL(x_k + t\Delta x_k, \pi_k + t\Delta\pi_k, s_k + t\Delta s_k, \lambda_k + t\Delta\lambda_k, \Lambda_k + t\Delta\Lambda_k)\|$
11: **if** $\phi_k(0) \leq \rho$ and $\Lambda_k \geq 0$ and ($\phi_k(t_k) \geq \phi_k(0)$ or $k = m$) **then**
12: **return** x_k with success status
13: $k \leftarrow k + 1$
14: **return** x_k with failure status

Let us make a few observations about this algorithm. First, note that if $\lambda > 0$, the matrix $2\lambda I + 4\pi^{-2}xx^\top + A^\top \text{Diag}(s^{-2})A$ is positive definite, and hence invertible. Thus, as long as $\lambda > 0$, the system (8.12) will have a (unique) solution Δx.

Second, the value for t in Line 9 of Algorithm 8.2 is chosen such that after the update, π, s, and λ will all remain positive. In principle, the value 0.9 could be

replaced by any real number from $(0,1)$. Note that we are not requiring that Λ remains positive in all iterations: numerical evidence suggests that the method is more likely to succeed if some elements of Λ are allowed to be negative in some iterations. Nevertheless, Algorithm 8.2 only returns a success status if the final Λ is nonnegative.

Third, the algorithm returns the current solution x with success status in two cases. In either case, the current solution should approximately be a stationary point of the Lagrangian, i.e. the norm of $DL(x,\pi,s,\lambda,\Lambda)$ has to be small, and we should have $\Lambda \geq 0$. Moreover, one of two conditions should hold. If the algorithm is in iteration m, we can return the current, approximately stationary point. Alternatively, if adding t times the Newton step leads to a larger norm of the Lagrangian gradient, we also return the current point. In other words, we keep taking Newton steps if it leads to a smaller gradient norm, and we are not yet in the final iteration. The reason to do so is that Newton's method converges very rapidly when the current point is near the optimum. By running just a few more iterations, we get a solution with much higher accuracy.

Finally, compared to the algorithm in Boyd et al. [20, Section 2], Algorithm 8.2 does not use backtracking line search. The reason is that for problem (8.7), the norm of the Lagrangian gradient does not seem to decrease monotonically during the algorithm's run. In fact, the norm of this gradient usually first decreases to the order 10^0, then increases slightly to the order 10^1, before decreasing rapidly to the order 10^{-8}. If one does backtracking line search on t to ensure that in every iteration the norm of the gradient decreases, the values of t can become very small (say, of the order 10^{-9}). Then, the number of iterations required to achieve convergence would be impractically large.

8.4 Pruning Constraints

The next question we should answer is how we can prune constraints from our outer approximation (8.2). Pruning is often used to reduce the number of constraints defining the outer approximation, which keeps the computational effort per iteration stable. Moreover, the linear system (8.12) will quickly become ill-conditioned if no constraints are dropped.

The idea we use is the same as in Boyd et al. [20, Section 3]. Since Φ is self-concordant, the *Dikin ellipsoid* around the analytic center z of $\mathcal{Q}$ is contained in $\mathcal{Q}$, that is,

$$\{x \in \mathbb{R}^n : (x-z)^\top D^2\Phi(z)(x-z) \leq 1\} \subseteq \mathcal{Q}, \tag{8.13}$$

where

$$D^2\Phi(z) = \frac{2}{R^2 - \|z\|^2} I + \frac{4}{(R^2 - \|z\|^2)^2} zz^\top + \sum_{i=1}^{M} \frac{1}{(b_i - a_i^\top z)^2} a_i a_i^\top. \tag{8.14}$$

Moreover, it will be shown at the end of this section that for our outer approximation $\mathcal{Q}$ it holds that

$$\mathcal{Q} \subseteq \{x \in \mathbb{R}^n : (x-z)^\top D^2\Phi(z)(x-z) \leq (M+2)^2\}. \tag{8.15}$$

Hence, following Boyd et al. [20], we define the relevance measure

$$\chi_i := \frac{b_i - a_i^\top z}{\sqrt{a_i^\top D^2\Phi(z)^{-1} a_i}}, \tag{8.16}$$

for all linear constraints $i \in \{1, ..., M\}$. By (8.13), all χ_i are at least one. Moreover, it follows from (8.15) that if $\chi_i \geq M+2$, the corresponding constraint is certainly redundant.

With this in mind, we propose Algorithm 8.3 to prune linear constraints from $\mathcal{Q}$. Note that the ball constraint $\|x\|^2 \leq R^2$ is never pruned.

As an alternative to Algorithm 8.3, one might consider dropping $M - M_{\max}$ constraints, possibly keeping some redundant constraints. The reason we do not adopt this strategy is that we noticed Algorithm 8.3 leads to slightly better numerical performance on our test sets.

We finish this section with a proof of the relation (8.15). It will use a result on *symmetric cones*, which are closed convex self-dual cones with a transitive automorphism group. Güler [47] proved that symmetric cones are the same as self-scaled cones, a class of cones better known to the optimization community at the time. In 1934, Jordan et al. [55] showed there are five irreducible symmetric cones (up to isomorphism), only two of which are used for optimization in practice: the second-order cone, and the cone of symmetric positive semidefinite matrices. Since linear programming is a special case of semidefinite programming, it can also be written as an optimization problem over a symmetric cone.

Algorithm 8.3 A pruning method for the intersection of a ball and a polyhedron

Input: convex body $\mathcal{Q} = \{x \in \mathbb{R}^n : \|x\|^2 \leq R^2, Ax \leq b\}$, where $A \in \mathbb{R}^{M\times n}$ and $b \in \mathbb{R}^M$;
analytic center z of $\mathcal{Q}$;
maximum number of linear inequalities $M_{\max} = 4n$.

Output: A convex body $\mathcal{Q}$ defined by at most $M_{\max}$ linear inequalities.

1: **if** $M > n$ **then**
2: Compute χ_i as in (8.16) for $i \in \{1, ..., M\}$
3: Remove all constraints $a_i^\top x \leq b_i$ with $\chi_i \geq M + 2$ from $\mathcal{Q}$
4: **if** $\mathcal{Q}$ still contains more than $M_{\max}$ linear inequalities **then**
5: Remove the constraints $a_i^\top x \leq b_i$ with the largest values of χ_i from $\mathcal{Q}$ such that $M_{\max}$ remain
6: **return** $\mathcal{Q}$

Proposition 8.2 ([10, Proposition 2]). *Let $A \in \mathbb{R}^{M\times n}$ have rows $a_1^\top, ..., a_M^\top$, and let $b \in \mathbb{R}^M$, and $R > 0$. Let $\mathcal{Q}$ be as defined in* (8.2)*, and assume that it has nonempty interior. Define Φ as in* (8.3)*, and let z be its minimizer. Then, for any $x \in \operatorname{dom}\Phi$, we have*

$$(x - z)^\top D^2\Phi(z)(x - z) \leq (M + 2)^2.$$

Proof. Define the barrier function

$$f(t, x, s) := -\log(t^2 - \|x\|^2) - \sum_{i=1}^{M} \log(s_i),$$

whose domain is a symmetric cone. The barrier parameter ϑ_f of f satisfies $\vartheta_f \leq M + 2$ (see for instance Renegar [95, Theorem 2.3.1]). Note that any $x \in \operatorname{dom}\Phi$ if and only if $(R, x, b - Ax) \in \operatorname{dom} f$. We will first show that the gradient of f at $(R, z, b - Az)$ is orthogonal to $(R, x, b - Ax) - (R, z, b - Az) = (0, x - z, A(z - x))$. The claim will then follow from a property of symmetric cones.

The gradient of f is

$$g(t, x, s) := \begin{bmatrix} -2t/(t^2 - \|x\|^2) \\ 2x/(t^2 - \|x\|^2) \\ -s^{-1} \end{bmatrix},$$

so it follows that

$$g(R,z,b-Az)^\top \begin{bmatrix} 0 \\ x-z \\ A(z-x) \end{bmatrix} = \frac{2z^\top(x-z)}{R^2-\|z\|^2} - \sum_{i=1}^{M} \frac{a_i^\top(z-x)}{b_i - a_i^\top z}. \tag{8.17}$$

Because z is the minimizer of the convex function Φ, we have

$$0 = D\Phi(z) = \frac{2}{R^2-\|z\|^2} z + \sum_{i=1}^{M} \frac{1}{b_i - a_i^\top z} a_i,$$

which implies that (8.17) is zero. Therefore, Theorem 3.5.9 in Renegar [95] shows that

$$\begin{bmatrix} 0 \\ x-z \\ A(z-x) \end{bmatrix}^\top H(R,z,b-Az) \begin{bmatrix} 0 \\ x-z \\ A(z-x) \end{bmatrix} \leq \vartheta_f^2, \tag{8.18}$$

where H is the Hessian of f. It is not hard to see that $H(t,x,s)$ equals

$$\frac{1}{(t^2-\|x\|^2)^2} \begin{bmatrix} 2t^2+\|x\|^2 & -4tx^\top & 0 \\ -4tx^\top & 2(t^2-\|x\|^2)I + 4xx^\top & 0 \\ 0 & 0 & (t^2-\|x\|^2)^2 \operatorname{Diag}(s^{-2}) \end{bmatrix}.$$

In other words, (8.18) is equivalent to

$$(x-z)^\top \left[\frac{2}{R^2-\|z\|^2} I + \frac{4}{(R^2-\|z\|^2)^2} zz^\top \right] (x-z) + \sum_{i=1}^{M} \frac{(a_i^\top(z-x))^2}{(b_i - a_i^\top z)^2} \leq \vartheta_f^2,$$

which proves the claim, since the left hand side is $(x-z)^\top D^2\Phi(z)(x-z)$ by (8.14), and $\vartheta_f \leq M+2$. □

8.5 Algorithm Statement

Recall that we are developing an analytic center cutting plane method to check complete positivity of a matrix, by solving an optimization problem over the copositive cone. Now that we have answered the major questions surrounding such a method, we move on to our final method. We start with a quite general analytic center cutting plane method, and then add a wrapper function that performs

the complete positivity check. The reason for making this split is that it makes our code easy to extend when solving other copositive optimization problems for which a bound on the norm of an optimal solution is known. We state our proposed analytic center cutting plane method to solve (8.1) in Algorithm 8.4.

We continue the algorithm even if we cannot find the analytic center to high accuracy. Late in the algorithm's run, the system (8.12) often becomes ill-conditioned. This is to be expected, since as Algorithm 8.4 progresses, the outer approximation $\mathcal{Q}_k$ becomes smaller and smaller. The distance from the analytic center to the linear constraints also goes to zero, but not at the same pace for every constraint. We may arrive in a situation where $b_i - a_i^\top x_k$ is of the order 10^{-4} for some constraints i, and of the order 10^{-8} for other constraints. This causes a considerable spread in the eigenvalues of the matrix in (8.12).

If the analytic center is not known to a decent accuracy, the pruning procedure in Algorithm 8.3 may remove constraints that are actually very important to the definition of $\mathcal{Q}_k$. One could of course still run the pruning function using the inaccurate analytic center approximation. However, because the problems in the analytic center computation only occur late in the algorithm's run, pruning or not pruning with the inaccurate approximation does not seem to have a major impact on total runtime.

Algorithm 8.4 is a (relatively) general analytic center cutting plane method. The problem (8.4) can be solved by calling Algorithm 8.4 with the right arguments, as is done by Algorithm 8.5.

Our aim in this chapter has been to propose an algorithm with good practical performance. This is why we placed emphasis on a robust copositivity check, constraint pruning, and efficient computation of the analytic center. However, such an algorithm does not lend itself well to a formal complexity analysis. For instance, to the best of our knowledge, the only analysis in the literature of an analytic center cutting plane method with constraint pruning is due to Atkinson and Vaidya [6]. Although the number of constraints in their algorithm is technically bounded by a polynomial of n, this bound is so large as to be uninteresting in practice.

The analysis that perhaps comes closest to covering our algorithm is the survey by Goffin and Vial [44], who find a polynomial number of iterations for an analytic center cutting plane method with deep cuts. Their method only uses linear

Algorithm 8.4 Analytic Center Cutting Plane method to solve (8.1)

Input: objective $c \in \mathbb{R}^n$;
oracle function ORACLE : $\mathbb{R}^n \to \{\text{TRUE}\} \cup \{\{x \in \mathbb{R}^n : a^\top x \leq b\} : a \in \mathbb{R}^n, b \in \mathbb{R}\}$;
radius $R > 0$;
optimality tolerance $\varepsilon = 10^{-6}$.

Output: A feasible solution x_* for which RELGAP$(c, x_*, \mathcal{Q}_k) \leq \varepsilon$. ▷ See Line 18

1: **function** ACCP(c, ORACLE, R)
2: $\mathcal{Q}_1 \leftarrow \{x \in \mathbb{R}^n : \|x\|^2 \leq R^2\}$
3: $x_0 \leftarrow 0$
4: $k \leftarrow 1$
5: **while** the best feasible solution so far x_* has RELGAP$(c, x_*, \mathcal{Q}_k) > \varepsilon$ **do**
6: Generate approximation x_k of the analytic center of $\mathcal{Q}_k$ through Algorithm 8.2, starting from x_{k-1}
7: **if** Algorithm 8.2 terminated with a failure status **then**
8: Check if $x_k \in \operatorname{int} \mathcal{Q}_k$. If not, throw an error.
9: **else**
10: Prune constraints from $\mathcal{Q}_k$ through Algorithm 8.3, assuming x_k is the analytic center of $\mathcal{Q}_k$
11: **if** ORACLE(x_k) returns TRUE **then**
12: $\mathcal{Q}_{k+1} \leftarrow \mathcal{Q}_k \cap \{x \in \mathbb{R}^n : c^\top x / \|c\| \leq c^\top x_k / \|c\|\}$
13: **else** ▷ ORACLE(x_k) returns a halfspace
14: $\mathcal{H}_k = \{x \in \mathbb{R}^n : a_k^\top x \leq b_k\}$ is the halfspace returned by ORACLE(x_k)
15: $\mathcal{Q}_{k+1} \leftarrow \mathcal{Q}_k \cap \{x \in \mathbb{R}^n : a_k^\top x / \|a_k\| \leq b_k / \|a_k\|\}$
16: $k \leftarrow k + 1$
17: **return** the best feasible solution found x_*
18: **function** RELGAP$(c, x_*, \mathcal{Q})$
19: $l \leftarrow \min_x \{c^\top x : x \in \mathcal{Q}\}$
20: **return** $(c^\top x_* - l)/(1 + \min\{|c^\top x_*|, |l|\})$

constraints, and does not prune cuts. Moreover, the method of recovering a feasible solution after adding a deep cut is different from the infeasible start Newton method we use.

Algorithm 8.5 A wrapper function to determine if a matrix is completely positive by solving (8.4)

Input: $C \in \mathbb{S}^d$ for which we want to determine if $C \in \mathcal{CP}^d$ or not.
Output: $X \in \mathcal{CO}^d$ such that $\langle C, X \rangle$ is approximately equal to (8.4).

1: $c \leftarrow \text{mat}^\top(C)$
2: $R \leftarrow 1$
3: ORACLE$(x) \leftarrow$ TESTCOPOSITIVE(mat(x))
4: **return** mat(ACCP(c, ORACLE, R))

Nevertheless, we compared our method numerically to Goffin and Vial's, and found that our method exhibits somewhat better numerical performance on our test set. In particular, Goffin and Vial's method struggles earlier to approximate the analytic center. Whereas we could solve the problems in our test set up to a relative gap of 10^{-6}, Goffin and Vial's method sometimes failed to recover a point in the feasible set when the relative gap was still of the order 10^{-5}. The condition number of their linear systems had become very large at this point, explaining the inaccuracy. At this level of the relative gap, the condition number of the system (8.12) in our algorithm was somewhat lower.

In short, while our method is not covered by a formal complexity analysis, we do prefer it over other algorithms in the literature for numerical reasons. The Julia implementation is available at `https://github.com/rileybadenbroek/CopositiveAnalyticCenter.jl`.

9 Numerical Experiments

So far, we have described three methods for optimization in the separation oracle setting: Algorithms 6.2, 7.2, and 8.4. In this chapter, we will compare these methods through numerical experiments. As a benchmark, we also include the ellipsoid method by Yudin and Nemirovski [114] in our experiments. Because of the applied nature of this chapter, below $\langle \cdot, \cdot \rangle$ refers to the Euclidean inner product on $\mathbb{R}^n$, and to the trace inner product on $\mathbb{S}^d$.

In Section 9.1, we establish that the high-quality covariance and mean approximations that Algorithm 6.2 needs take an impractical amount of time to generate. We proceed by comparing the remaining methods – Algorithms 7.2 and 8.4 – with the ellipsoid method in Section 9.2. It will be shown that Algorithm 7.2 requires significantly more oracle calls than Algorithm 8.4 or even the ellipsoid method. On the other hand, Algorithm 8.4 compares favorably to the ellipsoid method. Section 9.3 shows that Algorithm 8.4 also scales very reasonably.

This chapter is based on Sections 5.1 and 5.2 in Badenbroek and De Klerk [9] and Section 3 from Badenbroek and De Klerk [10]. The numerical results are slightly different from [9] because we use another test problem for the sake of

harmonization of this thesis (in [9], we used a different mapping from $\mathbb{S}^d$ to $\mathbb{R}^n$ than the operator vec). This does not affect our conclusions though.

9.1 Covariance and Mean Approximation with Hit-and-Run Sampling

The short-step interior point method Algorithm 6.2 required the approximation of certain covariance matrices and means by hit-and-run sampling. Let us investigate how well this works in practice. We will test this on the feasible set of (7.12), that is,

$$\left\{x \in \mathbb{R}^{d(d+1)/2} : \|x\| \leq 1, x \geq 0, \operatorname{mat}(x) \succeq 0\right\}, \tag{9.1}$$

where $d \in \{5, 10, 15, 20\}$. The membership test for this set is generally faster than that from Section 8.2 for the copositive cone, making it the more attractive option for this experiment.

First, we generate an approximation $\widehat{\Sigma}_0$ of the covariance matrix of the uniform distribution over (9.1) with hit-and-run sampling. This will use 20,000 hit-and-run samples with walk length 50,000, where the directions are drawn from $\mathcal{N}(0, I)$. We let $X = \frac{1}{4}(dI + ee^\top)/d^2 \in \mathbb{S}^d$ and take $x = \operatorname{vec}(X)$ as the starting point for all random walks.

Then, the experiment is repeated for $N \leq 20{,}000$ samples with walk length $\ell \leq 50{,}000$. We refer to these estimates as $\widehat{\Sigma}_{N,\ell}$. We would like to see for which $\epsilon \geq 0$ we have

$$\frac{1}{1+\epsilon}\widehat{\Sigma}_{N,\ell} \preceq \widehat{\Sigma}_0 \preceq (1+\epsilon)\widehat{\Sigma}_{N,\ell}.$$

Note that (2.3) shows that this condition is equivalent to

$$\widehat{\Sigma}_0^{-1/2}\widehat{\Sigma}_{N,\ell}\widehat{\Sigma}_0^{-1/2} - I \preceq \epsilon I \quad \text{and} \quad \widehat{\Sigma}_{N,\ell}^{-1/2}\widehat{\Sigma}_0\widehat{\Sigma}_{N,\ell}^{-1/2} - I \preceq \epsilon I.$$

Because similar matrices have the same eigenvalues, the smallest $\epsilon \geq 0$ that satisfies this condition is

$$\widehat{\epsilon}(N,\ell) := \max\left\{\lambda_{\max}(\widehat{\Sigma}_0^{-1}\widehat{\Sigma}_{N,\ell} - I), \lambda_{\max}(\widehat{\Sigma}_{N,\ell}^{-1}\widehat{\Sigma}_0 - I)\right\}.$$

The result is shown in Figure 9.1, where the covariance matrices are of size $n \times n$, that is, $\frac{1}{2}d(d+1) \times \frac{1}{2}d(d+1)$.

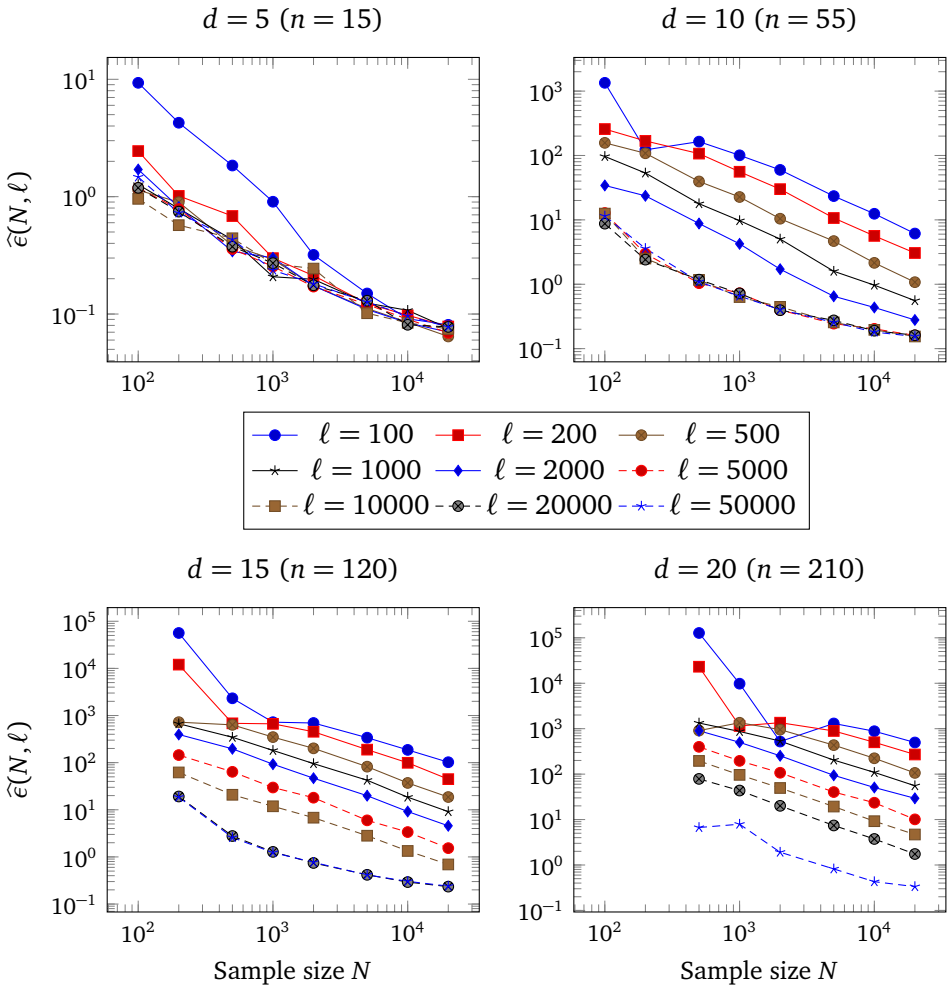

Figure 9.1: Effect of sample size N and walk length ℓ on covariance approximation quality over (9.1)

One major conclusion from Figure 9.1 is that the trajectory towards zero is relatively slow. To show that simply adding more samples with higher walk lengths will in practice not be feasible, we present the running times required to estimate a covariance matrix at the desired accuracy in Figure 9.2. Specifically, this figure shows the running times of the "efficient" combinations of N and ℓ: these are the

combinations of N and ℓ plotted in Figure 9.1 for which there are no N' and ℓ' such that $\widehat{\epsilon}(N',\ell') \leq \widehat{\epsilon}(N,\ell)$ and the running time for N' and ℓ' is lower than for N and ℓ. (The computer used has an Intel i7-6700 CPU with 16 GB RAM, and the code used eight threads.) Figure 9.2 shows that, even at low dimensions, approximating the covariance matrix to high accuracy will take an unpractical amount of time.

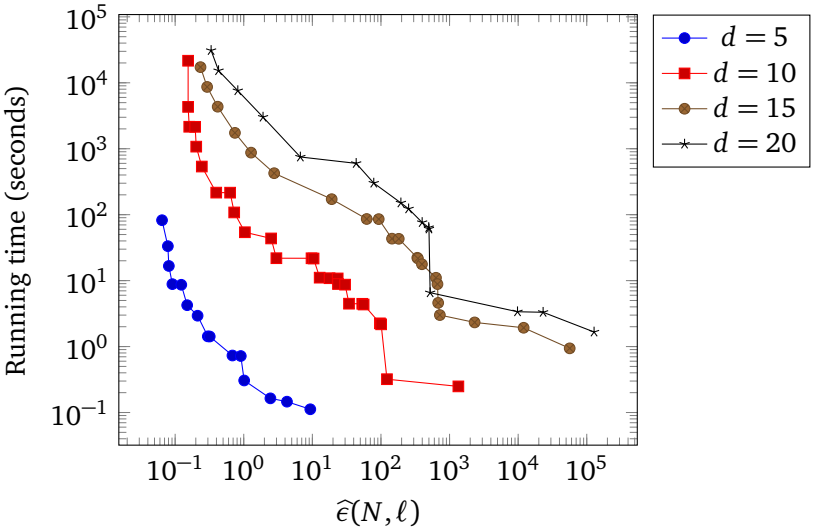

Figure 9.2: Running times required to find an approximation $\widehat{\Sigma}_{N,\ell}$ of the desired quality

To show that the slow trajectory towards zero in Figure 9.1 is a result of covariance estimation's fundamental difficulty, we consider a simpler problem. We will approximate the covariance matrix of the uniform distribution over the hypercube $[0,1]^n$ in $\mathbb{R}^n$. Note that the true covariance matrix of this distribution is known to be $\frac{1}{12}I$.

We will use hit-and-run with varying walk lengths and sample sizes to generate samples from the uniform distribution over $[0,1]^n$. The resulting covariance matrices $\widehat{\Sigma}_{N,\ell}$ will be compared with the true covariance $\frac{1}{12}I$ (comparing with a covariance estimate based on hit-and-run samples as in Figure 9.1 yields roughly

the same image). The analogue of $\widehat{\epsilon}(N,\ell)$ would be

$$\widehat{\xi}(N,\ell) := \max\left\{\lambda_{\max}(12\widehat{\Sigma}_{N,\ell} - I), \lambda_{\max}(\tfrac{1}{12}\widehat{\Sigma}_{N,\ell}^{-1} - I)\right\}.$$

The result is shown in Figure 9.3.

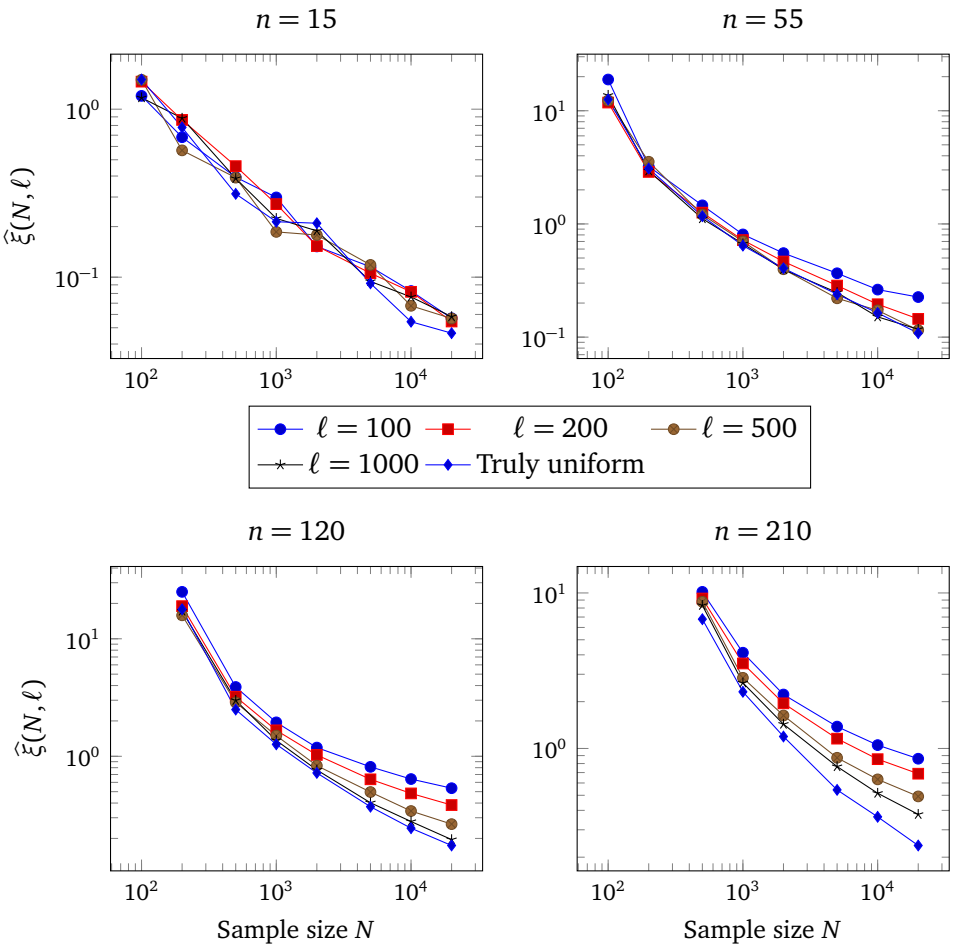

Figure 9.3: Effect of sample size N and walk length ℓ on covariance approximation quality over $[0,1]^n$

Figure 9.3 shows a pattern similar to that of Figure 9.1: as the problem size increases, the walk length should increase with the sample size to ensure the

estimate is as good as the sample size can guarantee. More importantly though, hit-and-run sampling does not perform significantly worse than true sampling. The problem is that approximating a covariance matrix to high accuracy – which we need for our interior point method – appears to be fundamentally hard.

Besides approximating covariance matrices, the interior point method from Chapter 6 also approximates means of certain distributions. One would expect this to be an easier problem: for instance, the number of samples required in Theorem 5.9 is linear in n, whereas that in Theorem 5.11 is quadratic in n. With the same samples that were used to create Figure 9.1, we create a mean estimate $\widehat{x}_0$ based on 20,000 hit-and-run samples with walk length 50,000. Then, for $N \leq$ 20,000 samples with walk length $\ell \leq 50{,}000$, we create the mean estimate $\widehat{x}_{N,\ell}$. Using the approximation $\widehat{\Sigma}_0$ of the uniform covariance matrix from the previous section, we compute $\|\widehat{x}_0 - \widehat{x}_{N,\ell}\|_{\widehat{\Sigma}_0^{-1}}$ and plot the results in Figure 9.4.

The results are comparable to those in Figures 9.1 and 9.2. It will take an impractical amount of time before the mean estimate approximates the true mean to high accuracy.

The conclusions above raise some questions about the practical viability of a sampling-based interior point method. The sampling would have to be parallelized massively to a get accurate approximations of the entropic barrier's derivatives in reasonable time. This is unlikely to be an attractive strategy. We therefore shift our focus to the other algorithms we discussed: the heuristic adaptation of Kalai and Vempala's algorithm (Algorithm 7.2), and the analytic center cutting plane method (Algorithm 8.4).

9.2 Separating from the 6×6 Completely Positive Cone

We will test our most promising algorithms, Algorithms 7.2 and 8.4, on instances of problem (8.4). After all, Algorithm 8.4 was developed with this problem in mind. To provide a benchmark, we will also solve the instances of problem (8.4) with the ellipsoid method from Yudin and Nemirovski [114].

We will use 6×6 doubly nonnegative matrices as test instances for (8.4). The reason for this choice of size is as follows. It has been known for decades that the doubly nonnegative cone coincides with $\mathcal{CP}^d$ for $d \leq 4$, as shown by Maxfield

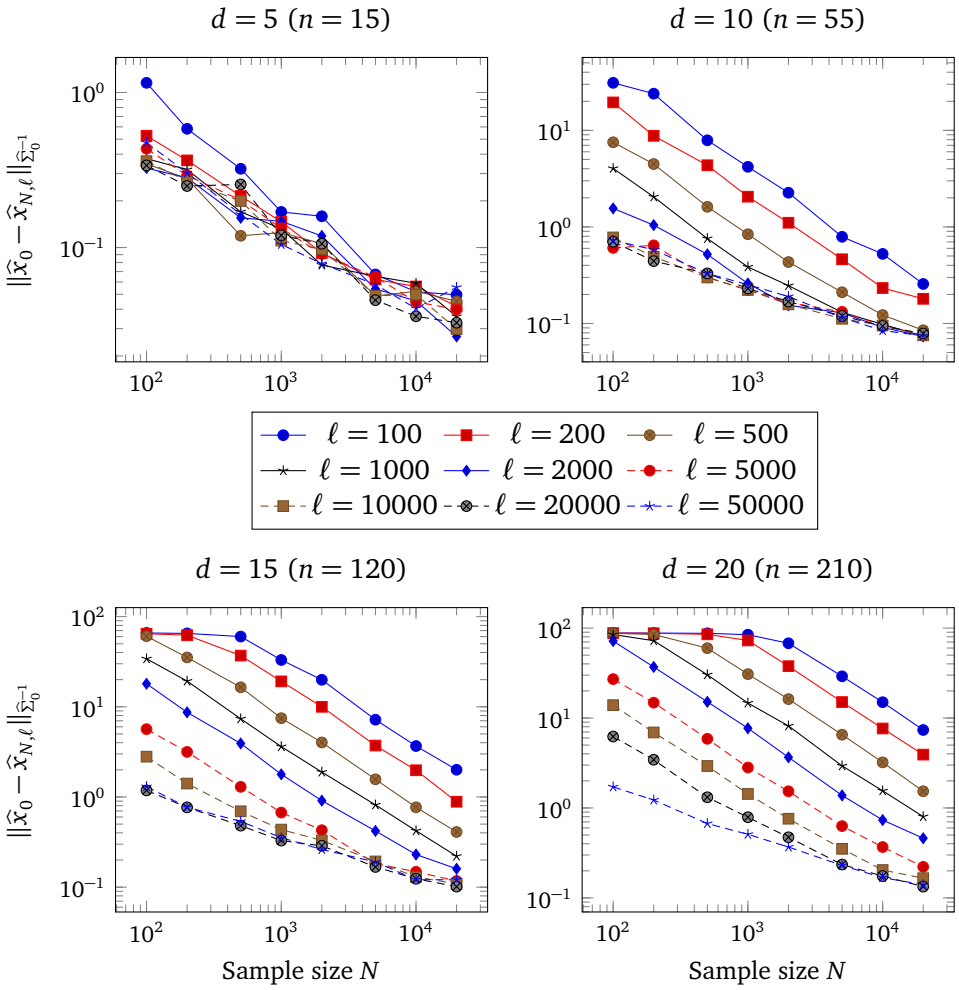

Figure 9.4: Effect of sample size N and walk length ℓ on mean approximation quality over (9.1)

and Minc [77]. Burer and Dong [26] proposed a method to separate matrices from $\mathcal{CP}^5$ which solves five optimization problems over the tractable $\mathcal{CO}^4$. This makes $d = 6$ the smallest size for which no algorithm is currently known that can separate from the completely positive cone in reasonable time.

We are interested in matrices on the boundary of the 6×6 doubly nonneg-

ative cone. (Randomly generating matrices in the interior of the 6×6 doubly nonnegative cone very often yields completely positive matrices, making separation irrelevant.) The extreme rays of this cone are described by Ycart [111, Proposition 6.1]. We generate random instances from the class of matrices described under case 3, graph 4 in Proposition 6.1 in [111]. These matrices are (up to permutation of the indices) doubly nonnegative matrices $C = [C_{ij}]$ with rank 3 satisfying $C_{i,i+1} = 0$ for $i \in \{1, ..., 5\}$. To generate such a matrix, we draw the elements of two vectors $v_1, v_2 \in \mathbb{R}^6$ and the first element $(v_3)_1 \in \mathbb{R}$ of a vector $v_3 \in \mathbb{R}^6$ from a Poisson distribution with rate 1, and multiply each of these elements by -1 with probability $\frac{1}{2}$. The remaining elements of v_3 are then chosen such that $C = \sum_{k=1}^{3} v_k v_k^\top$ satisfies $C_{i,i+1} = 0$ for $i \in \{1, ..., 5\}$. This procedure is repeated if the matrix C is not doubly nonnegative, or if BARON 15 [105] could find a nonnegative matrix $B \in \mathbb{R}^{6\times 9}$ such that $C = BB^\top$ in less than 30 seconds (for the cases where such a decomposition could be found, BARON terminated in less than a second). Thus, we are left with doubly nonnegative matrices for which it cannot quickly be shown that they are completely positive.

Ten of such random matrices are given in Appendix B in Badenbroek and De Klerk [9]. After scaling these matrices C such that $\|\operatorname{mat}^\top(C)\| = 1$, we run Algorithm 7.2 on these instances of problem (8.4). We let $X = \frac{1}{2}I/d \in \mathbb{S}^d$ and take $x_0 = \operatorname{vec}(X)$ as the starting point for this algorithm. The number of samples N and hit-and-run steps ℓ is given by (7.13), and the number of iterations is

$$m = \left\lceil \frac{\log\left(10^{-4}/n\right)}{\log\left(1 - 1/\sqrt{n}\right)} \right\rceil,$$

similar to (7.14). Note that for this m, the expected absolute gap in the final iteration is at most 10^{-4}. Not only does this gap coincide with that in Section 7.4, it is also large enough to guarantee that Algorithm 7.2 terminates within reasonable time.

We also ran Algorithm 8.5 (which calls Algorithm 8.4) on these matrices. However, the termination criterion in Algorithm 8.4 is phrased in terms of the relative gap, not the absolute gap. To allow for a fair comparison, we replace Line 5 in Algorithm 8.4 by the condition that the best feasible solution so far x_* satisfies

$$c^\top x_* - \min_{x \in \mathcal{Q}_k} c^\top x > 10^{-4}.$$

Finally, we also applied the ellipsoid method of Yudin and Nemirovski [114] to (8.4). The termination criterion for the ellipsoid method is similar to that for Algorithm 8.4, i.e. the absolute gap can be at most 10^{-4}. The only difference is that in the case of the ellipsoid method, the lower bound is computed through minimization over the current ellipsoid, not over some outer approximation $\mathcal{Q}$. We record the objective values of the solutions returned by these three algorithms in Table 9.1.

Instance	Algorithm 7.2	Ellipsoid method	Algorithm 8.5
`extremal_rand_1`	−0.00810	−0.00813	−0.00809
`extremal_rand_2`	−0.02112	−0.02116	−0.02111
`extremal_rand_3`	−0.03954	−0.03957	−0.03953
`extremal_rand_4`	−0.01027	−0.01031	−0.01027
`extremal_rand_5`	−0.00656	−0.00659	−0.00656
`extremal_rand_6`	−0.04473	−0.04476	−0.04472
`extremal_rand_7`	−0.02512	−0.02516	−0.02512
`extremal_rand_8`	−0.07365	−0.07368	−0.07364
`extremal_rand_9`	−0.04800	−0.04803	−0.04800
`extremal_rand_10`	−0.03030	−0.03033	−0.03029

Table 9.1: Objective value of solutions returned by Algorithm 7.2, the ellipsoid method, and Algorithm 8.5, applied to the normalized matrices from [9, Appendix B]. The termination criterion is an (expected) absolute gap of 10^{-4}.

It can be seen that all methods return a solution with approximately the same objective value. In particular, the randomized Algorithm 7.2 consistently returns a near-optimal solution. However, the number of calls to TESTCOPOSITIVE differs significantly between the algorithms, as can be seen in Table 9.2.

The reason to report this number of calls is that the oracle performs the theoretically intractable part of these methods: testing if a matrix is copositive. All other parts of the three methods complete in polynomial time for each oracle call. Hence, to get the best performance for larger matrices, one would like to minimize the number of oracle calls. It is clear from Table 9.2 that Algorithm 7.2 is significantly slower than the ellipsoid method, which in turn is outperformed by

Instance	Algorithm 7.2	Ellipsoid method	Algorithm 8.5
extremal_rand_1	6,684,932	2544	77
extremal_rand_2	6,739,177	2857	83
extremal_rand_3	6,811,093	3263	85
extremal_rand_4	6,627,005	2503	74
extremal_rand_5	6,599,481	2430	73
extremal_rand_6	6,809,453	3306	86
extremal_rand_7	6,726,332	2995	85
extremal_rand_8	6,897,368	3642	93
extremal_rand_9	6,847,610	3434	91
extremal_rand_10	6,714,194	2959	79

Table 9.2: Calls to the oracle TESTCOPOSITIVE by Algorithm 7.2, the ellipsoid method, and Algorithm 8.5, applied to the normalized matrices from [9, Appendix B]. The termination criterion is an (expected) absolute gap of 10^{-4}.

Algorithm 8.5. We conclude that Algorithm 7.2 is not going to be a competitive approach to solving convex programming problems.

Let us finish this section by arguing that Algorithm 8.5 can also solve problem (8.4) to somewhat higher accuracy. We now run Algorithm 8.5 on the matrices from Appendix B in Badenbroek and De Klerk [9] (without scaling them) until the original termination criterion in Algorithm 8.4 is met: the relative gap should be at most 10^{-6}. For the sake of comparison, we also run the ellipsoid method until the relative gap is at most 10^{-6}, where the lower bound is again computed through minimization over the current ellipsoid. The number of oracle calls these methods required is given in Table 9.3. Note that Algorithm 8.5 still requires significantly fewer oracle calls than the ellipsoid method.

9.3 Separating from the $d \times d$ Completely Positive Cone

To investigate how Algorithm 8.5 scales, we also generated test instances in higher dimensions. To the best of our knowledge, a complete characterization of the extremal rays of the $d \times d$ doubly nonnegative cone is unknown for $d > 6$. (See

Instance	Ellipsoid method	Algorithm 8.5
extremal_rand_1	8560	171
extremal_rand_2	8030	167
extremal_rand_3	8598	166
extremal_rand_4	7910	164
extremal_rand_5	8546	193
extremal_rand_6	8184	167
extremal_rand_7	9119	191
extremal_rand_8	8126	169
extremal_rand_9	8318	176
extremal_rand_10	7950	161

Table 9.3: Calls to the oracle TESTCOPOSITIVE by the Ellipsoid method and Algorithm 8.5, applied to the matrices from [9, Appendix B]. The termination criterion is a relative gap of 10^{-6}.

the corollary to Theorem 3.1, and Propositions 5.1 and 6.1 in Ycart [111] for the extremal matrices for $d \leq 6$.) Hence, we use a semidefinite programming heuristic to find doubly nonnegative matrices in these dimensions which are not completely positive.

The matrices used in Section 9.2 are 6×6 doubly nonnegative matrices C with rank 3 and the entries $C_{i,i+1} = 0$ for all $i \in \{1, ..., 5\}$. This pattern of zeros can of course be extended to higher dimensions, but the low rank criterion is not tractable in semidefinite programming. The standard trick to find a low-rank solution – which we also adopt – is to minimize the trace of the matrix variable, see for instance Fazel et al. [41] and the references therein. To create a $d \times d$ test instance, we thus run the procedure in Algorithm 9.1.

The objective in Line 3 of Algorithm 9.1 includes two terms: the term $\operatorname{tr} C$ to get a low-rank solution, and the term $\frac{1}{2}d\|C-R\|$ to get a solution close to our random matrix R. Without this last term, the optimal solution of the problem would be the zero matrix. The weight $\frac{1}{2}d$ was chosen because numerical experiments suggested this weight leads to solutions with low rank, but not rank zero, for the dimensions in our test set. The solution C_* computed in Line 3 by interior point

Algorithm 9.1 A heuristic procedure to generate random matrices on the boundary of the doubly nonnegative cone

Input: Dimension d of a random matrix $C \in \mathbb{S}^d$ to generate.

1: $R_0 \in \mathbb{R}^{d\times d}$ is a matrix whose elements are samples from a standard normal distribution

2: $R \leftarrow |R_0| + |R_0|^\top$, where $|R_0| = [|(R_0)_{ij}|]$ is the element-wise absolute value

3: Let C_* be an (approximately) optimal solution to

$$\begin{aligned} \inf_C \operatorname{tr} C + \tfrac{1}{2} d\|C - R\| & \\ \text{subject to } C_{i,i+1} = 0 & \qquad \forall i \in \{1,\ldots,d-1\} \\ C \succeq 0, C \geq 0. & \end{aligned}$$

4: **for** $j \in \{1,\ldots,10\}$ **do**

5: Set all eigenvalues of C_* smaller than 10^{-6} to zero

6: Set all elements of C_* smaller than 10^{-4} to zero

7: **return** $C_*/\|C_*\|$

methods still lies in the interior of the doubly nonnegative cone. To project this solution to the boundary of the doubly nonnegative cone, we run Lines 4 to 6. One could think of these lines as an alternating projection method to find a point close to the intersection of the boundaries of the positive semidefinite cone and the cone of nonnegative matrices.

For each $d \in \{6,7,8,9,10,15,20,25\}$, we generated ten test instances with Algorithm 9.1. Such an instance C is only included in the final test set if Algorithm 8.5 returns an X such that $\langle C, X\rangle < -0.01$, which was almost always the case. In those few cases where $\langle C, X\rangle \geq -0.01$, a new instance was generated. Hence, we end up with ten $d \times d$ doubly nonnegative matrices that are not completely positive, for each $d \in \{6,7,8,9,10,15,20,25\}$. These instances are also available online at `https://github.com/rileybadenbroek/CopositiveAnalyticCenter.jl/tree/master/test`.

Algorithm 8.5 is applied to each of these instances, and the total number of calls to TESTCOPOSITIVE is reported in Figure 9.5 alongside the total running time (as before, we used a computer an Intel i7-6700 CPU and 16 GB RAM). We do

not report these results as in Table 9.3 since there are 80 instances, and running the ellipsoid method for all of them would take too much time. We moreover sketch two functions, $d \mapsto 7d^{5/3}$ and $d \mapsto 0.0002d^5$, that roughly approximate the number of oracle calls and execution time, respectively. (The values 7, $\frac{5}{3}$, 0.0002, and 5 of the coefficients and exponents are found by rounding the results of a regression, and have no particular meaning.) The execution time grows rapidly with d, but this is not unexpected: every oracle call solves at least one mixed integer linear program whose size depends on d, which is theoretically intractable.

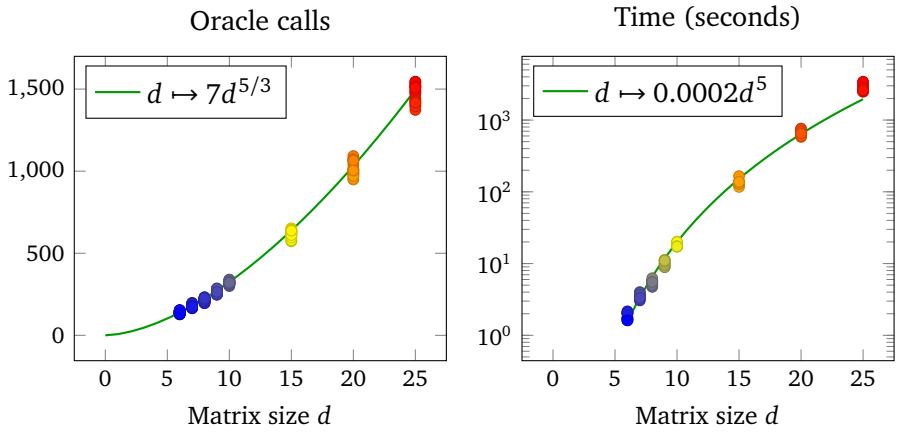

Figure 9.5: Number of oracle calls and execution times of Algorithm 8.5 for the $d \times d$ test instances generated with Algorithm 9.1

In conclusion, we have seen in Chapters 6 and 7 that a sampling based interior point method and a simulated annealing algorithm work in theory. In practice though, they do not even seem like viable alternatives to the ellipsoid method. The analytic center cutting plane method from Chapter 8 outperforms all of these approaches, and also scales very reasonably. In particular, the number of oracle calls to test matrix copositivity grows roughly like $O(d^2)$ for $d \times d$ matrices. We have therefore made some computational progress on an open problem formulated by Berman et al. [13]. It is worthwhile to recall that this algorithm can be applied to any copositive optimization problem, as long as an upper bound on the norm of the optimal solution is known. The implementation of the analytic center cutting plane method from Chapter 8 is available at `https:`

//github.com/rileybadenbroek/CopositiveAnalyticCenter.jl.

10

An Algorithm for Nonsymmetric Conic Optimization

The copositive cone is an example of a nonsymmetric cone. The main reason it was hard to optimize over the copositive cone is not the lack of symmetry – instead, the problem is that no self-concordant barrier with easily computable derivatives is known for this cone. Fortunately, certain other nonsymmetric cones do admit such a barrier.

A broader class of cones than the symmetric cones can be found by dropping the self-duality requirement: the resulting convex cones with a transitive automorphism group are called homogeneous (see Vinberg [108] for an example of a homogeneous cone that is not self-dual). Although Chua [27] showed that each optimization problem over a homogeneous cone can be rewritten as a semidefinite optimization problem, Chua [28] also proposed algorithms to exploit this structure directly. A larger class of cones is formed by the hyperbolicity cones, which Güler [48] showed contains the homogeneous cones. Moreover, Güler also proposed methods to solve optimization problems over these cones.

In this chapter, we consider an even broader class: proper cones that admit a logarithmically homogeneous self-concordant barrier (LHSCB). Interesting examples of such cones include the exponential cone

$$\left\{x \in \mathbb{R}^3 : x_1 \geq x_2 e^{x_3/x_2}, x_2 > 0\right\} \cup \left\{x \in \mathbb{R}^3 : x_1 \geq 0, x_2 = 0, x_3 \leq 0\right\}$$

and, for any $t \in (0,1)$, the three-dimensional power cone

$$\left\{x \in \mathbb{R}^3 : x_1^t x_2^{1-t} \geq |x_3|\right\}.$$

Many convex optimization problems occurring in practice can be modeled using these two cones and the (symmetric) second-order and semidefinite cones. For example, Lubin et al. [75] show that all convex problems from the MINLPLIB2 library can be expressed in this manner.

Dahl and Andersen [30] describe a method which is implemented in MOSEK 9 [78] that works very well on practical problems of this form. In this chapter, we aim to provide some theoretical foundation for their algorithm. Practical implementations will always differ from theoretical algorithms, so we focus on particular elements of Dahl and Andersen's algorithm: their scaling matrix, search direction, and neighborhood. With these ingredients, we will define an algorithm for nonsymmetric conic optimization that approximately solves the so-called homogeneous model in polynomial time.

This chapter is based on Badenbroek and Dahl [7], but here we define the dual problem in terms of the polar cone instead of the dual cone. (The conjugate of a cone's logarithmically homogeneous barrier, as defined in Chapter 2, has the polar cone as its domain.) This change only leads to a number of sign changes, and does not fundamentally change the results. We also derive Lemma 10.7 in a slightly more elegant manner than [7, Lemma 8], though this does not change the algorithm's complexity.

10.1 The Homogeneous Model and its Central Path

We will consider the problem

$$\inf_x \{\langle c, x\rangle : Ax = b, x \in \mathcal{K}\}, \tag{10.1}$$

and its dual

$$\sup_{y,s} \left\{ \langle b, y \rangle : s = A^\top y - c, s \in \mathcal{K}^\circ \right\}, \tag{10.2}$$

where $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{M \times n}$, $b \in \mathbb{R}^M$, $\mathcal{K} \subset \mathbb{R}^n$ is a proper cone, and

$$\mathcal{K}^\circ := \{ s \in \mathbb{R}^n : \langle x, s \rangle \leq 0 \, \forall x \in \mathcal{K} \}$$

is its polar cone. We assume that we have a LHSCB f for $\mathcal{K}$ with complexity parameter ϑ_f. As shown by Theorem 2.15, f^* is then a LHSCB for $\mathcal{K}^\circ$ with complexity parameter $\vartheta_{f^*} = \vartheta_f$. We remind the reader that we use g and H to denote the gradient and Hessian of f, and g^* and H^* to denote the gradient and Hessian of f^*, respectively.

The approaches we have seen until now are primal-only methods. However, researchers found that for linear optimization, primal-dual interior point methods generally outperformed their primal-only or dual-only counterparts. Naturally, they tried to extend these primal-dual methods to convex conic optimization. A major breakthrough in this area is due to Nesterov and Todd [87, 88], who introduced search directions for symmetric cones that perform well in practice. However, the Nesterov-Todd directions are defined at a primal-dual feasible point. Hence, given an optimization problem, one still needs to find such a feasible point, if it even exists. To circumvent this issue, Ye et al. [112] introduced a homogeneous model (also known as a self-dual embedding) for linear programming. Two major advantages of this homogeneous model are that no strictly feasible starting point is required, and that the algorithm can generate certificates for primal or dual infeasibility. Generalizations of this homogeneous model were proposed by e.g. Luo et al. [76], De Klerk et al. [34], Potra and Sheng [94], and Andersen and Ye [3].

To solve (10.1) and (10.2) with a homogeneous model, we define the linear operator

$$G(y, x, \tau, s, \kappa) := \begin{bmatrix} 0 & A & -b \\ -A^\top & 0 & c \\ b^\top & -c^\top & 0 \end{bmatrix} \begin{bmatrix} y \\ x \\ \tau \end{bmatrix} + \begin{bmatrix} 0 \\ s \\ \kappa \end{bmatrix}.$$

Then, the solutions to the *homogeneous self-dual model* are

$$\left\{ (y, x, \tau, s, \kappa) \in \mathbb{R}^M \times \mathcal{K} \times \mathbb{R}_+ \times \mathcal{K}^\circ \times \mathbb{R}_- : G(y, x, \tau, s, \kappa) = 0 \right\}, \tag{10.3}$$

and they have the following properties (see e.g. Skajaa and Ye [101, Lemma 1]):

1. $\langle x, s\rangle + \tau\kappa = 0$;
2. If $\tau > 0$, then x/τ is an optimal solution to (10.1) and $(y, s)/\tau$ is an optimal solution to (10.2);
3. If $\kappa < 0$, then either $\langle b, y\rangle > 0$ or $\langle c, x\rangle < 0$, or both. If $\langle b, y\rangle > 0$, (10.1) is infeasible. If $\langle c, x\rangle < 0$, (10.2) is infeasible.

In other words, finding an element of the set (10.3) where $\tau > 0$ or $\kappa < 0$ suffices to solve the primal-dual pair (10.1) and (10.2). We will therefore interpret $G(y, x, \tau, s, \kappa)$ as the residual associated with the solution (y, x, τ, s, κ), which we would like to be the zero vector.

Assume we have initial points $x_0 \in \operatorname{int} \mathcal{K}$ and $s_0 \in \operatorname{int} \mathcal{K}^\circ$, such that $x_0 = g^*(s_0)$, and hence $s_0 = g(x_0)$ by Theorem 2.12. Dahl and Andersen [30] choose x_0 and s_0, along with y_0, τ_0, and κ_0 satisfying

$$x_0 = s_0 = g(x_0) = g^*(s_0), \quad y_0 = 0, \quad \tau_0 = 1, \quad \kappa_0 = -1, \tag{10.4}$$

which admits a solution for the five cones that MOSEK 9 supports. Note that (2.22) implies that for logarithmically homogeneous f and $x \in \operatorname{dom} f$,

$$H(x)x = -g(x) \quad \text{and} \quad \langle x, g(x)\rangle = -\vartheta_f. \tag{10.5}$$

One of the perks of the choice (10.4) is therefore that $-\langle x_0, s_0\rangle = \langle -x_0, g(x_0)\rangle = \vartheta_f$, meaning that the initial complementarity is known. We define the central path for the homogeneous model as the $(y, x, \tau, s, \kappa) \in \mathbb{R}^M \times \mathcal{K} \times \mathbb{R}_+ \times \mathcal{K}^\circ \times \mathbb{R}_-$ for which there exists a $t \in (0, 1]$ such that

$$\begin{cases} G(y, x, \tau, s, \kappa) = tG(y_0, x_0, \tau_0, s_0, \kappa_0) \\ x = tg^*(s) \\ s = tg(x) \\ \kappa\tau = -t. \end{cases} \tag{10.6}$$

Informally, the condition $G(y, x, \tau, s, \kappa) = tG(y_0, x_0, \tau_0, s_0, \kappa_0)$ encodes that the residual norm should decrease as t decreases, and the other conditions assure the "centrality" of the solution.

Before we discuss how to measure proximity to this central path, we introduce some notation. To emphasize that $g(x) \in \mathcal{K}^\circ$ for all $x \in \operatorname{int}\mathcal{K}$ and $g^*(s) \in \mathcal{K}$ for all $s \in \operatorname{int}\mathcal{K}^\circ$, we define the *shadow iterates*

$$\tilde{s} := g(x) \quad \text{and} \quad \tilde{x} := g^*(s),$$

when $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$. We can then define the (shadow) complementarity gap as

$$\mu := -\frac{\langle x, s\rangle}{\vartheta_f} \geq 0 \quad \text{and} \quad \tilde{\mu} := -\frac{\langle \tilde{x}, \tilde{s}\rangle}{\vartheta_f} \geq 0. \tag{10.7}$$

As noted by Tunçel [106, Lemma 4.1], Nesterov and Todd [88, Remark 1] showed that for any $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$, we have

$$\mu\tilde{\mu} \geq 1, \tag{10.8}$$

with equality if and only if $x = \mu\tilde{x}$ (and hence $s = \mu\tilde{s}$).

Since any element of (10.3) satisfies $(x, \tau) \in \mathcal{K} \times \mathbb{R}_+$ and $(s, \kappa) \in \mathcal{K}^\circ \times \mathbb{R}_-$, it will prove useful to extend our barriers f and f^* to the domains $\mathcal{K} \times \mathbb{R}_+$ and $\mathcal{K}^\circ \times \mathbb{R}_-$, respectively. A straightforward way to do this is to define

$$f'(x, \tau) := f(x) - \log(\tau),$$

a $(\vartheta_f + 1)$-LHSCB for $\mathcal{K} \times \mathbb{R}_+$. With the inner product $\langle (x, \tau), (s, \kappa)\rangle = \langle x, s\rangle + \tau\kappa$, the conjugate of f' is

$$(f')^*(s, \kappa) = f^*(s) - \log(-\kappa) - 1,$$

which is a $(\vartheta_f + 1)$-LHSCB for $\mathcal{K}^\circ \times \mathbb{R}_-$. For these cones and barriers, the quantities analogous to (10.7) are

$$\mu' := -\frac{\langle x, s\rangle + \tau\kappa}{\vartheta_f + 1} \geq 0 \quad \text{and} \quad \tilde{\mu}' := -\frac{\langle \tilde{x}, \tilde{s}\rangle + 1/(\tau\kappa)}{\vartheta_f + 1} \geq 0.$$

Because $\mathcal{K} \times \mathbb{R}_+$ and $\mathcal{K}^\circ \times \mathbb{R}_-$ are each other's polar cones, the inequality (10.8) carries over to this setting. To be explicit, we must have $\mu'\tilde{\mu}' \geq 1$, with equality if and only if (x, τ) equals

$$\mu' D(f')^*(s, \kappa) = \begin{bmatrix} \mu' g^*(s) \\ -\mu'/\kappa \end{bmatrix} = \begin{bmatrix} \mu'\tilde{x} \\ -\mu'/\kappa \end{bmatrix},$$

in which case we also have $s = \mu'\tilde{s}$. Thus, if $\mu'\tilde{\mu}' = 1$, the centrality conditions in (10.6) are satisfied for $t = \mu'$. Since in general $\mu'\tilde{\mu}' \geq 1$, we could define a neighborhood of the central path as the points satisfying $\alpha\mu'\tilde{\mu}' \leq 1$ for some $\alpha \in (0,1]$. For the sake of simplicity, Dahl and Andersen [30, Section 3] instead assume

$$\frac{\alpha}{\tau\kappa}\frac{\langle x,s\rangle + \tau\kappa}{\vartheta_f + 1} \leq 1 \quad \text{and} \quad \alpha\langle \tilde{x},\tilde{s}\rangle \frac{\langle x,s\rangle + \tau\kappa}{\vartheta_f + 1} \leq \vartheta_f, \tag{10.9}$$

which implies $\alpha\mu'\tilde{\mu}' \leq 1$ for any $\alpha \in (0,1]$. Some other useful properties of the assumptions (10.9) are given in the next lemma.

Lemma 10.1. *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Let $x \in \operatorname{int}\mathcal{K}$, $s \in \operatorname{int}\mathcal{K}^\circ$, $\tau > 0$, and $\kappa < 0$. Assume $\tau\kappa \leq -\alpha\mu'$ and $\alpha\mu'\tilde{\mu} \leq 1$ for some $\alpha \in (0,1]$. Then,*

$$\frac{\mu}{2-\alpha} \leq \mu' \leq \frac{\mu}{\alpha}.$$

Proof. Since $-\tau\kappa \geq \alpha\mu'$, it holds that

$$\mu' = \frac{\mu\vartheta_f}{\vartheta_f + 1} - \frac{\tau\kappa}{\vartheta_f + 1} \geq \frac{\mu\vartheta_f}{\vartheta_f + 1} + \frac{\alpha\mu'}{\vartheta_f + 1},$$

which shows

$$\mu' \geq \left(1 - \frac{\alpha}{\vartheta_f + 1}\right)^{-1} \frac{\mu\vartheta_f}{\vartheta_f + 1} = \frac{\mu\vartheta_f}{\vartheta_f + 1 - \alpha} \geq \frac{\mu}{2-\alpha},$$

where the last inequality uses $\vartheta_f \geq 1$. To prove the second part of the claim, we use the assumption that $\alpha\tilde{\mu}\mu' \leq 1$. By (10.8), we have $\tilde{\mu} \geq 1/\mu$, and thus

$$1 \geq \alpha\tilde{\mu}\mu' \geq \frac{\alpha\mu'}{\mu}.$$

□

Thus, for high values of α, we have $\mu \approx \mu'$ under the assumptions (10.9), and therefore $x \approx \mu\tilde{x}$ and $s \approx \mu\tilde{s}$. We will often refer to the distance between x and $\mu\tilde{x}$, and between s and $\mu\tilde{s}$, so we introduce the following shorthand notation:

$$\zeta^{\mathrm{P}} := x - \mu\tilde{x} \quad \text{and} \quad \zeta^{\mathrm{D}} := s - \mu\tilde{s}.$$

10.2 Algorithm Statement

Nesterov et al. [86] provide a complexity analysis of a class of algorithms to solve the homogeneous model for convex conic optimization, where the cones do not have to be symmetric. However, in the nonsymmetric case the size of the linear systems to be solved doubles compared to the symmetric case, increasing the computation time by a factor of eight.

A more recent approach by Nesterov [84] splits each iteration in two phases. In the correction phase, a strictly feasible primal-dual pair and an associated scaling point are computed. These are used in the prediction phase to find a primal-dual direction that is approximately tangential to the central path. This algorithm has the drawback that it assumes the existence of a strictly feasible primal-dual point, and requires a strictly feasible primal starting point.

Skajaa and Ye [101] built on these two methods by proposing an algorithm that solves the homogeneous model and only uses the primal barrier, which means the size of the linear systems is the same as in the symmetric case. While theoretically attractive, this algorithm still requires centering steps. Serrano [99] proposed a variant of Skajaa and Ye's algorithm that no longer uses centering steps, and implements this for the exponential cone in the ECOS solver.

For two points x and s in a symmetric cone, we can always find a scaling point w such that the Hessian of the cone's barrier at w maps x to $-s$ and the gradient at $-s$ to the gradient at x. Moreover, the Hessian at w is bounded by the Hessians at x and $-s$ when x and $-s$ lie close to the central path. For a general convex cone, we can define a similar scaling which maps x to $-s$, but generally not the gradient at $-s$ to the gradient at x. Thus, the main hurdle in generalizing the Nesterov-Todd directions to nonsymmetric cones is to find a mapping from x to $-s$ and the gradient at $-s$ to the gradient at x, and to ensure that this mapping is in some sense close to the primal and dual Hessians to guarantee polynomial-time convergence. Tunçel [106] proposed to form a such scaling matrix by low-rank updates to an arbitrary positive definite matrix. Myklebust and Tunçel [82] provide explicit bounds on the scaling matrix if the current iterates x and s lie close to the central path.

Dahl and Andersen [30] expand on the ideas from Skajaa and Ye [101], but define their search direction using the scaling matrices analyzed by Tunçel [106] and

Myklebust and Tunçel [82]. The resulting algorithm is implemented in MOSEK 9 for the exponential and three-dimensional power cones.

We now proceed to the statement of the algorithm that will be analyzed in the remainder of this chapter. At the start of every iteration, we assume the following holds for some fixed $\alpha \in (0,1]$ and $\delta \in [0,1)$.

(A1) $x \in \operatorname{int} \mathcal{K}$ and $s \in \operatorname{int} \mathcal{K}^\circ$

(A2) $\tau\kappa \leq -\alpha\mu'$

(A3) $\tau > 0$ and $\kappa < 0$

(A4) $\alpha\mu'\tilde{\mu} \leq 1$

(A5) $\|\zeta^{\mathrm{P}}\|_x \leq \delta$.

Note that (A1) to (A4) are also imposed by MOSEK [30, Section 3]. Assumption (A5) is important to "sandwich" the primal-dual scaling matrix used by MOSEK.

Every iteration consists of two phases. In the first phase, we apply a simplified version of the search direction used in Dahl and Andersen [30]. The second phase consists of taking one corrector step to return to the assumptions (A1) to (A5). For the sake of brevity, let us collect all variables in a vector $z := (y, x, \tau, s, \kappa)$.

The first phase is started by computing a scaling matrix

$$W := \mu H(x) + \frac{ss^\top}{\vartheta_f \mu} - \frac{\mu \tilde{s}\tilde{s}^\top}{\vartheta_f} - \frac{\zeta^{\mathrm{D}}(\zeta^{\mathrm{D}})^\top}{\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}} \rangle} - \frac{\mu[H(x)\tilde{x} + \tilde{\mu}\tilde{s}][H(x)\tilde{x} + \tilde{\mu}\tilde{s}]^\top}{\|\tilde{x}\|_x^2 - \vartheta_f \tilde{\mu}^2}. \quad (10.10)$$

We refer to W as a scaling matrix because it is serves a similar purpose as the scaling point does for symmetric cones. Most importantly, we have

$$Wx = -s \quad \text{and} \quad W\tilde{x} = -\tilde{s}.$$

Dahl and Andersen [30, Section 5] derive a Cholesky factorization of W, thereby showing W is positive definite.

The scaling matrix W is used in the definition of the search direction in this first phase. The search direction consists of two parts: an affine direction Δz^{aff}

and a centering direction Δz^{cen}. The affine direction is the solution Δz^{aff} to

$$G(\Delta z^{\text{aff}}) = -G(z) \tag{10.11a}$$

$$\tau\Delta\kappa^{\text{aff}} + \kappa\Delta\tau^{\text{aff}} = -\tau\kappa \tag{10.11b}$$

$$W\Delta x^{\text{aff}} - \Delta s^{\text{aff}} = s. \tag{10.11c}$$

It follows from (10.11a) that moving in the direction Δz^{aff} decreases the norm of the residual, which amounts to progress in solving the self-dual homogeneous model. The centering direction Δz^{cen} is the solution to

$$G(\Delta z^{\text{cen}}) = G(z) \tag{10.12a}$$

$$\tau\Delta\kappa^{\text{cen}} + \kappa\Delta\tau^{\text{cen}} = -\mu' \tag{10.12b}$$

$$W\Delta x^{\text{cen}} - \Delta s^{\text{cen}} = -\mu'\tilde{s}. \tag{10.12c}$$

We see from (10.12a) that moving in direction Δz^{cen} increases the norm of the residual, but it serves to keep us close to the central path. We will combine these two directions to get the search direction in the first phase: for some $\varrho \in [0,1]$ to be fixed later, let

$$\Delta z^{\text{pred}} := \Delta z^{\text{aff}} + \varrho\Delta z^{\text{cen}}. \tag{10.13}$$

Then, for some $\gamma \in (0,1]$ also to be fixed later, we update z to the new iterate

$$z_+ := z + \gamma\Delta z^{\text{pred}} = z + \gamma(\Delta z^{\text{aff}} + \varrho\Delta z^{\text{cen}}). \tag{10.14}$$

After this predictor phase, we will need a corrector to ensure (A4) and (A5) hold. To define it, we will compute a scaling matrix similar to (10.10) defined as

$$\begin{aligned} W_+ := \mu_+ H(x_+) + \frac{s_+ s_+^\top}{\vartheta_f \mu_+} - \frac{\mu_+\tilde{s}_+\tilde{s}_+^\top}{\vartheta_f} - \frac{\zeta_+^{\text{D}}(\zeta_+^{\text{D}})^\top}{\langle \zeta_+^{\text{P}}, \zeta_+^{\text{D}}\rangle} \\ - \frac{\mu_+[H(x_+)\tilde{x}_+ + \tilde{\mu}_+\tilde{s}_+][H(x_+)\tilde{x}_+ + \tilde{\mu}_+\tilde{s}_+]^\top}{\|\tilde{x}_+\|_{x_+}^2 - \vartheta_f\tilde{\mu}_+^2}, \end{aligned} \tag{10.15}$$

where all quantities with a subscript "+" follow their original definition, but computed for the iterate z_+ instead of z. The corrector Δz_+^{cor} is the solution to

$$G(\Delta z_+^{\text{cor}}) = 0 \tag{10.16a}$$

$$\tau_+\Delta\kappa_+^{\text{cor}} + \kappa_+\Delta\tau_+^{\text{cor}} = 0 \tag{10.16b}$$

$$W_+\Delta x_+^{\text{cor}} - \Delta s_+^{\text{cor}} = s_+ - \mu_+\tilde{s}_+. \tag{10.16c}$$

It can be seen from (10.16a) that Δz_+^{cor} does not change the residuals, so the progress made by the predictor is maintained. (Skajaa and Ye [101] also use a corrector that satisfies (10.16a), but they take, in our notation, $\tau_+^2\Delta\kappa_+^{\text{cor}}+\mu'_+\Delta\tau_+^{\text{cor}} = -\kappa_+\tau_+^2 - \mu'_+\tau_+$ and $\mu'_+H(x_+)\Delta x_+^{\text{cor}} - \Delta s_+^{\text{cor}} = s_+ - \mu'_+\tilde{s}_+$ instead of (10.16b) and (10.16c).) We take one full corrector step to arrive at

$$z_{++} := z_+ + \Delta z_+^{\text{cor}}.$$

This z_{++} will be the starting point for the next iteration.

The algorithm in this section is summarized in Algorithm 10.1.

Algorithm 10.1 Algorithm for nonsymmetric conic optimization (based on Dahl and Andersen [30])

Input: predictor step size $\gamma \in (0,1]$;
centering parameter $\varrho \in [0,1]$;
optimality tolerance $\varepsilon > 0$.

Output: a solution z where $\mu' \le \varepsilon$ and $\|G(z)\| \le \varepsilon\|G(z_0)\|$

1: $z \leftarrow z_0 = (y_0, x_0, \tau_0, s_0, \kappa_0)$ as in (10.4)
2: **while** $\mu' > \varepsilon$ or $\|G(z)\| > \varepsilon\|G(z_0)\|$ **do**
3: Compute scaling matrix W as in (10.10)
4: Find the solution Δz^{aff} to (10.11a) to (10.11c), and the solution Δz^{cen} to (10.12a) to (10.12c)
5: $z_+ \leftarrow z + \gamma\Delta z^{\text{pred}} = z + \gamma(\Delta z^{\text{aff}} + \varrho\Delta z^{\text{cen}})$
6: Compute scaling matrix W_+ as in (10.15)
7: Find the solution Δz_+^{cor} to (10.16a) to (10.16c)
8: $z \leftarrow z_{++} = z_+ + \Delta z_+^{\text{cor}}$
9: **return** z

In the remainder of this chapter, we will give the outline of our analysis. The more technical proofs are deferred to Appendix C.

10.3 Scaling Matrix

The scaling matrix W is formed by low-rank updates to $\mu H(x)$. We would like that $W \approx \mu H(x)$ and $W \approx \frac{1}{\mu}H^*(s)^{-1}$ to derive further properties of Algorithm 10.1.

This section is concerned with finding positive scalars u^{P}, l^{P}, u^{D}, and l^{D} such that

$$l^{\mathrm{P}}\mu H(x) \preceq W \preceq u^{\mathrm{P}}\mu H(x) \quad \text{and} \quad \frac{l^{\mathrm{D}}}{\mu}H^*(s)^{-1} \preceq W \preceq \frac{u^{\mathrm{D}}}{\mu}H^*(s)^{-1}, \tag{10.17}$$

and similarly, positive scalars u_+^{P}, l_+^{P}, u_+^{D}, and l_+^{D} such that

$$l_+^{\mathrm{P}}\mu_+ H(x_+) \preceq W_+ \preceq u_+^{\mathrm{P}}\mu_+ H(x_+) \quad \text{and} \quad \frac{l_+^{\mathrm{D}}}{\mu_+}H^*(s_+)^{-1} \preceq W_+ \preceq \frac{u_+^{\mathrm{D}}}{\mu_+}H^*(s_+)^{-1}. \tag{10.18}$$

For instance, Myklebust and Tunçel [82, Theorem 6.8] derive such bounds for a different scaling matrix than the one by Dahl and Andersen [30] under the condition $\|s-\mu\tilde{s}\|_s^* \leq 1/64$. Note that through Lemma 2.4, (10.17) would also give us bounds on W^{-1} in terms of $\frac{1}{\mu}H(x)^{-1}$ and $\mu H^*(s)$, and (10.18) would give bounds on W_+^{-1} in terms of $\frac{1}{\mu_+}H(x_+)^{-1}$ and $\mu_+ H^*(s_+)$.

The bounds on the scaling matrix can be derived with the help of the following relation between Löwner orderings and operator norms.

Proposition 10.2 ([7, Lemma 2])**.** *Let $P,Q \in \mathbb{S}^n$ where $P \succ 0$, and $\epsilon > 0$. Then, $\|P^{-1}Q-I\|_P \leq \epsilon$ if and only if $(1-\epsilon)P \preceq Q \preceq (1+\epsilon)P$.*

Proof. Assume $\|P^{-1}Q-I\|_P \leq \epsilon$. To show $Q-(1-\epsilon)P \succeq 0$, it suffices to note that

$$\begin{aligned}
\inf_{\|u\|_P=1}\langle u,(Q-(1-\epsilon)P)\,u\rangle &\geq \inf_{\|u\|_P=1}\langle u,(Q-P)u\rangle + \inf_{\|u\|_P=1}\langle u,\epsilon Pu\rangle \\
&\geq \inf_{\|u\|_P=1} -\|u\|_P\|(Q-P)u\|_{P^{-1}} + \inf_{\|u\|_P=1}\epsilon\|u\|_P^2 \\
&= -\sup_{\|u\|_P=1}\|(P^{-1}Q-I)u\|_P + \epsilon \\
&\geq -\epsilon+\epsilon = 0.
\end{aligned}$$

Therefore, $\inf_{\|u\|_P\leq 1}\langle u,(Q-(1-\epsilon)P)\,u\rangle \geq 0$ as well. Proving $(1+\epsilon)P-Q \succeq 0$ can be done similarly.

Next, assume $(1-\epsilon)P \preceq Q \preceq (1+\epsilon)P$, i.e. $-\epsilon P \preceq Q-P \preceq \epsilon P$. Hence, for any $u \in \mathbb{R}^n$ with $\|u\|_P \leq 1$, we have $|\langle u,(Q-P)u\rangle| \leq \epsilon$. Using a transformation $v = P^{-1/2}u$,

$$\epsilon \geq \sup_{u\neq 0}\frac{|\langle u,(Q-P)u\rangle|}{\|u\|_P^2} = \sup_{v\neq 0}\frac{|\langle v,P^{-1/2}(Q-P)P^{-1/2}v\rangle|}{\|v\|^2}.$$

It is well known (see e.g. Horn and Johnson [52, Property 1.2.9]) that the supremum on the right hand side is attained at some eigenvector of $P^{-1/2}(Q-P)P^{-1/2}$ with norm one. Hence,

$$\epsilon \geq \sup_{v\neq 0} \frac{\|v\|\|P^{-1/2}(Q-P)P^{-1/2}v\|}{\|v\|^2} = \sup_{u\neq 0} \frac{\|P^{-1}(Q-P)u\|_P}{\|u\|_P} = \|P^{-1}Q-I\|_P. \quad \square$$

We are now ready to derive bounds on W as in (10.17), roughly following the approach by Myklebust and Tunçel [82]. We make the assumption $\|\zeta^{\mathrm{P}}\|_x \leq 0.18226$ to ensure that all denominators in these bounds are positive.

Theorem 10.3 ([7, Theorem 1])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Let $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$, and assume $\|\zeta^{\mathrm{P}}\|_x \leq 0.18226$. Let W be defined as in* (10.10)*. Then, the assumptions* (10.17) *are satisfied with values*

$$l^{\mathrm{P}} = 1-\epsilon-\xi, \quad u^{\mathrm{P}} = 1+\epsilon+\xi, \quad l^{\mathrm{D}} = l^{\mathrm{P}}(1-\|\zeta^{\mathrm{P}}\|_x)^2, \quad u^{\mathrm{D}} = \frac{u^{\mathrm{P}}}{(1-\|\zeta^{\mathrm{P}}\|_x)^2},$$

where

$$\epsilon := \frac{1}{\vartheta_f}\left(\|\zeta^{\mathrm{P}}\|_x + \frac{\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}\right)\left(\|\zeta^{\mathrm{P}}\|_x + \frac{\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + 2\sqrt{\vartheta_f}\right)$$

$$\xi := \frac{2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3 - \|\zeta^{\mathrm{P}}\|_x}\left(\frac{4\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + 2\|\zeta^{\mathrm{P}}\|_x + \frac{\left(\frac{3\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + \|\zeta^{\mathrm{P}}\|_x\right)^2}{\|\zeta^{\mathrm{P}}\|_x\left(1-\frac{3\|\zeta^{\mathrm{P}}\|_x}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}\right)}\right).$$

Proof. See Appendix C. $\square$

Of course, bounds on W_+ in terms of $\mu_+ H(x_+)$ and $\frac{1}{\mu_+}H^*(s_+)$ can also be found using Theorem 10.3 by replacing $\|\zeta^{\mathrm{P}}\|_x$ by $\|\zeta_+^{\mathrm{P}}\|_{x_+}$ in the definition of ϵ and ξ.

10.4 Properties of the Predictor

Now that we know that the scaling matrix W is approximately equal to $\mu H(x)$ and $\frac{1}{\mu}H^*(s)^{-1}$, we shift our focus to the predictor direction that it defines. We start with some simple properties of the predictor, followed by an upper bound on the local norm of the predictor. Thus, we will be able to derive sufficient conditions for (A1)

to hold after the predictor step. We then consider what happens to assumptions (A2) and (A3). It turns out we do not need to consider (A4), so we conclude with an analysis of (A5).

As we noted in Section 10.2, the affine direction Δz^{aff} decreases the norm of the residuals, and the centering direction Δz^{cen} increases it. Dahl and Andersen [30, Lemma 3] show by how much the residuals decrease, and what the value of μ'_+ is. For the sake of completeness, we prove this result using our notation, and we moreover show that $\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}} \rangle + \Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}}$ is zero.

Lemma 10.4 ([7, Lemma 5])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) and (A3) hold, and let $\gamma, \varrho \in \mathbb{R}$. Then, the following properties hold:*

(i) $G(z + \gamma\Delta z^{\text{pred}}) = (1 - \gamma(1-\varrho))G(z)$

(ii) $\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}} \rangle + \Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} = 0$

(iii) $\mu'_+ = (1 - \gamma(1-\varrho))\mu'$*, or equivalently,* $\langle x + \gamma\Delta x^{\text{pred}}, s + \gamma\Delta s^{\text{pred}} \rangle + (\tau + \gamma\Delta\tau^{\text{pred}})(\kappa + \gamma\Delta\kappa^{\text{pred}}) = (1 - \gamma(1-\varrho))[\langle x, s \rangle + \tau\kappa]$.

Proof. See Appendix C. □

Let us now consider what happens to (A1) after the predictor step. A question that needs answering is how big the local norms of the primal and dual predictors Δx^{pred} and Δs^{pred} can be. Without an upper bound on the norm of these predictors, it might be that taking the step from z to z_+ yields an $x_+ \notin \operatorname{int}\mathcal{K}$ or $s_+ \notin \operatorname{int}\mathcal{K}^\circ$.

Theorem 10.5 ([7, Theorem 2])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) to (A5) hold for some $\alpha \in (0, 1]$ and $\delta \in [0, 1)$. Let $l^{\text{P}}, u^{\text{D}} > 0$ be bounds such that* (10.17) *holds, and let $\varrho \in \mathbb{R}$. Then, the primal and dual predictors Δx^{pred} and Δs^{pred} satisfy*

$$\|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2 \leq \mu' \left[\vartheta_f \left(1 - 2\varrho + \frac{\varrho^2}{\alpha} \right) + 1 - \tfrac{1}{2}\alpha - \varrho + \frac{\varrho^2}{2\alpha} \right], \tag{10.19}$$

and

$$l^{\mathrm{P}}\|\Delta x^{\mathrm{pred}}\|_x^2 + \frac{1}{u^{\mathrm{D}}}(\|\Delta s^{\mathrm{pred}}\|_s^*)^2 \leq \frac{1}{\alpha}\left[\vartheta_f\left(1-2\varrho+\frac{\varrho^2}{\alpha}\right)+1-\tfrac{1}{2}\alpha-\varrho+\frac{\varrho^2}{2\alpha}\right]. \tag{10.20}$$

Proof. See Appendix C. □

We want to remark that both that the coefficient of ϑ_f and the constant term in (10.19) and (10.20) are nonnegative for all $\varrho \in \mathbb{R}$ and $\alpha \in (0,1]$. Concerning the coefficient, since $\varrho^2 \geq 0$, $\varrho^2/\alpha \geq \varrho^2$ for all $\alpha \in (0,1]$. Then,

$$1-2\varrho+\varrho^2/\alpha \geq 1-2\varrho+\varrho^2 = (\varrho-1)^2 \geq 0. \tag{10.21}$$

Next, we show that the constant terms in (10.19) and (10.20) are nonnegative. To see this, it suffices to show $\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2 \geq 0$ for all $\varrho \in \mathbb{R}$ and $\alpha \in (0,1]$. Since $\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2$ is concave in α, the claim must hold if $\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2 \geq 0$ for all $\alpha \in \{0,1\}$ and $\varrho \in \mathbb{R}$. For $\alpha = 0$, $\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2 = \frac{1}{2}\varrho^2 \geq 0$ for all $\varrho \in \mathbb{R}$, while for $\alpha = 1$, $\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2 = \frac{1}{2}\varrho^2-\varrho+\frac{1}{2} = \frac{1}{2}(\varrho-1)^2 \geq 0$. Hence,

$$1-\tfrac{1}{2}\alpha-\varrho+\frac{\varrho^2}{2\alpha} = \frac{\alpha-\frac{1}{2}\alpha^2-\varrho\alpha+\frac{1}{2}\varrho^2}{\alpha} \geq 0. \tag{10.22}$$

Moreover, the bounds (10.19) and (10.20) are tight in the simple case where $\alpha = \varrho = 1$: one can verify that the bounds are then both equal to zero, indicating that Δx^{pred} and Δs^{pred} are both zero.

To compress the notation of the upper bounds (10.19) and (10.20) somewhat, we define

$$\Pi := \left[\vartheta_f\left(1-2\varrho+\frac{\varrho^2}{\alpha}\right)+1-\tfrac{1}{2}\alpha-\varrho+\frac{\varrho^2}{2\alpha}\right], \tag{10.23}$$

such that $\|\Delta x^{\mathrm{pred}}\|_W^2 + \|\Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 \leq \mu'\Pi$ and $l^{\mathrm{P}}\|\Delta x^{\mathrm{pred}}\|_x^2 + (\|\Delta s^{\mathrm{pred}}\|_s^*)^2/u^{\mathrm{D}} \leq \Pi/\alpha$.

With Theorem 10.5, we can derive values for γ such that x_+ and s_+ lie in the Dikin ellipsoids around x and s respectively, which implies $x_+ \in \operatorname{int}\mathcal{K}$ and $s_+ \in \operatorname{int}\mathcal{K}^\circ$. This would show that (A1) is satisfied after the predictor step. We now move on to what happens to (A2) and (A3) after the predictor step.

Lemma 10.6 ([7, Lemma 7])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) to (A5) hold for some $\alpha \in (0, 1]$ and $\delta \in [0, 1)$. Let $\gamma \leq 1$ and $\varrho \in \mathbb{R}$. Then,*

$$\tau_+\kappa_+ \leq -\frac{\mu'_+}{1-\gamma(1-\varrho)}\left[\alpha(1-\gamma)+\gamma\varrho-\tfrac{1}{2}\gamma^2\Pi\right]. \tag{10.24}$$

If $\alpha < 1$ or $\varrho < 1$, and

$$0 \leq \gamma < \frac{\alpha-\varrho+\sqrt{(\alpha-\varrho)^2+2\alpha\Pi}}{\Pi}, \tag{10.25}$$

then $\tau_+ > 0$ and $\kappa_+ < 0$.

Proof. See Appendix C. □

One may wonder what happens to assumption (A4) after the predictor step. However, we did not find a satisfying way to bound $\mu'_+\tilde{\mu}_+$. This is the main reason we introduced a corrector in this analysis, which we consider in more detail in Section 10.5.

To complete the analysis of the predictor, we consider (A5). Compared to [7, Lemma 8], we use a somewhat more elegant bound on (C.13) in the proof of this result.

Lemma 10.7. *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) to (A5) hold for some $\alpha \in (0, 1]$ and $\delta \in [0, 1)$. Assume (10.17) holds with $u^{\mathrm{D}} = (1+\epsilon)/r$ and $l^{\mathrm{D}} = r(1-\epsilon)$ for some $r \in (0, 1]$ and $\epsilon \geq 0$. Let $\gamma \in [0, \sqrt{\alpha}\min\{l^{\mathrm{P}}, 1/u^{\mathrm{P}}\}/\Pi)$ and $\varrho \in \mathbb{R}$. Then,*

$$\begin{aligned}\|\zeta^{\mathrm{P}}_+\|_{x_+} \leq \frac{1}{1-\gamma\sqrt{\Pi/(l^{\mathrm{P}}\alpha)}}\Bigg[&(1-\gamma)\|\zeta^{\mathrm{P}}\|_x + \frac{\gamma^2\Pi}{2\alpha\sqrt{\vartheta_f}(1-\|\zeta^{\mathrm{P}}\|_x)} \\ &+ \frac{\gamma\sqrt{\Pi}}{\sqrt{l^{\mathrm{P}}\alpha}}\left(\frac{u^{\mathrm{D}}(1+\varsigma)}{1-\gamma\sqrt{u^{\mathrm{D}}\Pi/\alpha}}-1\right)\Bigg],\end{aligned}$$

where

$$\varsigma := \frac{\gamma^2\Pi}{2\alpha\vartheta_f} + \gamma\max\left\{1-\frac{\varrho}{2-\alpha}, \frac{\varrho}{\alpha}-1\right\}.$$

Proof. See Appendix C. □

10.5 Properties of the Corrector

We have analyzed what happens to the assumptions (A1) to (A3) and (A5) after the predictor step, but we have not investigated (A4). Moreover, it is not clear from Lemma 10.7 that we can pick values for γ, δ, α, and ϱ such that $\|\zeta_+^{\mathrm{P}}\|_{x_+} \leq \|\zeta^{\mathrm{P}}\|_x$. As we will see, the corrector introduced in this work fixes both these problems.

We start with some simple properties of the corrector (10.16a) to (10.16c). These will allow us – among other things – to argue that (A1) to (A3) hold after the corrector step.

Lemma 10.8 ([7, Lemma 9])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+ = (y_+, x_+, \tau_+, s_+, \kappa_+)$ such that $x_+ \in \operatorname{int}\mathcal{K}$, $s_+ \in \operatorname{int}\mathcal{K}^\circ$, $\tau_+ > 0$, and $\kappa_+ < 0$. Then,*

(i) $G(z_+ + \Delta z_+^{\mathrm{cor}}) = G(z_+)$

(ii) $\langle x_+, \Delta s_+^{\mathrm{cor}}\rangle + \langle \Delta x_+^{\mathrm{cor}}, s_+\rangle = 0$

(iii) $\langle \Delta x_+^{\mathrm{cor}}, \Delta s_+^{\mathrm{cor}}\rangle + \Delta\tau_+^{\mathrm{cor}}\Delta\kappa_+^{\mathrm{cor}} = 0$

(iv) $\langle x_+ + \Delta x_+^{\mathrm{cor}}, s_+ + \Delta s_+^{\mathrm{cor}}\rangle + (\tau_+ + \Delta\tau_+^{\mathrm{cor}})(\kappa_+ + \Delta\kappa_+^{\mathrm{cor}}) = \langle x_+, s_+\rangle + \tau_+\kappa_+$. *In other words,* $\mu'_{++} = \mu'_+$

(v) $\|\Delta x_+^{\mathrm{cor}}\|_{W_+}^2 + \|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2 \leq \|\zeta_+^{\mathrm{P}}\|_{W_+}^2$

(vi) $|\langle \Delta x_+^{\mathrm{cor}}, \Delta s_+^{\mathrm{cor}}\rangle| \leq \frac{1}{2}\|\zeta_+^{\mathrm{P}}\|_{W_+}^2$

(vii) $(\tau_+ + \Delta\tau_+^{\mathrm{cor}})(\kappa_+ + \Delta\kappa_+^{\mathrm{cor}}) \leq \tau_+\kappa_+ + \frac{1}{2}\|\zeta_+^{\mathrm{P}}\|_{W_+}^2$. *If* $\tau_+\kappa_+ + \frac{1}{2}\|\zeta_+^{\mathrm{P}}\|_{W_+}^2 < 0$, *then* $\tau_{++} > 0$ *and* $\kappa_{++} < 0$.

Proof. See Appendix C. □

Moving on to (A4), the following result will show that the corrector step leads to a small $\mu_+\tilde{\mu}_{++}$. In Section 10.6, we will show that a small $\mu_+\tilde{\mu}_{++}$ implies a small value of $\mu'_{++}\tilde{\mu}_{++}$.

Lemma 10.9 ([7, Lemma 10])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+ = (y_+, x_+, \tau_+, s_+, \kappa_+)$ such that $x_+ \in \operatorname{int}\mathcal{K}$, $s_+ \in \operatorname{int}\mathcal{K}^\circ$, $\tau_+ > 0$, and $\kappa_+ < 0$. Assume* (10.18) *holds with $u_+^{\mathrm{D}} = (1+\epsilon)/r$ and $l_+^{\mathrm{D}} = r(1-\epsilon)$ for some $r \in (0,1]$ and $\epsilon \geq 0$. Suppose $\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+} < \sqrt{\min\{l_+^{\mathrm{D}}, 1/u_+^{\mathrm{D}}\}}$. Then,*

$$\begin{aligned}\mu_+\tilde{\mu}_{++} \leq 1 + \|\zeta_+^{\mathrm{P}}\|_{W_+} \Bigg[& \frac{u_+^{\mathrm{D}}}{\sqrt{\mu_+\vartheta_f}}\left(\frac{1}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}} - 1\right) \\ & + \frac{\|\tilde{x}_+\|_{W_+}}{\vartheta_f}\left(\frac{1}{l_+^{\mathrm{D}}(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{l_+^{\mathrm{D}}\mu_+})} - 1\right)\Bigg] \\ & + \frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}^2 u_+^{\mathrm{D}}}{\mu_+\vartheta_f l_+^{\mathrm{D}}(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{l_+^{\mathrm{D}}\mu_+})(1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+})}.\end{aligned}$$

Proof. See Appendix C. □

Note that the bound in the lemma above still depends on $\|\tilde{x}_+\|_{W_+}/\vartheta_f$. Although we chose not to analyze $\langle \tilde{x}_+, \tilde{s}_+ \rangle$, we can still crudely bound this quantity as

$$\frac{\|\tilde{x}_+\|_{W_+}}{\vartheta_f} = \frac{\|\mu_+\tilde{x}_+ - x_+ + x_+\|_{W_+}}{\mu_+\vartheta_f} \leq \frac{\|\zeta_+^{\mathrm{P}}\|_{W_+} + \|x_+\|_{W_+}}{\mu_+\vartheta_f} = \frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{\mu_+\vartheta_f} + \frac{1}{\sqrt{\mu_+\vartheta_f}}. \tag{10.26}$$

Of course, better bounds could be found through a thorough analysis of $\langle \tilde{x}_+, \tilde{s}_+ \rangle$.

We end this section by considering (A5). The corrector (10.16a) to (10.16c) was designed with the goal of reducing the distance $\|\zeta_+^{\mathrm{P}}\|_{x_+}$. The following lemma shows that this goal is indeed attained, provided $\|\zeta_+^{\mathrm{P}}\|_{W_+}$ is itself not too large (in which case, u_+^{D} is close to one).

Lemma 10.10 ([7, Lemma 11])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+ = (y_+, x_+, \tau_+, s_+, \kappa_+)$ such that $x_+ \in \operatorname{int}\mathcal{K}$, $s_+ \in \operatorname{int}\mathcal{K}^\circ$, $\tau_+ > 0$, and $\kappa_+ < 0$. Assume* (10.18) *holds with $u_+^{\mathrm{D}} = (1+\epsilon)/r$ and $l_+^{\mathrm{D}} = r(1-\epsilon)$ for some $r \in (0,1]$ and $\epsilon \geq 0$. Suppose $\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+} < \sqrt{\min\{l_+^{\mathrm{P}}, 1/u_+^{\mathrm{P}}\}}$. Then, $\|\zeta_{++}^{\mathrm{P}}\|_{x_{++}}$*

is at most

$$\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+ l_+^{\mathrm{P}}})\sqrt{\mu_+ l_+^{\mathrm{P}}}}\left(\frac{u_+^{\mathrm{D}}}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}}-1\right)$$
$$+\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}^2}{2\mu_+\sqrt{\vartheta_f}}\left[1-\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+ l_+^{\mathrm{P}}})\sqrt{\mu_+ l_+^{\mathrm{P}}}}\left(\frac{u_+^{\mathrm{D}}}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}}-1\right)\right]^{-1}.$$

Proof. See Appendix C. □

10.6 Complexity Analysis

In the previous two sections, we saw how the predictor and corrector step impacted the starting assumptions (A1) to (A5) for general values of the parameters γ, α, ϱ, and δ. Below, we will fix

$$\gamma=\frac{1}{100\vartheta_f},\quad \alpha=0.9,\quad \varrho=0.9,\quad \text{and}\quad \delta=\frac{1}{400\sqrt{\vartheta_f}}. \tag{10.27}$$

It follows from (10.23) and Theorem 10.3 that

$$\Pi=0.1(\vartheta_f+1),\quad l^{\mathrm{P}}\geq 0.97966,\quad \text{and}\quad u^{\mathrm{D}}\leq 1.02546.$$

Moreover, Lemma 10.7 shows that

$$\|\zeta_+^{\mathrm{P}}\|_{x_+}\leq\frac{0.00268}{\sqrt{\vartheta_f}}, \tag{10.28}$$

and consequently Theorem 10.3 implies that

$$l_+^{\mathrm{P}}\geq 0.97819,\quad l_+^{\mathrm{D}}\geq 0.97296,\quad u_+^{\mathrm{P}}\leq 1.02181,\quad \text{and}\quad u_+^{\mathrm{D}}\leq 1.02731.$$

With these values fixed, we can show that Algorithm 10.1 converges to a near-optimal solution of the homogeneous model in $O(\vartheta_f\log(1/\varepsilon))$ iterations.

Theorem 10.11 ([7, Theorem 3])**.** *Let $\mathcal{K}\subset\mathbb{R}^n$ be a proper cone admitting a LH-SCB. Assume we start Algorithm 10.1 from a starting point satisfying* (10.4)*, with*

parameter values as in (10.27). *For any* $\varepsilon \in (0,1]$*, the algorithm produces a solution* z *satisfying*

$$\mu' \le \varepsilon \quad \textit{and} \quad \|G(z)\| \le \varepsilon \|G(z_0)\|,$$

in $O(\vartheta_f \log(1/\varepsilon))$ *iterations.*

Proof. We will show that for the parameter values in (10.27), the point z_{++} satisfies (A1) to (A5) if z satisfies them, and that some progress is made in moving from z to z_{++}.

(A1): Assumption (A1) states that $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$. By Theorem 10.5, we have $\|\gamma\Delta x^{\mathrm{pred}}\|_x \le \gamma\sqrt{\Pi/(\alpha l^{\mathrm{P}})}$, which, for the parameter values in (10.27) and $\vartheta_f \ge 1$, is at most $0.01\sqrt{0.1(\vartheta_f+1)/0.88169}/\vartheta_f \le 0.00477 < 1$. Hence, $x_+ \in \operatorname{int}\mathcal{K}$. Similarly, $\|\gamma\Delta s^{\mathrm{pred}}\|_s^* \le \gamma\sqrt{\Pi u^{\mathrm{D}}/\alpha} \le 0.01\sqrt{0.1(\vartheta_f+1)1.1394}/\vartheta_f \le 0.00478 < 1$, implying that $s_+ \in \operatorname{int}\mathcal{K}^\circ$. Having established that $x_+ \in \operatorname{int}\mathcal{K}$ and $s_+ \in \operatorname{int}\mathcal{K}^\circ$, we consider the corrector step. It follows from (10.18) and Lemma 10.8(v) that

$$\begin{aligned} l_+^{\mathrm{P}}\mu_+\|\Delta x_+^{\mathrm{cor}}\|_{x_+}^2 + \frac{\mu_+}{u_+^{\mathrm{D}}}(\|\Delta s_+^{\mathrm{cor}}\|_{s_+}^*)^2 &\le \|\Delta x_+^{\mathrm{cor}}\|_{W_+}^2 + \|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2 \\ &\le \|\zeta_+^{\mathrm{P}}\|_{W_+}^2 \le u_+^{\mathrm{P}}\mu_+\|\zeta_+^{\mathrm{P}}\|_{x_+}^2 \le u_+^{\mathrm{P}}\mu_+(0.00268)^2, \end{aligned}$$

where the final inequality is due to (10.28). We therefore have $\|\Delta x_+^{\mathrm{cor}}\|_{x_+} \le \|\zeta_+^{\mathrm{P}}\|_{x_+}\sqrt{u_+^{\mathrm{P}}/l_+^{\mathrm{P}}} \le 0.00274 < 1$ and $\|\Delta s_+^{\mathrm{cor}}\|_{s_+}^* \le \|\zeta_+^{\mathrm{P}}\|_{x_+}\sqrt{u_+^{\mathrm{P}}u_+^{\mathrm{D}}} \le 0.00275 < 1$. In conclusion, $x_{++} \in \operatorname{int}\mathcal{K}$ and $s_{++} \in \operatorname{int}\mathcal{K}^\circ$.

(A2): By Lemma 10.6 and Lemma 10.8(vii),

$$\tau_{++}\kappa_{++} \le -\frac{\mu'_+}{1-\gamma(1-\varrho)}\left(\alpha(1-\gamma)+\gamma\varrho-\tfrac{1}{2}\gamma^2\Pi\right)+\tfrac{1}{2}\|\zeta_+^{\mathrm{P}}\|_{W_+}^2. \tag{10.29}$$

Since $\mu'_+ = \mu'_{++}$ by Lemma 10.8(iv), our next step is to bound $\|\zeta_+^{\mathrm{P}}\|_{W_+}^2$ in terms of μ'_{++}. To this end, note that Corollary C.4 shows

$$\frac{\mu_+}{\mu} \le 1 + \frac{\gamma^2\Pi}{2\alpha\vartheta_f} + \gamma\left(\frac{\varrho}{\alpha}-1\right) = 1 + \frac{\vartheta_f+1}{180000\vartheta_f^3} \le 1 + \tfrac{1}{90000}.$$

By (10.18), we can therefore write

$$\|\zeta_+^{\mathrm{P}}\|_{W_+}^2 \le u_+^{\mathrm{P}}\mu_+\|\zeta_+^{\mathrm{P}}\|_{x_+}^2 \le u_+^{\mathrm{P}}\mu\left(1+\tfrac{1}{90000}\right)\|\zeta_+^{\mathrm{P}}\|_{x_+}^2.$$

Now Lemma 10.1 and Lemma 10.4(iii) show

$$\|\zeta_+^{\mathrm{P}}\|_{W_+}^2 \le u_+^{\mathrm{P}}(2-\alpha)\mu'\left(1+\tfrac{1}{90000}\right)\|\zeta_+^{\mathrm{P}}\|_{x_+}^2 = \frac{u_+^{\mathrm{P}}(2-\alpha)\left(1+\frac{1}{90000}\right)}{1-\gamma(1-\varrho)}\mu'_+\|\zeta_+^{\mathrm{P}}\|_{x_+}^2.$$

Plugging the above into (10.29) yields

$$\tau_{++}\kappa_{++} \le \frac{\mu'_+}{1-\gamma(1-\varrho)}\Big[\tfrac{1}{2}\gamma^2\Pi-\alpha+\gamma(\alpha-\varrho)+\tfrac{1}{2}u_+^{\mathrm{P}}(2-\alpha)\left(1+\tfrac{1}{90000}\right)\|\zeta_+^{\mathrm{P}}\|_{x_+}^2\Big].$$

This bound is at most $-\alpha\mu'_{++} = -\alpha\mu'_+$ if and only if

$$\tfrac{1}{2}\gamma^2\Pi-\alpha+\gamma(\alpha-\varrho)+\tfrac{1}{2}u_+^{\mathrm{P}}(2-\alpha)\left(1+\tfrac{1}{90000}\right)\|\zeta_+^{\mathrm{P}}\|_{x_+}^2 \le -\alpha[1-\gamma(1-\varrho)].$$

Eliminating $-\alpha$ from both sides, and multiplying by ϑ_f yields the sufficient condition

$$\frac{\vartheta_f+1}{200000\vartheta_f}+\tfrac{1}{2}1.02181\times 1.1\left(1+\tfrac{1}{90000}\right)(0.00268)^2 \le \tfrac{9}{10000},$$

which is true for all $\vartheta_f \ge 1$. Hence, (A2) is satisfied for z_{++}.

(A3): To verify that (A3) holds for z_{++}, we first turn to Lemma 10.6. It is not hard to verify that for the values in (10.27),

$$\frac{\varrho-\alpha+\sqrt{(\alpha-\varrho)^2+2\alpha\Pi}}{\Pi} = \sqrt{\frac{2\alpha}{\Pi}} = \sqrt{\frac{18}{\vartheta_f+1}} > \frac{1}{100\vartheta_f} = \gamma,$$

so $\tau_+ > 0$ and $\kappa_+ < 0$. Lemma 10.8(vii) shows that $\tau_{++} > 0$ and $\kappa_{++} < 0$ as well, since it was shown above that $\tau_{++}\kappa_{++} \le -\alpha\mu'_{++} < 0$.

(A4): Lemma 10.9 gives us an upper bound on $\mu_+\tilde{\mu}_{++}$, while we want an upper bound on $\alpha\mu'_{++}\tilde{\mu}_{++}$. Note that Lemma 10.8(iv) and Lemma 10.4(iii) show

$$\alpha\mu'_{++}\tilde{\mu}_{++} = \alpha(1-\gamma(1-\varrho))\mu'\tilde{\mu}_{++} = \alpha(1-\gamma(1-\varrho))\frac{\mu'}{\mu_+}\mu_+\tilde{\mu}_{++}. \tag{10.30}$$

To find an upper bound on μ'/μ_+, note that by definition (10.14),

$$\begin{aligned}\frac{\mu'}{\mu_+} &= \frac{\mu'\vartheta_f}{-\langle x+\gamma\Delta x^{\mathrm{pred}}, s+\gamma\Delta s^{\mathrm{pred}}\rangle}\\ &= \frac{\mu'\vartheta_f}{\mu\vartheta_f+\gamma\langle x, W\Delta x^{\mathrm{pred}}-\Delta s^{\mathrm{pred}}\rangle-\gamma^2\langle\Delta x^{\mathrm{pred}}, \Delta s^{\mathrm{pred}}\rangle}.\end{aligned}$$

It follows from (10.11c), (10.12c), and (10.13) that $W\Delta x^{\mathrm{pred}} - \Delta s^{\mathrm{pred}} = s - \varrho\mu'\tilde{s}$. Hence, by Corollary C.3 and Lemma 10.1,

$$\begin{aligned}\frac{\mu'}{\mu_+} &\le \frac{\mu'\vartheta_f}{\mu\vartheta_f + \gamma(-\mu\vartheta_f + \varrho\mu'\vartheta_f) - \frac{1}{2}\gamma^2\mu'\Pi} \\ &\le \frac{\mu'\vartheta_f}{(1-\gamma)\alpha\mu'\vartheta_f + \gamma\varrho\mu'\vartheta_f - \frac{1}{2}\gamma^2\mu'\Pi} = \frac{1}{(1-\gamma)\alpha + \gamma\varrho - \frac{1}{2}\gamma^2\Pi/\vartheta_f}. \quad (10.31)\end{aligned}$$

Next, note that $\|\zeta_+^{\mathrm{p}}\|_{W_+} \le \sqrt{u_+^{\mathrm{p}}\mu_+}\|\zeta_+^{\mathrm{p}}\|_{x_+} \le 0.00271\sqrt{\mu_+/\vartheta_f}$ by (10.18). Consequently, by Lemma 10.9 and (10.26),

$$\alpha(1-\gamma(1-\varrho))(\mu_+\tilde{\mu}_{++}-1) \le \frac{0.0001}{\vartheta_f} \le \frac{0.9}{1000\vartheta_f} - \frac{\vartheta_f+1}{200000\vartheta_f^3} = \gamma\varrho(1-\alpha) - \frac{\gamma^2\Pi}{2\vartheta_f}. \quad (10.32)$$

Plugging (10.31) and (10.32) into (10.30) yields

$$\begin{aligned}\alpha\mu'_{++}\tilde{\mu}_{++} &\le \frac{\alpha(1-\gamma(1-\varrho))}{(1-\gamma)\alpha + \gamma\varrho - \frac{1}{2}\gamma^2\Pi/\vartheta_f}[(\mu_+\tilde{\mu}_{++}-1)+1] \\ &\le \frac{\alpha(1-\gamma(1-\varrho)) + \gamma\varrho(1-\alpha) - \frac{1}{2}\gamma^2\Pi/\vartheta_f}{(1-\gamma)\alpha + \gamma\varrho - \frac{1}{2}\gamma^2\Pi/\vartheta_f} = 1.\end{aligned}$$

(A5): It follows from Lemma 10.10 that for the parameter values in (10.27),

$$\|\zeta_{++}^{\mathrm{p}}\|_{x_{++}} \le \frac{0.00009}{\sqrt{\vartheta_f}} < \frac{0.0025}{\sqrt{\vartheta_f}} = \frac{1}{400\sqrt{\vartheta_f}} = \delta.$$

The discussion above demonstrated that for the parameter values (10.27), an iteration of Algorithm 10.1 starting at a solution z satisfying (A1) to (A5) ends at a solution z_{++} for which (A1) to (A5) also hold. By Lemmas 10.4(i), 10.4(iii), 10.8(i), and 10.8(iv), the residuals and complementarity reduce at a rate of $1-\gamma(1-\varrho)$ per iteration. If we start at an initial point z_0 as in (10.4), then $\mu' = 1$ and (A1) to (A5) all hold. Thus, after k iterations of Algorithm 10.1, the complementarity gap is exactly $(1-\gamma(1-\varrho))^k$, and the residuals are $G(z_0)(1-\gamma(1-\varrho))^k$. This completes the proof. □

11

Conclusions and Future Work

Let us highlight the main insights that we gained throughout this thesis, and point out possible improvements that future research could focus on. This thesis covered four approaches to convex programming: the sampling-based interior point method from Chapter 6, the simulated annealing algorithm by Kalai and Vempala [56] in Chapter 7, the analytic center cutting plane method in Chapter 8, and the nonsymmetric conic algorithm in Chapter 10. We will briefly discuss each of these.

To analyze the first two methods, we needed the prerequisites from Chapters 2 to 5. Where Chapters 2 and 3 contained mostly well-known background material on interior point theory, Chapters 4 and 5 concerned the quality of approximations of the mean and covariance of Boltzmann distributions, based on hit-and-run sampling. The bounds we derived there are likely not tight though.

The first reason is that we cited Theorem 1.1 from Lovász and Vempala [71], which states a walk length that ensures a hit-and-run sample's distribution is close to the target distribution. This number of steps contains an astronomical constant 10^{30}, which makes this walk length, and the walk length in our Theorem 4.14, far

too big to be used in practice. However, experiments show that hit-and-run does seem like a viable strategy to generate samples, which suggests the theoretical analysis is overly pessimistic.

As a second reason, Theorem 5.11 uses $O(n^2)$ samples to approximate a covariance matrix, which may be too conservative. Results such as Theorem 4.1 in Adamczak et al. [2] suggest that a covariance matrix may be approximated with $O(n)$ samples. However, their result depends on the assumption that all samples are drawn independently from the target distribution. Whether this result can be extended to near-independent samples from distributions close to the target distribution is left for future research.

Even with these (possibly) non-tight bounds on the walk length and sample size, it was shown in Chapter 5 that we can approximate the mean and covariance of a Boltzmann distribution within polynomial time. Chapter 6 then proposed a sampling-based interior point method to compute a solution that is near-optimal with probability at least $1 - q^*$, where the number of oracle calls is $O^*(n^{8.5}/q^*)$. The same complexity was found in Chapter 7 for Kalai and Vempala's simulated annealing algorithm [56]. It might be that both these complexity results can be strengthened for the reasons also discussed in Section 7.3. The first reason was already raised above: the number of samples required to approximate a covariance may be linear in n, not quadratic. It was moreover described in Section 7.3 that a lower bound on the spectrum of Boltzmann covariance matrices which is not exponential in n would improve the algorithms' complexity.

But such theoretical improvements would not change these methods' practical perspectives. As we saw in Chapter 9, approximating the mean and covariance of a Boltzmann distribution to high accuracy with hit-and-run sampling takes an impractically long time. This raises concerns about the applicability of the sampling-based interior point method, since it depends heavily on these approximations. The simulated annealing algorithm performs worse than the ellipsoid method, even after applying some improvements and taking a heuristic number of steps and samples. It seems massive parallelization would be necessary to make these approaches competitive. This does not appear to be an attractive strategy, especially since there are viable alternatives.

The analytic center cutting plane method that was introduced in Chapter 8 is such an alternative. Even if we did not formally analyze the number of oracle calls

this method makes, this quantity seems to scale well in practice (see Section 9.3). The method was successfully applied to copositive programming, using the copositivity oracle from Section 8.2. This oracle solves a mixed integer linear program, which is theoretically NP-hard, but quite fast in practice. Our implementation is available online.

Besides the lack of theoretical guarantees, there is another downside to this method of solving copositive optimization problems: it requires an upper bound on the norm of an optimal solution. This was easy for our testing problem, since the entire feasible set was contained in a unit ball. However, it is not clear how such a bound could be determined ex-ante in general.

The last algorithm we discussed focused on a slightly more structured problem: convex programming on proper cones that admit a readily computable logarithmically homogeneous barrier. In Chapter 10, we analyzed an algorithm that is closely related to that of Dahl and Andersen [30], which was implemented in MOSEK 9 [78]. We showed that our algorithm returns a near-optimal solution to the homogeneous model in $O(\vartheta_f \log(1/\varepsilon))$ iterations. Future work could focus on improving this bound, or analyzing an algorithm that has fewer differences with the method by Dahl and Andersen [30]. For instance, we disregarded the higher-order corrector in their work, and introduced a corrector of our own for the sake of simplicity.

We have thus covered four algorithms for convex programming – two randomized, two deterministic. The randomized algorithms do not appear attractive in practice, because they call the membership oracle of the feasible set too many times. This seems to be caused by their consisting of many layers, as depicted in Figures 6.1 and 7.1. The randomized methods use the oracle calls to find the end points of line segments, which yield one hit-and-run step. After many such steps, we have a hit-and-run sample. With many samples, we can create an estimate of a covariance matrix, and with many of these estimated covariances, we can run our randomized methods. By contrast, the analytic center cutting plane method from Chapter 8 uses each and every oracle call to shrink the outer approximation of the optimal set. We therefore argue that a practically competitive randomized method for convex programming would use fewer layers than the methods from this thesis.

A

Fréchet Derivatives for Self-Concordance

The definitions of the gradient, Hessian, and third derivative of a function, as stated in Section 2.1, are all based on Fréchet derivatives. In this appendix, we provide more details on this type of derivative. This will allow us to fill in some details in the proof of Theorem 2.6.

Following Dieudonné [39], we adopt the notation that the Fréchet derivative of a function f is Df, the second Fréchet derivative is D^2f, etcetera. The reader will find that Definitions 2.1, 2.2, and 2.5 can be recovered by identifying g with Df, H with D^2f, and T with D^3f.

After providing the formal definition of Fréchet derivatives in Appendix A.1, we provide the analogues of the well-known chain rule, product rule, and quotient rule in Appendix A.2. Appendix A.3 will then show that the first two Fréchet derivatives correspond to vectors and linear operators, respectively (in the simplest case, these linear operators are just square matrices). To prove Theorem 2.6, we will also need to understand the third Fréchet derivative; this topic is covered in Appendix A.4. We conclude this appendix with a proof of Theorem 2.6 in Appendix A.5.

A.1 Definition of Fréchet Derivatives

Recall that $\mathcal{L}(V;W)$ denotes the space of bounded linear operators from V to W, where V and W are Banach spaces. Moreover, below $\mathcal{L}(V_1,...,V_m;W)$ will denote the space of bounded multilinear operators from $V_1 \times \cdots \times V_m$ to W.

The formal definition of Fréchet derivatives is phrased in terms of Banach spaces, i.e. complete normed vector spaces.

Definition A.1. Let V, W be Banach spaces, and let $V' \subseteq V$ be an open (with respect to the norm topology) subset of V. Then $f : V' \to W$ is *Fréchet differentiable* at $\theta \in V'$ if there exists a bounded linear operator $Df(\theta) : V \to W$ with

$$\lim_{\|w\|\downarrow 0} \frac{\|f(\theta+w)-f(\theta)-Df(\theta)[w]\|}{\|w\|} = 0,$$

where we use the brackets to emphasize that we are applying a linear operator to a vector. If such an operator exists, it is unique. f is said to be *continuously differentiable* if the function $Df : V' \to \mathcal{L}(V;W)$, that is $\theta \mapsto Df(\theta)$, is continuous.

One should note that $\mathcal{L}(V;W)$ is also a Banach space (whose norm is the operator norm), so we could define the derivative of the function $Df : V' \to \mathcal{L}(V,W)$ at $\theta \in V'$, if it exists. We denote this derivative by $D^2f : V' \to \mathcal{L}(V;\mathcal{L}(V;W))$. However, the space $\mathcal{L}(V;\mathcal{L}(V,W))$ can be identified with the space of bounded bilinear operators $\mathcal{L}(V,V;W)$: this can be done by identifying with each $\phi \in \mathcal{L}(V;\mathcal{L}(V;W))$ the bilinear operator $(v,w) \mapsto (\phi[v])[w]$, where $v, w \in V$. In particular, we let $D^2f(\theta)[v,w] \equiv (D^2f(\theta)[v])[w]$.

We can apply this argument once more. The third derivative is denoted by $D^3f : V' \to \mathcal{L}(V;\mathcal{L}(V;\mathcal{L}(V;W)))$. The space $\mathcal{L}(V;\mathcal{L}(V;\mathcal{L}(V;W)))$ can be identified with the space of bounded trilinear operators $\mathcal{L}(V,V,V;W)$ by identifying each $\phi \in \mathcal{L}(V;\mathcal{L}(V;\mathcal{L}(V;W)))$ with $(u,v,w) \mapsto ((\phi(\theta)[u])[v])[w]$, where $u, v, w \in V$. In particular, we let $D^3f(\theta)[u,v,w] \equiv ((D^3f(\theta)[u])[v])[w]$.

Generally, the n-th Fréchet derivative can be identified with the unique multilinear operator $D^nf(\theta)$ such that, for all $w_1,...,w_{n-1} \in V$,

$$\frac{\|D^{n-1}f(\theta+w_n)[w_{n-1},...,w_1]-D^{n-1}f(\theta)[w_{n-1},...,w_1]-D^nf(\theta)[w_n,...,w_1]\|}{\|w_n\|}$$

tends to zero when $\|w_n\| \downarrow 0$.

A.2 Calculus Rules for Fréchet Derivatives

We will need the analogues of the chain rule, product rule, and quotient rule for Fréchet derivatives. We start by citing the chain rule from Dieudonné [39].

Theorem A.2 ([39, Theorem 8.2.1])**.** *Let U, V, W be three Banach spaces, U' an open neighborhood of $\theta \in U$, f a continuous function from U' into V, V' an open neighborhood of $f(\theta) \in V$, and $\tilde{f}$ a continuous function from V into W. Then, if f is differentiable at θ and $\tilde{f}$ is differentiable at $f(\theta)$, the function $\phi : U' \to W$ defined by $\phi(y) = \tilde{f}(f(y))$ is differentiable at θ and*

$$D\phi(\theta) = D\tilde{f}(f(\theta)) \circ Df(\theta),$$

that is, $D\phi(\theta)[w] = D\tilde{f}(f(\theta))[Df(\theta)[w]]$ for all $w \in U$.

Note that within the setting of the theorem, $Df(\theta)$ is defined as a linear operator from U to V, and $D\tilde{f}(f(\theta))$ is a linear operator from V to W. Hence their composition is a linear operator from U to W, as one would expect from $D\phi(\theta)$.

Next, we prove the product rule for Fréchet derivatives.

Theorem A.3. *Let V and W be Banach spaces, V' an open neighborhood of $\theta \in V$, $f : V' \to W$ and $\tilde{f} : V' \to \mathbb{R}$ continuous functions. If f and $\tilde{f}$ are differentiable at θ, then the function $\phi : V' \to W$ defined by $\phi(y) = \tilde{f}(y)f(y)$ is differentiable at θ and for all $w \in V$,*

$$D\phi(\theta)[w] = \tilde{f}(\theta)Df(\theta)[w] + D\tilde{f}(\theta)[w]f(\theta). \tag{A.1}$$

Proof. The proof runs along the lines of well-known calculus. If we substitute (A.1),

$$\begin{aligned}
&\|\tilde{f}(\theta+w)f(\theta+w) - \tilde{f}(\theta)f(\theta) - D\phi(\theta)[w]\| \\
&= \|\tilde{f}(\theta+w)\big(f(\theta+w) - f(\theta)\big) + \big(\tilde{f}(\theta+w) - \tilde{f}(\theta)\big)f(\theta) - D\phi(\theta)[w]\| \\
&\le \|\tilde{f}(\theta+w)\big(f(\theta+w) - f(\theta)\big) - \tilde{f}(\theta)Df(\theta)[w]\| \\
&\quad + \|\big(\tilde{f}(\theta+w) - \tilde{f}(\theta) - D\tilde{f}(\theta)[w]\big)f(\theta)\| \\
&\le \|\tilde{f}(\theta)\big(f(\theta+w) - f(\theta) - Df(\theta)[w]\big)\| \\
&\quad + \|\big(\tilde{f}(\theta+w) - \tilde{f}(\theta)\big)\big(f(\theta+w) - f(\theta)\big)\| \\
&\quad + \|\big(\tilde{f}(\theta+w) - \tilde{f}(\theta) - D\tilde{f}(\theta)[w]\big)f(\theta)\|.
\end{aligned}$$

Thus, the algebraic limit theorem shows

$$\begin{aligned}0 &\le \lim_{\|w\|\downarrow 0} \frac{\|\tilde{f}(\theta+w)f(\theta+w)-\tilde{f}(\theta)f(\theta)-D\phi(\theta)[w]\|}{\|w\|}\\ &\le |\tilde{f}(\theta)| \lim_{\|w\|\downarrow 0} \frac{\|f(\theta+w)-f(\theta)-Df(\theta)[w]\|}{\|w\|}\\ &\quad + \lim_{\|w\|\downarrow 0} \frac{|\tilde{f}(\theta+w)-\tilde{f}(\theta)|}{\|w\|}\|f(\theta+w)-f(\theta)\|\\ &\quad + \|f(\theta)\| \lim_{\|w\|\downarrow 0} \frac{|\tilde{f}(\theta+w)-\tilde{f}(\theta)-D\tilde{f}(\theta)[w]|}{\|w\|} = 0.\end{aligned}$$

where the final equality holds because $D\tilde{f}(\theta)$ is a bounded linear operator. □

Finally, we prove the quotient rule.

Theorem A.4. *Let V and W be Banach spaces, V' an open neighborhood of $\theta \in V$, $f : V' \to W$ and $\tilde{f} : V' \to \mathbb{R}$ continuous functions such that $\tilde{f}(\theta) \neq 0$. If f and $\tilde{f}$ are differentiable at θ, the function $\phi : V' \to W$ defined by $\phi(y) = f(y)/\tilde{f}(y)$ is differentiable at θ and for all $w \in V$,*

$$D\phi(\theta)[w] = \frac{1}{\tilde{f}(\theta)^2}\big(\tilde{f}(\theta)Df(\theta)[w] - D\tilde{f}(\theta)[w]f(\theta)\big).$$

Proof. We apply the product and chain rule to $\phi(\theta) = (\tilde{f}(\theta))^{-1}f(\theta)$ to find

$$D\phi(\theta)[w] = (\tilde{f}(\theta))^{-1}Df(\theta)[w] + \big(-\tilde{f}(\theta)^{-2}D\tilde{f}(\theta)[w]\big)f(\theta).$$ □

A.3 Associations of Fréchet Derivatives

In this section, we will assume that V is a finite-dimensional Hilbert space, and $W = \mathbb{R}$. We saw in Appendix A.1 that $Df(\theta)$ is formally a linear operator from V to $\mathbb{R}$, and $D^2f(\theta)$ is formally a linear operator from V to $\mathcal{L}(V;\mathbb{R})$. However, Definitions 2.1 and 2.2 defined the gradient and Hessian as a vector and a linear operator from V to V, respectively. In this section, we argue that these interpretations can be used interchangeably.

Depending on the context, we would like to interpret the Fréchet derivative $Df(\theta)$ as either a vector in V, or as a linear operator from V to $\mathbb{R}$. The following

result demonstrates that every vector corresponds to a unique linear operator, and vice versa.

Proposition A.5. *Let V be a finite-dimensional inner product space.*

(i) For every $a \in \mathcal{L}(V;\mathbb{R})$ and inner product $\langle\cdot,\cdot\rangle$ on V, there exists a unique $\overline{a} \in V$ such that $\langle \overline{a}, x\rangle = a[x]$ for all $x \in V$.

(ii) For every $\overline{a} \in V$ and inner product $\langle\cdot,\cdot\rangle$ on V, the $a \in \mathcal{L}(V;\mathbb{R})$ defined by $a[x] = \langle \overline{a}, x\rangle$ for all $x \in V$ is the only operator in $\mathcal{L}(V;\mathbb{R})$ with this property.

Moreover, the pairings between $\mathcal{L}(V;\mathbb{R})$ and V in (i) and (ii) are each other's inverses.

Proof. Let $\{e_1, ..., e_n\}$ be an orthonormal basis for V with respect to $\langle\cdot,\cdot\rangle$.

(i): Define $\overline{a} = \sum_{i=1}^n a[e_i]e_i$, and note

$$\langle \overline{a}, x\rangle = \sum_{i=1}^n a[e_i]\langle e_i, x\rangle = a\left[\sum_{i=1}^n \langle e_i, x\rangle e_i\right] = a[x]. \tag{A.2}$$

Suppose there is some other $\overline{b} \in V$ such that $\langle \overline{b}, x\rangle = a[x]$. Then $\langle \overline{a} - \overline{b}, x\rangle = 0$ for all $x \in V$. Hence $\overline{a} - \overline{b} = 0$, which proves uniqueness of $\overline{a}$.

(ii): The argument for uniqueness is similar to (i).

Finally, it is clear from (ii) and (A.2) that if we start with an $a \in \mathcal{L}(V;\mathbb{R})$ and find its associated vector $\overline{a} = \sum_{i=1}^n a[e_i]e_i$, then the linear operator induced by $\overline{a}$ is again a. □

We would like to do something similar for the second derivative $D^2 f(\theta)$. It will be shown below that this linear operator from V to $\mathcal{L}(V;\mathbb{R})$ can be identified with a linear operator from V to V.

Proposition A.6. *Let V be a finite-dimensional inner product space.*

(i) For every $A \in \mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ and inner product $\langle\cdot,\cdot\rangle$ on V, there exists a unique $\overline{A} \in \mathcal{L}(V;V)$ such that $\langle \overline{A}[x], y\rangle = (A[x])[y]$ for all $x, y \in V$.

(ii) For every $\overline{A} \in \mathcal{L}(V;V)$ and inner product $\langle\cdot,\cdot\rangle$, the $A \in \mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ defined by $(A[x])[y] = \langle \overline{A}[x], y\rangle$ for all $x, y \in V$ is the only operator in $\mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ with this property.

Moreover, the pairings between $\mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ and $\mathcal{L}(V;V)$ in (i) and (ii) are each other's inverses.

Proof. Let $\{e_1,...,e_n\}$ be an orthonormal basis for V with respect to $\langle\cdot,\cdot\rangle$.

(i): Define $\overline{A}[x]=\sum_{i=1}^n (A[x])[e_i]e_i$, and note

$$\langle\overline{A}[x],y\rangle=\sum_{i=1}^n (A[x])[e_i]\langle e_i,y\rangle=(A[x])\left[\sum_{i=1}^n\langle e_i,y\rangle e_i\right]=(A[x])[y]. \tag{A.3}$$

Suppose there is some other $\overline{B}:V\to V$ such that $\langle\overline{B}[x],y\rangle=(A[x])[y]$. Then $\langle(\overline{A}-\overline{B})[x],y\rangle=0$ for all $x,y\in V$. Hence $\overline{A}-\overline{B}=0$, which proves uniqueness of $\overline{A}$.

(ii): The argument for uniqueness is similar to (i).

Finally, it is clear from (ii) and (A.3) that if we start with an $A\in\mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ and find its associated $\overline{A}\in\mathcal{L}(V;V)$ with $\overline{A}[x]=\sum_{i=1}^n (A[x])[e_i]e_i$, then the linear operator induced by $\overline{A}$ is again A. □

Propositions A.5 and A.6 show that, given an inner product on V, the space $\mathcal{L}(V;\mathbb{R})$ is isomorphic to V, and $\mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))$ is isomorphic to $\mathcal{L}(V;V)$. Hence, if $V=\mathbb{R}^n$, we can think of $Df(\theta)$ as a vector in $\mathbb{R}^n$, and of $D^2f(\theta)$ as a linear operator from $\mathbb{R}^n$ to $\mathbb{R}^n$. If moreover $\langle\cdot,\cdot\rangle$ is the Euclidean inner product, the gradient is the usual vector of partial derivatives, and the Hessian is the usual matrix of second order partial derivatives.

A.4 Computing the Third Derivative

While we now have some feeling for the gradient and Hessian, the third derivative $D^3f:\mathcal{L}(V;\mathcal{L}(V;\mathbb{R}))\to\mathbb{R}$ remains a bit mysterious. We will rephrase its definition in terms of Renegar's notation [95] of the Hessian (cf. Definition 2.2) below, and provide its elements explicitly when $V=\mathbb{R}^n$ and $\langle\cdot,\cdot\rangle$ is the Euclidean inner product.

According to Definition A.1, D^3f is the unique linear operator such that

$$0=\lim_{\|u\|\downarrow 0}\frac{\|D^2f(\theta+u)-D^2f(\theta)-D^3f(\theta)[u]\|}{\|u\|}, \tag{A.4}$$

where the norm in the numerator is the operator norm on $\mathcal{L}(V;\mathcal{L}(V;W))$. By the definition of the operator norm,

$$\begin{aligned}
&\|D^2 f(\theta+u) - D^2 f(\theta) - D^3 f(\theta)[u]\| \\
&= \max_{v:\|v\|=1} \|(D^2 f(\theta+u) - D^2 f(\theta) - D^3 f(\theta)[u])[v]\| \\
&= \max_{v:\|v\|=1} \max_{w:\|w\|=1} \|((D^2 f(\theta+u) - D^2 f(\theta) - D^3 f(\theta)[u])[v])[w]\|.
\end{aligned}$$

If $W = \mathbb{R}$, then the norm on W in the last expression is equal to the absolute value up to scaling. Recall that we can think of every linear operator in $\mathcal{L}(V;\mathcal{L}(V;W))$ as an operator in $\mathcal{L}(V,V;W)$ such that $(D^2 f(\theta)[v])[w] \equiv D^2 f(\theta)[v,w]$, and similar for $D^3 f(\theta)$. It follows that we may rewrite (A.4) as the condition that for all $v, w \in V$ with $\|v\|, \|w\| = 1$,

$$\begin{aligned}
0 &= \lim_{\|u\|\to 0} \frac{|D^2 f(\theta+u)[v,w] - D^2 f(\theta)[v,w] - D^3 f(\theta)[u,v,w]|}{\|u\|} \\
&= \lim_{\|u\|\to 0} \frac{|\langle w, (H(\theta+u) - H(\theta))v\rangle - D^3 f(\theta)[u,v,w]|}{\|u\|}.
\end{aligned}$$

In other words, $D^3 f$ is the unique trilinear operator such that for each $u, v, w \in V$, it holds that

$$D^3 f(\theta)[u,v,w] = \lim_{t\to 0} \frac{\langle w, (H(\theta+tu) - H(\theta))v\rangle}{t}. \tag{A.5}$$

Thus (A.5) establishes the relationship between the Fréchet definition of $D^3 f$ and Renegar's notation of the Hessian as in Definition 2.2. Still, it is not immediately clear how to compute (A.5), even in the simple case where $V = \mathbb{R}^n$ and $\langle\cdot,\cdot\rangle$ is the Euclidean inner product. The key lemma is the following.

Lemma A.7. *Let $\langle\cdot,\cdot\rangle$ be the Euclidean inner product on $\mathbb{R}^n$, which induces the Euclidean norm $\|\cdot\|$, and let $e_i \in \mathbb{R}^n$ be the i-th standard basis vector. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a three times Fréchet differentiable functional, and $\theta \in \operatorname{dom} f$. Then,*

$$D^3 f(\theta)[e_i, e_j, e_k] = \frac{\partial^3 f(\theta)}{\partial x_i \partial x_j \partial x_k} \qquad \forall i, j, k \in \{1, \ldots, n\}.$$

Proof. From (A.5), it follows that

$$\begin{aligned} D^3 f(\theta)[e_i, e_j, e_k] &= \lim_{t\to 0} \frac{\langle e_k, (H(\theta + te_i) - H(\theta))e_j\rangle}{t} \\ &= \lim_{t\to 0} \frac{1}{t}\left(\frac{\partial^2 f(\theta + te_i)}{\partial x_j \partial x_k} - \frac{\partial^2 f(\theta)}{\partial x_j \partial x_k}\right) = \frac{\partial^3 f(\theta)}{\partial x_i \partial x_j \partial x_k}. \end{aligned}$$ □

Because $D^3 f(\theta)$ is (identified with) a tri-linear operator, we can compute (A.5) easily for arbitrary $u, v, w \in \mathbb{R}^n$:

$$\begin{aligned} D^3 f(\theta)[u, v, w] &= D^3 f(\theta)\left[\sum_{i=1}^n u_i e_i, \sum_{j=1}^n v_j e_j, \sum_{k=1}^n w_k e_k\right] \\ &= \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n u_i v_j w_k D^3 f(\theta)\big[e_i, e_j, e_k\big] \\ &= \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n u_i v_j w_k \frac{\partial^3 f(\theta)}{\partial x_i \partial x_j \partial x_k}. \end{aligned}$$

A.5 Proof of Theorem 2.6

We end this appendix with the proof of Theorem 2.6, which shows that Renegar's definition of self-concordance coincides with that of Nesterov and Nemirovskii [85] for three times continuously differentiable functionals. We follow Renegar's proof [95], but we provide some details in separate lemmas. For the reader's convenience, we restate the theorem first.

Theorem 2.6 ([95, Theorem 2.5.3])**.** *Let f be a three times continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open subset of $\mathbb{R}^n$. Then, f is self-concordant if and only if the following two properties hold:*

(i) For any sequence $\{\theta_k\} \subset \operatorname{dom} f$ that converges to a point on the boundary of $\operatorname{dom} f$*, we have $f(\theta_k) \to \infty$.*

(ii) For any $\theta \in \operatorname{dom} f$ and $\Delta\theta \in \mathbb{R}^n$, the function $\phi(t) := f(\theta + t\Delta\theta)$ satisfies $\phi'''(t) \le 2\phi''(t)^{3/2}$ for all $t \in \operatorname{dom}\phi$.

Proof. The "only if" part follows from Theorem 2.2.9 and page 61 in Renegar [95]. To show the "if" part, it suffices to prove conditions (1c) and (2c) in Theorem 2.5.2 in Renegar [95]. Since (2c) is the same as (i), it remains to show

$$\limsup_{\Delta\theta\to 0} \frac{\|I - H_\theta(\theta+\Delta\theta)\|_\theta}{\|\Delta\theta\|_\theta} \le 2, \tag{A.6}$$

for all $\theta \in \operatorname{dom} f$ whenever (i) and (ii) hold.

By Lemma A.8, Condition (ii) is equivalent to

$$|D^3 f(\theta)[u,u,u]| \le 2 \qquad \forall \theta \in \operatorname{dom} f, u \in \mathbb{R}^n : \|u\|_\theta \le 1.$$

Since Lemma A.9 shows that for any $\theta \in \operatorname{dom} f$,

$$\max_{\substack{u,v,w:\\ \|u\|_\theta,\|v\|_\theta,\|w\|_\theta=1}} |D^3 f(\theta)[u,v,w]| = \max_{\substack{u:\\ \|u\|_\theta=1}} |D^3 f(\theta)[u,u,u]|,$$

it follows that $|D^3 f(\theta)[u,v,w]| \le 2$ for all $\theta \in \operatorname{dom} f$ and $u,v,w \in \mathbb{R}^n$ such that $\|u\|_\theta, \|v\|_\theta, \|w\|_\theta \le 1$ (and in particular for $v = w$). Then, Lemma A.10 shows (A.6), completing the proof. □

We now state the remaining lemmas that were used in the proof of Theorem 2.6.

Lemma A.8. *Let f be a three times continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open subset of $\mathbb{R}^n$. Then, the following are equivalent:*

(i) For any $\theta \in \operatorname{dom} f$ and $\Delta\theta \in \mathbb{R}^n$, the function $\phi(t) = f(\theta + t\Delta\theta)$ satisfies $\phi'''(t) \le 2\phi''(t)^{3/2}$ for all $t \in \operatorname{dom}\phi$.

(ii) For any $\theta \in \operatorname{dom} f$ and $u \in \mathbb{R}^n$ with $\|u\|_\theta \le 1$, $|D^3 f(\theta)[u,u,u]| \le 2$.

Proof. We can assume without loss of generality that $t = 0$: the given inequality should hold for $t = 0$ in particular, and if we want to evaluate f at some $\theta + t\Delta\theta$ with $t \neq 0$, we can always change θ to the desired point. By Definitions 2.1 and A.1,

$$\begin{aligned}\phi'(0) = \frac{\partial}{\partial t} f(\theta + t\Delta\theta)\Big|_{t=0} &= \lim_{t\to 0} \frac{f(\theta+t\Delta\theta) - f(\theta)}{t} \\ &= \langle \Delta\theta, g(\theta)\rangle = Df(\theta)[\Delta\theta].\end{aligned}$$

Moreover, by Definition 2.2,

$$\phi''(0) = \lim_{t\to 0} \frac{\langle \Delta\theta, g(\theta + t\Delta\theta) - g(\theta)\rangle}{t} = \langle \Delta\theta, H(\theta)\Delta\theta\rangle = D^2 f(\theta)[\Delta\theta, \Delta\theta],$$

and finally it follows from (A.5) that

$$\phi'''(0) = \lim_{t\to 0} \frac{\langle \Delta\theta, (H(\theta + t\Delta\theta) - H(\theta))\Delta\theta\rangle}{t} = D^3 f(\theta)[\Delta\theta, \Delta\theta, \Delta\theta].$$

Hence (i) is equivalent to f satisfying the following for all $\theta \in \operatorname{dom} f, \Delta\theta \in \mathbb{R}^n$:

$$D^3 f(\theta)[\Delta\theta, \Delta\theta, \Delta\theta] \le 2(D^2 f(\theta)[\Delta\theta, \Delta\theta])^{3/2} = 2\|\Delta\theta\|_\theta^3.$$

This condition should also hold for $-\Delta\theta$, so by the multilinearity of $D^3 f(\theta)$, it follows that $-D^3 f(\theta)[\Delta\theta, \Delta\theta, \Delta\theta] \le 2\|\Delta\theta\|_\theta^3$ as well. We may therefore also write $|D^3 f(\theta)[\Delta\theta, \Delta\theta, \Delta\theta]|$ on the left hand side of the equation above. Finally, we divide by $\|\Delta\theta\|_\theta^3$ on both sides, and get our desired result:

$$\begin{aligned} 2 &\ge \frac{1}{\|\Delta\theta\|_\theta^3} |D^3 f(\theta)[\Delta\theta, \Delta\theta, \Delta\theta]| \\ &= \left| D^3 f(\theta)\left[\frac{\Delta\theta}{\|\Delta\theta\|_\theta}, \frac{\Delta\theta}{\|\Delta\theta\|_\theta}, \frac{\Delta\theta}{\|\Delta\theta\|_\theta}\right]\right| = |D^3 f(\theta)[u,u,u]|, \end{aligned}$$

where $\|u\|_\theta = 1$. □

In his proof of [95, Theorem 2.5.3], Renegar claims that for any three times continuously differentiable function f, any $\theta \in \operatorname{dom} f$, and any inner product norm $\|\cdot\| = \langle\cdot,\cdot\rangle^{1/2}$,

$$\max_{\substack{u,v,w:\\ \|u\|,\|v\|,\|w\|=1}} |D^3 f(\theta)[u,v,w]| = \max_{\substack{u:\\ \|u\|=1}} |D^3 f(\theta)[u,u,u]|.$$

The next lemma is less general than this result used by Renegar. We restrict ourselves to the local inner product to clearly distinguish the reference inner product.

Lemma A.9. *Let f be a three times continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open subset of $\mathbb{R}^n$, and fix $\theta \in \operatorname{dom} f$. Then,*

$$\max_{\substack{u,v,w:\\ \|u\|_\theta,\|v\|_\theta,\|w\|_\theta=1}} |D^3 f(\theta)[u,v,w]| = \max_{\substack{u:\\ \|u\|_\theta=1}} |D^3 f(\theta)[u,u,u]| \tag{A.7}$$

Proof. Let us first show that we can take $v = w$ in (A.7). Pick $t \neq 0$. The Cauchy-Schwarz inequality shows

$$\begin{aligned}|\langle w, (H(\theta+tu)-H(\theta))v\rangle| &= |\langle w, (H_\theta(\theta+tu)-H_\theta(\theta))v\rangle_\theta| \\ &\leq \|w\|_\theta \|(H_\theta(\theta+tu)-H_\theta(\theta))v\|_\theta,\end{aligned}$$

with equality attained when w is collinear with $(H_\theta(\theta+tu)-H_\theta(\theta))v$. In other words,

$$\max_{\substack{v,w:\\ \|v\|_\theta,\|w\|_\theta=1}} |\langle w, (H(\theta+tu)-H(\theta))v\rangle| = \max_{\substack{v:\\ \|v\|_\theta=1}} \|(H_\theta(\theta+tu)-H_\theta(\theta))v\|_\theta. \quad \text{(A.8)}$$

Because $H_\theta(\theta+tu)-H_\theta(\theta)$ is a self-adjoint operator with respect to $\langle\cdot,\cdot\rangle_\theta$, it has a spectral decomposition: $(H_\theta(\theta+tu)-H_\theta(\theta))v = \sum_{i=1}^n \lambda_i \langle y_i, v\rangle_\theta y_i$, where the y_i are orthonormal eigenvectors with respect to $\langle\cdot,\cdot\rangle_\theta$. If $v = \sum_{i=1}^n \alpha_i y_i$, then $\|v\|_\theta^2 = \sum_{i=1}^n \alpha_i^2$. It can also be shown that $\langle v, (H_\theta(\theta+tu)-H_\theta(\theta))v\rangle_\theta = \sum_{i=1}^n \alpha_i^2\lambda_i$. Then,

$$\begin{aligned}\max_{\substack{v:\\ \|v\|=1}} |\langle v, (H_\theta(\theta+tu)-H_\theta(\theta))v\rangle_\theta| &= \max_{\substack{\alpha_1,\ldots,\alpha_n:\\ \sum_i \alpha_i^2=1}} \left|\sum_{i=1}^n \alpha_i^2\lambda_i\right| = \max_{i\in\{1,\ldots,n\}} |\lambda_i| \\ &= \max_{\substack{v:\\ \|v\|_\theta=1}} \|(H_\theta(\theta+tu)-H_\theta(\theta))v\|_\theta \\ &= \max_{\substack{v,w:\\ \|v\|_\theta,\|w\|_\theta=1}} |\langle w, (H(\theta+tu)-H(\theta))v\rangle|,\end{aligned}$$

where the final equality is due to (A.8). Since the relation above holds for all $t \neq 0$, it also holds in the limit as $t \to 0$. Thus, we can show that one may take $v = w$ in (A.7) as follows:

$$\begin{aligned}\max_{\substack{u,v,w:\\ \|u\|_\theta,\|v\|_\theta,\|w\|_\theta=1}} |D^3 f(\theta)[u,v,w]| &= \max_{\substack{u,v,w:\\ \|u\|_\theta,\|v\|_\theta,\|w\|_\theta=1}} \lim_{t\to 0} \frac{|\langle w, (H(\theta+tu)-H(\theta))v\rangle|}{|t|} \\ &= \max_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} \lim_{t\to 0} \frac{|\langle v, (H(\theta+tu)-H(\theta))v\rangle|}{|t|} \\ &= \max_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} |D^3 f(\theta)[u,v,v]|. \quad \text{(A.9)}\end{aligned}$$

By Theorem 8.12.4 in Dieudonné [39], $D^3f(\theta)[u,v,v] = D^3f(\theta)[v,u,v]$. Hence,

$$\begin{aligned}\max_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} |D^3f(\theta)[u,v,v]| &= \max_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} |D^3f(\theta)[v,u,v]| \\ &= \max_{\substack{u:\\ \|u\|_\theta=1}} |D^3f(\theta)[u,u,u]|,\end{aligned}$$

where the final equality follows from applying (A.9) again. □

The final lemma needed for the proof of Theorem 2.6 is the following.

Lemma A.10. *Let f be a three times continuously differentiable, strictly convex functional such that* $\operatorname{dom} f$ *is an open subset of $\mathbb{R}^n$, and fix $\theta \in \operatorname{dom} f$. Then,*

$$\limsup_{\Delta\theta\to 0} \frac{\|I - H_\theta(\theta+\Delta\theta)\|_\theta}{\|\Delta\theta\|_\theta} \le 2, \tag{A.10}$$

if and only if $|D^3f(\theta)[u,v,v]| \le 2$ for all $u,v \in \mathbb{R}^n$ such that $\|u\|_\theta, \|v\|_\theta \le 1$.

Proof. Since $H_\theta(\theta) = I$,

$$\begin{aligned}\frac{\|I - H_\theta(\theta+\Delta\theta)\|_\theta}{\|\Delta\theta\|_\theta} &= \frac{\|H_\theta(\theta+\Delta\theta) - H_\theta(\theta)\|_\theta}{\|\Delta\theta\|_\theta} \\ &= \sup_{v:\|v\|_\theta=1} \frac{|\langle v, (H_\theta(\theta+\Delta\theta) - H_\theta(\theta))v\rangle_\theta|}{\|\Delta\theta\|_\theta}.\end{aligned}$$

If (A.10) holds, we have by the max-min inequality

$$\begin{aligned}2 &\ge \inf_{\epsilon>0} \sup_{t:|t|\le\epsilon} \sup_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} \frac{|\langle v, (H_\theta(\theta+tu) - H_\theta(\theta))v\rangle_\theta|}{|t|} \\ &\ge \sup_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} \inf_{\epsilon>0} \sup_{t:|t|\le\epsilon} \frac{|\langle v, (H(\theta+tu) - H(\theta))v\rangle|}{|t|} \\ &= \sup_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} |D^3f(\theta)[u,v,v]|.\end{aligned}$$

Conversely, if (A.10) does not hold, there exists some $\delta > 0$ such that for every $\epsilon > 0$,

$$\sup_{t:|t|\le\epsilon} \sup_{\substack{u,v:\\ \|u\|_\theta,\|v\|_\theta=1}} \frac{|\langle v, (H(\theta+tu) - H(\theta))v\rangle|}{|t|} \ge 2 + \delta,$$

which shows there exist $u, v \in \mathbb{R}^n$ such that $\|u\|_\theta, \|v\|_\theta \leq 1$ and

$$|D^3 f(\theta)[u,v,v]| = \lim_{t\to 0} \frac{|\langle v, (H(\theta+tu) - H(\theta))v\rangle|}{|t|} > 2. \qquad \square$$

B

Spectra of Boltzmann Covariance Matrices

As it turns out, we can use interior point theory to derive bounds on the spectra of covariance matrices of the Boltzmann distribution. Of course, covariance matrices have nonnegative eigenvalues, but for our analysis we need a strictly positive lower bound on the eigenvalues of $\Sigma(\theta)$ for $\theta \in \mathbb{R}^n$. (Recall that we use $\Sigma(\theta)$ to denote the covariance operator of the Boltzmann distribution with parameter θ, see Table 3.1 on page 32.) The analysis below has appeared as Section 3.1 in Badenbroek and De Klerk [8], with only minor differences.

We will denote the smallest and largest eigenvalue of a self-adjoint linear operator A by $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$, respectively. Note that these quantities are independent of the inner product. Recall that for self-adjoint linear operators A, we have $\lambda_{\min}(A) = \min_{v:\|v\|=1} \langle v, Av \rangle$ and $\lambda_{\max}(A) = \max_{v:\|v\|=1} \langle v, Av \rangle$. Moreover, we remind the reader that when we discuss balls, they are presumed to be balls with respect to the reference inner product.

One should note that an upper bound of the spectrum of $\Sigma(\theta)$ is trivial to derive for any $\theta \in \mathbb{R}^n$. If the distribution's support $\mathcal{S}$ is contained in a ball with

radius R, i.e. the diameter of $\mathcal{S}$ is at most $2R$,

$$\lambda_{\max}(\Sigma(\theta)) = \max_{v:\|v\|=1} \mathbb{E}_\theta[\langle X - \mathbb{E}_\theta[X], v\rangle^2] \le (2R)^2, \tag{B.1}$$

where the equality uses Proposition 3.3(ii). Thus, we will focus on bounding the smallest eigenvalue of $\Sigma(\theta)$ from below. Our starting point is the following result from Kannan et al. [57].

Lemma B.1 ([57, Theorem 4.1]). *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $\langle\cdot,\cdot\rangle$ be the Euclidean inner product. If the covariance matrix $\Sigma(0)$ of the uniform distribution over $\mathcal{S}$ satisfies $\Sigma(0) = I$, then $\mathcal{S}$ is contained in a ball with radius $n+1$.*

Through a transformation, we can use this lemma to bound the spectrum of $\Sigma(0)$ from below.

Lemma B.2 ([8, Lemma 3.2]). *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $\langle\cdot,\cdot\rangle$ be the Euclidean inner product. Assume $\mathcal{S}$ contains a ball with radius $r > 0$. Then, $\lambda_{\min}(\Sigma(0)) \ge \frac{1}{4}(\frac{r}{n+1})^2$.*

Proof. The convex body $\mathcal{S}' = \Sigma(0)^{-1/2}\mathcal{S}$ has the property that the uniform distribution over $\mathcal{S}'$ has identity covariance. By Lemma B.1, $\mathcal{S}'$ is contained in a ball of radius $n+1$.

Let $x \in \mathcal{S}$ be the center of the ball with radius r contained in $\mathcal{S}$, and let v be a unit vector such that $\Sigma(0)^{-1/2}v = \lambda_{\max}(\Sigma(0)^{-1/2})v$. Since v is a unit vector, the point $x + rv$ lies in $\mathcal{S}$. Because $\Sigma(0)^{-1/2}x$ and $\Sigma(0)^{-1/2}(x+rv)$ lie in $\mathcal{S}'$, we find $\|\Sigma(0)^{-1/2}((x+rv)-x)\| \le 2(n+1)$, where $2(n+1)$ is the diameter of a ball containing $\mathcal{S}'$. In conclusion,

$$2(n+1) \ge \|r\Sigma(0)^{-1/2}v\| = r\,\lambda_{\max}(\Sigma(0)^{-1/2}) = \frac{r}{\sqrt{\lambda_{\min}(\Sigma(0))}}. \qquad \square$$

With the spectrum of the uniform covariance matrix bounded, we can continue to analyze the smallest eigenvalue of $\Sigma(\theta)$, where $\theta \in \mathbb{R}^n$. To clarify the dependence on the smallest eigenvalue of $\Sigma(0)$, we derive this result for general inner products. This was first done for the Euclidean inner product in [8], where the exponent of the lower bound was slightly worse ($4\sqrt{\vartheta_{f^*}}+1$ instead of $4\sqrt{\vartheta_{f^*}}$).

Theorem B.3 (Based on [8, Theorem 3.3]). *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let f and f^* be its associated log-partition function and entropic barrier, respectively. Assume $\mathcal{S}$ is contained in a ball of radius $R > 0$. Then, for any $\theta \in \mathbb{R}^n$ with $\|\theta\| \le \frac{1}{4R}$,*

$$\lambda_{\min}(\Sigma(\theta)) \ge \tfrac{1}{4}\,\lambda_{\min}(\Sigma(0)),$$

and for all $\theta \in \mathbb{R}^n$ with $\|\theta\| > \frac{1}{4R}$,

$$\lambda_{\min}(\Sigma(\theta)) \ge \tfrac{1}{16}\left(\frac{1}{4R\|\theta\|}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)).$$

Proof. We want to find a lower bound on $\|v\|_\theta$, where $v \in \mathbb{R}^n$ is an arbitrary unit vector. The main idea is to move θ to 0, and use the self-concordance of the log-partition function to bound the change in $\Sigma(\theta)$ during this shift.

If $\|\theta\| \le \frac{1}{4R}$, then (B.1) shows

$$\|\theta - 0\|_0 \le \sqrt{\lambda_{\max}(\Sigma(0))}\|\theta\| \le 2R\|\theta\| \le \tfrac{1}{2} < 1,$$

and thus we may apply the first inequality in (2.1) to show that

$$\|v\|_\theta \ge \|v\|_0(1 - \|\theta - 0\|_0) \ge \tfrac{1}{2}\sqrt{\lambda_{\min}(\Sigma(0))}\|v\|. \tag{B.2}$$

It then follows from (B.2) that

$$\lambda_{\min}(\Sigma(\theta)) = \min_{v:\|v\|=1}\|v\|_\theta^2 \ge \tfrac{1}{4}\,\lambda_{\min}(\Sigma(0)).$$

Next, suppose that $\|\theta\| > \frac{1}{4R}$. Let $\theta_0 := \theta$ and recursively define

$$\theta_k := \left(1 - \frac{1}{2\sqrt{\vartheta_{f^*}}}\right)\theta_{k-1}.$$

Observe that by (3.1), for all k,

$$\|\theta_{k-1} - \theta_k\|_{\theta_{k-1}} = \frac{\|\theta_{k-1}\|_{\theta_{k-1}}}{2\sqrt{\vartheta_{f^*}}} \le \frac{\sqrt{\vartheta_{f^*}}}{2\sqrt{\vartheta_{f^*}}} = \tfrac{1}{2} < 1.$$

Since θ_k and θ_{k-1} are close in the sense above, we can apply self-concordance. By the second inequality of (2.1), for all k, $\|v\|_{\theta_{k-1}} \ge \big(1 - \|\theta_{k-1} - \theta_k\|_{\theta_{k-1}}\big)\|v\|_{\theta_k} \ge \frac{1}{2}\|v\|_{\theta_k}$. Thus, after m steps, we have

$$\|v\|_\theta = \|v\|_{\theta_0} \ge 2^{-m}\|v\|_{\theta_m}. \tag{B.3}$$

Setting

$$m = \left\lceil \frac{\log_2(\frac{1}{4R\|\theta\|})}{\log_2(1-\frac{1}{2\sqrt{\vartheta_{f^*}}})} \right\rceil,$$

we obtain

$$\|\theta_m\| = \left(1-\frac{1}{2\sqrt{\vartheta_{f^*}}}\right)^m \|\theta_0\| \leq \frac{1}{4R\|\theta\|}\|\theta_0\| = \frac{1}{4R}.$$

We may now apply (B.2) to see that $\|v\|_{\theta_m} \geq \frac{1}{2}\sqrt{\lambda_{\min}(\Sigma(0))}\|v\|$. Combined with (B.3), it follows that

$$\|v\|_\theta \geq 2^{-m}\|v\|_{\theta_m} \geq \frac{2^{-m}}{2}\sqrt{\lambda_{\min}(\Sigma(0))}\|v\| = 2^{-m-1}\sqrt{\lambda_{\min}(\Sigma(0))}\|v\|. \tag{B.4}$$

Because m is an integer, we arrive at the following lower bound for 2^{-m-1}:

$$2^{-m-1} \geq \tfrac{1}{4}(4R\|\theta\|)^{1/\log_2(1-1/(2\sqrt{\vartheta_{f^*}}))}.$$

Since $4R\|\theta\| > 1$ by assumption, and $1/\log_2(1-t) \geq -1/t$ for all $t \in (0,1)$, this bound can be developed to

$$2^{-m-1} \geq \tfrac{1}{4}(4R\|\theta\|)^{1/\log_2(1-1/(2\sqrt{\vartheta_{f^*}}))} \geq \tfrac{1}{4}(4R\|\theta\|)^{-2\sqrt{\vartheta_{f^*}}},$$

and we can conclude from (B.4) that

$$\lambda_{\min}(\Sigma(\theta)) = \min_{v:\|v\|=1}\|v\|_\theta^2 \geq \tfrac{1}{16}\left(\frac{1}{4R\|\theta\|}\right)^{4\sqrt{\vartheta_{f^*}}}\lambda_{\min}(\Sigma(0)). \qquad \square$$

For the Euclidean inner product, we can then plug in our lower bound on $\lambda_{\min}(\Sigma(0))$ from Lemma B.2 to obtain the following.

Corollary B.4 (Based on [8, Theorem 3.3]). *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $\langle\cdot,\cdot\rangle$ be the Euclidean inner product. Let f and f^* be the log-partition function and entropic barrier associated with $\mathcal{S}$, respectively. Assume $\mathcal{S}$ contains a ball with radius $r > 0$ and is contained in a ball of radius R. Then, for any $\theta \in \mathbb{R}^n$ with $\|\theta\| \leq \frac{1}{4R}$,*

$$\lambda_{\min}(\Sigma(\theta)) \geq \tfrac{1}{16}\left(\frac{r}{n+1}\right)^2,$$

and for all $\theta \in \mathbb{R}^n$ with $\|\theta\| > \frac{1}{4R}$,

$$\lambda_{\min}(\Sigma(\theta)) \geq \tfrac{1}{64}\left(\frac{1}{4R\|\theta\|}\right)^{4\sqrt{\vartheta_{f^*}}}\left(\frac{r}{n+1}\right)^2.$$

Note that the lower bounds from Theorem B.3 and Corollary B.4 are exponential in $\vartheta_{f^*} = n + o(n)$ (see Theorem 3.4). We can in fact derive a stronger lower bound on $\|\theta\|_\theta = \sqrt{\langle \theta, \Sigma(\theta)\theta \rangle}$ than the one obtained from Theorem B.3 by setting $\nu = \theta/\|\theta\|$. The following result gives such a lower bound that is not exponential in n.

Theorem B.5 (Based on [8, Lemma 3.4])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let f be its associated log-partition function. Then, for all $\theta \in \mathbb{R}^n$,*

$$\|\theta\|_\theta \geq \frac{\sqrt{\lambda_{\min}(\Sigma(0))}\|\theta\|}{1 + \sqrt{\lambda_{\min}(\Sigma(0))}\|\theta\|} \tag{B.5}$$

Proof. Note that the right hand side of (B.5) is always strictly smaller than one. The claim therefore holds automatically for all θ with $\|\theta\|_\theta \geq 1$, and we can assume in the remainder that $\|\theta\|_\theta < 1$. The second inequality in (2.1) gives us

$$\sqrt{\lambda_{\min}(\Sigma(0))}\|\theta\| \leq \|\theta\|_0 \leq \frac{\|\theta\|_\theta}{1 - \|\theta\|_\theta},$$

which can be rewritten as (B.5). □

Again, we can find a more explicit bound for the Euclidean inner product by applying Lemma B.2.

Corollary B.6 ([8, Lemma 3.4])**.** *Let $\mathcal{S} \subset \mathbb{R}^n$ be a convex body, and let $\langle \cdot, \cdot \rangle$ be the Euclidean inner product. Assume $\mathcal{S}$ contains a ball with radius $r > 0$. Let f be the log-partition function associated with $\mathcal{S}$. Then, for all $\theta \in \mathbb{R}^n$,*

$$\|\theta\|_\theta \geq \frac{r\|\theta\|}{2(n+1) + r\|\theta\|}.$$

C

Proofs for the Nonsymmetric Conic Algorithm

In this appendix, we collect the more technical proofs that we omitted in Chapter 10 for the sake of brevity. The results in Section 10.3 are proven in Appendix C.1, the results from Section 10.4 are proven in Appendix C.2, and the results from Section 10.5 are proven in Appendix C.3. Like Chapter 10, this appendix is based on Badenbroek and Dahl [7], but changes various signs without fundamentally changing the results.

C.1 Scaling Matrix

The following lemma from Myklebust and Tunçel [82] is crucial to our proof of Theorem 10.3. Some minor details are different in our setting.

Lemma C.1 ([82, Theorem B.1(4)]). *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a*

self-concordant barrier f. Let $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$. If $\|\zeta^{\mathrm{P}}\|_x < 1$, then

$$\|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} \leq \frac{\mu\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}. \tag{C.1}$$

Proof. Let $v \in \mathbb{R}^n$ be an arbitrary vector, and consider the function $\phi : [0,1] \to \mathbb{R}$ defined as

$$\phi(t) := \langle v, g(x - t\zeta^{\mathrm{P}})\rangle.$$

By Taylor's theorem, we have $\phi(1) = \phi(0) + \phi'(0) + \frac{1}{2}\phi''(r)$ for some $r \in [0,1]$. We first derive an upper bound on $\phi''(r)$. Note that by the Cauchy-Schwarz inequality,

$$\begin{aligned}
\phi''(r) &= \lim_{t\to 0} \frac{\langle v, [H(x-(r+t)\zeta^{\mathrm{P}}) - H(x-r\zeta^{\mathrm{P}})]\zeta^{\mathrm{P}}\rangle}{t} \\
&\leq \lim_{t\to 0} \frac{\|v\|_{x-r\zeta^{\mathrm{P}}}\|[H_{x-r\zeta^{\mathrm{P}}}(x-(r+t)\zeta^{\mathrm{P}}) - I]\zeta^{\mathrm{P}}\|_{x-r\zeta^{\mathrm{P}}}}{t} \\
&\leq \|v\|_{x-r\zeta^{\mathrm{P}}}\|\zeta^{\mathrm{P}}\|_{x-r\zeta^{\mathrm{P}}} \lim_{t\to 0} \frac{\|H_{x-r\zeta^{\mathrm{P}}}(x - r\zeta^{\mathrm{P}} - t\zeta^{\mathrm{P}}) - I\|_{x-r\zeta^{\mathrm{P}}}}{t}.
\end{aligned}$$

Using Theorem 2.2.1 in Renegar [95], it follows that

$$\begin{aligned}
\phi''(r) &\leq \|v\|_{x-r\zeta^{\mathrm{P}}}\|\zeta^{\mathrm{P}}\|_{x-r\zeta^{\mathrm{P}}} \lim_{t\to 0} \frac{1}{t}\left(\frac{1}{(1-t\|\zeta^{\mathrm{P}}\|_{x-r\zeta^{\mathrm{P}}})^2} - 1\right) \\
&= 2\|v\|_{x-r\zeta^{\mathrm{P}}}\|\zeta^{\mathrm{P}}\|_{x-r\zeta^{\mathrm{P}}}^2 \\
&\leq \frac{2\|v\|_x\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3},
\end{aligned}$$

where the final inequality uses self-concordance and $r \leq 1$. Hence,

$$\langle v, H(x)\zeta^{\mathrm{P}} + s/\mu - \tilde{s}\rangle = -\phi'(0) + \phi(1) - \phi(0) = \tfrac{1}{2}\phi''(r) \leq \frac{\|v\|_x\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}.$$

With this upper bound, we can show

$$\|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} = \sup_{v:\|v\|_x\leq 1} \langle v, \mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\rangle \leq \sup_{v:\|v\|_x\leq 1} \mu\|v\|_x \frac{\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3},$$

which proves the claim. □

To prove Theorem 10.3, we will use Proposition 10.2 to relate the desired Löwner orderings to operator norms. We first establish some straightforward properties of the operator norm. For any vectors v, w and invertible linear operator P, we have

$$\|P^{-1}vw^\top\|_P = \sup_{\|u\|_P \le 1} \|P^{-1}v\langle w,u\rangle\|_P = \|v\|_{P^{-1}} \sup_{\|u\|_P\le 1} \langle w,u\rangle = \|v\|_{P^{-1}}\|w\|_{P^{-1}},$$

and therefore, as Myklebust and Tunçel [82] showed,

$$\begin{aligned}\|P^{-1}\left[vv^\top - ww^\top\right]\|_P &= \left\|P^{-1}\left[\tfrac{1}{2}(v+w)(v-w)^\top + \tfrac{1}{2}(v-w)(v+w)^\top\right]\right\|_P \\ &\le \|P^{-1}(v+w)(v-w)^\top\|_P = \|v+w\|_{P^{-1}}\|v-w\|_{P^{-1}}.\end{aligned} \tag{C.2}$$

Moreover, for any $t > 0$ and $Q \in \mathbb{S}^n$,

$$\|(tP)^{-1}Q\|_{tP} = \sup_{\|\sqrt{t}u\|_P \le 1} \frac{\|\sqrt{t}P^{-1}Qu\|_P}{t} = \sup_{\|v\|_P\le 1} \frac{\|P^{-1}Qv\|_P}{t} = \frac{\|P^{-1}Q\|_P}{t}. \tag{C.3}$$

We are now ready to prove Theorem 10.3.

Theorem 10.3 ([7, Theorem 1])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Let $x \in \operatorname{int}\mathcal{K}$ and $s \in \operatorname{int}\mathcal{K}^\circ$, and assume $\|\zeta^{\mathrm{P}}\|_x \le 0.18226$. Let W be defined as in* (10.10)*. Then, the assumptions* (10.17) *are satisfied with values*

$$l^{\mathrm{P}} = 1-\epsilon-\xi, \quad u^{\mathrm{P}} = 1+\epsilon+\xi, \quad l^{\mathrm{D}} = l^{\mathrm{P}}(1-\|\zeta^{\mathrm{P}}\|_x)^2, \quad u^{\mathrm{D}} = \frac{u^{\mathrm{P}}}{(1-\|\zeta^{\mathrm{P}}\|_x)^2},$$

where

$$\epsilon := \frac{1}{\vartheta_f}\left(\|\zeta^{\mathrm{P}}\|_x + \frac{\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}\right)\left(\|\zeta^{\mathrm{P}}\|_x + \frac{\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + 2\sqrt{\vartheta_f}\right)$$

$$\xi := \frac{2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3 - \|\zeta^{\mathrm{P}}\|_x}\left(\frac{4\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + 2\|\zeta^{\mathrm{P}}\|_x + \frac{\left(\frac{3\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3} + \|\zeta^{\mathrm{P}}\|_x\right)^2}{\|\zeta^{\mathrm{P}}\|_x\left(1-\frac{3\|\zeta^{\mathrm{P}}\|_x}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}\right)}\right).$$

Proof. We will try to bound $W - \mu H(x)$ in two steps, each considering two terms from (10.10). First, observe that by (C.2),

$$\begin{aligned}\left\|H(x)^{-1}\left[\frac{ss^\top}{\vartheta_f\mu} - \frac{\mu\tilde{s}\tilde{s}^\top}{\vartheta_f}\right]\right\|_x &\le \frac{\|s-\mu\tilde{s}\|_x^{-1}\|s+\mu\tilde{s}\|_x^{-1}}{\mu\vartheta_f} \\ &\le \frac{\|\zeta^{\mathrm{D}}\|_x^{-1}(\|\zeta^{\mathrm{D}}\|_x^{-1} + 2\mu\|\tilde{s}\|_x^{-1})}{\mu\vartheta_f},\end{aligned} \tag{C.4}$$

where it can be shown that $\|\tilde{s}\|_x^{-1} = \|\tilde{s}\|_{\tilde{s}}^* = \sqrt{\vartheta_f}$ by Theorem 2.12 and (10.5). Moreover, by Lemma C.1,

$$\|\zeta^{\mathrm{D}}\|_x^{-1} \le \|\mu H(x)\zeta^{\mathrm{P}}\|_x^{-1} + \|\mu H(x)\zeta^{\mathrm{P}} - \zeta^{\mathrm{D}}\|_x^{-1} \le \mu\|\zeta^{\mathrm{P}}\|_x + \frac{\mu\|\zeta^{\mathrm{P}}\|_x^2}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}, \quad \text{(C.5)}$$

and therefore, by using (C.3) and (C.4), we can show

$$\left\| [\mu H(x)]^{-1}\left[\frac{ss^\top}{\vartheta_f\mu} - \frac{\mu\tilde{s}\tilde{s}^\top}{\vartheta_f}\right]\right\|_{\mu H(x)} \le \frac{\|\zeta^{\mathrm{D}}\|_x^{-1}(\|\zeta^{\mathrm{D}}\|_x^{-1} + 2\mu\|\tilde{s}\|_x^{-1})}{\mu^2\vartheta_f} \le \epsilon. \quad \text{(C.6)}$$

For the second step, let

$$R \coloneqq \mu H(x) + \frac{ss^\top}{\vartheta_f\mu} - \frac{\mu\tilde{s}\tilde{s}^\top}{\vartheta_f},$$

be a rank-two update to $\mu H(x)$ such that $Rx = -s$ but $R\tilde{x} \neq -\tilde{s}$ in general. Then, as was noted in Myklebust and Tunçel [82, Theorem 6.6], we can write

$$\begin{aligned}
&\frac{\zeta^{\mathrm{D}}(\zeta^{\mathrm{D}})^\top}{\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle} + \frac{\mu[H(x)\tilde{x}+\tilde{\mu}\tilde{s}][H(x)\tilde{x}+\tilde{\mu}\tilde{s}]^\top}{\|\tilde{x}\|_x^2 - \vartheta_f\tilde{\mu}^2} \\
&= \frac{\zeta^{\mathrm{D}}(\zeta^{\mathrm{D}})^\top - R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R}{\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle} + \left(\frac{1}{\|\zeta^{\mathrm{P}}\|_R^2} + \frac{1}{\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle}\right)R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R. \quad \text{(C.7)}
\end{aligned}$$

Since

$$\left|\frac{1}{\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle} + \frac{1}{\|\zeta^{\mathrm{P}}\|_R^2}\right| = \left|\frac{\langle\zeta^{\mathrm{P}},R\zeta^{\mathrm{P}}+\zeta^{\mathrm{D}}\rangle}{\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle\|\zeta^{\mathrm{P}}\|_R^2}\right| \le \frac{\|\zeta^{\mathrm{P}}\|_x\|R\zeta^{\mathrm{P}}+\zeta^{\mathrm{D}}\|_x^{-1}}{|\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle|\|\zeta^{\mathrm{P}}\|_R^2},$$

it will suffice to know upper bounds on $\|\zeta^{\mathrm{D}}-R\zeta^{\mathrm{P}}\|_x^{-1}$, $\|\zeta^{\mathrm{D}}+R\zeta^{\mathrm{P}}\|_x^{-1}$, $\|R\zeta^{\mathrm{P}}\|_x^{-1}$, and $\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle = \mu\vartheta(1-\mu\tilde{\mu}) \le 0$, as well as a lower bound on $\|\zeta^{\mathrm{P}}\|_R^2$. We derive these bounds in a manner similar to [82, Lemma B.4], although minor details again differ.

Using Lemma C.1, is it easy to show, similar to [82, Lemma B.4(3)],

$$\begin{aligned}
\langle\zeta^{\mathrm{P}},\zeta^{\mathrm{D}}\rangle &= \langle\zeta^{\mathrm{P}},-\mu H(x)\zeta^{\mathrm{P}} + \mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\rangle \\
&\le -\mu\|\zeta^{\mathrm{P}}\|_x^2 + \|\zeta^{\mathrm{P}}\|_x\|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} \\
&\le -\mu\|\zeta^{\mathrm{P}}\|_x^2\left(1 - \frac{\|\zeta^{\mathrm{P}}\|_x}{(1-\|\zeta^{\mathrm{P}}\|_x)^3}\right). \quad \text{(C.8)}
\end{aligned}$$

Moreover, as in [82, Lemma B.4(7)],

$$|\langle x, \mu H(x)\zeta^{\mathrm{P}}\rangle| \le |\langle x, \zeta^{\mathrm{D}}\rangle| + \|x\|_x \|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} = 0 + \sqrt{\vartheta_f}\,\|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1},$$

where we used $\langle x, \zeta^{\mathrm{D}}\rangle = \langle x, s - \mu\tilde{s}\rangle = -\mu\vartheta_f + \mu\vartheta_f$ and (10.5). Thus, Lemma C.1 shows (cf. [82, Lemma B.4(8)])

$$\begin{aligned}
\|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} &= \left\| \mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}} - \frac{\mu\langle \tilde{s}, \zeta^{\mathrm{P}}\rangle}{\vartheta_f}\tilde{s} \right\|_x^{-1} \\
&\le \|\mu H(x)\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} + \frac{|\langle x, \mu H(x)\zeta^{\mathrm{P}}\rangle|}{\vartheta_f}\|\tilde{s}\|_{\tilde{s}}^* \\
&\le \frac{2\mu\|\zeta^{\mathrm{P}}\|_x^2}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3}. \qquad \text{(C.9)}
\end{aligned}$$

Combining (C.8) and (C.9) as in [82, Lemma B.4(11)],

$$\begin{aligned}
\|\zeta^{\mathrm{P}}\|_R^2 &= \langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle + \langle \zeta^{\mathrm{P}}, R\zeta^{\mathrm{P}} - \zeta^{\mathrm{D}}\rangle \\
&\ge \mu\|\zeta^{\mathrm{P}}\|_x^2 \left(1 - \frac{\|\zeta^{\mathrm{P}}\|_x}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3}\right) - \frac{2\mu\|\zeta^{\mathrm{P}}\|_x^3}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3} \\
&= \mu\|\zeta^{\mathrm{P}}\|_x^2 \left(1 - \frac{3\|\zeta^{\mathrm{P}}\|_x}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3}\right).
\end{aligned}$$

Finally, as in [82, Lemma B.4(9-10)], it follows from (C.5) and (C.9) that

$$\|R\zeta^{\mathrm{P}}\|_x^{-1} \le \|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} + \|\zeta^{\mathrm{D}}\|_x^{-1} \le \frac{3\mu\|\zeta^{\mathrm{P}}\|_x^2}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3} + \mu\|\zeta^{\mathrm{P}}\|_x,$$

and similarly,

$$\|R\zeta^{\mathrm{P}} - \zeta^{\mathrm{D}}\|_x^* \le \|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1} + 2\|\zeta^{\mathrm{D}}\|_x^{-1} \le \frac{4\mu\|\zeta^{\mathrm{P}}\|_x^2}{(1 - \|\zeta^{\mathrm{P}}\|_x)^3} + 2\mu\|\zeta^{\mathrm{P}}\|_x.$$

We now have the tools to bound the operator norm of (C.7). By (C.2),

$$\begin{aligned}
&\left\| H(x)^{-1}\left[\frac{\zeta^{\mathrm{D}}(\zeta^{\mathrm{D}})^\top - R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R}{\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle} + \left(\frac{1}{\|\zeta^{\mathrm{P}}\|_R^2} + \frac{1}{\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle}\right) R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R \right] \right\|_x \\
&\le \frac{\|R\zeta^{\mathrm{P}} - \zeta^{\mathrm{D}}\|_x^{-1}\|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1}}{|\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle|} + \frac{\|\zeta^{\mathrm{P}}\|_x\|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1}}{|\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle|\|\zeta^{\mathrm{P}}\|_R^2}(\|R\zeta^{\mathrm{P}}\|_x^{-1})^2 \\
&= \frac{\|R\zeta^{\mathrm{P}} + \zeta^{\mathrm{D}}\|_x^{-1}}{|\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}}\rangle|}\left(\|R\zeta^{\mathrm{P}} - \zeta^{\mathrm{D}}\|_x^{-1} + \|\zeta^{\mathrm{P}}\|_x \frac{(\|R\zeta^{\mathrm{P}}\|_x^{-1})^2}{\|\zeta^{\mathrm{P}}\|_R^2} \right) \le \xi\mu.
\end{aligned}$$

Therefore, (C.3) shows that

$$\left\| [\mu H(x)]^{-1} \left[\frac{\zeta^{\mathrm{D}}(\zeta^{\mathrm{D}})^\top - R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R}{\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}} \rangle} + \left(\frac{1}{\|\zeta^{\mathrm{P}}\|_R^2} + \frac{1}{\langle \zeta^{\mathrm{P}}, \zeta^{\mathrm{D}} \rangle} \right) R\zeta^{\mathrm{P}}(\zeta^{\mathrm{P}})^\top R \right] \right\|_{\mu H(x)}$$

is at most ξ. Hence, we see from the triangle inequality and (C.6) that

$$\|[\mu H(x)]^{-1}[W - \mu H(x)]\|_{\mu H(x)} \leq \epsilon + \xi.$$

Proposition 10.2 thus shows

$$(1 - \epsilon - \xi)\mu H(x) \preceq W \preceq (1 + \epsilon + \xi)\mu H(x).$$

Finally, we can use (2.2) to bound $\frac{1}{\mu} H^*(s)^{-1} = \mu H(\mu \tilde{x})$ as

$$(1 - \epsilon - \xi)(1 - \|\zeta^{\mathrm{P}}\|_x)^2 \tfrac{1}{\mu} H^*(s)^{-1} \preceq W \preceq \frac{1 + \epsilon + \xi}{(1 - \|\zeta^{\mathrm{P}}\|_x)^2} \tfrac{1}{\mu} H^*(s)^{-1},$$

similar to [82, Theorem 6.8]. □

C.2 Properties of the Predictor

The simple properties of the predictor can be derived mostly through substitution of various definitions.

Lemma 10.4 ([7, Lemma 5])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) and (A3) hold, and let $\gamma, \varrho \in \mathbb{R}$. Then, the following properties hold:*

(i) $G(z + \gamma \Delta z^{\mathrm{pred}}) = (1 - \gamma(1 - \varrho))G(z)$

(ii) $\langle \Delta x^{\mathrm{pred}}, \Delta s^{\mathrm{pred}} \rangle + \Delta\tau^{\mathrm{pred}} \Delta\kappa^{\mathrm{pred}} = 0$

(iii) $\mu'_+ = (1 - \gamma(1 - \varrho))\mu'$, *or equivalently,* $\langle x + \gamma \Delta x^{\mathrm{pred}}, s + \gamma \Delta s^{\mathrm{pred}} \rangle + (\tau + \gamma \Delta\tau^{\mathrm{pred}})(\kappa + \gamma \Delta\kappa^{\mathrm{pred}}) = (1 - \gamma(1 - \varrho))[\langle x, s \rangle + \tau\kappa]$.

Proof. (i): Follows directly from (10.11a), (10.12a), and the fact that G is a linear operator.

(ii): Using (i) and the linearity of G, we have

$$0 = G(z + \gamma\Delta z^{\text{pred}} - (1-\gamma(1-\varrho))z) = \gamma G(\Delta z^{\text{pred}} + (1-\varrho)z).$$

A skew-symmetry argument shows

$$\begin{aligned} 0 &= \left\langle \begin{bmatrix} \Delta y^{\text{pred}} + (1-\varrho)y \\ \Delta x^{\text{pred}} + (1-\varrho)x \\ \Delta\tau^{\text{pred}} + (1-\varrho)\tau \end{bmatrix}, G(\Delta z^{\text{pred}} + (1-\varrho)z) \right\rangle \\ &= \langle \Delta x^{\text{pred}} + (1-\varrho)x, \Delta s^{\text{pred}} + (1-\varrho)s \rangle \\ &\quad + (\Delta\tau^{\text{pred}} + (1-\varrho)\tau)(\Delta\kappa^{\text{pred}} + (1-\varrho)\kappa). \end{aligned}$$

Therefore, we can write

$$\begin{aligned} \langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}} \rangle + \Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} = -(1-\varrho)^2[\langle x, s\rangle + \tau\kappa] - (1-\varrho)[\langle x, \Delta s^{\text{pred}}\rangle \\ + \langle \Delta x^{\text{pred}}, s\rangle + \tau\Delta\kappa^{\text{pred}} + \Delta\tau^{\text{pred}}\kappa]. \end{aligned} \tag{C.10}$$

From (10.11c) and (10.12c), we can see that

$$\begin{aligned} \langle x, \Delta s^{\text{pred}} \rangle + \langle \Delta x^{\text{pred}}, s\rangle &= \langle x, \Delta s^{\text{aff}} + \varrho\Delta s^{\text{cen}}\rangle - \langle \Delta x^{\text{aff}} + \varrho\Delta x^{\text{cen}}, Wx\rangle \\ &= \langle x, \Delta s^{\text{aff}} - W\Delta x^{\text{aff}}\rangle + \varrho\langle x, \Delta s^{\text{cen}} - W\Delta x^{\text{cen}}\rangle \\ &= \langle x, -s\rangle + \varrho\langle x, \mu'\tilde{s}\rangle = -\varrho\mu'\vartheta_f - \langle x, s\rangle. \end{aligned}$$

Moreover, (10.11b) and (10.12b) show that

$$\begin{aligned} \tau\Delta\kappa^{\text{pred}} + \Delta\tau^{\text{pred}}\kappa &= \tau(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}}) + (\Delta\tau^{\text{aff}} + \varrho\Delta\tau^{\text{cen}})\kappa \\ &= \tau\Delta\kappa^{\text{aff}} + \Delta\tau^{\text{aff}}\kappa + \varrho(\tau\Delta\kappa^{\text{cen}} + \Delta\tau^{\text{cen}}\kappa) \\ &= -\tau\kappa - \varrho\mu'. \end{aligned}$$

Combining the above, we get

$$\begin{aligned} \langle x, \Delta s^{\text{pred}} \rangle + \langle \Delta x^{\text{pred}}, s\rangle + \tau\Delta\kappa^{\text{pred}} + \Delta\tau^{\text{pred}}\kappa &= -\varrho\mu'\vartheta_f - \langle x, s\rangle - \tau\kappa - \varrho\mu' \\ &= (\varrho - 1)[\langle x, s\rangle + \tau\kappa], \end{aligned} \tag{C.11}$$

by definition of μ'. Hence, (C.10) must be zero.

(iii): Using (ii) to substitute $\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}} \rangle + \Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}}$, we get

$$\begin{aligned}
&\langle x + \gamma\Delta x^{\text{pred}}, s + \gamma\Delta s^{\text{pred}} \rangle + (\tau + \gamma\Delta\tau^{\text{pred}})(\kappa + \gamma\Delta\kappa^{\text{pred}}) \\
&= \langle x, s \rangle + \tau\kappa + \gamma[\langle x, \Delta s^{\text{pred}} \rangle + \langle \Delta x^{\text{pred}}, s \rangle + \tau\Delta\kappa^{\text{pred}} + \Delta\tau^{\text{pred}}\kappa] + \gamma^2 0 \\
&= (1 - \gamma(1-\varrho))[\langle x, s \rangle + \tau\kappa],
\end{aligned}$$

where the final equality is due to (C.11). □

As we will see, the norms of the predictors depend on $\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}}$. We first show that $\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} \geq (\tau\kappa + \varrho\mu')^2/(4\tau\kappa)$.

Lemma C.2 ([7, Lemma 6]). *Let $\tau, \mu' > 0$, $\kappa < 0$, and $\varrho \geq 0$. Then, the optimization problem*

$$\begin{aligned}
\min_{\Delta\kappa^{\text{aff}}, \Delta\kappa^{\text{cen}}, \Delta\tau^{\text{aff}}, \Delta\tau^{\text{cen}}} \quad & (\Delta\tau^{\text{aff}} + \varrho\Delta\tau^{\text{cen}})(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}}) \\
\text{subject to} \quad & \tau\Delta\kappa^{\text{aff}} + \kappa\Delta\tau^{\text{aff}} = -\tau\kappa \\
& \tau\Delta\kappa^{\text{cen}} + \kappa\Delta\tau^{\text{cen}} = -\mu',
\end{aligned}$$

has optimal value $(\tau\kappa + \varrho\mu')^2/(4\tau\kappa)$.

Proof. The constraints show that $\Delta\tau^{\text{aff}} = -\tau - \frac{\tau}{\kappa}\Delta\kappa^{\text{aff}}$ and $\Delta\tau^{\text{cen}} = -\frac{\mu'}{\kappa} - \frac{\tau}{\kappa}\Delta\kappa^{\text{cen}}$. Then, the objective is equal to

$$\begin{aligned}
&(\Delta\tau^{\text{aff}} + \varrho\Delta\tau^{\text{cen}})(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}}) \\
&= \left(-\tau - \frac{\tau}{\kappa}\Delta\kappa^{\text{aff}} + \varrho\left(-\frac{\mu'}{\kappa} - \frac{\tau}{\kappa}\Delta\kappa^{\text{cen}}\right)\right)(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}}) \\
&= -\frac{\tau}{\kappa}(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}})^2 - (\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}})\left(\tau + \varrho\frac{\mu'}{\kappa}\right).
\end{aligned}$$

This expression is minimized if and only if the first order condition

$$-\frac{2\tau}{\kappa}(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}}) - \left(\tau + \varrho\frac{\mu'}{\kappa}\right) = 0$$

holds. Hence, all minimizers satisfy $\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}} = -\frac{1}{2}(\varrho\mu'/\tau + \kappa)$. Therefore, the optimal value is

$$\begin{aligned}
&-\frac{\tau}{\kappa}(\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}})^2 - (\Delta\kappa^{\text{aff}} + \varrho\Delta\kappa^{\text{cen}})\left(\tau + \varrho\frac{\mu'}{\kappa}\right) \\
&= -\frac{\tau}{4\kappa}\left(\frac{\varrho\mu'}{\tau} + \kappa\right)^2 + \tfrac{1}{2}\left(\frac{\varrho\mu'}{\tau} + \kappa\right)\left(\tau + \varrho\frac{\mu'}{\kappa}\right) = \frac{(\tau\kappa + \varrho\mu')^2}{4\tau\kappa}.
\end{aligned}$$

□

We are now ready to bound the norm of the predictor.

Theorem 10.5 ([7, Theorem 2])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y, x, \tau, s, \kappa)$ such that (A1) to (A5) hold for some $\alpha \in (0, 1]$ and $\delta \in [0, 1)$. Let $l^{\mathrm{P}}, u^{\mathrm{D}} > 0$ be bounds such that* (10.17) *holds, and let $\varrho \in \mathbb{R}$. Then, the primal and dual predictors Δx^{pred} and Δs^{pred} satisfy*

$$\|\Delta x^{\mathrm{pred}}\|_W^2 + \|\Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 \leq \mu' \left[\vartheta_f \left(1 - 2\varrho + \frac{\varrho^2}{\alpha} \right) + 1 - \tfrac{1}{2}\alpha - \varrho + \frac{\varrho^2}{2\alpha} \right], \tag{10.19}$$

and

$$l^{\mathrm{P}} \|\Delta x^{\mathrm{pred}}\|_x^2 + \frac{1}{u^{\mathrm{D}}} (\|\Delta s^{\mathrm{pred}}\|_s^*)^2 \leq \frac{1}{\alpha} \left[\vartheta_f \left(1 - 2\varrho + \frac{\varrho^2}{\alpha} \right) + 1 - \tfrac{1}{2}\alpha - \varrho + \frac{\varrho^2}{2\alpha} \right]. \tag{10.20}$$

Proof. Note that for any $v, w \in \mathbb{R}^n$ with $\langle v, w \rangle = 0$, we have $\|v - w\|^2 = \|v\|^2 + \|w\|^2$. As shown by Lemma 10.4(ii), $\langle (W^{1/2} \Delta x^{\mathrm{pred}}, \Delta\tau^{\mathrm{pred}}), (W^{-1/2} \Delta s^{\mathrm{pred}}, \Delta\kappa^{\mathrm{pred}}) \rangle = 0$, so

$$\begin{aligned} &\|W \Delta x^{\mathrm{pred}} - \Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 + (\Delta\tau^{\mathrm{pred}} - \Delta\kappa^{\mathrm{pred}})^2 \\ &= \|\Delta x^{\mathrm{pred}}\|_W^2 + \|\Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 + (\Delta\tau^{\mathrm{pred}})^2 + (\Delta\kappa^{\mathrm{pred}})^2. \end{aligned}$$

By (10.11c), (10.12c), and (10.13), $W \Delta x^{\mathrm{pred}} - \Delta s^{\mathrm{pred}} = s - \varrho\mu' \tilde{s}$. Therefore,

$$\begin{aligned} \|\Delta x^{\mathrm{pred}}\|_W^2 + \|\Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 &= \|s - \varrho\mu'\tilde{s}\|_{W^{-1}}^2 - 2\Delta\tau^{\mathrm{pred}} \Delta\kappa^{\mathrm{pred}} \\ &= -\langle x, s \rangle - 2\varrho\mu'\vartheta_f + \varrho^2 (\mu')^2 \tilde{\mu} \vartheta_f - 2\Delta\tau^{\mathrm{pred}} \Delta\kappa^{\mathrm{pred}}, \end{aligned}$$

where the final equality used $\langle x, \tilde{s} \rangle = \langle x, g(x) \rangle = -\vartheta_f$ and the definition of $\tilde{\mu}$. By Lemma C.2,

$$\begin{aligned} &\|\Delta x^{\mathrm{pred}}\|_W^2 + \|\Delta s^{\mathrm{pred}}\|_{W^{-1}}^2 \\ &\leq -\langle x, s \rangle - 2\varrho\mu'\vartheta_f + \varrho^2 (\mu')^2 \tilde{\mu} \vartheta_f - \frac{(\tau\kappa + \varrho\mu')^2}{2\tau\kappa} \\ &= -\langle x, s \rangle - 2\varrho\mu'\vartheta_f + \varrho^2 (\mu')^2 \tilde{\mu} \vartheta_f - \tfrac{1}{2}\tau\kappa - \varrho\mu' - \frac{\varrho^2 (\mu')^2}{2\tau\kappa}. \end{aligned}$$

To bound all the above in terms of μ', we use (A2) and (A4):

$$\begin{aligned}
&\|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2 \\
&\leq -(\langle x,s\rangle + \tau\kappa) + \tfrac{1}{2}\tau\kappa - 2\varrho\mu'\vartheta_f + \varrho^2\mu'\frac{\vartheta_f}{\alpha} - \varrho\mu' + \frac{\varrho^2\mu'}{2\alpha} \\
&\leq \mu'\left[(\vartheta_f+1) - \tfrac{1}{2}\alpha - 2\varrho\vartheta_f + \varrho^2\frac{\vartheta_f}{\alpha} - \varrho + \frac{\varrho^2}{2\alpha}\right],
\end{aligned}$$

which proves (10.19). Towards proving (10.20), we note that by (10.17) and Lemma 2.4,

$$l^{\text{P}}\|\Delta x^{\text{pred}}\|_x^2 + \frac{1}{u^{\text{D}}}(\|\Delta s^{\text{pred}}\|_s^*)^2 \leq \frac{\|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2}{\mu}.$$

The claim now follows from Lemma 10.1 and (10.19). □

The following is a straightforward consequence of Theorem 10.5.

Corollary C.3 ([7, Corollary 2]). *Under the conditions of Theorem 10.5,*

$$|\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle| \leq \tfrac{1}{2}\mu'\Pi \leq \frac{\Pi\mu}{2\alpha}.$$

Proof. Note that

$$0 \leq \|W\Delta x^{\text{pred}} + \Delta s^{\text{pred}}\|_{W^{-1}}^2 = \|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2 + 2\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle,$$

which implies $-\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle \leq \frac{1}{2}[\|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2]$. The bound then follows from (10.19). By considering $\|W\Delta x^{\text{pred}} - \Delta s^{\text{pred}}\|_{W^{-1}}^2$, one can show similarly that $\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle \leq \frac{1}{2}[\|\Delta x^{\text{pred}}\|_W^2 + \|\Delta s^{\text{pred}}\|_{W^{-1}}^2]$. The final inequality is due to Lemma 10.1. □

As a second consequence, we can bound the difference between μ_+ and μ, in the following sense.

Corollary C.4 ([7, Corollary 3]). *Under the conditions of Theorem 10.5,*

$$\left|1 - \frac{\mu_+}{\mu} + \gamma\left(\varrho\frac{\mu'}{\mu} - 1\right)\right| = \left|\frac{\gamma^2}{\mu\vartheta_f}\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle\right| \leq \frac{\gamma^2\Pi}{2\alpha\vartheta_f}.$$

Proof. By the definition (10.13),

$$\begin{aligned}\frac{\mu_+}{\mu} &= -\frac{\langle x+\gamma\Delta x^{\text{pred}}, s+\gamma\Delta s^{\text{pred}}\rangle}{\mu\vartheta_f} \\ &= 1+\frac{\gamma}{\mu\vartheta_f}\langle x, W\Delta x^{\text{pred}}-\Delta s^{\text{pred}}\rangle - \frac{\gamma^2}{\mu\vartheta_f}\langle \Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle.\end{aligned}$$

It follows from (10.11c), (10.12c), and (10.13) that $W\Delta x^{\text{pred}}-\Delta s^{\text{pred}} = s-\varrho\mu'\tilde{s}$. This proves the desired equality. The inequality follows from Corollary C.3. □

We now analyze τ_+ and κ_+, which covers assumptions (A2) and (A3).

Lemma 10.6 ([7, Lemma 7])**.** *Let $\mathcal{K}\subset\mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z=(y,x,\tau,s,\kappa)$ such that (A1) to (A5) hold for some $\alpha\in(0,1]$ and $\delta\in[0,1)$. Let $\gamma\le 1$ and $\varrho\in\mathbb{R}$. Then,*

$$\tau_+\kappa_+ \le -\frac{\mu'_+}{1-\gamma(1-\varrho)}\left[\alpha(1-\gamma)+\gamma\varrho-\tfrac{1}{2}\gamma^2\Pi\right]. \tag{10.24}$$

If $\alpha<1$ or $\varrho<1$, and

$$0\le\gamma<\frac{\alpha-\varrho+\sqrt{(\alpha-\varrho)^2+2\alpha\Pi}}{\Pi}, \tag{10.25}$$

then $\tau_+>0$ and $\kappa_+<0$.

Proof. Recall that $z_+ = z+\gamma\Delta z^{\text{pred}}$. By (10.11b), (10.12b), and (10.13),

$$\begin{aligned}\tau_+\kappa_+ &= \tau\kappa+\gamma(\tau\Delta\kappa^{\text{pred}}+\kappa\Delta\tau^{\text{pred}})+\gamma^2\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} \\ &= \tau\kappa+\gamma(-\tau\kappa-\varrho\mu')+\gamma^2\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} \\ &\le -(1-\gamma)\alpha\mu'-\gamma\varrho\mu'+\gamma^2\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}},\end{aligned}$$

where the inequality is due to (A2). Hence, the main remaining task is to upper bound $\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}}$. By Lemma 10.4(ii), $\Delta\tau^{\text{pred}}\Delta\kappa^{\text{pred}} = -\langle\Delta x^{\text{pred}}, \Delta s^{\text{pred}}\rangle$. It therefore follows from Corollary C.3 that $\tau_+\kappa_+\le -\mu'[\alpha(1-\gamma)+\gamma\varrho-\frac{1}{2}\gamma^2\Pi]$. Lemma 10.4(iii) then proves the bound (10.24).

It can be seen from (10.21) that $1-2\varrho+\varrho^2/\alpha\le 0$ only if $\alpha=\varrho=1$. To avoid trivial difficulties, we therefore assume that $\alpha<1$ or $\varrho<1$. Then,

$\Pi = \vartheta_f\left(1-2\varrho+\varrho^2/\alpha\right)+1-\frac{1}{2}\alpha-\varrho+\frac{1}{2}\varrho^2/\alpha$ is positive by (10.22). The zeros of the right hand side of (10.24) in γ are

$$\frac{\alpha-\varrho \pm \sqrt{(\alpha-\varrho)^2+2\alpha\Pi}}{\Pi}.$$

We see that the square root above is greater than $|\alpha-\varrho|$, and the denominator is positive. Thus, for all γ satisfying (10.25), the upper bound (10.24) on $\tau_+\kappa_+$ is negative.

If $\tau_+\kappa_+ < 0$, then $\tau_+ > 0$ and $\kappa_+ < 0$, or $\tau_+ < 0$ and $\kappa_+ > 0$. For the sake of contradiction, suppose that $\tau_+ < 0$ and $\kappa_+ > 0$. Since $\gamma_0 \mapsto \tau + \gamma_0\Delta\tau^{\text{pred}}$ is continuous and $\tau > 0$, the intermediate value theorem implies that there exists some $\gamma_0 \in (0,\gamma)$ where $\tau+\gamma_0\Delta\tau^{\text{pred}} = 0$. But for this γ_0, we have $(\tau+\gamma_0\Delta\tau^{\text{pred}})(\kappa+\gamma_0\Delta\kappa^{\text{pred}}) = 0$, while the upper bound (10.24) is negative for all $\gamma_0 \in (0,\gamma)$. Thus, we have a contradiction, and therefore $\tau_+ > 0$ and $\kappa_+ < 0$. □

We close this section with the upper bound on $\|\zeta_+^{\text{P}}\|_{x_+}$, which relates to assumption (A5).

Lemma 10.7. *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z = (y,x,\tau,s,\kappa)$ such that (A1) to (A5) hold for some $\alpha \in (0,1]$ and $\delta \in [0,1)$. Assume* (10.17) *holds with $u^{\text{D}} = (1+\epsilon)/r$ and $l^{\text{D}} = r(1-\epsilon)$ for some $r \in (0,1]$ and $\epsilon \geq 0$. Let $\gamma \in [0, \sqrt{\alpha\min\{l^{\text{P}}, 1/u^{\text{P}}\}/\Pi})$ and $\varrho \in \mathbb{R}$. Then,*

$$\|\zeta_+^{\text{P}}\|_{x_+} \leq \frac{1}{1-\gamma\sqrt{\Pi/(l^{\text{P}}\alpha)}}\Bigg[(1-\gamma)\|\zeta^{\text{P}}\|_x + \frac{\gamma^2\Pi}{2\alpha\sqrt{\vartheta_f}(1-\|\zeta^{\text{P}}\|_x)} + \frac{\gamma\sqrt{\Pi}}{\sqrt{l^{\text{P}}\alpha}}\left(\frac{u^{\text{D}}(1+\varsigma)}{1-\gamma\sqrt{u^{\text{D}}\Pi/\alpha}}-1\right)\Bigg],$$

where

$$\varsigma := \frac{\gamma^2\Pi}{2\alpha\vartheta_f} + \gamma\max\left\{1-\frac{\varrho}{2-\alpha}, \frac{\varrho}{\alpha}-1\right\}.$$

Proof. By definition, we have

$$\zeta_+^{\text{P}} = x_+ - \mu_+\tilde{x}_+ = x+\gamma\Delta x^{\text{pred}} - \mu_+ g^*\left(s+\gamma\Delta s^{\text{pred}}\right).$$

It can be shown using (10.11c), (10.12c), and (10.13) that $\Delta x^{\text{pred}} = \varrho\mu'\tilde{x} - x + W^{-1}\Delta s^{\text{pred}}$. Therefore,

$$\begin{aligned} x + \gamma\Delta x^{\text{pred}} &= x + \gamma\left(\varrho\mu'\tilde{x} - x\right) + \gamma W^{-1}\Delta s^{\text{pred}} \\ &= (1-\gamma)(x - \mu\tilde{x}) + \left((1-\gamma)\mu + \gamma\varrho\mu'\right)\tilde{x} + \gamma W^{-1}\Delta s^{\text{pred}}. \end{aligned}$$

Moreover, the fundamental theorem of calculus (see e.g. Renegar [95, Theorem 1.5.6]) implies

$$\begin{aligned} &\mu_+ g^*\left(s + \gamma\Delta s^{\text{pred}}\right) \\ &= \mu_+\left[g^*(s) + \int_0^1 H^*\left(s + t\gamma\Delta s^{\text{pred}}\right)\gamma\Delta s^{\text{pred}}\,\mathrm{d}t\right] \\ &= \mu_+\tilde{x} + \gamma\int_0^1 \left[\mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) - W^{-1}\right]\Delta s^{\text{pred}}\,\mathrm{d}t + \gamma W^{-1}\Delta s^{\text{pred}}. \end{aligned}$$

Combining the above observations yields

$$\begin{aligned} \zeta_+^{\text{P}} &= (1-\gamma)(x - \mu\tilde{x}) + \left((1-\gamma)\mu + \gamma\varrho\mu' - \mu_+\right)\tilde{x} \\ &\quad - \gamma\int_0^1 \left[\mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) - W^{-1}\right]\Delta s^{\text{pred}}\,\mathrm{d}t \\ &= (1-\gamma)\zeta^{\text{P}} + \left(1 - \gamma + \gamma\varrho\frac{\mu'}{\mu} - \frac{\mu_+}{\mu}\right)\mu\tilde{x} \qquad \text{(C.12)} \\ &\quad - \gamma\int_0^1 \left[\mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) - W^{-1}\right]\Delta s^{\text{pred}}\,\mathrm{d}t. \qquad \text{(C.13)} \end{aligned}$$

We will bound each of the three terms in (C.12) and (C.13) separately in $\|\cdot\|_x$. Of course, $\|\zeta^{\text{P}}\|_x$ is known to be bounded by assumption (A5).

To bound the second term of (C.12), note that by Corollary C.4,

$$\left|1 - \gamma + \gamma\varrho\frac{\mu'}{\mu} - \frac{\mu_+}{\mu}\right| \le \frac{\gamma^2\Pi}{2\alpha\vartheta_f}.$$

Since $\|\mu\tilde{x}\|_x \le \|\mu\tilde{x}\|_{\mu\tilde{x}}/(1 - \|\zeta^{\text{P}}\|_x) = \sqrt{\vartheta_f}/(1 - \|\zeta^{\text{P}}\|_x)$ by self-concordance and logarithmic homogeneity,

$$\left\|\left(1 - \gamma + \gamma\varrho\frac{\mu'}{\mu} - \frac{\mu_+}{\mu}\right)\mu\tilde{x}\right\|_x \le \frac{\gamma^2\Pi}{2\alpha\sqrt{\vartheta_f}(1 - \|\zeta^{\text{P}}\|_x)}. \qquad \text{(C.14)}$$

To bound (C.13), we will bound $\mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right)$ in terms of W^{-1} to invoke Proposition 10.2. First, note that by Corollary C.4 and Lemma 10.1,

$$\left|\frac{\mu_+}{\mu} - 1\right| \leq \frac{\gamma^2\Pi}{2\alpha\vartheta_f} + \gamma\left|\varrho\frac{\mu'}{\mu} - 1\right| \leq \frac{\gamma^2\Pi}{2\alpha\vartheta_f} + \gamma\max\left\{1 - \frac{\varrho}{2-\alpha}, \frac{\varrho}{\alpha} - 1\right\} = \varsigma.$$

Hence, we have

$$(1-\varsigma)\mu H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) \preceq \mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) \preceq (1+\varsigma)\mu H^*\left(s + t\gamma\Delta s^{\text{pred}}\right).$$

Next, we apply self-concordance as in (2.2) to see that

$$H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) \preceq \frac{1}{(1 - t\gamma\|\Delta s^{\text{pred}}\|_s^*)^2} H^*(s) \preceq \frac{1}{(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2} H^*(s),$$

by Theorem 10.5, and similarly $H^*(s + t\gamma\Delta s^{\text{pred}}) \succeq (1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2 H^*(s)$. Combined with (10.17), we thus get

$$\begin{aligned}(1-\varsigma)\left(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha}\right)^2 l^{\text{D}} W^{-1} &\preceq \mu_+ H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) \\ &\preceq \frac{u^{\text{D}}(1+\varsigma)}{(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2} W^{-1}.\end{aligned}$$

With these bounds, it follows from Proposition 10.2 that

$$\begin{aligned}&\left\|\mu_+ W H^*\left(s + t\gamma\Delta s^{\text{pred}}\right) - I\right\|_{W^{-1}} \\ &\leq \max\left\{1 - (1-\varsigma)\left(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha}\right)^2 l^{\text{D}}, \frac{u^{\text{D}}(1+\varsigma)}{(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2} - 1\right\} \\ &= \frac{u^{\text{D}}(1+\varsigma)}{(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2} - 1,\end{aligned}$$

where the value of the maximization is determined by the fact that for all $\epsilon, \varsigma \geq 0$ and $r \in (0, 1]$,

$$1 - r(1-\varsigma)(1-\epsilon) \leq \frac{(1+\varsigma)(1+\epsilon)}{r} - 1.$$

Using (10.17) and Theorem 10.5, we can thus bound the local norm of (C.13) as

follows:

$$\begin{aligned}
&\left\| \gamma \int_0^1 \left[\mu_+ H^*\left(s + t\gamma \Delta s^{\text{pred}}\right) - W^{-1} \right] \Delta s^{\text{pred}} \, \mathrm{d}t \right\|_x \\
&\leq \frac{\gamma}{\sqrt{l^{\text{P}}\mu}} \int_0^1 \left\| \left[\mu_+ H^*\left(s + t\gamma \Delta s^{\text{pred}}\right) - W^{-1} \right] \Delta s^{\text{pred}} \right\|_W \mathrm{d}t \\
&\leq \frac{\gamma}{\sqrt{l^{\text{P}}\mu}} \int_0^1 \left\| \mu_+ W H^*\left(s + t\gamma \Delta s^{\text{pred}}\right) - I \right\|_{W^{-1}} \|\Delta s^{\text{pred}}\|_{W^{-1}} \, \mathrm{d}t \\
&\leq \frac{\gamma\sqrt{\mu'\Pi}}{\sqrt{l^{\text{P}}\mu}} \int_0^1 \left(\frac{u^{\text{D}}(1+\varsigma)}{(1 - t\gamma\sqrt{u^{\text{D}}\Pi/\alpha})^2} - 1 \right) \mathrm{d}t \leq \frac{\gamma\sqrt{\Pi}}{\sqrt{l^{\text{P}}\alpha}} \left(\frac{u^{\text{D}}(1+\varsigma)}{1 - \gamma\sqrt{u^{\text{D}}\Pi/\alpha}} - 1 \right),
\end{aligned}$$

where the final inequality uses Lemma 10.1.

If we combine the above with the bound (C.14), it can be seen from (C.12) and (C.13) that

$$\|\zeta_+^{\text{P}}\|_x \leq (1-\gamma)\|\zeta^{\text{P}}\|_x + \frac{\gamma^2\Pi}{2\alpha\sqrt{\vartheta_f}(1 - \|\zeta^{\text{P}}\|_x)} + \frac{\gamma\sqrt{\Pi}}{\sqrt{l^{\text{P}}\alpha}} \left(\frac{u^{\text{D}}(1+\varsigma)}{1 - \gamma\sqrt{u^{\text{D}}\Pi/\alpha}} - 1 \right).$$

Since $\|x - x_+\|_x = \gamma\|\Delta x^{\text{pred}}\|_x \leq \gamma\sqrt{\Pi/(l^{\text{P}}\alpha)}$ by Theorem 10.5, the proof is completed by applying self-concordance. □

C.3 Properties of the Corrector

As for the predictor, some properties of the corrector can be derived directly from the definitions.

Lemma 10.8 ([7, Lemma 9])**.** *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+ = (y_+, x_+, \tau_+, s_+, \kappa_+)$ such that $x_+ \in \operatorname{int}\mathcal{K}$, $s_+ \in \operatorname{int}\mathcal{K}^\circ$, $\tau_+ > 0$, and $\kappa_+ < 0$. Then,*

(i) $G(z_+ + \Delta z_+^{\text{cor}}) = G(z_+)$

(ii) $\langle x_+, \Delta s_+^{\text{cor}} \rangle + \langle \Delta x_+^{\text{cor}}, s_+ \rangle = 0$

(iii) $\langle \Delta x_+^{\text{cor}}, \Delta s_+^{\text{cor}} \rangle + \Delta\tau_+^{\text{cor}}\Delta\kappa_+^{\text{cor}} = 0$

(iv) $\langle x_+ + \Delta x_+^{\rm cor}, s_+ + \Delta s_+^{\rm cor}\rangle + (\tau_+ + \Delta\tau_+^{\rm cor})(\kappa_+ + \Delta\kappa_+^{\rm cor}) = \langle x_+, s_+\rangle + \tau_+\kappa_+$. *In other words,* $\mu'_{++} = \mu'_+$

(v) $\|\Delta x_+^{\rm cor}\|_{W_+}^2 + \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}^2 \le \|\zeta_+^{\rm P}\|_{W_+}^2$

(vi) $|\langle \Delta x_+^{\rm cor}, \Delta s_+^{\rm cor}\rangle| \le \frac{1}{2}\|\zeta_+^{\rm P}\|_{W_+}^2$

(vii) $(\tau_+ + \Delta\tau_+^{\rm cor})(\kappa_+ + \Delta\kappa_+^{\rm cor}) \le \tau_+\kappa_+ + \frac{1}{2}\|\zeta_+^{\rm P}\|_{W_+}^2$. *If* $\tau_+\kappa_+ + \frac{1}{2}\|\zeta_+^{\rm P}\|_{W_+}^2 < 0$, *then* $\tau_{++} > 0$ *and* $\kappa_{++} < 0$.

Proof. (i): Follows directly from (10.16a) and the fact that G is a linear operator.

(ii): By (10.16c) and the fact that $W_+x_+ = -s_+$,

$$\begin{aligned}\langle x_+, \Delta s_+^{\rm cor}\rangle + \langle \Delta x_+^{\rm cor}, s_+\rangle &= \langle x_+, W_+\Delta x_+^{\rm cor} + \mu_+\tilde{s}_+ - s_+\rangle + \langle \Delta x_+^{\rm cor}, s_+\rangle \\ &= \langle x_+, \mu_+\tilde{s}_+ - s_+\rangle,\end{aligned}$$

which is zero because $\langle x_+, \tilde{s}_+\rangle = -\vartheta_f$.

(iii): From (10.16a) and skew-symmetry, it can be seen that

$$0 = \left\langle \begin{bmatrix} \Delta y_+^{\rm cor} \\ \Delta x_+^{\rm cor} \\ \Delta\tau_+^{\rm cor}\end{bmatrix}, G(\Delta z_+^{\rm cor}) \right\rangle = \langle \Delta x_+^{\rm cor}, \Delta s_+^{\rm cor}\rangle + \Delta\tau_+^{\rm cor}\Delta\kappa_+^{\rm cor}.$$

(iv): A simple expansion shows

$$\langle x_+ + \Delta x_+^{\rm cor}, s_+ + \Delta s_+^{\rm cor}\rangle + (\tau_+ + \Delta\tau_+^{\rm cor})(\kappa_+ + \Delta\kappa_+^{\rm cor}) - [\langle x_+, s_+\rangle + \tau_+\kappa_+]$$

equals

$$[\langle x_+, \Delta s_+^{\rm cor}\rangle + \langle \Delta x_+^{\rm cor}, s_+\rangle] + [\tau_+\Delta\kappa_+^{\rm cor} + \kappa_+\Delta\tau_+^{\rm cor}] + [\langle \Delta x_+^{\rm cor}, \Delta s_+^{\rm cor}\rangle + \Delta\tau_+^{\rm cor}\Delta\kappa_+^{\rm cor}],$$

where the first term is zero by (ii), the second term is zero by (10.16b), and the third term is zero by (iii).

(v): Recall that for any $v, w \in \mathbb{R}^n$ such that $\langle v, w\rangle = 0$, we have $\|v - w\|^2 = \|v\|^2 + \|w\|^2$. By (iii), we have $\langle (W_+^{1/2}\Delta x_+^{\rm cor}, \Delta\tau_+^{\rm cor}), (W_+^{-1/2}\Delta s_+^{\rm cor}, \Delta\kappa_+^{\rm cor})\rangle = 0$, so

$$\begin{aligned}&\|W_+\Delta x_+^{\rm cor} - \Delta s_+^{\rm cor}\|_{W_+^{-1}}^2 + (\Delta\tau_+^{\rm cor} - \Delta\kappa_+^{\rm cor})^2 \\ &= \|\Delta x_+^{\rm cor}\|_{W_+}^2 + \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}^2 + (\Delta\tau_+^{\rm cor})^2 + (\Delta\kappa_+^{\rm cor})^2.\end{aligned}$$

Subtracting $(\Delta\tau_+^{\mathrm{cor}})^2+(\Delta\kappa_+^{\mathrm{cor}})^2$ from both sides and using $W_+\Delta x_+^{\mathrm{cor}}-\Delta s_+^{\mathrm{cor}}=-\zeta_+^{\mathrm{D}}$, we get

$$\|\zeta_+^{\mathrm{D}}\|_{W_+^{-1}}^2-2\Delta\tau_+^{\mathrm{cor}}\Delta\kappa_+^{\mathrm{cor}}=\|\Delta x_+^{\mathrm{cor}}\|_{W_+}^2+\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2. \tag{C.15}$$

Since $\tau_+\Delta\kappa_+^{\mathrm{cor}}+\kappa_+\Delta\tau_+^{\mathrm{cor}}=0$ by (10.16b), we can derive the upper bound

$$-\Delta\kappa_+^{\mathrm{cor}}\Delta\tau_+^{\mathrm{cor}}=\Delta\tau_+^{\mathrm{cor}}\frac{\kappa_+\Delta\tau_+^{\mathrm{cor}}}{\tau_+}\leq 0.$$

Hence, (v) follows from (C.15) and the observation $\|\zeta_+^{\mathrm{D}}\|_{W_+^{-1}}^2=\|\zeta_+^{\mathrm{P}}\|_{W_+}^2$.

(vi): Can be proven similar to Corollary C.3 using (v).

(vii): From (10.16b) and (iii), we get

$$(\tau_++\Delta\tau_+^{\mathrm{cor}})(\kappa_++\Delta\kappa_+^{\mathrm{cor}})=\tau_+\kappa_++\Delta\tau_+^{\mathrm{cor}}\Delta\kappa_+^{\mathrm{cor}}=\tau_+\kappa_+-\langle\Delta x_+^{\mathrm{cor}},\Delta s_+^{\mathrm{cor}}\rangle.$$

The upper bound now follows from (vi). If this upper bound on $(\tau_++\Delta\tau_+^{\mathrm{cor}})(\kappa_++\Delta\kappa_+^{\mathrm{cor}})$ is negative, then either $\tau_{++}>0$ and $\kappa_{++}<0$, or $\tau_{++}<0$ and $\kappa_{++}>0$. Suppose for the sake of contradiction that $\tau_{++}<0$ and $\kappa_{++}>0$. Then, $\Delta\tau_+^{\mathrm{cor}}<0$ and $\Delta\kappa_+^{\mathrm{cor}}>0$. However, it follows from (10.16b) that these cannot hold at the same time if $\tau_+>0$ and $\kappa_+<0$. Hence, $\tau_{++}>0$ and $\kappa_{++}<0$. □

We move on to an analysis of (A4) after the corrector step.

Lemma 10.9 ([7, Lemma 10])**.** *Let $\mathcal{K}\subset\mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+=(y_+,x_+,\tau_+,s_+,\kappa_+)$ such that $x_+\in\operatorname{int}\mathcal{K}$, $s_+\in\operatorname{int}\mathcal{K}^\circ$, $\tau_+>0$, and $\kappa_+<0$. Assume* (10.18) *holds with $u_+^{\mathrm{D}}=(1+\epsilon)/r$ and $l_+^{\mathrm{D}}=r(1-\epsilon)$ for some $r\in(0,1]$ and $\epsilon\geq 0$. Suppose $\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+}<\sqrt{\min\{l_+^{\mathrm{D}},1/u_+^{\mathrm{D}}\}}$. Then,*

$$\begin{aligned}\mu_+\tilde{\mu}_{++}\leq 1+\|\zeta_+^{\mathrm{P}}\|_{W_+}&\left[\frac{u_+^{\mathrm{D}}}{\sqrt{\mu_+\vartheta_f}}\left(\frac{1}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}}-1\right)\right.\\&\left.+\frac{\|\tilde{x}_+\|_{W_+}}{\vartheta_f}\left(\frac{1}{l_+^{\mathrm{D}}(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{l_+^{\mathrm{D}}\mu_+})}-1\right)\right]\\&+\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}^2u_+^{\mathrm{D}}}{\mu_+\vartheta_f l_+^{\mathrm{D}}(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{l_+^{\mathrm{D}}\mu_+})(1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+})}.\end{aligned}$$

Proof. We are interested in finding a lower bound on $\langle g(x_+ + \Delta x_+^{\rm cor}), g^*(s_+ + \Delta s_+^{\rm cor})\rangle$. It follows from (10.16c) that $x_+ + \Delta x_+^{\rm cor} = \mu_+ \tilde{x}_+ + W_+^{-1}\Delta s_+^{\rm cor}$. By the fundamental theorem of calculus,

$$\begin{aligned} g(x_+ + \Delta x_+^{\rm cor}) &= g(\mu_+\tilde{x}_+ + W_+^{-1}\Delta s_+^{\rm cor}) \\ &= g(\mu_+\tilde{x}_+) + \int_0^1 H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\rm cor})W_+^{-1}\Delta s_+^{\rm cor}\,{\rm d}t \\ &= \frac{1}{\mu_+}s_+ + \int_0^1 H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\rm cor})W_+^{-1}\Delta s_+^{\rm cor}\,{\rm d}t, \end{aligned}$$

where the final equality uses (2.20) and Theorem 2.12 to see that $g(\mu_+\tilde{x}_+) = g(g^*(s_+))/\mu_+ = s_+/\mu_+$. Another application of the fundamental theorem of calculus yields

$$g^*(s_+ + \Delta s_+^{\rm cor}) = g^*(s_+) + \int_0^1 H^*(s_+ + t\Delta s_+^{\rm cor})\Delta s_+^{\rm cor}\,{\rm d}t.$$

Consequently, it can be seen that

$$\begin{aligned} &\langle g(x_+ + \Delta x_+^{\rm cor}), g^*(s_+ + \Delta s_+^{\rm cor})\rangle \\ &= -\frac{\vartheta_f}{\mu_+} + \int_0^1 \left\langle \Delta s_+^{\rm cor}, \frac{1}{\mu_+}H^*(s_+ + t\Delta s_+^{\rm cor})s_+ + W_+^{-1}H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\rm cor})\tilde{x}_+ \right\rangle {\rm d}t \qquad \text{(C.16)} \\ &\quad + \int_0^1\int_0^1 \langle \Delta s_+^{\rm cor}, W_+^{-1}H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\rm cor})H^*(s_+ + r\Delta s_+^{\rm cor})\Delta s_+^{\rm cor}\rangle\,{\rm d}t\,{\rm d}r. \qquad \text{(C.17)} \end{aligned}$$

Using the Cauchy-Schwartz inequality, it follows that the inner product in (C.16) is at least

$$-\|\Delta s_+^{\rm cor}\|_{W_+^{-1}} \left\| \frac{1}{\mu_+}H^*(s_+ + t\Delta s_+^{\rm cor})s_+ + W_+^{-1}H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\rm cor})\tilde{x}_+ \right\|_{W_+}.$$

The latter norm can be further bounded by the triangle inequality and the fact

that $-H^*(s_+)s_+ = g^*(s_+) = \tilde{x}_+$:

$$\begin{aligned}
&\left\| \frac{1}{\mu_+} H^*(s_+ + t\Delta s_+^{\mathrm{cor}})s_+ + W_+^{-1} H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}})\tilde{x}_+ \right\|_{W_+} \\
&\leq \left\| \frac{1}{\mu_+} [H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)]s_+ \right\|_{W_+} && \text{(C.18)} \\
&\quad + \frac{1}{\mu_+} \left\| W_+^{-1}[\mu_+ H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) - W_+]\tilde{x}_+ \right\|_{W_+}. && \text{(C.19)}
\end{aligned}$$

Starting with the norm in (C.18), note that by (10.18) and Lemma 2.4,

$$\begin{aligned}
\mu_+[H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)] &\preceq \left(\frac{1}{(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} - 1 \right) \mu_+ H^*(s_+) \\
&\preceq \left(\frac{u_+^{\mathrm{D}}}{(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} - u_+^{\mathrm{D}} \right) W_+^{-1}.
\end{aligned} \tag{C.20}$$

Similarly,

$$\begin{aligned}
\mu_+[H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)] &\succeq \left((1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2 - 1 \right) \mu_+ H^*(s_+) \\
&\succeq \left(l_+^{\mathrm{D}}(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2 - l_+^{\mathrm{D}} \right) W_+^{-1}.
\end{aligned} \tag{C.21}$$

Hence, by Proposition 10.2,

$$\begin{aligned}
&\frac{1}{\mu_+^2} \left\| \mu_+[H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)]s_+ \right\|_{W_+} \\
&= \frac{1}{\mu_+^2} \left\| \left[W_+ \left(\mu_+[H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)] + W_+^{-1} \right) - I \right] s_+ \right\|_{W_+^{-1}} \\
&\leq \frac{\|s_+\|_{W_+^{-1}}}{\mu_+^2} \left\| W_+ \left(\mu_+[H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) - H^*(s_+)] + W_+^{-1} \right) - I \right\|_{W_+^{-1}} \\
&\leq \frac{\|s_+\|_{W_+^{-1}}}{\mu_+^2} \max \left\{ \frac{u_+^{\mathrm{D}}}{(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} - u_+^{\mathrm{D}}, l_+^{\mathrm{D}} - l_+^{\mathrm{D}}(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2 \right\} \\
&= \frac{\sqrt{\vartheta_f}}{\mu_+\sqrt{\mu_+}} \left(\frac{u_+^{\mathrm{D}}}{(1 - t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} - u_+^{\mathrm{D}} \right),
\end{aligned} \tag{C.22}$$

since $1/(1-r)^2 - 1 \geq 1 - (1-r)^2$ for all $r \in [0, 1)$.

To bound the norm in (C.19) with Proposition 10.2, we first note that by self-concordance and the observation that $\mu_+ H(\mu_+\tilde{x}_+) = H^*(s_+)^{-1}/\mu_+$,

$$\begin{aligned}\mu_+ H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) &\preceq \frac{1}{(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}\mu_+ H(\mu_+\tilde{x}_+)\\ &\preceq \frac{1}{l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}W_+,\end{aligned} \tag{C.23}$$

where the last step used (10.18). Similarly,

$$\begin{aligned}\mu_+ H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) &\succeq (1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2\mu_+ H(\mu_+\tilde{x}_+)\\ &\succeq \frac{(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}{u_+^{\mathrm{D}}}W_+,\end{aligned} \tag{C.24}$$

such that Proposition 10.2 shows

$$\begin{aligned}&\frac{1}{\mu_+}\left\|W_+^{-1}[\mu_+ H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) - W_+]\tilde{x}_+\right\|_{W_+}\\ &\le \frac{\|\tilde{x}_+\|_{W_+}}{\mu_+}\left\|\mu_+ W_+^{-1}H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) - I\right\|_{W_+}\\ &\le \frac{\|\tilde{x}_+\|_{W_+}}{\mu_+}\max\left\{\frac{1}{l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2} - 1, 1 - \frac{(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}{u_+^{\mathrm{D}}}\right\}\\ &= \frac{\|\tilde{x}_+\|_{W_+}}{\mu_+}\left(\frac{1}{l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2} - 1\right),\end{aligned} \tag{C.25}$$

since $1/[(1-\epsilon)r]-1 \ge 1-r/(1+\epsilon)$ for all $r\in(0,1]$ and $\epsilon \ge 0$.

In summary, the inner product in (C.16) is, using the bounds (C.22) and (C.25) on (C.18) and (C.19), at least

$$\begin{aligned}-\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}\Bigg[&\frac{\sqrt{\vartheta_f}}{\mu_+\sqrt{\mu_+}}\left(\frac{u_+^{\mathrm{D}}}{(1-t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} - u_+^{\mathrm{D}}\right)\\ &+\frac{\|\tilde{x}_+\|_{W_+}}{\mu_+}\left(\frac{1}{l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2} - 1\right)\Bigg].\end{aligned} \tag{C.26}$$

By the properties of the operator norm, the inner product in (C.17) is at least

$$\begin{aligned}
&-\frac{\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2}{\mu_+^2}\|H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}})H^*(s_+ + r\Delta s_+^{\mathrm{cor}})\|_{W_+^{-1}} \\
&\geq -\frac{\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2}{\mu_+^2}\|H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}})W_+^{-1}\|_{W_+^{-1}}\|W_+H^*(s_+ + r\Delta s_+^{\mathrm{cor}})\|_{W_+^{-1}}.
\end{aligned} \tag{C.27}$$

To bound the first norm in (C.27), we note that for any linear operator P,

$$\|PW_+^{-1}\|_{W_+^{-1}} = \sup_{\|u\|_{W_+^{-1}}\leq 1}\|PW_+^{-1}u\|_{W_+^{-1}} = \sup_{\|v\|_{W_+}\leq 1}\|Pv\|_{W_+^{-1}} = \|W_+^{-1}P\|_{W_+}.$$

Therefore, $\|H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}})W_+^{-1}\|_{W_+^{-1}}$ equals

$$\frac{\|W_+^{-1}[\mu_+H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) + W_+] - I\|_{W_+}}{\mu_+}.$$

Using the bounds (C.23) and (C.24), it can be shown that

$$\begin{aligned}
\left(\frac{(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}{u_+^{\mathrm{D}}} + 1\right)W_+ &\preceq \mu_+H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) + W_+ \\
&\preceq \left(\frac{1}{l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2} + 1\right)W_+.
\end{aligned}$$

Hence, Proposition 10.2 shows

$$\begin{aligned}
&\|H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}})W_+^{-1}\|_{W_+^{-1}} \\
&= \frac{\|W_+^{-1}[\mu_+H(\mu_+\tilde{x}_+ + tW_+^{-1}\Delta s_+^{\mathrm{cor}}) + W_+] - I\|_{W_+}}{\mu_+} \\
&\leq \frac{1}{\mu_+l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2}.
\end{aligned} \tag{C.28}$$

Similarly, one can show along the lines of (C.20) and (C.21) that

$$\begin{aligned}
\left(l_+^{\mathrm{D}}(1-r\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2 + 1\right)W_+^{-1} &\preceq \mu_+H^*(s_+ + r\Delta s_+^{\mathrm{cor}}) + W_+^{-1} \\
&\preceq \left(\frac{u_+^{\mathrm{D}}}{(1-r\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} + 1\right)W_+^{-1},
\end{aligned} \tag{C.29}$$

such that Proposition 10.2 shows

$$\|\mu_+ H^*(s_+ + r\Delta s_+^{\mathrm{cor}})\|_{W_+^{-1}} \leq \frac{u_+^{\mathrm{D}}}{(1-r\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2}. \tag{C.30}$$

In summary, the inner product in (C.17) is, using the bounds (C.27), (C.28), and (C.30), at least

$$-\frac{\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2 u_+^{\mathrm{D}}}{\mu_+^2 l_+^{\mathrm{D}}(1-t\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})^2(1-r\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2}. \tag{C.31}$$

Combining the bounds (C.26) and (C.31) on the inner products in (C.16) and (C.17) respectively yields

$$\begin{aligned}
&\langle g(x_+ + \Delta x_+^{\mathrm{cor}}), g^*(s_+ + \Delta s_+^{\mathrm{cor}})\rangle \\
&\geq -\frac{\vartheta_f}{\mu_+} - \|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}\left[\frac{\sqrt{\vartheta_f}}{\mu_+\sqrt{\mu_+}}\left(\frac{u_+^{\mathrm{D}}}{1-\|\Delta s_+^{\mathrm{cor}}\|_{s_+}} - u_+^{\mathrm{D}}\right)\right. \\
&\quad \left. + \frac{\|\tilde{x}_+\|_{W_+}}{\mu_+}\left(\frac{1}{l_+^{\mathrm{D}}(1-\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})} - 1\right)\right] \\
&\quad - \frac{\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}^2 u_+^{\mathrm{D}}}{\mu_+^2 l_+^{\mathrm{D}}(1-\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+})(1-\|\Delta s_+^{\mathrm{cor}}\|_{s_+})}.
\end{aligned}$$

The proof is complete after a multiplication by $-\mu_+/\vartheta_f$ and bounding the remaining norms. Lemma 10.8(v) shows $\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}} \leq \|\zeta_+^{\mathrm{P}}\|_{W_+}$. Moreover, $H(\mu_+\tilde{x}_+) = H^*(s_+)^{-1}/\mu_+^2$, so

$$\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{\mu_+\tilde{x}_+} = \frac{\|W_+^{-1}\Delta s_+^{\mathrm{cor}}\|_{s_+}^{-1}}{\mu_+} \leq \frac{\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}}}{\sqrt{l_+^{\mathrm{D}}\mu_+}} \leq \frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{\sqrt{l_+^{\mathrm{D}}\mu_+}},$$

by (10.18). Finally, $\|\Delta s_+^{\mathrm{cor}}\|_{s_+} \leq \sqrt{u_+^{\mathrm{D}}/\mu_+}\|\Delta s_+^{\mathrm{cor}}\|_{W_+^{-1}} \leq \sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}$. □

We end this section with an analysis of (A5) after the corrector step.

Lemma 10.10 ([7, Lemma 11]). *Let $\mathcal{K} \subset \mathbb{R}^n$ be a proper cone admitting a LHSCB f. Pick $z_+ = (y_+, x_+, \tau_+, s_+, \kappa_+)$ such that $x_+ \in \operatorname{int}\mathcal{K}$, $s_+ \in \operatorname{int}\mathcal{K}^\circ$, $\tau_+ > 0$, and $\kappa_+ < 0$. Assume* (10.18) *holds with $u_+^{\mathrm{D}} = (1+\epsilon)/r$ and $l_+^{\mathrm{D}} = r(1-\epsilon)$ for some*

$r \in (0,1]$ and $\epsilon \geq 0$. Suppose $\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+} < \sqrt{\min\{l_+^{\mathrm{P}}, 1/u_+^{\mathrm{P}}\}}$. Then, $\|\zeta_{++}^{\mathrm{P}}\|_{x_{++}}$ is at most

$$\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+ l_+^{\mathrm{P}}})\sqrt{\mu_+ l_+^{\mathrm{P}}}}\left(\frac{u_+^{\mathrm{D}}}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}}-1\right)$$
$$+\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}^2}{2\mu_+\sqrt{\vartheta_f}}\left[1-\frac{\|\zeta_+^{\mathrm{P}}\|_{W_+}}{(1-\|\zeta_+^{\mathrm{P}}\|_{W_+}/\sqrt{\mu_+ l_+^{\mathrm{P}}})\sqrt{\mu_+ l_+^{\mathrm{P}}}}\left(\frac{u_+^{\mathrm{D}}}{1-\sqrt{u_+^{\mathrm{D}}/\mu_+}\|\zeta_+^{\mathrm{P}}\|_{W_+}}-1\right)\right]^{-1}.$$

Proof. By the triangle inequality, self-concordance, and (10.18),

$$\begin{aligned}
\|\zeta_{++}^{\mathrm{P}}\|_{x_{++}} &= \|x_{++}-\mu_{++}\tilde{x}_{++}\|_{x_{++}} \\
&\leq \|x_{++}-\mu_+\tilde{x}_{++}\|_{x_{++}} + \left|\frac{\mu_{++}}{\mu_+}-1\right|\|\mu_+\tilde{x}_{++}\|_{x_{++}} \\
&\leq \frac{\|x_{++}-\mu_+\tilde{x}_{++}\|_{x_+}}{1-\|\Delta x_+^{\mathrm{cor}}\|_{x_+}} + \left|\frac{\mu_{++}}{\mu_+}-1\right|\frac{\|\mu_+\tilde{x}_{++}\|_{\mu_+\tilde{x}_{++}}}{1-\|x_{++}-\mu_+\tilde{x}_{++}\|_{x_{++}}} \\
&\leq \frac{\|x_{++}-\mu_+\tilde{x}_{++}\|_{W_+}}{(1-\|\Delta x_+^{\mathrm{cor}}\|_{x_+})\sqrt{\mu_+ l_+^{\mathrm{P}}}} + \left|\frac{\mu_{++}}{\mu_+}-1\right|\frac{\sqrt{\vartheta_f}}{1-\frac{\|x_{++}-\mu_+\tilde{x}_{++}\|_{W_+}}{(1-\|\Delta x_+^{\mathrm{cor}}\|_{x_+})\sqrt{\mu_+ l_+^{\mathrm{P}}}}}. \qquad \text{(C.32)}
\end{aligned}$$

We continue by bounding $\|x_{++}-\mu_+\tilde{x}_{++}\|_{W_+}$. Note that by the fundamental theorem of calculus and (10.16c),

$$\begin{aligned}
x_{++}-\mu_+\tilde{x}_{++} &= (x_+ + \Delta x_+^{\mathrm{cor}}) - \mu_+ g^*(s_+ + \Delta s_+^{\mathrm{cor}}) \\
&= x_+ + \Delta x_+^{\mathrm{cor}} - \mu_+\left(g^*(s_+) + \int_0^1 H^*(s_+ + t\Delta s_+^{\mathrm{cor}})\Delta s_+^{\mathrm{cor}}\,\mathrm{d}t\right) \\
&= \mu_+\tilde{x}_+ + W_+^{-1}\Delta s_+^{\mathrm{cor}} - \mu_+\tilde{x}_+ - \int_0^1 \mu_+ H^*(s_+ + t\Delta s_+^{\mathrm{cor}})\Delta s_+^{\mathrm{cor}}\,\mathrm{d}t \\
&= \int_0^1 \left(W_+^{-1} - \mu_+ H^*(s_+ + t\Delta s_+^{\mathrm{cor}})\right)\Delta s_+^{\mathrm{cor}}\,\mathrm{d}t. \qquad \text{(C.33)}
\end{aligned}$$

To bound the integrand of (C.33) in the norm induced by W_+, we will bound the operator norm of $W_+^{-1} - \mu_+ H^*(s_+ + t\Delta s_+^{\mathrm{cor}})$. One can show similarly to (C.29) that

$$(1-t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2 l_+^{\mathrm{D}} W_+^{-1} \preceq \mu_+ H^*(s_+ + t\Delta s_+^{\mathrm{cor}}) \preceq \frac{u_+^{\mathrm{D}}}{(1-t\|\Delta s_+^{\mathrm{cor}}\|_{s_+})^2} W_+^{-1}.$$

It then follows from Proposition 10.2 that

$$\begin{aligned}
&\left\|\left(W_+^{-1}-\mu_+H^*(s_+ + t\Delta s_+^{\rm cor})\right)\Delta s_+^{\rm cor}\right\|_{W_+}\\
&= \left\|W_+\left(W_+^{-1}-\mu_+H^*(s_+ + t\Delta s_+^{\rm cor})\right)\Delta s_+^{\rm cor}\right\|_{W_+^{-1}}\\
&\le \left\|\mu_+W_+H^*(s_+ + t\Delta s_+^{\rm cor})-I\right\|_{W_+^{-1}}\|\Delta s_+^{\rm cor}\|_{W_+^{-1}}\\
&\le \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}\max\left\{\frac{u_+^{\rm D}}{(1-t\|\Delta s_+^{\rm cor}\|_{s_+})^2}-1, 1-(1-t\|\Delta s_+^{\rm cor}\|_{s_+})^2 l_+^{\rm D}\right\}\\
&= \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}\left(\frac{u_+^{\rm D}}{(1-t\|\Delta s_+^{\rm cor}\|_{s_+})^2}-1\right),
\end{aligned}$$

where the final equality uses $1/[(1-\epsilon)r]-1 \ge 1-r/(1+\epsilon)$ for all $r\in(0,1]$ and $\epsilon\ge 0$. We can therefore bound the W_+-norm of (C.33) by

$$\begin{aligned}
\|x_{++}-\mu_+\tilde{x}_{++}\|_{W_+} &\le \int_0^1 \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}\left(\frac{u_+^{\rm D}}{(1-t\|\Delta s_+^{\rm cor}\|_{s_+})^2}-1\right)\mathrm{d}t\\
&= \|\Delta s_+^{\rm cor}\|_{W_+^{-1}}\left(\frac{u_+^{\rm D}}{1-\|\Delta s_+^{\rm cor}\|_{s_+}}-1\right)\\
&\le \|\zeta_+^{\rm P}\|_{W_+}\left(\frac{u_+^{\rm D}}{1-\sqrt{u_+^{\rm D}/\mu_+}\|\zeta_+^{\rm P}\|_{W_+}}-1\right), \qquad \text{(C.34)}
\end{aligned}$$

where the final inequality uses Lemma 10.8(v) and (10.18).

The next factor from (C.32) we look at is $|\mu_{++}/\mu_+-1|$. Lemma 10.8(ii) implies that $\langle x_+ + \Delta x_+^{\rm cor}, s_+ + \Delta s_+^{\rm cor}\rangle = \langle x_+, s_+\rangle + \langle \Delta x_+^{\rm cor}, \Delta s_+^{\rm cor}\rangle$. Therefore, it follows from Lemma 10.8(vi) that

$$\left|\frac{\mu_{++}}{\mu_+}-1\right| = \frac{|\langle \Delta x_+^{\rm cor}, \Delta s_+^{\rm cor}\rangle|}{\mu_+\vartheta_f} \le \frac{\|\zeta_+^{\rm P}\|_{W_+}^2}{2\mu_+\vartheta_f}. \qquad \text{(C.35)}$$

The last quantity in (C.32) that we have yet to bound is $\|\Delta x_+^{\rm cor}\|_{x_+}$. By (10.18) and Lemma 10.8(v),

$$\|\Delta x_+^{\rm cor}\|_{x_+} \le \frac{\|\Delta x_+^{\rm cor}\|_{W_+}}{\sqrt{\mu_+ l_+^{\rm P}}} \le \frac{\|\zeta_+^{\rm P}\|_{W_+}}{\sqrt{\mu_+ l_+^{\rm P}}}. \qquad \text{(C.36)}$$

The proof can be completed by using (C.34), (C.35), and (C.36) to develop (C.32). □

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Riley Badenbroek (Rheden, the Netherlands, 1994) received his Bachelor's degree from Tilburg University in 2015, followed by a Master's degree (2016) and a Research Master degree (2017), both in Operations Research. He became a PhD candidate in Operations Research at Tilburg University in 2017. During the PhD period, he spent two weeks at Mosek ApS as a visiting scholar.

This thesis explores four methods for convex optimization. The first two are an interior point method and a simulated annealing algorithm that share a theoretical foundation. This connection is due to the interior point method's use of the so-called entropic barrier, whose derivatives can be approximated through sampling. Here, the sampling will be carried out with a technique known as hit-and-run. By carefully analyzing the properties of hit-and-run sampling, it is shown that both the interior point method and the simulated annealing algorithm can solve a convex optimization problem in the membership oracle setting. The number of oracle calls made by these methods is bounded by a polynomial in the input size.

The third method is an analytic center cutting plane method that shows promising performance for copositive optimization. It outperforms the first two methods by a significant margin on the problem of separating a matrix from the completely positive cone.

The final method is based on Mosek's algorithm for nonsymmetric conic optimization. With their scaling matrix, search direction, and neighborhood, we define a method that converges to a near-optimal solution in polynomial time.

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