# Mixed Laplace approximation for marginal posterior and Bayesian inference in error-in-operator model

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#### Abstract

Laplace approximation is a very useful tool in Bayesian inference and it claims a nearly Gaussian behavior of the posterior. Spokoiny (2023) established some rather accurate finite sample results about the quality of Laplace approximation in terms of the so called effective dimension **p** under the critical dimension constraint  $\mathbf{p}^3 \ll n$ . However, this condition can be too restrictive for many applications like error-in-operator problem or Deep Neuronal Networks. This paper addresses the question whether the dimensionality condition can be relaxed and the accuracy of approximation can be improved if the target of estimation is low dimensional while the nuisance parameter is high or infinite dimensional. Under mild conditions, the marginal posterior can be approximated by a Gaussian mixture and the accuracy of the approximation only depends on the target dimension. Under the condition  $\mathbf{p}^2 \ll n$  or in some special situation like semi-orthogonality, the Gaussian mixture can be replaced by one Gaussian distribution leading to a classical Laplace result. The second result greatly benefits from the recent advances in Gaussian comparison from Götze et al. (2019). The results are illustrated and specified for the case of error-in-operator model.

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#### MIXED LAPLACE APPROXIMATION

# Contents

1	$\operatorname{Intr}$	oducti	on	3		
2	Laplace approximation of the marginal					
	2.1	Full di	mensional bounds	10		
	2.2	Orthog	gonal case	11		
	2.3	Condit	tional Laplace approximation	11		
	2.4	Conce	ntration of the conditional and marginal distribution	12		
	2.5	Appro	ximation by a Gaussian mixture	13		
	2.6	Laplac	e approximation	15		
	2.7	Gaussi	ian comparison and elliptic credible sets	17		
	2.8	Varian	ce homogenization	18		
	2.9	A bou	nd for the bias under one-point orthogonality	19		
	2.10	Laplac	e approximation: a general bound	20		
	2.11	Critica	al dimension in marginal Laplace approximation	22		
3	Error-in-operator model					
	3.1	Identif	fability, warm start, efficient information matrix	23		
	3.2	2 Full and target efficient dimension		25		
	3.3	Full dimensional concentration of the posterior		27		
	3.4	Marginal posterior: concentration and Laplace approximation		27		
	3.5	Critical dimension		30		
A	Loca	al smo	othness conditions	31		
	A.1	Smoot	hness and self-concordance in Gateaux sense	31		
	A.2	Fréchet derivatives and smoothness of the Hessian				
	A.3	A.3 Optimization after linear or quadratic perturbation		35		
		A.3.1	A linear perturbation	35		
		A.3.2	Quadratic penalization	39		
	A.4 Conditional and marginal optimization		tional and marginal optimization	42		
		A.4.1	Partial optimization and local partial smoothness	42		
		A.4.2	Conditional optimization and a bound on the bias $\ldots \ldots \ldots$	44		
		A.4.3	One-point orthogonality by a linear transform	47		
		A.4.4	Composite nuisance variable	50		

В	Din	Dimension free bounds for Laplace approximation				
	B.1	Setup and conditions				
		B.1.1	Concavity	53		
		B.1.2	Laplace effective dimension	53		
		B.1.3	Local smoothness conditions	54		
	B.2	bounds for Laplace approximation	54			
		B.2.1	Critical dimension $\ldots \ldots \ldots$	56		
	B.3	Tools	and proofs	56		
		B.3.1	Overall error of Laplace approximation	56		
		B.3.2	Lower and upper Gaussian measures	58		
		B.3.3	Gaussian moments	58		
		B.3.4	Local approximation $\ldots$	59		
		B.3.5	Tail integrals	64		
		B.3.6	${\rm Local\ concentration}  . \ . \ . \ . \ . \ . \ . \ . \ . \ .$	66		
		B.3.7	Finalizing the proof of Theorem B.1 and B.2	67		
С	Examples of priors					
	C.1	Truncation and smooth priors				
	C.2	Effective dimension				
	C.3	Sobolev classes and smooth priors				
	C.4	Properties of the sub-projector $P_G$				
D	Some results for Gaussian quadratic forms					
	D.1	D.1 Moments of a Gaussian quadratic form				
	D.2	2 Deviation bounds for Gaussian quadratic forms				
$\mathbf{E}$	Gaı	aussian comparison 7				

# 1 Introduction

Laplace approximation is one of the most powerful instruments in Bayesian inference. Let  $f(\cdot)$  be a non-normalized posterior log-density, usually of the form

$$f(\boldsymbol{v}) = L(\boldsymbol{v}) + \log \pi(\boldsymbol{v})$$

for the log-likelihood function L(v) and a prior density  $\pi(v)$ . Laplace approximation claims that, for a strongly concave function f(x), the posterior measure  $\mathbb{P}_f$  with a density proportional to  $e^{f(v)}$  can be well approximated by a Gaussian distribution  $\mathcal{N}(\boldsymbol{v}^*, \mathbb{F}^{-1})$ , where  $\boldsymbol{v}^* = \operatorname{argmax}_{\boldsymbol{v}} f(\boldsymbol{v})$  and  $\mathbb{F} = -\nabla^2 f(\boldsymbol{v}^*)$ . The original Laplace result was stated for the univariate case. Recently this topic attracted a lot of attention in connection with statistical inference for complex high dimensional model such as nonlinear inverse problems, Deep Neuronal Networks, optimal transport, etc. We refer to recent papers Helin and Kretschmann (2022), Kasprzak et al. (2022), Katsevich and Rigollet (2023), Nickl (2022), and references therein. Classical asymptotic setup with the fixed prior and a growing sample size leads to the prominent Bernstein–von Mises Theorem that claims prior free asymptotic normal posterior distribution centered at the MLE  $\widetilde{\boldsymbol{v}} = \operatorname{argmax}_{\boldsymbol{v}} L(\boldsymbol{v})$ . We refer to (Ghosal and van der Vaart, 2017, Chapter 12) for a detailed presentation and literature overview. However, the case of large or even huge parameter dimension requires a separate study, the Bernstein–von Mises phenomenon does not apply any more, the prior impact could be significant. A particular issue is the *critical dimension* meaning the dimensionality constraint under which the Laplace approximation still applies. Spokoiny (2023) established rather precise nonasymptotic bounds on the quality of Laplace approximation in terms of the so called *Laplace effec*tive dimension  $\bar{\mathbf{p}}$ ; see Section B.1.2 for a precise definition. The main result of Spokoiny (2023) requires  $\overline{\mathbf{p}}^3 \ll n$ , where n is the sample size; see e.g. Theorem B.2. For high dimensional models this constraint appears to be very limiting. Unfortunately, it seems to be impossible to relax this condition in a general situation. This paper focuses on a slightly different problem. Let the parameter vector  $\boldsymbol{v}$  be high dimensional but we are only interested in its low dimensional component  $\boldsymbol{x}$ . The main question under consideration is whether the accuracy of approximation of the marginal x-posterior can be controlled in terms of the x-dimension  $p_e$  thus relaxing the dimensionality constraint. The whole study can be split into two big steps. The first result of Theorem 2.5 describes an approximation of the marginal distribution of the subvector  $\boldsymbol{x}$  by a Gaussian mixture. A nice feature of this result is that the accuracy of approximation only depends on the effective dimension  $\mathbf{p}_{\mathrm{e}}$  of the target variable x only. The next step of the study aims at addressing the question if the obtained mixture can be replaced by one Gaussian distribution. The main tools include Gaussian comparison Götze et al. (2019) and a bias reduction in conditional optimization based on one-point orthogonalization. It appears that even in a rather general situation, one can relax the condition  $\overline{p}^3 \ll n$  to  $\overline{p}^2 \ll n$ . In some special cases like semi-orthogonality, the full parameter dimension does not show up and the marginal x-posterior can be approximated by Gaussian law with accuracy  $\sqrt{p_e^3/n}$ .

#### Motivation 1: error-in-operator problem

Let A be a linear mapping (operator) of the source signal  $\boldsymbol{x} \in \mathbb{R}^p$  to the image space  $\mathbb{R}^q$ . We consider the problem of inverting the relation  $\boldsymbol{z} = A\boldsymbol{x}$ : given an image vector  $\boldsymbol{z} \in \mathbb{R}^q$ , recover the corresponding source  $\boldsymbol{x} \in \mathbb{R}^p$ . This leads to the linear least square problem of maximizing the negative fidelity function  $\ell(\cdot)$  of the form

$$\ell(\boldsymbol{x}) = -\frac{1}{2\sigma^2} \|\boldsymbol{z} - A\boldsymbol{x}\|^2, \qquad (1.1)$$

where  $\sigma^2$  describes the image noise. However, this approach assumes the operator A to be precisely known. In many applications, this assumption is not fulfilled and the operator A is known up to some error. This means that only an estimate  $\hat{A}$  of A is available. Particular examples include all kinds of tomography, regression with random design, instrumental regression, error-in-variable regression, functional data analysis, etc. A pragmatic plug-in approach just replaces A in (1.1) by its estimate  $\hat{A}$  leading to the solution

$$\widehat{\boldsymbol{x}} = \operatorname*{argmin}_{\boldsymbol{x}} \|\boldsymbol{z} - \widehat{A}\boldsymbol{x}\|^2 = (\widehat{A}^{\top}\widehat{A})^{-1}\widehat{A}^{\top}\boldsymbol{z}.$$

Unfortunately, inverting a large matrix  $\widehat{A}^{\top}\widehat{A}$  can be tricky, especially if the operator A is smooth. Hoffmann and Reiss (2008) considered simultaneous wavelet estimation of the signal  $\boldsymbol{x}$  and the operator A. Trabs (2018) extended these results to Bayesian inference using a parametric assumption about the unknown operator  $A = A_{\theta}$  and provided some examples from imaging and linear PDE/SDEs. In that paper, one can also find a literature overview and more references on this topic. This paper treats the original problem in a semiparametric setup by including the operator A in the parameter set  $\boldsymbol{v} = (\boldsymbol{x}, A)$ . This leads to the new fidelity function

$$-rac{1}{2\sigma^2}\|m{z}-Am{x}\|^2 - rac{\mu^2}{2\sigma^2}\|\widehat{A}-A\|_{
m Fr}^2\,,$$

where  $\mu$  describes the level of the operator noise and  $||A||_{\text{Fr}}^2 = \text{tr}(A^{\top}A)$  stands for the squared Frobenius norm. The use of a Gaussian prior on  $\boldsymbol{x}$  leads to the posterior log-density

$$f(\boldsymbol{v}) = -\frac{1}{2\sigma^2} \|\boldsymbol{z} - A\boldsymbol{x}\|^2 - \frac{\mu^2}{2\sigma^2} \|\widehat{A} - A\|_{\rm Fr}^2 - \frac{1}{2} \|G(\boldsymbol{x} - \boldsymbol{x}_0)\|^2,$$
(1.2)

where the precision operator  $G^2$  is responsible for the smoothness of the source signal while  $\boldsymbol{x}_0$  stands for a starting guess. The quadratic term  $-\mu^2 (2\sigma^2)^{-1} \|\hat{A} - A\|_{\text{Fr}}^2$  can be viewed as a Gaussian log-density on A. The function f is not concave in the set of variables  $\boldsymbol{v} = (\boldsymbol{x}, A)$ . However, it is locally concave in a vicinity of the point  $(\boldsymbol{x}_0, \hat{A})$  under "warm start" condition which requires a reasonable quality of the guess  $\boldsymbol{x}_0$  and of the pilot  $\hat{A}$ ; see Section 3 later. The main objective is the marginal of the full dimensional posterior distribution related to the target parameter  $\boldsymbol{x}$ . Some results about semiparametric Bernstein–von Mises Theorem are available; see e.g. Castillo (2012), Bickel and Kleijn (2012), L'Huillier et al. (2023), and references therein. Castillo and Rousseau (2015) considered the BvM result for smooth functionals. However, the results focused on asymptotic rate of contraction and asymptotic Gaussian approximation of the posterior in some metric like  $\ell_2$ -Wasserstein. This paper, similarly to Spokoiny (2022), rather attempts to explore the quality of Laplace approximation and to address the issue of critical dimension of the nuisance parameters. The results of Section 2 state a surprising phase-transition result: an increase of the dimensionality of the nuisance parameter may lead to a mixed Laplace approximation in place of usual Laplace approximation. This requires to extend the results from Spokoiny (2023) to the marginal distribution.

#### Motivation 2. Random design regression

In many applications, the design  $X_1, \ldots, X_n$  in regression models  $Y_i = f(X_i) + \varepsilon_i$  may be naturally assumed to be random, often i.i.d. This particularly concerns econometric, biological, chemical, sociological studies etc. Under linear parametric assumption  $f(\boldsymbol{x}) = \sum_j \theta_j \psi_j(\boldsymbol{x}) = \Psi(\boldsymbol{x})^\top \boldsymbol{\theta}$  and noise homogeneity, the model log-likelihood reads exactly as in the case of a deterministic design

$$L(\boldsymbol{\theta}) = -\frac{1}{2\sigma^2} \|\boldsymbol{Y} - \boldsymbol{\Psi}(\boldsymbol{X})^{\top} \boldsymbol{\theta}\|^2 + \mathtt{C},$$

where  $\Psi(\mathbf{X})$  is the  $p \times n$  matrix with entries  $\psi_j(X_i)$ . The corresponding MLE  $\tilde{\boldsymbol{\theta}}$  is again given by

$$\widetilde{\boldsymbol{\theta}} = \left\{ \boldsymbol{\Psi}(\boldsymbol{X}) \boldsymbol{\Psi}(\boldsymbol{X})^{\top} \right\}^{-1} \boldsymbol{\Psi}(\boldsymbol{X}) \boldsymbol{Y}.$$

However, a study of this estimator is quite involved due to the random nature of the matrix  $\Psi(\mathbf{X})$ , especially in the case of a high design dimension d; see recent papers Bartlett et al. (2020), Cheng and Montanari (2022), and references therein for the case of linear regression with d = n.

Now we describe our semiparametric approach. Suppose to be given another collection of features  $(\phi_k)$  for  $k = 1, \ldots, q$ . The use of  $(\phi_k) = (\psi_j)$  is one of possible options. However, one can use many others including biorthogonal bases, regression trees and forests, last layer neurones of Deep Neuronal Networks, etc. Define  $\boldsymbol{\Phi}(X_i) = (\phi_k(X_i)) \in \mathbb{R}^q$  and  $\boldsymbol{\Phi}(\boldsymbol{X}) = (\boldsymbol{\Phi}(X_1), \dots, \boldsymbol{\Phi}(X_n))$ . Introduce two linear operators (design kernels) A and  $\hat{A}: \mathbb{R}^p \to \mathbb{R}^q$  by

$$\widehat{A} \stackrel{\text{def}}{=} \boldsymbol{\Phi}(\boldsymbol{X}) \boldsymbol{\Psi}(\boldsymbol{X})^{\top} = \sum_{i=1}^{n} \boldsymbol{\Phi}(X_{i}) \boldsymbol{\Psi}(X_{i})^{\top},$$
$$A^{*} \stackrel{\text{def}}{=} \boldsymbol{E} \boldsymbol{\Phi}(\boldsymbol{X}) \boldsymbol{\Psi}(\boldsymbol{X})^{\top} = \sum_{i=1}^{n} \boldsymbol{E} \boldsymbol{\Phi}(X_{i}) \boldsymbol{\Psi}(X_{i})^{\top}$$

Clearly  $\mathbb{E}\widehat{A} = A^*$ , so  $\widehat{A}$  might be viewed as an empirical version of  $A^*$ . If the  $X_i$ 's are i.i.d. and  $f_X$  is the design density then

$$A^* = n \mathbb{E} \boldsymbol{\Phi}(X_1) \boldsymbol{\Psi}(X_1)^{\top} = n \int \boldsymbol{\Phi}(\boldsymbol{x}) \boldsymbol{\Psi}(\boldsymbol{x})^{\top} f_X(\boldsymbol{x}) d\boldsymbol{x},$$

In general, with  $\widehat{A}_i = n \mathbf{\Phi}(X_i) \mathbf{\Psi}(X_i)^\top$ , it holds  $\widehat{A} = n^{-1} \sum_{i=1}^n \widehat{A}_i$  and also

$$\sum_{i=1}^{n} \|\widehat{A}_{i} - A\|_{\mathrm{Fr}}^{2} = \sum_{i=1}^{n} \|\widehat{A}_{i} - \widehat{A}\|_{\mathrm{Fr}}^{2} + n\|\widehat{A} - A\|_{\mathrm{Fr}}^{2}.$$

As the term  $\sum_{i=1}^{n} \|\widehat{A}_{i} - \widehat{A}\|_{\mathrm{Fr}}^{2}$  only depends on the design X, one may equally use  $\sum_{i=1}^{n} \|\widehat{A}_{i} - A\|_{\mathrm{Fr}}^{2}$  and  $n\|\widehat{A} - A\|_{\mathrm{Fr}}^{2}$  to measure the data misfit of a possible guess A.

Further, denote

$$Z_k \stackrel{\text{def}}{=} \sum_{i=1}^n Y_i \, \phi_k(X_i)$$

and let Z be the vector in  $\mathbb{R}^p$  with entries  $Z_k$ . The LPA  $f(x) = \Psi(x)^\top \theta$  together with  $Y = f + \varepsilon$  and  $U = \Phi(X)\varepsilon$  implies

$$oldsymbol{Z} = oldsymbol{\Phi}(oldsymbol{X})oldsymbol{f} + oldsymbol{\Phi}(oldsymbol{X})oldsymbol{arepsilon} = oldsymbol{\Phi}(oldsymbol{X})oldsymbol{arepsilon} = oldsymbol{\Phi}(oldsymbol{X})oldsymbol{arepsilon} = oldsymbol{A}oldsymbol{ heta} + oldsymbol{U}.$$

The vector  $\mathbf{Z}$  might be viewed as new "observations" of the "response"  $\boldsymbol{\eta} = A\boldsymbol{\theta}$  corrupted by two sources of errors: the additive error  $\mathbf{U}$  and the error in operator  $\widehat{A} - A$ . Due to definition, these errors are not independent, however,  $\mathbf{E}(\mathbf{U} \mid \mathbf{X}) = 0$ . If the errors  $\varepsilon_i = Y_i - f(X_i)$  are Gaussian independent of the design variables  $X_i$ , then the new "noise"  $\mathbf{U}$  is Gaussian conditionally on  $\mathbf{X}$ . This enables us to decouple these sources in the likelihood by considering in place of  $\|\mathbf{Z} - \widehat{A}\boldsymbol{\theta}\|^2$  two fidelity terms  $\|\mathbf{Z} - \boldsymbol{\eta}\|^2$  and  $n\|\widehat{A} - A\|_{\mathrm{Fr}}^2$  subject to the structural equation  $\boldsymbol{\eta} = A\boldsymbol{\theta}$ . Using the Lagrange multiplier idea, we put all together in one expression

$$\mathscr{L}(\boldsymbol{\theta},\boldsymbol{\eta},A) \stackrel{\text{def}}{=} -\frac{1}{2\sigma^2} \|\boldsymbol{Z}-\boldsymbol{\eta}\|^2 - \frac{n}{2\sigma_X^2} \|\widehat{A}-A\|_{\text{Fr}}^2 - \frac{\lambda}{2\sigma^2} \|\boldsymbol{\eta}-A\boldsymbol{\theta}\|^2.$$

The first term specifies the quality of fitting the "data" Z by the "response"  $\eta$ . The second term is a similar fidelity term for the operator A observed with the operator noise of variance  $\sigma_A^2 = n^{-1}\sigma_X^2$ . Note that the operator noise is only related to the design density  $f_X$ , the observation noise  $\varepsilon$  does not show up here. The last term transfers the structural equation  $\eta = A\theta$  into a penalty term. For the parameter  $\lambda$ , a natural choice is  $\lambda = 1$ . Note that this equation is a special case of (1.2).

#### This paper contribution

Laplace approximation claiming near normality of the posterior is the basic result in Bayesian inference. However, its validity requires some constraints on the dimensionality of the parameter space of the sort  $\bar{\mathbf{p}}^3 \ll n$  for the effective dimension  $\bar{\mathbf{p}}$  of the parameter; Spokoiny (2023). This paper studies an important special case when only a p-dimensional target of the posterior is of interest. We present two new results. The first one only requiring  $\bar{\mathbf{p}} \ll n$  and  $\mathbf{p}_e^3 \ll n$  ensures a full dimensional concentration of the posterior and approximation of the marginal posterior by a *Gaussian mixture* with the accuracy of order  $\sqrt{\mathbf{p}_e^3/n}$ . This result reduces the original problem to some analysis for high dimensional Gaussian measures. The second result provides some sufficient conditions for the classical *Laplace approximation* of the posterior. Recent advances in high dimensional Gaussian probability Götze et al. (2019) help to relax the condition  $\bar{\mathbf{p}}^3 \ll n$  to  $\bar{\mathbf{p}}^2 \ll$ n. An interesting open question is a possibility of getting a multimodal non-Gaussian approximation of the marginal posterior for the range  $n^{1/2} \ll \bar{\mathbf{p}} \ll n$ . The general results are illustrated on the particular example of *error-in-operator* model.

Some issues important for statistical inference are not addressed in this paper. In particular, we do not discuss the bias induced by the prior, the use of credible sets as frequentist confidence sets, contraction rate over smoothness classes. However, all these issues can been addressed similarly to Spokoiny (2022, 2023), the calculus from Section C can be well used for the corresponding analysis. Necessary finite sample guarantees for penalized estimation in error-in-operator or high dimensional random design models require a careful derivation and will be provided in the forthcoming paper.

#### Organization of the paper

Section 2 considers a general semiparametric framework and presents some results on marginal Laplace approximation including Theorem 2.5 about mixed Laplace approximation and Theorem 2.12 about Laplace approximation on the class of elliptic sets. We also provide some sufficient conditions in terms of the efficient dimension of the full parameter, under which the mixed Laplace approximation can be reduced back to the standard Laplace Theorem. Section 3 specifies the result to the case of an error-in-operator problem. The appendix collects some very useful facts about Laplace approximation for the integral  $\int e^{f(v)} dv$  for a smooth concave function f as well as some useful bounds from high-dimensional probability. For reference convenience we include the general results on Laplace approximation from Spokoiny (2023) in Section B and the technical results on Gaussian quadratic forms in Section D.

## 2 Laplace approximation of the marginal

This section considers the problem of Laplace approximation when the argument v of the function f(v) is high dimensional,  $v \in \mathbb{R}^{\overline{p}}$ , but we are interested only in the subvector x of v,  $x \in \mathbb{R}^p$ . We state several results about marginal posterior. Theorem 2.3 explains concentration properties of the marginal posterior under the bound  $\overline{p}_G \ll n$  on the effective dimension of the full parameter v. Further, Theorem 2.5 presents our main result about mixed Laplace approximation of the marginal distribution. Later Theorem 2.7 and Theorem 2.8 provide some sufficient condition which allow to replace the mixed Laplace approximation by a single Gaussian distribution. The most advanced Theorem 2.11 combines the obtained bounds with the standard trick in semiparametric estimation based on one-point orthogonality; see e.g. Bickel et al. (1993). The latter result allows to improve the bound on the critical dimension from  $\overline{p}^3 \ll n$  to  $\overline{p}^2 \ll n$ for establishing a Laplace approximation for the low-dimensional marginal distribution. However, we guess that in zone  $n^{1/2} \ll \overline{p} \ll n$ , a mixed Laplace approximation is possible; see Section 2.11 for details.

We write  $\boldsymbol{v} = (\boldsymbol{x}, \boldsymbol{a})$ , where  $\boldsymbol{a}$  stands for the nuisance component taking its values in some set  $\mathsf{A} \subseteq \mathbb{R}^q$ , so that  $\overline{p} = p + q$ . Denote  $\Upsilon = \mathbb{R}^p \times \mathsf{A}$ ,

$$\boldsymbol{v}^* = \operatorname*{argmax}_{\boldsymbol{v}} f(\boldsymbol{v}), \qquad \boldsymbol{v}^* = (\boldsymbol{x}^*, \boldsymbol{a}^*).$$

The full dimensional approach of Spokoiny (2023) considers the measure  $\mathbb{P}_f$  on  $\Upsilon$  whose density is proportional to  $e^{f(\boldsymbol{v})}$ , and approximates it by a Gaussian measure. To be more specific, assume the concavity condition  $(\mathcal{C}_0)$  with the decomposition

$$f(\boldsymbol{v}) = \ell(\boldsymbol{v}) - \|\mathcal{G}\boldsymbol{v}\|^2/2$$
(2.1)

for a concave function  $\ell(\boldsymbol{v})$  and a symmetric positive full dimensional matrix  $\mathcal{G}^2$ . Define  $\mathscr{F} = -\nabla^2 f(\boldsymbol{v}^*), \ \mathscr{F}_0 = -\nabla^2 \ell(\boldsymbol{v}^*).$ 

#### 2.1 Full dimensional bounds

This section states full dimensional about the parameter  $\,\boldsymbol{\upsilon}\,.\,$  The full Laplace effective dimension is

$$\overline{\mathbf{p}} \stackrel{\text{def}}{=} \operatorname{tr}(\mathscr{F}^{-1}\mathscr{F}_0)$$

With x fixed, define

$$\overline{\mathbf{r}} = 2\sqrt{\overline{\mathbf{p}}} + \sqrt{2\mathbf{x}} \,. \tag{2.2}$$

Theorem B.2 yields the following result.

**Proposition 2.1.** Let  $f(\boldsymbol{v})$  follow (2.1) and satisfy  $(\boldsymbol{\mathcal{S}}_3)$  with  $\boldsymbol{v} = \boldsymbol{v}^*$ ,  $\mathbf{m}^2 = n^{-1} \mathscr{F}_0 = -n^{-1} \nabla^2 \ell(\boldsymbol{v}^*)$ , and  $\mathbf{r} = \nu^{-1} \overline{\mathbf{r}}$ ; see (2.2). With  $\nu = 2/3$ , let

$$\omega^+ \stackrel{\text{def}}{=} \frac{\mathsf{c}_3 \,\nu^{-1}\overline{\mathsf{r}}}{n^{1/2}} \le \frac{3}{4} \,. \tag{2.3}$$

Then

$$\mathbb{P}_f(\|\mathscr{F}_0^{1/2}(\boldsymbol{v}-\boldsymbol{v}^*)\| > \nu^{-1}\overline{\mathbf{r}}) \leq \mathrm{e}^{-\mathrm{x}}.$$

Moreover, if

$$\frac{\mathsf{c}_3\,\nu^{-1}\overline{\mathsf{r}}\,\overline{\mathsf{p}}}{n^{1/2}}\leq 2$$

then

$$\sup_{A \in \mathscr{B}(\mathbb{R}^p)} \left| \mathbb{P}_f(\boldsymbol{v} - \boldsymbol{v}^* \in A) - \mathbb{P}(\mathscr{F}^{-1/2}\boldsymbol{\gamma} \in A) \right| \le 4(\diamondsuit_3 + \mathrm{e}^{-\mathtt{x}})$$

with  $\gamma$  standard normal in  $\mathbb{R}^{\overline{p}}$  and

$$\diamondsuit_3 = \frac{\mathsf{c}_3(\overline{\mathsf{p}}+1)^{3/2}}{4(1-\omega^+/3)^{3/2}n^{1/2}} \le \frac{\mathsf{c}_3(\overline{\mathsf{p}}+1)^{3/2}}{2n^{1/2}} \,. \tag{2.4}$$

Let  $\check{\mathbb{F}}^{-1} = (\mathscr{F}^{-1})_{xx}$  be the xx-block of  $\mathscr{F}^{-1}$ . If  $Z \sim \mathbb{P}_f$  and  $(X, \mathbb{A})$  are the components of Z, then the marginal X of Z is also nearly Gaussian  $\mathcal{N}(x^*, \check{\mathbb{F}}^{-1})$ . However, due to (2.4), the accuracy of the full dimensional approximation deteriorates polynomially with the total effective dimension  $\bar{p} = \bar{p}(v^*)$  and requires  $\bar{p} \ll n^{1/3}$ . The value  $\bar{p}$  can be large even after dimensionality reduction caused by a penalty term. Unfortunately, one cannot drop the condition  $\bar{p} \ll n^{1/3}$ , it seems to be inherent for the problem at hand. However, if we are interested in the low dimensional component x only, one can try to integrate out the remaining components and to relax the condition on the full parameter dimension.

#### 2.2 Orthogonal case

This section illustrates the principal idea on the special *orthogonal* case when the function  $f(\boldsymbol{v}) = f(\boldsymbol{x}, \boldsymbol{a})$  satisfies the condition

$$\nabla_{\boldsymbol{a}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{a}) \equiv 0. \tag{2.5}$$

In this case the function f can be decomposed as  $f(x, a) = f_1(x) + f_2(a)$  for some functions  $f_1(x)$  and  $f_2(a)$ . When considering the x-marginal distribution of  $\mathbb{P}_f$ , the nuisance variable a can be ignored.

**Lemma 2.2.** Let f be twice continuously differentiable and satisfy (2.5). Then for any  $A \in \mathscr{B}(\mathbb{R}^p)$ , it holds  $\mathbb{P}_f(\mathbf{x} \in A) = \mathbb{P}_{f_1}(\mathbf{x} \in A)$ .

*Proof.* The condition  $\nabla_{\boldsymbol{a}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{a}) \equiv 0$  implies the decomposition  $f(\boldsymbol{x}, \boldsymbol{a}) = f_1(\boldsymbol{x}) + f_2(\boldsymbol{a})$ . Now the result follows by the Fubini Theorem.

This result allows to apply the result about Laplace approximation of  $\mathbb{P}_f$  to the function  $f_1(\mathbf{x})$  of the target variable  $\mathbf{x}$ , the corresponding accuracy depends also on the target dimension only. Unfortunately the orthogonality condition (2.5) is too restrictive. Later we discuss what can be stated if this condition is violated.

#### 2.3 Conditional Laplace approximation

The basic idea of our approach is, for any fixed value of the nuisance variable a, to consider the Laplace approximation of  $f_a(x) = f(x, a)$  as a function of x only. We follow the line of Section B. Define

$$\begin{split} \boldsymbol{x_a} &\stackrel{\text{def}}{=} \operatorname*{argmax}_{\boldsymbol{x}} f_{\boldsymbol{a}}(\boldsymbol{x}), \\ \mathbb{F}_{\boldsymbol{a}} &\stackrel{\text{def}}{=} -\nabla^2 f_{\boldsymbol{a}}(\boldsymbol{x_a}) = -\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x_a}, \boldsymbol{a}) \end{split}$$

First we state a conditional result: for each a, the measure  $\mathbb{P}_{f,a}$  on  $\mathbb{R}^p$  with the density proportional to  $e^{f_a(x)}$  can be well approximated by the Gaussian measure  $\mathcal{N}(x_a, \mathbb{F}_a^{-1})$ . The accuracy of approximation corresponds to the dimension of the target variable xonly. Moreover, under natural conditions, this result can be stated uniformly over the set  $a \in A$ . This implies that the x-marginal of  $\mathbb{P}_f$  can be well approximated by the mixture of  $\mathcal{N}(x_a, \mathbb{F}_a^{-1})$ . Under the additional conditions  $x_a \approx x_{a^*}$ ,  $\mathbb{F}_a \approx \mathbb{F} \stackrel{\text{def}}{=} \mathbb{F}_{a^*}$ , this mixture can be replaced by the Gaussian distribution  $\mathcal{N}(x^*, \mathbb{F}^{-1})$ .

Now we present our conditions. The first one replaces the strong concavity of the full dimensional function f by concavity of each partial function  $f_a$ ,  $a \in A$ .

 $(\mathcal{C}_a)$  For any  $a \in \mathsf{A}$ , there exists an operator  $\mathsf{D}_a^2 \leq \mathbb{F}_a$  in  $\mathbb{R}^p$  such that the function

$$\ell_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}+\boldsymbol{u}) \stackrel{\text{def}}{=} f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}+\boldsymbol{u}) + \frac{1}{2} \|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2 - \frac{1}{2} \|\mathbb{D}_{\boldsymbol{a}}\boldsymbol{u}\|^2$$

is concave in  $\boldsymbol{u} \in \mathbb{R}^p$ .

If  $f(\boldsymbol{v}) = \ell(\boldsymbol{v}) - \|\mathcal{G}\boldsymbol{v}\|^2/2$  with  $\|\mathcal{G}\boldsymbol{v}\|^2 = \|G\boldsymbol{x}\|^2 + \|\boldsymbol{\Gamma}\boldsymbol{a}\|^2$  and  $\ell(\boldsymbol{x}, \boldsymbol{a})$  concave in  $\boldsymbol{x}$ , then one can use  $\mathsf{D}_{\boldsymbol{a}}^2 = -\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \ell(\boldsymbol{x}_{\boldsymbol{a}}, \boldsymbol{a})$  while  $\mathbb{F}_{\boldsymbol{a}} = \mathsf{D}_{\boldsymbol{a}}^2 + G^2$ . ( $\mathcal{C}_{\boldsymbol{a}}$ ) enables us to define for each  $\boldsymbol{a} \in \mathsf{A}$  the effective target dimension  $\mathsf{p}_{\boldsymbol{a}}$ , the corresponding radius  $\mathsf{r}_{\boldsymbol{a}}$ , and the local vicinity  $\mathcal{U}_{\boldsymbol{a}}$ :

$$\begin{split} \mathbf{p}_{a} &= \operatorname{tr} \left( \mathsf{D}_{a}^{2} \mathbb{F}_{a}^{-1} \right), \\ \mathbf{r}_{a} &= 2 \sqrt{\mathbf{p}_{a}} + \sqrt{2 \mathbf{x}}, \\ \mathcal{U}_{a} &= \left\{ \boldsymbol{u} \colon \| \mathsf{D}_{a} \boldsymbol{u} \| \leq \mathbf{r}_{a} \right\} \end{split}$$

Later we assume that each function  $f_a$  satisfies the smoothness conditions  $(S_{3|a})$ ,  $(S_{3|a}^+)$ , and, if necessary,  $(S_{4|a})$  with  $\mathbf{r} = \nu^{-1}\mathbf{r}_a$  for  $\nu \ge 2/3$ ; see Section A.4.

#### 2.4 Concentration of the conditional and marginal distribution

We start with a concentration property for the target component. (B.9) of Theorem B.1 applied to each  $f_a$  yields the conditional bound on the tail probability: for the measure  $\mathbb{P}_{f,a}$  with the density proportional to  $\exp f_a(x)$ , it holds

$$\mathbb{P}_{f,a}(\|\mathsf{D}_{a}(X-x_{a})\| > \nu^{-1}\mathsf{r}_{a}) \le \mathrm{e}^{-\mathsf{x}}, \qquad a \in \mathsf{A}.$$
(2.6)

If we also succeed to control the variability of  $\mathsf{D}_a^2$  and  $\|\mathsf{D}_a(x_a - x^*)\|$  in a, then the conditional bound (2.6) would imply an unconditional one. With  $\mathsf{D}^2 = \mathsf{D}_{a^*}^2$ , global Fréchet smoothness (A.32) of  $(\mathcal{S}_{3,a}^+)$  implies  $\|\mathsf{D}^{-1}\mathsf{D}_a^2\mathsf{D}^{-1}\| \leq 1 + \omega^+$  for a in A and  $\omega^+$  from (A.38); see Lemma A.15. In the next result we do not require global Fréchet smoothness. Instead, we simply bound the variability of  $\mathsf{D}_a^2$ : for some fixed  $\mathsf{C}_0 \geq 1$ 

$$\mathbf{C}_0^{-2}\,\mathbf{D}^2 \le \mathbf{D}_a^2 \le \mathbf{C}_0^2\,\mathbf{D}^2, \qquad \boldsymbol{a} \in \mathbf{A}.$$

**Theorem 2.3.** Suppose  $(\mathcal{C}_a)$ ,  $(\mathcal{S}_{3|a})$ , and (2.7) for all  $a \in A$ . Let also

$$\sup_{\boldsymbol{a}\in\mathsf{A}}\|\mathsf{D}(\boldsymbol{x}_{\boldsymbol{a}}-\boldsymbol{x}^{*})\|\leq\mathsf{s}\,,\tag{2.8}$$

and for any  $a \in A$ 

$$\omega_{3,a} = \frac{\mathsf{c}_3 \, \mathsf{r}_a}{n^{1/2}} \le 1/3. \tag{2.9}$$

Then

$$\mathbb{P}_f(\|\mathsf{D}(\boldsymbol{X}-\boldsymbol{x}^*)\| > \mathsf{C}_0^2 \nu^{-1} \mathsf{r}_{\boldsymbol{a}^*} + \mathsf{s}) \le \mathrm{e}^{-\mathsf{x}}.$$
(2.10)

*Proof.* Note first that by (2.7) and (2.8)

$$\begin{split} \|\mathsf{D}(oldsymbol{X}-oldsymbol{x}^*)\| &\leq \|\mathsf{D}\,\mathsf{D}_{oldsymbol{a}}^{-1}\,\mathsf{D}_{oldsymbol{a}}\,(oldsymbol{X}-oldsymbol{x}_{oldsymbol{a}})\| + \|\mathsf{D}(oldsymbol{x}_{oldsymbol{a}}-oldsymbol{x}^*)\| \ &\leq \mathsf{C}_0\,\|\mathsf{D}_{oldsymbol{a}}\,(oldsymbol{X}-oldsymbol{x}_{oldsymbol{a}})\| + \mathsf{s}. \end{split}$$

Moreover, (2.7) implies  $\mathbf{r}_{a} \leq C_0 \mathbf{r}_{a^*}$  and the statement follows from (2.6).

1

A nice feature of the bound (2.10) is that the concentration radius  $\mathbf{r}_{a^*}$  corresponds to the dimension of the target variable X only. Also, under  $(S_{3|a})$ , the condition  $\mathbf{p}_a \ll n$ implies  $\mathbf{c}_3 \mathbf{r}_a n^{-1/2} \ll 1$ . However, the result (2.10) becomes meaningful only if we can bound the semiparametric bias term  $\mathbf{s}$ ; see (2.8). The condition  $\mathbf{s} \lesssim \mathbf{r}_{a^*}$  yields the following corollary.

Corollary 2.4. Suppose the conditions of Theorem 2.3 and let  $s \leq C_{\text{bias}} r_{a^*}$ . Then

$$\mathbb{P}_f ig( \| \mathsf{D}(\mathbf{X} - \mathbf{x}_{\mathbf{a}}) \| > (\mathsf{C}_0^2 \, \nu^{-1} + \mathsf{C}_{\mathrm{bias}}) \, \mathtt{r}_{\mathbf{a}^*} ig) \leq \mathrm{e}^{-\mathtt{x}}$$

Usually this result is applied in combination with the so called "one-point orthogonality" condition; see Section 2.9 later.

#### 2.5 Approximation by a Gaussian mixture

Now we turn to approximation of the marginal distribution of X by a Gaussian mixture. (B.10) of Theorem B.1 yields a TV-bound for each condition distribution of X given a: for the measure  $\mathbb{P}_{f,a}$  with the density proportional to  $\exp f_a(x)$ , it holds

$$\mathrm{TV}(\mathbb{P}_{f,a}, \mathcal{N}(\boldsymbol{x}_{a}, \mathbb{F}_{a}^{-1})) \leq \frac{2(\diamondsuit_{a} + \mathrm{e}^{-\mathrm{x}})}{1 - \diamondsuit_{a} - \mathrm{e}^{-\mathrm{x}}} \leq 4(\diamondsuit_{a} + \mathrm{e}^{-\mathrm{x}}),$$

where with  $\omega_a$  from (2.9)

$$\diamondsuit_{\boldsymbol{a}} = \frac{0.75\,\omega_{\boldsymbol{a}}\,\mathtt{p}_{\boldsymbol{a}}}{1-\omega_{\boldsymbol{a}}};$$

see (B.11). Moreover, under the self-concordance condition  $(\mathcal{S}_{3|a})$ , one can use

$$\diamondsuit_{\boldsymbol{a}} = \frac{\mathsf{c}_3}{2} \sqrt{\frac{(\mathsf{p}_{\boldsymbol{a}}+1)^3}{n}}; \qquad (2.11)$$

cf. (B.13). This is again a nice bound which only involves the target dimension  $p_a$ . However, the approximating Gaussian distribution varies with a. Introduce

$$\phi_{\boldsymbol{a}} \stackrel{\text{def}}{=} \max_{\boldsymbol{x}} f_{\boldsymbol{a}}(\boldsymbol{x}) - f(\boldsymbol{v}^*) = f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}) - f(\boldsymbol{v}^*) = f(\boldsymbol{x}_{\boldsymbol{a}}, \boldsymbol{a}) - f(\boldsymbol{v}^*),$$
  
$$\delta_{\boldsymbol{a}} \stackrel{\text{def}}{=} \frac{1}{2} \log \det(\mathbb{F}_{\boldsymbol{a}}^{-1}\mathbb{F}).$$
(2.12)

By definition, the *deficiency*  $-\phi_a$  between the global maximum of f(v) and the partial maximum of f(x, a) w.r.t. x for a fixed is always nonnegative. Later we show that the study can be limited to  $a \in A$  with  $\phi_a$  not too big in absolute value. The first result states an approximation of the x-marginal by a mixture of normals.

**Theorem 2.5.** Let  $f(v^*) = \sup_{v} f(v)$ . Suppose  $(\mathcal{C}_a)$  and  $(\mathcal{S}_{3|a})$  for all  $a \in A$  and assume that

$$\sup_{\boldsymbol{a}\in\mathsf{A}}\frac{\mathsf{c}_3\,\mathsf{r}_{\boldsymbol{a}}\,\mathsf{p}_{\boldsymbol{a}}}{n^{1/2}}\leq\frac{3}{4}\,.$$

Define  $\Diamond_{a}$  by (2.11) and let also with  $\phi_{a}$  and  $\delta_{a}$  from (2.12)

$$\Diamond_{\mathsf{A}} \stackrel{\text{def}}{=} \frac{\int_{\mathsf{A}} \Diamond_{\boldsymbol{a}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}}{\int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}} < \frac{1}{2} - e^{-\mathsf{x}} \,. \tag{2.13}$$

Then for any function g(x) satisfying  $|g(x)| \leq 1$ , it holds with  $\gamma$  standard normal

$$\left|\frac{\int_{\Upsilon} \mathrm{e}^{f(\boldsymbol{v})} g(\boldsymbol{x}) \, d\boldsymbol{v}}{\int_{\Upsilon} \mathrm{e}^{f(\boldsymbol{v})} \, d\boldsymbol{v}} - \frac{\int_{\mathsf{A}} \mathrm{e}^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} \, \mathbb{E}g(\boldsymbol{x}_{\boldsymbol{a}} + \mathbb{F}_{\boldsymbol{a}}^{-1/2} \boldsymbol{\gamma}) \, d\boldsymbol{a}}{\int_{\mathsf{A}} \mathrm{e}^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} \, d\boldsymbol{a}}\right| \leq \frac{2(\diamondsuit_{\mathsf{A}} + \mathrm{e}^{-\mathbf{x}})}{1 - \diamondsuit_{\mathsf{A}} - \mathrm{e}^{-\mathbf{x}}}.$$
 (2.14)

**Remark 2.1.** Obviously  $\diamond_A$  from (2.13) satisfies

$$\diamondsuit_{\mathsf{A}} \leq \diamondsuit^* \stackrel{\mathrm{def}}{=} \sup_{a \in \mathsf{A}} \diamondsuit_a$$

However, the term  $\phi_a$  is always negative and it may decrease almost quadratically as a deviates from zero. Thus, bound (2.13) on  $\diamond_A$  is weaker than the bound on  $\diamond^*$ .

*Proof.* For any v = (x, a), the definitions of  $f_a(x) = f(x, a)$  and of  $\phi_a = f_a(x_a) - f(v^*)$  yield a nice decomposition

$$f(\boldsymbol{v}) - f(\boldsymbol{v}^*) = \phi_{\boldsymbol{a}} + f_{\boldsymbol{a}}(\boldsymbol{x}) - f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}})$$

which enables us to operate with each function  $f_a(x)$  for  $a \in A$  independently:

$$\int_{\Upsilon} e^{f(\boldsymbol{v}) - f(\boldsymbol{v}^*)} g(\boldsymbol{u}) d\boldsymbol{v} = \int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}}} \left( \int e^{f_{\boldsymbol{a}}(\boldsymbol{x}) - f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}})} g(\boldsymbol{x}) d\boldsymbol{x} \right) d\boldsymbol{a}$$
$$= \int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}}} \left( \int e^{f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}) - f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}})} g(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}) d\boldsymbol{u} \right) d\boldsymbol{a}$$
$$= \int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}}} \left( \int e^{f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}};\boldsymbol{u})} g(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}) d\boldsymbol{u} \right) d\boldsymbol{a}. \tag{2.15}$$

By the arguments from the proof of Theorem B.1, see (B.19) and (B.20), for any  $a \in A$ 

$$\left|\frac{\int e^{f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}};\boldsymbol{u})} g(\boldsymbol{x}_{\boldsymbol{a}}+\boldsymbol{u}) \, d\boldsymbol{u} - \int e^{-\|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^{2}/2} g(\boldsymbol{x}_{\boldsymbol{a}}+\boldsymbol{u}) \, d\boldsymbol{u}}{\int e^{-\|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u}}\right| \le \diamondsuit_{\boldsymbol{a}} + e^{-\mathbf{x}}$$

Integrating w.r.t.  $\boldsymbol{a}$  yields by (2.15)

$$\left| \int e^{f(\boldsymbol{v}) - f(\boldsymbol{v}^*)} g(\boldsymbol{u}) \, d\boldsymbol{u} \, d\boldsymbol{a} - \iint e^{\phi_{\boldsymbol{a}}} e^{-\|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2/2} g(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}) \, d\boldsymbol{u} \, d\boldsymbol{a} \right|$$
  
$$\leq \iint e^{\phi_{\boldsymbol{a}}} e^{-\|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2/2} \left( \diamondsuit_{\boldsymbol{a}} + e^{-\mathbf{x}} \right) d\boldsymbol{x} \, d\boldsymbol{a} \,.$$
(2.16)

The same bound applies with  $g(u) \equiv 1$ . By definition,

$$\int e^{-\|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u} = e^{\delta_{\boldsymbol{a}}} \int e^{-\|\mathbb{F}^{1/2}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}$$

and (2.14) follows.

The full dimensional concentration result of Theorem B.2 enables us to limit v to the local vicinity of the point  $v^*$ 

$$\Upsilon_0 = \left\{ oldsymbol{v} \colon \|\mathscr{F}_0^{1/2}(oldsymbol{v} - oldsymbol{v}^*)\| \leq 
u^{-1} \overline{\mathbf{r}} 
ight\}$$

for  $\nu = 2/3$  and some specific  $\overline{\mathbf{r}}$ . By  $A_0$  we denote the projection of  $\Upsilon_0$  on A:

$$\mathsf{A}_0 = \{ \boldsymbol{a} \in \mathsf{A} \colon (\boldsymbol{x}, \boldsymbol{a}) \in \Upsilon_0 \text{ for some } \boldsymbol{x} \}.$$
(2.17)

**Theorem 2.6.** Suppose the conditions of Theorem 2.5 and of Theorem B.2. Then mixed Laplace approximation (2.14) applies with  $A_0$  in place of A.

#### 2.6 Laplace approximation

The result of Theorem 2.5 is very useful because it replaces the original problem by a very particular problem for Gaussian measures only. Namely, we are now interested in

approximating a Gaussian mixture by one Gaussian distribution. The Gaussian mixture in the approximation (2.14) is characterized by the collection of the conditional mean  $x_a$ , variance  $\mathbb{F}_a^{-1}$ , and of the deficiencies  $\phi_a$  for each  $a \in A$ . Moreover, Theorem 2.6 enables us to consider only  $a \in A_0$ . The next question is about possibility of using one Gaussian distribution  $\mathcal{N}(x^*, \mathbb{F}^{-1})$  instead of the mixture of  $\mathcal{N}(x_a, \mathbb{F}_a^{-1})$ . For this, we have to control variability of the parameters  $x_a$  and  $\mathbb{F}_a^{-1}$ . Given a test function g(u), introduce in addition to  $\phi_a$  and  $\delta_a$  from (2.12) one more function of the argument a:

$$\Delta_{g,a} \stackrel{\text{def}}{=} \mathbb{E}g(\mathbf{x}_a + \mathbb{F}_a^{-1/2} \boldsymbol{\gamma}) - \mathbb{E}g(\mathbf{x}_{a^*} + \mathbb{F}_{a^*}^{-1/2} \boldsymbol{\gamma}).$$
(2.18)

Clearly the value  $\Delta_{g,a}$  is uniquely determined by  $x_a - x^*$  and  $\delta_a$  from (2.12).

**Theorem 2.7.** Suppose the conditions of Theorem 2.5. Fix a function  $g(\mathbf{x})$  with  $|g(\mathbf{x})| \leq 1$ . With  $\Delta_{g,\mathbf{a}}$  from (2.18),  $\phi_{\mathbf{a}}$  and  $\delta_{\mathbf{a}}$  from (2.12), define

$$\Delta_g \stackrel{\text{def}}{=} \left| \frac{\int_{\mathsf{A}} \Delta_{g, \boldsymbol{a}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}}{\int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}} \right|,$$

and let  $\diamondsuit_A + \Delta_g < 1/2 - e^{-x}$ ; see (2.13). Then

$$\left| \frac{\int_{\Upsilon} e^{f(\boldsymbol{v})} g(\boldsymbol{x}) d\boldsymbol{v}}{\int_{\Upsilon} e^{f(\boldsymbol{v})} d\boldsymbol{v}} - \mathbb{E}g(\boldsymbol{x}^* + \mathbb{F}_{\boldsymbol{a}^*}^{-1/2} \boldsymbol{\gamma}) \right| \leq \frac{2(\diamondsuit_{\mathsf{A}} + \varDelta_g + e^{-\mathbf{x}})}{1 - \diamondsuit_{\mathsf{A}} - \varDelta_g - e^{-\mathbf{x}}}.$$
 (2.19)

Under the conditions of Theorem B.2, the result applies with  $\mathsf{A}_0$  in place of  $\mathsf{A}$  .

*Proof.* Bound (2.16) and definition (2.18) imply

$$\begin{aligned} \left| \frac{1}{\int \mathrm{e}^{-\|\mathbb{F}^{1/2}\boldsymbol{u}\|^{2}/2}\,d\boldsymbol{u}} \int_{\boldsymbol{\Upsilon}} \mathrm{e}^{f(\boldsymbol{\upsilon})-f(\boldsymbol{\upsilon}^{*})}\,g(\boldsymbol{u})\,d\boldsymbol{\upsilon} - \boldsymbol{E}g(\boldsymbol{x}^{*} + \mathbb{F}_{\boldsymbol{a}^{*}}^{-1/2}\boldsymbol{\gamma})\int_{\mathsf{A}} \mathrm{e}^{\phi_{\boldsymbol{a}}+\delta_{\boldsymbol{a}}}\,d\boldsymbol{a} \right| \\ &\leq \left| \int_{\mathsf{A}} (\diamondsuit_{\boldsymbol{a}} + \mathrm{e}^{-\mathbf{x}} + \Delta_{g,\boldsymbol{a}})\,\mathrm{e}^{\phi_{\boldsymbol{a}}+\delta_{\boldsymbol{a}}}\,d\boldsymbol{a} \right| \leq (\diamondsuit_{\mathsf{A}} + \Delta_{g} + \mathrm{e}^{-\mathbf{x}})\int_{\mathsf{A}} \mathrm{e}^{\phi_{\boldsymbol{a}}+\delta_{\boldsymbol{a}}}\,d\boldsymbol{a}. \end{aligned}$$

The same bound applies to  $g(\mathbf{x}) \equiv 1$  and the result follows as in the proof of Proposition B.4.

The bound of Theorem 2.5 only assumes  $|g(\boldsymbol{x})| \leq 1$ , otherwise  $g(\cdot)$  can be any measurable function of the target parameter  $\boldsymbol{x}$ . In the contrary, the error term  $\Diamond_{g,\boldsymbol{a}}$ in (2.18) strongly relies on the function  $g(\cdot)$ . One way for stating auniform result can be based on Pinsker's inequality. For two measures  $\mathcal{N}_{\boldsymbol{a}^*} = \mathcal{N}(\boldsymbol{x}^*, \mathbb{F}_{\boldsymbol{a}^*}^{-1})$  and  $\mathcal{N}_{\boldsymbol{a}} =$  $\mathcal{N}(\boldsymbol{x}_{\boldsymbol{a}}, \mathbb{F}_{\boldsymbol{a}}^{-1})$  and for any function  $g(\cdot)$  bounded by 1, it holds

$$|\Delta_{g,a}| \leq \mathrm{TV}(\mathcal{N}_{a^*}, \mathcal{N}_{a}) \leq \sqrt{\mathscr{K}(\mathcal{N}_{a^*}, \mathcal{N}_{a})/2}, \qquad (2.20)$$

where  $\operatorname{TV}(\mathcal{N}_{a^*}, \mathcal{N}_a)$  is the total variation distance between  $\mathcal{N}_{a^*}$  and  $\mathcal{N}_a$ , while  $\mathscr{K}(\mathcal{N}_{a^*}, \mathcal{N}_a)$  is the Kullback-Leibler divergence. For two Gaussian measures  $\mathcal{N}_{a^*}, \mathcal{N}_a$ , it holds with  $\mathbb{F} = \mathbb{F}_{a^*}$ 

$$\mathscr{K}(\mathcal{N}_{\boldsymbol{a}^*}, \mathcal{N}_{\boldsymbol{a}}) = \frac{1}{2} \big\{ \|\mathbb{F}^{1/2}(\boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^*)\|^2 + \operatorname{tr}(\mathbb{F}_{\boldsymbol{a}}^{-1}\mathbb{F} - I_p) + \log \det(\mathbb{F}_{\boldsymbol{a}}^{-1}\mathbb{F}) \big\}.$$
(2.21)

Moreover, if the matrix  $\mathcal{B}_a = \mathbb{F}_a^{-1/2} \mathbb{F} \mathbb{F}_a^{-1/2} - I_p$  satisfies  $||\mathcal{B}_a|| \le 2/3$  then

$$\operatorname{TV}(\mathcal{N}_{a^*}, \mathcal{N}_{a}) \leq \frac{1}{2} \Big( \|\mathbb{F}^{1/2}(\boldsymbol{x}_a - \boldsymbol{x}^*)\| + \sqrt{\operatorname{tr} \mathbb{B}_a^2} \Big).$$

This statement and Theorem 2.7 imply a bound for the total variation distance between the  $\boldsymbol{x}$ -marginal of  $\mathbb{P}_f$  and the Gaussian approximation  $\mathcal{N}(\boldsymbol{x}^*, \mathbb{F}^{-1})$ . However, Pinsker's inequality might be too rough. Particularly, dependence on  $\|\mathbb{F}^{1/2}(\boldsymbol{x}_a - \boldsymbol{x}^*)\|$  can be problematic.

#### 2.7 Gaussian comparison and elliptic credible sets

Bound (2.20) can be drastically improved by using recent results on Gaussian comparison if we limit ourselves to some special class of functions g of the form  $g(\boldsymbol{u}) = \mathbb{1}(\|Q\boldsymbol{u}\| \leq r)$ ; see Section E. Define

$$\Delta_{\boldsymbol{a}} = \frac{1}{\|Q \mathbb{F}^{-1} Q^{\top}\|_{\mathrm{Fr}}} \left( \|Q (\mathbb{F}^{-1} - \mathbb{F}_{\boldsymbol{a}}^{-1}) Q^{\top}\|_{1} + \|Q (\boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^{*})\|^{2} \right), \qquad (2.22)$$

$$\Delta_{\mathsf{A}} \stackrel{\text{def}}{=} \frac{\int_{\mathsf{A}} \Delta_{\boldsymbol{a}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}}{\int_{\mathsf{A}} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} d\boldsymbol{a}}.$$
(2.23)

**Theorem 2.8.** Suppose the conditions of Theorem 2.5. For any  $Q: \mathbb{R}^p \to \mathbb{R}^q$ , it holds with  $\gamma \sim \mathcal{N}(0, I)$ 

$$\sup_{\mathbf{r}>0} \left| \mathbb{P}_f \left( \|Q(\mathbf{X} - \mathbf{x}^*)\| \le \mathbf{r} \right) - \mathbb{P} \left( \|Q \mathbb{F}^{-1/2} \boldsymbol{\gamma}\| \le \mathbf{r} \right) \right| \le \frac{2(\diamondsuit_Q + e^{-\mathbf{x}})}{1 - \diamondsuit_Q - e^{-\mathbf{x}}}, \quad (2.24)$$

where

$$\Diamond_Q = \Diamond_\mathsf{A} + \mathsf{C} \varDelta_\mathsf{A}$$

with  $\diamondsuit_A$  from (2.13),  $\varDelta_A$  from (2.23), and some absolute constant C. Under conditions of Theorem B.2, one can use  $A_0$  from (2.17) in place of A.

As a characteristic example, consider  $Q = \mathsf{D}$ . Then Laplace approximation (2.24) requires small values of  $\|\mathsf{D}(\mathbb{F}^{-1} - \mathbb{F}_a^{-1})\mathsf{D}\|_1/\sqrt{\mathsf{p}_{a^*}}$  and  $\|\mathsf{D}(\boldsymbol{x}_a - \boldsymbol{x}^*)\|$  for all  $a \in \mathsf{A}_0$ .

#### 2.8 Variance homogenization

To make the result of Theorem 2.8 meaningful, we have to get the rid of the bias  $s_a = x_a - x^* = x_a - x_{a^*}$  and of the varying precision matrix  $\mathbb{F}_a$ . This section focuses on the latter. Variability of  $\mathbb{F}_a$  is measured by the first term  $\|Q(\mathbb{F}^{-1} - \mathbb{F}_a^{-1})Q^{\top}\|_1$  in (2.22). Now we can restate the approximation bounds (2.14) and (2.19) using Gaussian mixture with a homogeneous variance  $\mathbb{F}^{-1}$ .

**Theorem 2.9.** Suppose the conditions of Theorem 2.5 and of Theorem B.2. For any  $Q: \mathbb{R}^p \to \mathbb{R}^q$ , it holds with  $\gamma$  standard normal and  $A_0$  from (2.17)

$$\sup_{\mathbf{r}>0} \left| \frac{\int_{\Upsilon} e^{f(\boldsymbol{v})} \, \mathbb{I}(\|Q\boldsymbol{x}\| \leq \mathbf{r}) \, d\boldsymbol{v}}{\int_{\Upsilon} e^{f(\boldsymbol{v})} \, d\boldsymbol{v}} - \frac{\int_{\mathsf{A}_0} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} \, \mathcal{P}(\|\boldsymbol{x}_{\boldsymbol{a}} + \mathbb{F}^{-1/2} \boldsymbol{\gamma}\| \leq \mathbf{r}) \, d\boldsymbol{a}}{\int_{\mathsf{A}_0} e^{\phi_{\boldsymbol{a}} + \delta_{\boldsymbol{a}}} \, d\boldsymbol{a}} \right| \\
\leq \frac{2(\diamondsuit_{\mathsf{A}_0} + \mathbb{C} \, \boldsymbol{\Delta}_{\mathbb{F}} + e^{-\mathbf{x}})}{1 - \diamondsuit_{\mathsf{A}_0} - \mathbb{C} \, \boldsymbol{\Delta}_{\mathbb{F}} - e^{-\mathbf{x}}} \leq 4(\diamondsuit_{\mathsf{A}_0} + \mathbb{C} \, \boldsymbol{\Delta}_{\mathbb{F}} + e^{-\mathbf{x}}),$$
(2.25)

where C is an absolute constant while with  $\omega^+$  from (2.3)

$$\Delta_{\mathbb{F}} = \frac{1}{\|Q \,\mathbb{F}^{-1} \,Q^{\top}\|_{\mathrm{Fr}}} \, \frac{\int_{\mathsf{A}_0} \|Q(\mathbb{F}^{-1} - \mathbb{F}_a^{-1}) Q^{\top}\|_1 \,\mathrm{e}^{\phi_a + \delta_a} \,da}{\int_{\mathsf{A}_0} \mathrm{e}^{\phi_a + \delta_a} \,da} \leq \frac{\omega^+}{1 - \omega^+} \, \frac{\mathrm{tr}(Q \,\mathbb{F}^{-1} Q^{\top})}{\|Q \,\mathbb{F}^{-1} \,Q^{\top}\|_{\mathrm{Fr}}}$$

Furthermore, define

$$\mathbb{B}_Q = \frac{1}{\|Q \mathbb{F}^{-1} Q^\top\|} Q \mathbb{F}^{-1} Q^\top, \qquad \mathbf{p}_Q = \operatorname{tr}(\mathbb{B}_Q),$$

and suppose that

$$|\mathbf{B}_Q||_{\mathrm{Fr}}^2 = \operatorname{tr} \mathbf{B}_Q^2 \ge \mathsf{C}_0^2 \operatorname{tr} \mathbf{B}_Q = \mathsf{C}_0^2 \operatorname{p}_Q \tag{2.26}$$

with some fixed positive constant  $C_0$ . Then the result (2.25) applies with

$$\Delta_{\mathbb{F}} \leq \frac{\omega^+ \sqrt{p_Q}}{\mathsf{C}_0(1-\omega^+)} = \frac{\mathsf{c}_3 \, \nu^{-1} \, \overline{\mathsf{r}} \, \sqrt{p_Q}}{\mathsf{C}_0(1-\omega^+) \sqrt{n}} \, .$$

*Proof.* The first statement follows from Theorem 2.5 similarly to the proof of Theorem 2.8 using Gaussian comparison results from Section E. It remains to evaluate  $||Q(\mathbb{F}^{-1} - \mathbb{F}_a^{-1})Q^{\top}||_1$ . We present a simple upper bound.

**Lemma 2.10.** Assume the conditions of Proposition 2.1. Let  $\mathbf{a} \in A_0$ . Then for any  $Q: \mathbb{R}^p \to \mathbb{R}^q$ , it holds with  $\mathbb{F} = \mathbb{F}_{\mathbf{a}^*}$ 

$$\|Q(\mathbb{F}^{-1} - \mathbb{F}_{a}^{-1})Q^{\top}\|_{1} \le \frac{\omega^{+}}{1 - \omega^{+}} \operatorname{tr}(Q \mathbb{F}^{-1}Q^{\top}).$$
(2.27)

$$\|\mathsf{D}(\mathbb{F}^{-1} - \mathbb{F}_{\boldsymbol{a}}^{-1})\mathsf{D}\|_1 \le \frac{\omega^+ \operatorname{p}_{\boldsymbol{a}^*}}{1 - \omega^+} \ .$$

*Proof.* Lemma A.3 implies for  $v_a = (x_a, a)$  and  $\mathscr{F}_a = \mathscr{F}(v_a)$ 

$$\frac{1}{1+\omega^+} \mathscr{F}^{-1} \leq \mathscr{F}_a^{-1} \leq \frac{1}{1-\omega^+} \mathscr{F}^{-1} \,.$$

Clearly the same bound applies to the xx-blocks  $\mathbb{F}^{-1}$  and  $\mathbb{F}_{a}^{-1}$ :

$$\frac{1}{1+\omega^{+}} \mathbb{F}^{-1} \le \mathbb{F}_{a}^{-1} \le \frac{1}{1-\omega^{+}} \mathbb{F}^{-1}.$$
(2.28)

Now

$$\|Q(\mathbb{F}_{a}^{-1} - \mathbb{F}^{-1})Q^{\top}\|_{1} \leq \left\|Q\left(\frac{\mathbb{F}^{-1}}{1 - \omega^{+}} - \mathbb{F}^{-1}\right)Q^{\top}\right\|_{1} \leq \frac{\omega^{+}}{1 - \omega^{+}}\operatorname{tr}(Q \mathbb{F}^{-1}Q^{\top}),$$

and (2.27) follows.

**Remark 2.2.** Lemma 2.10 demonstrates advantage of using the Gaussian comparison bound in terms of (2.22) instead of KL-bound (2.20) and (2.21). The quantities  $\log \det(\mathbb{F}_{a}^{-1}\mathbb{F}_{a^*})$  or  $\operatorname{tr}(\mathbb{F}_{a}^{-2}\mathbb{F}_{a^*}^2)$  can be evaluated using (2.28), however the related bound would involve the target dimension p in place of the effective dimension  $\mathbf{p}_{a^*}$ . If the target variable is low dimensional and p is small, this difference is not critical.

**Remark 2.3.** In an important special case of a finite dimensional target x, the value  $p_Q$  is bounded accordingly. Therefore, the result (2.25) only requires  $\omega^+ \ll 1$  or  $\overline{p} \ll n$ .

#### 2.9 A bound for the bias under one-point orthogonality

The result of Theorem 2.9 claims an approximation of the posterior measure  $\mathbb{P}_f$  by a homogeneous mixture of Gaussian distributions  $\mathcal{N}(\mathbf{x}_a, \mathbb{F}^{-1})$  with mean  $\mathbf{x}_a$  and a constant variance  $\mathbb{F}^{-1}$ . This section focuses on the bias component  $\mathbf{s}_a = \mathbf{x}_a - \mathbf{x}^*$ . The main problem in establishing a sensitive bound for marginal Laplace approximation is that the bias vector  $\mathbf{s}_a$  is nearly linear in  $\mathbf{a}$ ; see Lemma A.12 for the case of a quadratic function  $f(\mathbf{v})$ . The use of the one-point orthogonality device described Section 2.10, allows to kill the linear term and yields a better bound on the norm of the bias  $\mathbf{s}_a$ . *One-point* orthogonality condition reads

This condition can always be enforced by a linear transform of the nuisance parameter; see Section A.4.3, Lemma A.18. It obviously yields that the negative Hessian  $\mathscr{F} = -\nabla^2 f(\boldsymbol{v}^*)$  is block-diagonal and the  $\boldsymbol{x}\boldsymbol{x}$ -block  $\check{\mathbb{F}}^{-1}$  of  $\mathscr{F}^{-1}$  coincides with  $\mathbb{F}^{-1}$ .

**Theorem 2.11.** Let  $f(\boldsymbol{v})$  follow (2.1) and condition (2.29) be fulfilled. Assume ( $\mathcal{C}_0$ ) and ( $\mathcal{S}_3^+$ ) with  $\boldsymbol{v} = \boldsymbol{v}^*$ ,  $\mathbf{m}^2 = n^{-1} \mathscr{F}_0$ , and  $\mathbf{r} = \nu^{-1} \overline{\mathbf{r}}$ . Let also

$$\omega^{+} \stackrel{\text{def}}{=} \frac{\mathsf{c}_{3} \,\nu^{-1} \,\overline{\mathsf{r}}}{n^{1/2}} \le 1/3. \tag{2.30}$$

Given Q, assume (2.26). Then with  $\gamma_{\mathbb{F}} \sim \mathcal{N}(0, \mathbb{F}^{-1})$ 

$$\begin{split} \sup_{\mathbf{r}>0} & \left| \mathcal{P}_f \left( \|Q(\boldsymbol{X}-\boldsymbol{x}^*)\| \leq \mathbf{r} \right) - \mathcal{P} \left( \|Q\,\boldsymbol{\gamma}_{\mathsf{F}}\| \leq \mathbf{r} \right) \right| \\ & \lesssim \frac{\mathsf{c}_3\,\mathsf{r}_{a^*}\,\mathsf{p}_{a^*}}{\sqrt{n}} + \frac{\mathsf{c}_3\,\overline{\mathsf{r}}\,\sqrt{\mathsf{p}_Q}}{\sqrt{n}} + \frac{\mathsf{c}_3^2\,\overline{\mathsf{r}}^4}{n\,\sqrt{\mathsf{p}_Q}} + \mathrm{e}^{-\mathsf{x}}. \end{split}$$

*Proof.* It holds by (2.27) of Lemma 2.10 and (2.26)

$$\frac{\|Q(\mathbb{F}^{-1} - \mathbb{F}_{a}^{-1})Q^{\top}\|_{1}}{\|Q\,\mathbb{F}^{-1}\,Q\|_{\mathrm{Fr}}} \le \frac{\omega^{+}}{1 - \omega^{+}} \frac{\operatorname{tr}(Q\,\mathbb{F}^{-1}\,Q)}{\|Q\,\mathbb{F}^{-1}\,Q\|_{\mathrm{Fr}}} \le \frac{\omega^{+}\sqrt{\mathtt{P}Q}}{\mathtt{C}_{0}(1 - \omega^{+})} = \frac{\mathtt{c}_{3}\,\nu^{-1}\,\overline{\mathtt{r}}\,\sqrt{\mathtt{P}Q}}{\nu\,\mathtt{C}_{0}(1 - \omega^{+})\sqrt{n}}$$

Proposition A.16 in Section A.4.2 implies with  $\mathbf{r}_{\circ} = \nu^{-1} \overline{\mathbf{r}}$ 

$$\|Q s_{a}\| \leq \frac{\mathsf{c}_{3} \,\mathsf{r}_{\circ}^{2}}{\sqrt{n}} \|Q \,\mathbb{F}^{-1} Q^{\top}\|^{1/2}$$

and

$$\frac{\|Q \, \boldsymbol{s}_{\boldsymbol{a}}\|^2}{\|Q \, \mathbb{F}^{-1} \, Q\|_{\mathrm{Fr}}} \leq \frac{\mathsf{c}_3^2 \, \mathsf{r}_\circ^2 \, \|Q \, \mathbb{F}^{-1} \, Q\|}{n \, \|Q \, \mathbb{F}^{-1} \, Q\|_{\mathrm{Fr}}} \leq \frac{\mathsf{c}_3^2 \, \mathsf{r}_\circ^2}{n \, \mathsf{C}_0 \, \sqrt{\mathsf{p}_Q}}$$

This yields the assertion by Theorem 2.5 and Theorem 2.9.

#### 2.10 Laplace approximation: a general bound

One-point orthogonality condition (2.29) plays an important role in the results of Section 2.9. Unfortunately, this condition is rarely fulfilled for the original model function  $f(\boldsymbol{v})$ . However, a simple trick based on a linear transform of the nuisance variable allows to ensure this condition in a rather general situation. We again consider the setup (2.1). Instead of (2.29), we only impose a mild *separability condition*: the full dimensional information matrix  $\mathscr{F} = \mathscr{F}(\boldsymbol{v}^*) = -\nabla^2 f(\boldsymbol{v}^*)$  can be bounded from below by the block-diagonal matrix with the blocks  $-\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{v}^*)$  and  $-\nabla^2_{\boldsymbol{aa}} f(\boldsymbol{v}^*)$ . For a precise

formulation, consider the block representation of  $\mathscr{F}$ :

$$\mathscr{F} = egin{pmatrix} \mathscr{F}_{oldsymbol{x} oldsymbol{a}} \\ \mathscr{F}_{oldsymbol{a} oldsymbol{x}} & \mathscr{F}_{oldsymbol{a} oldsymbol{a}} \end{pmatrix}, \qquad \mathscr{F}_{oldsymbol{a} oldsymbol{x}} = \mathscr{F}_{oldsymbol{x} oldsymbol{a}}^\top$$

( $\mathscr{F}$ ) It holds  $\mathscr{F}_{xx} > 0$ ,  $\mathscr{F}_{aa} > 0$ , and for some  $\rho = \rho(\mathscr{F}) < 1$ 

$$\|\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\mathscr{F}_{\boldsymbol{x}\boldsymbol{a}}\,\mathscr{F}_{\boldsymbol{a}\boldsymbol{a}}^{-1}\,\mathscr{F}_{\boldsymbol{a}\boldsymbol{x}}\,\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\|\leq\rho.$$

Define the efficient semiparametric Fisher matrix

$$\check{\mathbb{F}} \stackrel{\text{def}}{=} \mathscr{F}_{xx} - \mathscr{F}_{xa} \,\mathscr{F}_{aa}^{-1} \,\mathscr{F}_{ax}; \qquad (2.31)$$

see (A.44). Lemma A.17 implies

$$(1-\rho)\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} \le \check{\mathbb{F}} \le \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} \,. \tag{2.32}$$

Moreover,  $(\mathscr{F})$  can be written as  $\mathscr{F}_{xa} \mathscr{F}_{aa}^{-1} \mathscr{F}_{ax} \leq \rho \mathscr{F}_{xx}$ , that is, (2.32) is equivalent to  $(\mathscr{F})$ . Define also  $\mathscr{C} = \mathscr{F}_{aa}^{-1} \mathscr{F}_{ax}$ . Lemma A.18 explains how the linear transform

$$\tau = \mathbf{a} + \mathscr{F}_{\mathbf{a}\mathbf{a}}^{-1} \mathscr{F}_{\mathbf{a}\mathbf{x}} \left( \mathbf{x} - \mathbf{x}^* \right) = \mathbf{a} + \mathscr{C} \left( \mathbf{x} - \mathbf{x}^* \right),$$
  
$$\breve{f}(\mathbf{x}, \tau) = f(\mathbf{x}, \mathbf{a}) = f(\mathbf{x}, \tau - \mathscr{C} \left( \mathbf{x} - \mathbf{x}^* \right)).$$
(2.33)

ensures one-point orthogonality of the transformed function  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau})$ . Moreover, all the important concavity and smoothness conditions on the function  $f(\boldsymbol{v})$  are transferred to the function  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau})$ . In particular, the self-concordance condition  $(\mathcal{S}_3^+)$  is not dramatically affected by the linear transform (2.33), perhaps, the constant  $c_3$  has to be slightly updated due to a change of the shape of the local elliptic vicinity of  $\boldsymbol{v}^*$ . The same holds for the Laplace effective dimensions  $\bar{\mathbf{p}}$  and  $\mathbf{p}_a$ . Now everything is prepared for applying the result of Theorem 2.11 to the function  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau})$ . The major change is in using the Gaussian approximation  $\mathcal{N}(\boldsymbol{x}^*, \check{\mathbf{F}}^{-1})$  in place of  $\mathcal{N}(\boldsymbol{x}^*, \mathbf{F}^{-1})$ .

**Theorem 2.12.** Let  $f(\boldsymbol{v})$  follow (2.1). Assume  $(\mathcal{C}_0)$ ,  $(\mathscr{F})$ , and  $(\mathcal{S}_3^+)$  with  $\boldsymbol{v} = \boldsymbol{v}^*$ ,  $\mathbf{m}^2 = n^{-1}\mathscr{F}_0$ , and  $\mathbf{r} = \nu^{-1}\overline{\mathbf{r}}$  following (2.30). For Q satisfying (2.26), it holds with  $\gamma_{\breve{F}} \sim \mathcal{N}(0, \breve{F}^{-1})$ 

$$\begin{split} \sup_{\mathbf{r}>0} & \left| \mathcal{P}_f \big( \|Q(\mathbf{X}-\mathbf{x}^*)\| \leq \mathbf{r} \big) - \mathcal{P} \big( \|Q\,\boldsymbol{\gamma}_{\breve{\mathsf{F}}}\| \leq \mathbf{r} \big) \right| \\ & \lesssim \frac{\mathsf{c}_3\,\mathbf{r}_{a^*}\,\mathbf{p}_{a^*}}{\sqrt{n}} + \frac{\mathsf{c}_3\,\overline{\mathbf{r}}\,\sqrt{\mathsf{p}_Q}}{\sqrt{n}} + \frac{\mathsf{c}_3^2\,\overline{\mathbf{r}}^4}{n\,\sqrt{\mathsf{p}_Q}} + \mathrm{e}^{-\mathsf{x}}. \end{split}$$

#### 2.11 Critical dimension in marginal Laplace approximation

The result of Theorem 2.11 yields an important conclusion. With  $\bar{r} \simeq \bar{p}^{1/2}$ , the condition  $\Delta_a \ll 1$  from (2.22) means that

$$c_3^2 p_Q \overline{p} \ll n, \qquad c_3^2 \overline{p}^2 \ll n \sqrt{p_Q}.$$
 (2.34)

The marginal Laplace approximation requires in addition  $c_3 r_{a^*} p_{a^*} \approx c_3 p_{a^*}^{3/2} \ll n^{1/2}$ . In particular, if the target component is low dimensional and the factors  $p_{a^*}, p_Q$  can be ignored, condition (2.34) reads as  $c_3^2 \bar{p}^2 \ll n$  which improves the full dimensional condition  $c_3^2 \bar{p}^3 \ll n$ . This improvement is obtained by a non-trivial combination of the Gaussian mixture approximation of Theorem 2.5 and the Gaussian comparison bound used in Theorem 2.8.

### 3 Error-in-operator model

This section aims at applying the general results of Section 2 to the special case of error-in-operator model. The main focus is on the properties of the marginal posterior such as concentration and Laplace approximation under possibly weak conditions on the full parameter dimension. In the contrary to Trabs (2018), the issues like contraction rate under smoothness conditions on the source signal  $\boldsymbol{x}$  and the operator A are not discussed. However, the main result from Theorem 3.4 claims that the marginal posterior behaves as in the classical linear inverse problem with the true known operator. This enables us to reduce the remaining questions to the well studied case of a linear inverse problem; see e.g. Knapik et al. (2011), Knapik et al. (2016).

Given a vector  $\boldsymbol{z} \in \mathbb{R}^n$ , the task is to invert the relation  $\boldsymbol{z} = A\boldsymbol{x} + \boldsymbol{\varepsilon}$  when the linear operation A is not known and only a pilot  $\hat{A}$  is available. Following the suggestion in Section 1, we treat this task as a semiparametric problem of recovering  $\boldsymbol{x}$  while Aserves as nuisance parameter. Given an image vector  $\boldsymbol{z} \in \mathbb{R}^q$  and a pilot  $\hat{A} \colon \mathbb{R}^p \to \mathbb{R}^q$ , consider the function

$$f(\boldsymbol{x}, A) = -\frac{1}{2} \|\boldsymbol{z} - A\boldsymbol{x}\|^2 - \frac{\mu^2}{2} \|\widehat{A} - A\|_{\rm Fr}^2 - \frac{1}{2} \|G\boldsymbol{x}\|^2 - \frac{1}{2} \|A\|_{\mathcal{K}}^2.$$
(3.1)

Here  $\boldsymbol{x} \in \mathbb{R}^p$  is the variable of interest while  $A \in \mathbb{R}^{q \times p}$  is an operator from  $\mathbb{R}^p$  to  $\mathbb{R}^q$ serving as a nuisance variable. The factor  $\mu$  in the fidelity term  $\mu^2 \|\hat{A} - A\|_{\text{Fr}}^2$  scales the operator noise. As usual, smoothness of the source signal  $\boldsymbol{x}$  is controlled by the penalty term  $\|G\boldsymbol{x}\|^2$ . One can easily extend the derivation for a penalty  $\|G(\boldsymbol{x}-\boldsymbol{x}_0)\|^2/2$  in which  $\boldsymbol{x}_0$  is an initial guess for  $\boldsymbol{x}$ . Equivalently, one can treat this penalty as log-density of the Gaussian prior  $\mathcal{N}(\boldsymbol{x}_0, G^{-2})$  on  $\boldsymbol{x}$ . The norm  $\|\cdot\|_{\mathcal{K}}$  reflects our prior information about operator smoothness. Note that the fidelity  $\mu^2 \|\widehat{A} - A\|_{\mathrm{Fr}}^2$  already collects some prior information about A, so an additional penalization is not ultimate. However, this term does not mimic any smoothness of the operator A. We apply a construction reflecting the standard "approximation spaces" approach; see Hoffmann and Reiss (2008), Trabs (2018). Consider  $\mathcal{K} = \mathrm{block}\{\mathcal{K}_1, \ldots, \mathcal{K}_q\}$ , where  $\mathcal{K}_m$  is a positive symmetric operator in  $\mathbb{R}^p$ . For  $A = (A_1, \ldots, A_q)^{\top}$ , this yields

$$||A||_{\mathcal{K}}^2 = \sum_{m=1}^q ||\mathcal{K}_m A_m||^2.$$

The ridge regression case corresponds to  $G^2 = g^2 I_p$  and  $\mathcal{K}_m^2 \equiv 0$ .

The main question under study is the set of sufficient conditions ensuring Laplace approximation for the marginal distribution for the target parameter  $\boldsymbol{x}$  when considering the unknown operator A as nuisance. Define

$$(\boldsymbol{x}^*, A^*) = \operatorname*{argmax}_{(\boldsymbol{x}, A)} f(\boldsymbol{x}, A).$$

Because of the product term  $A\mathbf{x}$  in (3.1), this problem is not quadratic in the scope of parameters  $\mathbf{v} = (\mathbf{x}, A)$  and a closed form solution is not available. In particular,  $\mathbf{x}^*$  does not coincide with the plug-in solution  $\mathbf{x}_{\widehat{A}}$ 

$$\boldsymbol{x}_{\widehat{A}} = \left(\widehat{A}^{\top}\widehat{A} + G^{2}\right)^{-1}\widehat{A}^{\top}\boldsymbol{z}.$$

#### 3.1 Identifiability, warm start, efficient information matrix

The original relation  $\mathbf{z} = A\mathbf{x}$  does not allow to recover  $\mathbf{x}$  when A is unknown. The additional information about A in form of a pilot  $\widehat{A}$  or, alternatively, a prior on A, improves this lack of identifiability. However, the quality of the pilot measured by the multiplicative factor  $\mu$  in (3.1) is important. The smaller is the operator noise, or, equivalently, the better is the accuracy of the pilot  $\widehat{A}$ , the larger  $\mu$  should be. Still we have an issue with identifiability for  $\mathbf{x}$  very large due to multiplicative term  $A\mathbf{x}$  in  $\|\mathbf{z} - A\mathbf{x}\|^2/2$ : even a small error in the operator A may result in a large shift of the solution  $\mathbf{x}$ . Proposition 3.1 later in this section helps to address the identifiability question using the so called "warm start" condition. We also compute the efficient semiparametric matrix  $\breve{F}$  and check condition ( $\mathscr{F}$ ).

**Proposition 3.1.** Let  $G^2 \ge G_0^2$  for some  $G_0^2$  positive semi-definite. Define for  $\rho < 1$ 

$$\Upsilon^{\circ} \stackrel{\text{def}}{=} \Big\{ (\boldsymbol{x}, A) \colon 4 \| \boldsymbol{x} \|^2 \le \rho \, \mu^2, \ 4 \| A \boldsymbol{x} - \boldsymbol{z} \|^2 I_p \le \rho \, \mu^2 \left( A^\top A + 2G_0^2 \right) \Big\}.$$
(3.2)

Let the point  $(\mathbf{x}^*, A^*)$  belong to a set  $\Upsilon^{\circ}$ . Then  $(\mathscr{F})$  is fulfilled for  $\mathscr{F} = \mathscr{F}(\mathbf{v})$  and all  $\mathbf{v} \in \Upsilon^{\circ}$  with the same  $\rho$ , and  $f(\mathbf{v})$  is strongly concave on  $\Upsilon^{\circ}$ .

*Proof.* Let  $\boldsymbol{v} = (\boldsymbol{x}, A)$  and  $A_m^{\top}$  be the rows of A. The function  $f(\boldsymbol{x}, A)$  from (3.1) can be represented as

$$f(\boldsymbol{x}, A) = -\frac{1}{2} \sum_{m=1}^{q} \left( |z_m - A_m^{\top} \boldsymbol{x}|^2 + \|\widehat{A}_m - A_m\|^2 + \|\mathcal{K}_m A_m\|^2 \right) - \frac{1}{2} \|G\boldsymbol{x}\|^2.$$

It holds

$$\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v}) = -\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 f(\boldsymbol{x}, A) = A^{\top}A + G^2 = \sum_{m=1}^q A_m A_m^{\top} + G^2$$
(3.3)

and for each  $m = 1, \dots, q$  with  $H_m^2 = \mu^2 I_p + \mathcal{K}_m^2$ 

$$-\nabla_{A_m A_m}^2 f(\boldsymbol{x}, A) = \boldsymbol{x} \boldsymbol{x}^\top + \mu^2 I_p + \mathcal{K}_m^2 \stackrel{\text{def}}{=} \boldsymbol{x} \boldsymbol{x}^\top + H_m^2,$$
  
$$-\nabla_{\boldsymbol{x}} \nabla_{A_m} f(\boldsymbol{x}, A) = (A_m^\top \boldsymbol{x} - z_m) I_p + A_m \, \boldsymbol{x}^\top \stackrel{\text{def}}{=} J_m(\boldsymbol{x}, A_m).$$
(3.4)

Block-diagonal structure of  $\mathscr{F}_{AA}(\boldsymbol{v})$  yields

$$\mathscr{F}_{\boldsymbol{x}A}(\boldsymbol{v}) \, \mathscr{F}_{AA}^{-1}(\boldsymbol{v}) \, \mathscr{F}_{A\boldsymbol{x}}(\boldsymbol{v}) = \sum_{m=1}^{q} J_m(\boldsymbol{x}, A_m) \, \mathscr{F}_{A_m A_m}^{-1}(\boldsymbol{v}) \, J_m^{\top}(\boldsymbol{x}, A_m) \,.$$
Moreover,  $\mathscr{F}_{A_m A_m}^{-1}(\boldsymbol{v}) = (\boldsymbol{x}\boldsymbol{x}^{\top} + \mu^2 I_p + \mathcal{K}_m^2)^{-1} \leq (\mu^2 I_p + \mathcal{K}_m^2)^{-1} \leq \mu^{-2} I_p \,\text{ and}$ 

$$J_m(\boldsymbol{x}, A_m) \, \mathscr{F}_{A_m A_m}^{-1}(\boldsymbol{v}) \, J_m^{\top}(\boldsymbol{x}, A_m) \leq 2(A_m^{\top}\boldsymbol{x} - z_m)^2 (\mu^2 I_p + \mathcal{K}_m^2)^{-1}$$

$$+ 2 \, \boldsymbol{x}^{\top} (\boldsymbol{x}\boldsymbol{x}^{\top} + \mu^2 I_p + \mathcal{K}_m^2)^{-1} \boldsymbol{x} \, A_m \, A_m^{\top}$$

$$\leq \frac{2(A_m^{\top}\boldsymbol{x} - z_m)^2}{\mu^2} \, I_p + \frac{2\|\boldsymbol{x}\|^2}{\|\boldsymbol{x}\|^2 + \mu^2} \, A_m \, A_m^{\top}$$

yielding by (3.2)

$$\begin{aligned} \mathscr{F}_{\boldsymbol{x}A}(\boldsymbol{v}) \, \mathscr{F}_{AA}^{-1}(\boldsymbol{v}) \, \mathscr{F}_{A\boldsymbol{x}}(\boldsymbol{v}) &\leq \frac{2}{\mu^2} \|\boldsymbol{z} - A\boldsymbol{x}\|^2 I_p + \frac{2\|\boldsymbol{x}\|^2}{\|\boldsymbol{x}\|^2 + \mu^2} \, A^\top A \\ &\leq \frac{\rho}{2} (A^\top A + 2G_0^2) + \frac{\rho}{2(\rho/4 + 1)} \, A^\top A \end{aligned}$$

and for any  $v \in \Upsilon^{\circ}$ 

$$\breve{\mathbb{F}}(\boldsymbol{v}) \ge (1-\rho)\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v}).$$
(3.5)

By (2.32), this yields  $(\mathscr{F})$ . Moreover,  $\mathscr{F}_{xx}(v) \geq G^2$  by (3.3), and also by (3.4), it holds  $\mathscr{F}_{AA} \geq \operatorname{block}\{H_1^2, \ldots, H_q^2\}$  with  $H_m^2 = \mu^2 I_p + \mathcal{K}_m^2 \geq \mu^2 I_p$ . This and  $(\mathscr{F})$  yields strong concavity of f(v) on  $\Upsilon^\circ$ ; see Lemma A.17. We already mentioned that the fidelity term  $\|\boldsymbol{z} - A\boldsymbol{x}\|^2$  is not convex in the scope of variables  $\boldsymbol{x}, A$ . Proposition 3.1 shows that adding the quadratic penalties helps to improve the situation, at least, locally. Introduce the function

$$\ell(\boldsymbol{v}) = \ell(\boldsymbol{x}, A) = -\frac{1}{2} \|\boldsymbol{z} - A\boldsymbol{x}\|^2 - \frac{\mu^2}{2} \|\widehat{A} - A\|_{\rm Fr}^2 - \frac{1}{2} \|G_0\boldsymbol{x}\|^2$$
(3.6)

with  $G_0^2 \leq G^2$ . In fact, we proved in Proposition 3.1 that it is strongly concave in  $(\boldsymbol{x}, A)$  on the set  $\Upsilon^\circ$  from (3.2). Later we denote

$$\mathscr{F}_0(\boldsymbol{v}) = -\nabla^2 \ell(\boldsymbol{v}).$$

#### 3.2 Full and target efficient dimension

The results about posterior concentration heavily rely on the *full effective dimension*  $\bar{\mathbf{p}}(\boldsymbol{v})$  and the *target effective dimension*  $\mathbf{p}_{e}(\boldsymbol{v})$  defined as

$$\overline{\mathbf{p}}(\boldsymbol{v}) = \operatorname{tr}\left\{\mathscr{F}_{0}(\boldsymbol{v})\,\mathscr{F}^{-1}(\boldsymbol{v})\right\},\tag{3.7}$$

$$\mathbf{p}_{\mathbf{e}}(\boldsymbol{v}) = \operatorname{tr}\left\{\mathscr{F}_{0,\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v})\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1}(\boldsymbol{v})\right\} = \operatorname{tr}\left\{(A^{\top}A + G_{0}^{2})(A^{\top}A + G^{2})^{-1}\right\}.$$
 (3.8)

As  $p_{e}(\boldsymbol{v})$  only depends on A, we write  $p_{e}(A)$  instead of  $p_{e}(\boldsymbol{v})$ . It appears that the full effective dimension  $\overline{p}(\boldsymbol{v})$  can be bounded from above by the sum of the target effective dimension and the *nuisance effective dimension*  $q_{e}$  defined as

$$q_{\rm e} \stackrel{\rm def}{=} \sum_{m=1}^{q} \mu^2 \operatorname{tr}(\mu^2 I_p + \mathcal{K}_m^2)^{-1}.$$
(3.9)

The next lemma quantifies this statement.

**Lemma 3.2.** Let  $\Upsilon^{\circ}$  be given by (3.2). It holds for  $\overline{p}(\upsilon)$  from (3.7) and any  $\upsilon = (\boldsymbol{x}, A) \in \Upsilon^{\circ}$  with  $q_{e}$  from (3.9)

$$\begin{split} \overline{\mathtt{p}}(\boldsymbol{\upsilon}) &\leq \frac{\mathtt{p}_{\mathrm{e}}(A)}{1-\rho} + \frac{1}{1-\rho} \sum_{m=1}^{q} \mathrm{tr} \big\{ (\boldsymbol{x} \boldsymbol{x}^{\top} + \mu^{2} I_{p}) (\boldsymbol{x} \boldsymbol{x}^{\top} + \mu^{2} I_{p} + \mathcal{K}_{m}^{2})^{-1} \big\} \\ &\leq \frac{\mathtt{p}_{\mathrm{e}}(A)}{1-\rho} + \frac{(1+\rho/4)\mathtt{q}_{\mathrm{e}}}{1-\rho} \,. \end{split}$$

Proof. Proposition 3.1 and Lemma A.17 yield

$$\begin{split} \overline{\mathbf{p}}(\boldsymbol{v}) &\leq \frac{1}{1-\rho} \operatorname{tr} \left\{ \mathscr{F}_{0}(\boldsymbol{v}) \operatorname{ block} \left\{ \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1}(\boldsymbol{v}), \mathscr{F}_{AA}^{-1}(\boldsymbol{v}) \right\} \right\} \\ &\leq \frac{1}{1-\rho} \operatorname{tr} \left\{ \mathscr{F}_{0,\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v}) \operatorname{\mathscr{F}}_{\boldsymbol{x}\boldsymbol{x}}^{-1}(\boldsymbol{v}) \right\} + \frac{1}{1-\rho} \operatorname{tr} \left\{ \mathscr{F}_{0,AA}(\boldsymbol{v}) \operatorname{\mathscr{F}}_{AA}^{-1}(\boldsymbol{v}) \right\} \end{split}$$

Block structure of  $\mathscr{F}_{AA}(\boldsymbol{v})$  and  $\mathscr{F}_{0,AA}(\boldsymbol{v})$  due to (3.4) yields

$$\operatorname{tr} \big\{ \mathscr{F}_{0,AA}(\boldsymbol{v}) \, \mathscr{F}_{AA}^{-1}(\boldsymbol{v}) \big\} \leq \sum_{m=1}^{q} \operatorname{tr} \big\{ (\boldsymbol{x} \boldsymbol{x}^{\top} + \mu^{2} I_{p}) (\boldsymbol{x} \boldsymbol{x}^{\top} + \mu^{2} I_{p} + \mathcal{K}_{m}^{2})^{-1} \big\}$$

and the assertions follow in view of the bound  $||x||^2 \le \rho \mu^2/4$ .

By Lemma 3.2, the full effective dimension exceeds the target effective dimension by the value of order  $q_e$ . An important message from this result is as follows: if the value  $q_e$  from (3.9) and thus, the full effective dimension  $\overline{p}(\boldsymbol{v})$  is of the same order as the target effective dimension  $p_e(\boldsymbol{v})$ , then even full dimensional concentration and Laplace approximation deliver the desired quality corresponding to the target effective dimension. In particular, the plug-in procedure with  $\hat{A}$  in place of A is nearly efficient.

Without penalization of the operator A or for a small penalization with  $\max_m \|\mathcal{K}_m^2\| \ll \mu^2$ , one can bound

$$q_e \approx p \, q. \tag{3.10}$$

Although  $\mu^2$  can be large, as in the random regression case with  $\mu^2 \approx n$ , the bound (3.10) is not satisfactory because it is not dimension free and involve the ambient dimension p, q. The value  $\mathbf{q}_e$  and hence,  $\mathbf{\bar{p}}$  can be drastically reduced by using smoothness properties of the signal  $\boldsymbol{x}$  and of the operator A given in terms of the penalty  $||A||_{\mathcal{K}}^2/2$  for  $\mathcal{K} = \text{block}\{\mathcal{K}_1, \ldots, \mathcal{K}_q\}$ . As smoothness of  $\boldsymbol{x}$  is anyway described by the penalty term  $||G\boldsymbol{x}||^2/2$ , it is natural to take  $\mathcal{K}_m^2 = \varkappa_m^2 G^2$ . The growth of the factors  $\varkappa_m^2$  describes smoothness properties of the image of A.

As usual, suppose that  $\varkappa_m^2$  grow sufficiently fast, e.g. polynomially or exponentially, and similarly for the ordered eigenvalues  $g_j^2$  of  $G^2$ . Then for each m we can define  $j_m$ as the largest index j with  $g_j^2 \leq \mu^2 \varkappa_m^{-2}$ . For a polynomial growth of the  $g_j^2$ , simple calculus show that

$$\operatorname{tr}(\mu^2 I_p + \mathcal{K}_m^2)^{-1} = \mu^{-2} \,\mu^2 \,\varkappa_m^{-2} \operatorname{tr}(\mu^2 \varkappa_m^{-2} I_p + G^2)^{-1} \asymp \mu^{-2} j_m \,;$$

see Section C.2. Therefore,

$$\mathsf{q}_{\mathrm{e}} \asymp \sum_{m} j_{m}$$
 .

#### 3.3 Full dimensional concentration of the posterior

We are now about to state the main results for the error-in-operator model. Denote  $\mathscr{F}_0 = \mathscr{F}_0(\boldsymbol{v}^*), \ \bar{\mathbf{p}} = \bar{\mathbf{p}}(\boldsymbol{v}^*)$  and define for  $\nu = 2/3$  the concentration set

$$\mathcal{A} = \left\{ \boldsymbol{\upsilon} \colon \|\mathscr{F}_0^{1/2}(\boldsymbol{\upsilon} - \boldsymbol{\upsilon}^*)\| \le \nu^{-1} \overline{\mathbf{r}} \right\},$$
  
$$\overline{\mathbf{r}} = 2 \overline{\mathbf{p}}^{1/2} + (2\mathbf{x})^{1/2}.$$
(3.11)

**Theorem 3.3.** Let the set  $\mathcal{A}$  from (3.11) satisfy  $\mathcal{A} \subset \Upsilon^{\circ}$  for  $\Upsilon^{\circ}$  from (3.2). If  $c_3 \overline{r} n^{-1/2} \leq 1/3$  with  $c_3 = 6\mu^{-1}$ , then

$$\mathbb{P}_f(\|\mathscr{F}_0^{1/2}(\boldsymbol{v}-\boldsymbol{v}^*)\| > \nu^{-1}\mathbf{\bar{r}}) \leq \mathrm{e}^{-\mathbf{x}}.$$

Moreover,

$$\mathbb{P}_f((1-\rho)\mu \|A - A^*\|_{\mathrm{Fr}} > \nu^{-1}\overline{\mathbf{r}}) \le \mathrm{e}^{-\mathbf{x}}.$$

*Proof.* Later we show that  $\ell(v)$  fulfills the full dimensional smoothness condition  $(S_3)$  on the set  $\Upsilon^{\circ}$  with  $c_3 = 6\mu^{-1}$ , and the result follows from (B.9) of Theorem B.1.

#### 3.4 Marginal posterior: concentration and Laplace approximation

This section presents our main results about Laplace approximation of the marginal posterior. We apply the general results of Section 2.10 to the considered setup after restricting the parameter space to  $\Upsilon^{\circ}$ . Remind the notation  $\mathbb{F}(\boldsymbol{v}) = \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v}) = A^{\top}A + G^2$ ; see (3.5). As in Section 2.10, for  $p_e(A) = p_e(\boldsymbol{v})$  from (3.8), define

$$\mathbf{r}(A) = 2\sqrt{\mathbf{p}_{\mathrm{e}}(A)} + \sqrt{2\mathbf{x}}$$

Notation  $\mathbb{F} = \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}(\boldsymbol{v}^*)$  and  $\check{\mathbb{F}} = \check{\mathbb{F}}(\boldsymbol{v}^*)$  will be used. One good news is that the efficient semiparametric matrix  $\check{\mathbb{F}} = \check{\mathbb{F}}(\boldsymbol{v}^*)$  from (2.31) satisfies  $(1-\rho)\mathbb{F} \leq \check{\mathbb{F}} \leq \mathbb{F}$ .

With  $G_0$  shown in (3.6), define the *effective sample size* n by the equation

$$n^{-1} = \| (A^{*\top}A^{*} + G_0^2)^{-1} \|.$$
(3.12)

Note that this value does not depend on  $\mu$ . For a linear mapping Q in  $\mathbb{R}^p$ , define

$$\mathbb{B}_Q = \frac{1}{\|Q \mathbb{F}^{-1} Q^{\top}\|} Q \mathbb{F}^{-1} Q^{\top}, \qquad \mathbf{p}_Q = \operatorname{tr}(\mathbb{B}_Q)$$

Theorem 2.12 implies the following bound.

**Theorem 3.4.** Assume the conditions of Theorem 3.3. Let Q be such that

$$\|\boldsymbol{\mathcal{B}}_Q\|_{\mathrm{Fr}}^2 = \operatorname{tr} \boldsymbol{\mathcal{B}}_Q^2 \ge \mathsf{C}_0^2 \operatorname{tr} \boldsymbol{\mathcal{B}}_Q = \mathsf{C}_0^2 \operatorname{p}_Q$$

with some fixed positive constant  $\mathtt{C}_0$ . For  $\breve{\mathtt{F}}=\breve{\mathtt{F}}(\upsilon^*)$ , it holds with  $\gamma_{\breve{\mathtt{F}}}\sim\mathcal{N}(0,\breve{\mathtt{F}}^{-1})$ 

$$\sup_{\mathbf{r}>0} \left| \mathcal{P}_{f} \left( \| Q(\mathbf{X} - \mathbf{x}^{*}) \| \leq \mathbf{r} \right) - \mathcal{P} \left( \| Q \gamma_{\breve{F}} \| \leq \mathbf{r} \right) \right| \\
\lesssim \frac{\mu^{-1} \mathbf{r}(A^{*}) \mathbf{p}_{e}(A^{*})}{\sqrt{n}} + \frac{\mu^{-1} \overline{\mathbf{r}} \sqrt{\mathbf{p}Q}}{\sqrt{n}} + \frac{\mu^{-2} \overline{\mathbf{r}}^{4}}{n \sqrt{\mathbf{p}Q}} + e^{-\mathbf{x}}.$$
(3.13)

*Proof.* Consider  $\ell(v)$  from (3.6). It obviously holds

$$-\nabla^2_{\boldsymbol{x}\boldsymbol{x}}\ell(\boldsymbol{x},A) = \mathsf{D}^2(A) = A^\top A + G_0^2,$$
  
$$-\nabla^2_{AA}\ell(\boldsymbol{x},A) = \operatorname{block}\{\boldsymbol{x}\boldsymbol{x}^\top + \mu^2 I_p, \dots, \boldsymbol{x}\boldsymbol{x}^\top + \mu^2 I_p\};$$

see (3.4). It is natural to describe the local geometry at  $\boldsymbol{v} = (\boldsymbol{x}, A)$  by

$$\mathbf{m}^{2}(\boldsymbol{v}) = n^{-1}\operatorname{block}\{\mathsf{D}^{2}(A), \mu^{2}I\}$$
(3.14)

with n from (3.12). The next step is in checking  $(S_3)$  and  $(S_4)$ .

**Lemma 3.5.** Let  $\mu \leq \mu$ . For the functions  $f(\boldsymbol{v})$  and  $\ell(\boldsymbol{v})$ , conditions  $(S_3)$  and  $(S_4)$ hold at any  $\boldsymbol{v} \in \Upsilon^{\circ}$  with  $m^2(\boldsymbol{v})$  from (3.14) and

$$c_3 = 6\mu^{-1}, \qquad c_4 = 3\mu^{-2}.$$
 (3.15)

*Proof.* Fix  $\boldsymbol{u} = (\boldsymbol{\xi}, \boldsymbol{U})$  with  $\boldsymbol{U}^{\top} = (\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_q)$  such that

$$n \boldsymbol{u}^{\top} \boldsymbol{\mathsf{m}}^{2}(\boldsymbol{v}) \boldsymbol{u} = \boldsymbol{\xi}^{\top} (A^{\top} A + G_{0}^{2}) \boldsymbol{\xi} + \sum_{m=1}^{q} \left( |\boldsymbol{x}^{\top} \boldsymbol{\omega}_{m}|^{2} + \mu^{2} \|\boldsymbol{\omega}_{m}\|^{2} \right) = \boldsymbol{\mathsf{r}}^{2}.$$
(3.16)

Consider  $\ell(\boldsymbol{v} + t\boldsymbol{u}) = \ell(\boldsymbol{x} + t\boldsymbol{\xi}, A + t\boldsymbol{U})$ . The fourth derivative  $\nabla^4 \ell(\boldsymbol{v} + t\boldsymbol{u})$  in t does not depend on  $\boldsymbol{v}$  and it holds for any t

$$-\frac{d^4}{dt^4}\ell(\boldsymbol{\upsilon}+t\boldsymbol{u}) = \langle \nabla^4\ell(\boldsymbol{\upsilon}), \boldsymbol{u}^{\otimes 4} \rangle = 12\sum_{m=1}^q (\boldsymbol{\xi}^\top \boldsymbol{\omega}_m)^2.$$

By (3.16), (3.12), and the inequality  $4ab \leq (a+b)^2$ , it holds

$$4\mu^{2} \sum_{m=1}^{q} (\boldsymbol{\xi}^{\top} \boldsymbol{\omega}_{m})^{2} \leq 4 \|\boldsymbol{\xi}\|^{2} \sum_{m=1}^{q} \mu^{2} \|\boldsymbol{\omega}_{m}\|^{2}$$
  
$$\leq 4 \| (A^{\top} A + G_{0}^{2})^{-1} \| \boldsymbol{\xi}^{\top} (A^{\top} A + G_{0}^{2}) \boldsymbol{\xi} \sum_{m=1}^{q} \mu^{2} \|\boldsymbol{\omega}_{m}\|^{2}$$
  
$$\leq \| (A^{\top} A + G_{0}^{2})^{-1} \| \mathbf{r}^{4} = \mathbf{r}^{4} / n .$$
(3.17)

This easily implies  $(\mathcal{S}_4)$  with  $c_4$  from (3.15).

Now we proceed with  $(S_3)$ . Definition yields

$$-\frac{d^3}{dt^3}\ell(\boldsymbol{x}+t\boldsymbol{\xi},A+t\boldsymbol{U})\Big|_{t=0} = 6\sum_{m=1}^q (\boldsymbol{x}^\top\boldsymbol{\omega}_m+A_m^\top\boldsymbol{\xi})\boldsymbol{\xi}^\top\boldsymbol{\omega}_m.$$

The use of (3.16) yields similarly to (3.17) with  $s = \mu^{-1} \mathbf{r} n^{-1/2}/2$ 

$$2\sum_{m=1}^{q} \boldsymbol{x}^{\top} \boldsymbol{\omega}_{m} \, \boldsymbol{\xi}^{\top} \boldsymbol{\omega}_{m} \leq s \sum_{m=1}^{q} (\boldsymbol{x}^{\top} \boldsymbol{\omega}_{m})^{2} + s^{-1} \sum_{m=1}^{q} (\boldsymbol{\xi}^{\top} \boldsymbol{\omega}_{m})^{2}$$
$$\leq s \, \mathbf{r}^{2} + s^{-1} \mu^{-2} \mathbf{r}^{4} / (4n) \leq \mu^{-1} \, \mathbf{r}^{3} \, n^{-1/2}.$$

Similarly,

$$2\sum_{m=1}^{q} A_{m}^{\top} \boldsymbol{\xi} \ \boldsymbol{\xi}^{\top} \boldsymbol{\omega}_{m} \leq s \sum_{m=1}^{q} (A_{m}^{\top} \boldsymbol{\xi})^{2} + s^{-1} \sum_{m=1}^{q} (\boldsymbol{\xi}^{\top} \boldsymbol{\omega}_{m})^{2}$$
$$\leq s \ \boldsymbol{\xi}^{\top} A^{\top} A \ \boldsymbol{\xi} + s^{-1} \mu^{-2} \mathbf{r}^{4} / (4n)$$
$$\leq s \ \mathbf{r}^{2} + s^{-1} \mu^{-2} \mathbf{r}^{4} / (4n) \leq \mu^{-1} \ \mathbf{r}^{3} n^{-1/2}.$$

Summing up the latter bounds yields

$$\left|\langle 
abla^3 \ell(oldsymbol{v}), oldsymbol{u}^{\otimes 3} 
angle 
ight| \leq 6 \mu^{-1} \, \mathtt{r}^3 \, n^{-1/2}$$

and  $(\mathcal{S}_3)$  follows with  $c_3 = 6\mu^{-1}$ .

Lemma 3.5 ensures  $(S_3)$  with  $c_3 \simeq \mu^{-1}$  and the accuracy bound (3.13) of the theorem follows from Theorem 2.12.

#### 3.5 Critical dimension

Now we discuss the issue of critical dimension. With n from (3.12) and  $\overline{p}$  from Lemma 3.2, Theorem 3.3 requires  $\mu^{-1}\overline{\mathbf{r}} \ll n^{1/2}$  or

$$\mu^{-2}\,\overline{\mathbf{r}}^2\approx\mu^{-2}\,\overline{\mathbf{p}}\asymp\mu^{-2}(\mathbf{p}_{\mathrm{e}}+\mathbf{q}_{\mathrm{e}})\ll n.$$

For the unpenalized case with  $\mathcal{K} = 0$ , it leads to  $\mu^{-2} q_e = \mu^{-2} p q \ll n$ ; see (3.10). A particular case with  $\mu^{-2} = p = q = n$  as in random design regression is nearly included up to a small factor. The use of penalization by  $||A||_{\mathcal{K}}^2$  results in the updated condition

$$\sum_{m=1}^{q} \operatorname{tr}(\mu^{2} I_{p} + \mathcal{K}_{m}^{2})^{-1} \ll n.$$

This penalization allows to incorporate the cases with  $p = q \gg n$  and even  $p = q = \infty$ .

The condition on critical dimension in Theorem 3.4 is even more striking. Suppose that  $Q = \mathsf{D}$  and  $\mathsf{p}_Q \approx \mathsf{p}_{\mathsf{e}}$ . Theorem 3.4 applies under the conditions

$$\mu^{-2}\,\overline{\mathbf{r}}^2\,\mathbf{p}_{\mathrm{e}} \ll n, \qquad \mu^{-2}\,\overline{\mathbf{r}}^4 \ll n\sqrt{\mathbf{p}_{\mathrm{e}}}\,.$$

The use of  $\mu^{-2} \overline{r}^2 \approx \mu^{-2} \overline{p} \simeq \mu^{-2} (p_e + q_e)$  and (3.9) leads to

$$p_{e} \sum_{m=1}^{q} tr(\mu^{2}I_{p} + \mathcal{K}_{m}^{2})^{-1} \ll n,$$
$$\frac{\mu}{p_{e}^{1/4}} \sum_{m=1}^{q} tr(\mu^{2}I_{p} + \mathcal{K}_{m}^{2})^{-1} \ll \sqrt{n}$$

Without operator penalty, that is, for  $\mathcal{K}_m \equiv 0$  this becomes

$$\mathbf{p}_{\rm e} \, \mu^{-2} \, p \, q \ll n,$$
  
 $\mathbf{p}_{\rm e}^{1/4} \, \mu^{-1} \, p \, q \ll \sqrt{n} \, .$ 

While the first condition can be nearly fulfilled for  $\mathbf{p}_{e}$  bounded and  $p = q \times n$ , the second condition fails completely when n is large. However, the use of a proper operator  $\mathcal{K}^{2}$  ensures the required "critical dimension" condition; see Section C for more details.

# A Local smoothness conditions

This section discusses different local smoothness characteristics of a multivariate function  $f(v) = \mathbb{E}L(v), v \in \mathbb{R}^p$ .

#### A.1 Smoothness and self-concordance in Gateaux sense

Below we assume the function  $f(\boldsymbol{v})$  to be strongly concave with the negative Hessian  $\mathbb{F}(\boldsymbol{v}) \stackrel{\text{def}}{=} -\nabla^2 f(\boldsymbol{v}) \in \mathfrak{M}_p$  positive definite. Also assume  $f(\boldsymbol{v})$  three or sometimes even four times Gateaux differentiable in  $\boldsymbol{v} \in \boldsymbol{\Upsilon}$ . For any particular direction  $\boldsymbol{u} \in \mathbb{R}^p$ , we consider the univariate function  $f(\boldsymbol{v} + t\boldsymbol{u})$  and measure its smoothness in t. Local smoothness of f will be described by the relative error of the Taylor expansion of the third or four order. Namely, define

$$\delta_3(\boldsymbol{v}, \boldsymbol{u}) = f(\boldsymbol{v} + \boldsymbol{u}) - f(\boldsymbol{v}) - \langle \nabla f(\boldsymbol{v}), \boldsymbol{u} \rangle - \frac{1}{2} \langle \nabla^2 f(\boldsymbol{v}), \boldsymbol{u}^{\otimes 2} \rangle,$$
  
$$\delta'_3(\boldsymbol{v}, \boldsymbol{u}) = \langle \nabla f(\boldsymbol{v} + \boldsymbol{u}), \boldsymbol{u} \rangle - \langle \nabla f(\boldsymbol{v}), \boldsymbol{u} \rangle - \langle \nabla^2 f(\boldsymbol{v}), \boldsymbol{u}^{\otimes 2} \rangle,$$

and

$$\delta_4(\boldsymbol{\upsilon},\boldsymbol{u}) \stackrel{\text{def}}{=} f(\boldsymbol{\upsilon}+\boldsymbol{u}) - f(\boldsymbol{\upsilon}) - \langle \nabla f(\boldsymbol{\upsilon}),\boldsymbol{u} \rangle - \frac{1}{2} \langle \nabla^2 f(\boldsymbol{\upsilon}),\boldsymbol{u}^{\otimes 2} \rangle - \frac{1}{6} \langle \nabla^3 f(\boldsymbol{\upsilon}),\boldsymbol{u}^{\otimes 3} \rangle.$$

Now, for each  $\boldsymbol{v}$ , suppose to be given a positive symmetric operator  $\mathsf{D}(\boldsymbol{v}) \in \mathfrak{M}_p$  with  $\mathsf{D}^2(\boldsymbol{v}) \leq \mathbb{F}(\boldsymbol{v}) = -\nabla^2 f(\boldsymbol{v})$  defining a local metric and a local vicinity around  $\boldsymbol{v}$ :

$$\mathcal{U}(\boldsymbol{v}) = \left\{ \boldsymbol{u} \in {I\!\!R}^p \colon \|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\| \le \mathsf{r} \right\}$$

for some radius r.

Local smoothness properties of f are given via the quantities

$$\omega(\boldsymbol{v}) \stackrel{\text{def}}{=} \sup_{\boldsymbol{u}: \|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\| \le \mathbf{r}} \frac{2|\delta_3(\boldsymbol{v}, \boldsymbol{u})|}{\|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\|^2}, \qquad \omega'(\boldsymbol{v}) \stackrel{\text{def}}{=} \sup_{\boldsymbol{u}: \|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\| \le \mathbf{r}} \frac{2|\delta'_3(\boldsymbol{v}, \boldsymbol{u})|}{\|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\|^2}.$$
(A.1)

The Taylor expansion yields for any  $\boldsymbol{u}$  with  $\|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\| \leq r$ 

$$\left| \delta_3(\boldsymbol{v}, \boldsymbol{u}) \right| \le \frac{\omega(\boldsymbol{v})}{2} \| \mathsf{D}(\boldsymbol{v}) \boldsymbol{u} \|^2, \qquad \left| \delta_3'(\boldsymbol{v}, \boldsymbol{u}) \right| \le \frac{\omega'(\boldsymbol{v})}{2} \| \mathsf{D}(\boldsymbol{v}) \boldsymbol{u} \|^2.$$
 (A.2)

The introduced quantities  $\omega(v)$ ,  $\omega'(v)$  strongly depend on the radius  $\mathbf{r}$  of the local vicinity  $\mathcal{U}(v)$ . The results about Laplace approximation can be improved provided a homogeneous upper bound on the error of Taylor expansion. Assume a subset  $\Upsilon^{\circ}$  of  $\Upsilon$  to be fixed.

 $(\mathcal{T}_3)$  There exists  $au_3$  such that for all  $v \in \Upsilon^\circ$ 

$$\left|\delta_3(\boldsymbol{v}, \boldsymbol{u})\right| \leq rac{ au_3}{6} \|\mathsf{D}(\boldsymbol{v})\, \boldsymbol{u}\|^3, \quad \left|\delta_3'(\boldsymbol{v}, \boldsymbol{u})\right| \leq rac{ au_3}{2} \|\mathsf{D}(\boldsymbol{v})\, \boldsymbol{u}\|^3, \quad \boldsymbol{u} \in \mathcal{U}(\boldsymbol{v}).$$

 $(\mathcal{T}_4)$  There exists  $au_4$  such that for all  $v \in \Upsilon^\circ$ 

$$\left|\delta_4(\boldsymbol{v}, \boldsymbol{u})
ight| \leq rac{ au_4}{24} \|\mathsf{D}(\boldsymbol{v})\, \boldsymbol{u}\|^4\,, \qquad \boldsymbol{u}\in\mathcal{U}(\boldsymbol{v}).$$

**Lemma A.1.** Under  $(\mathcal{T}_3)$ , the values  $\omega(v)$  and  $\omega'(v)$  from (A.1) satisfy

$$\omega(\boldsymbol{v}) \leq rac{ au_3\,\mathbf{r}}{3}\,, \qquad \omega'(\boldsymbol{v}) \leq au_3\,\mathbf{r}\,, \qquad \boldsymbol{v}\in arY^\circ.$$

*Proof.* For any  $u \in \mathcal{U}(v)$  with  $\|\mathsf{D}(v)u\| \leq r$ 

$$\left|\delta_3(\boldsymbol{\upsilon}, \boldsymbol{u})\right| \leq rac{ au_3}{6} \|\mathsf{D}(\boldsymbol{\upsilon})\boldsymbol{u}\|^3 \leq rac{ au_3\,\mathbf{r}}{6} \,\|\mathsf{D}(\boldsymbol{\upsilon})\boldsymbol{u}\|^2,$$

and the bound for  $\omega(v)$  follows. The proof for  $\omega'(v)$  is similar.

The values  $\tau_3$  and  $\tau_4$  are usually very small. Some quantitative bounds are given later in this section under the assumption that the function  $f(\boldsymbol{v}) = \mathbb{E}L_G(\boldsymbol{v})$  can be written in the form  $-f(\boldsymbol{v}) = nh(\boldsymbol{v})$  for a fixed smooth function  $h(\boldsymbol{v})$  with the Hessian  $\nabla^2 h(\boldsymbol{v})$ . The factor n has meaning of the sample size.

$$\begin{aligned} (\mathcal{S}_3) \quad -f(\boldsymbol{\upsilon}) &= nh(\boldsymbol{\upsilon}) \ \text{for } h(\boldsymbol{\upsilon}) \ \text{convex with } \nabla^2 h(\boldsymbol{\upsilon}) \geq \mathsf{m}^2(\boldsymbol{\upsilon}) = \mathsf{D}^2(\boldsymbol{\upsilon})/n \ \text{and} \\ & \sup_{\boldsymbol{u}: \ \|\mathsf{m}(\boldsymbol{\upsilon})\boldsymbol{u}\| \leq \mathsf{r}/\sqrt{n}} \frac{\left| \langle \nabla^3 h(\boldsymbol{\upsilon}+\boldsymbol{u}), \boldsymbol{u}^{\otimes 3} \rangle \right|}{\|\mathsf{m}(\boldsymbol{\upsilon})\boldsymbol{u}\|^3} &\leq \mathsf{c}_3 \,. \end{aligned}$$

 $(\mathcal{S}_4)$  the function  $h(\cdot)$  satisfies  $(\mathcal{S}_3)$  and

$$\sup_{\boldsymbol{u}: \, \|\boldsymbol{\mathsf{m}}(\boldsymbol{v})\boldsymbol{u}\| \leq \mathbf{r}/\sqrt{n}} \frac{\left| \langle \nabla^4 h(\boldsymbol{v}+\boldsymbol{u}), \boldsymbol{u}^{\otimes 4} \rangle \right|}{\|\boldsymbol{\mathsf{m}}(\boldsymbol{v})\boldsymbol{u}\|^4} \leq \mathsf{c}_4 \, .$$

 $(\mathcal{S}_3)$  and  $(\mathcal{S}_4)$  are local versions of the so called self-concordance condition; see Nesterov (1988). In fact, they require that each univariate function  $h(\boldsymbol{v} + t\boldsymbol{u})$  of  $t \in \mathbb{R}$  is selfconcordant with some universal constants  $c_3$  and  $c_4$ . Under  $(\mathcal{S}_3)$  and  $(\mathcal{S}_4)$ , we can use  $\mathsf{D}^2(\boldsymbol{v}) = n \,\mathsf{m}^2(\boldsymbol{v})$  and easily bound the values  $\delta_3(\boldsymbol{v}, \boldsymbol{u})$ ,  $\delta_4(\boldsymbol{v}, \boldsymbol{u})$ , and  $\omega(\boldsymbol{v})$ ,  $\omega'(\boldsymbol{v})$ .

**Lemma A.2.** Suppose  $(S_3)$ . Then  $(T_3)$  follows with  $\tau_3 = c_3 n^{-1/2}$ . Moreover, for  $\omega(v)$  and  $\omega'(v)$  from (A.1), it holds

$$\omega(\boldsymbol{v}) \leq \frac{\mathsf{c}_3\,\mathsf{r}}{3n^{1/2}}, \qquad \omega'(\boldsymbol{v}) \leq \frac{\mathsf{c}_3\,\mathsf{r}}{n^{1/2}}. \tag{A.3}$$

Also  $(\mathcal{T}_4)$  follows from  $(\mathcal{S}_4)$  with  $\tau_4 = c_4 n^{-1}$ .

*Proof.* For any  $u \in \mathcal{U}(v)$  and  $t \in [0,1]$ , by the Taylor expansion of the third order

$$\begin{split} |\delta(\boldsymbol{\upsilon},\boldsymbol{u})| &\leq \frac{1}{6} \left| \langle \nabla^3 f(\boldsymbol{\upsilon} + t\boldsymbol{u}), \boldsymbol{u}^{\otimes 3} \rangle \right| = \frac{n}{6} \left| \langle \nabla^3 h(\boldsymbol{\upsilon} + t\boldsymbol{u}), \boldsymbol{u}^{\otimes 3} \rangle \right| \leq \frac{n \, \mathsf{c}_3}{6} \, \|\mathsf{m}(\boldsymbol{\upsilon})\boldsymbol{u}\|^3 \\ &= \frac{n^{-1/2} \, \mathsf{c}_3}{6} \, \|\mathsf{D}(\boldsymbol{\upsilon})\boldsymbol{u}\|^3 \leq \frac{n^{-1/2} \, \mathsf{c}_3 \, \mathsf{r}}{6} \, \|\mathsf{D}(\boldsymbol{\upsilon})\boldsymbol{u}\|^2 \, . \end{split}$$

This implies  $(\mathcal{T}_3)$  as well as (A.3); see (A.2). The statement about  $(\mathcal{T}_4)$  is similar.  $\Box$ 

#### A.2 Fréchet derivatives and smoothness of the Hessian

For evaluation of the bias, we also need stronger smoothness conditions in the Fréchet sense. Let f be a strongly concave function. Essentially we need some continuity of the negative Hessian  $\mathbb{F}(\boldsymbol{v}) = -\nabla^2 f(\boldsymbol{v})$ . For  $\boldsymbol{v} \in \boldsymbol{\Upsilon}$ , define  $\mathsf{D}(\boldsymbol{v}) = \mathbb{F}^{1/2}(\boldsymbol{v})$  and

$$\omega^{+}(\boldsymbol{v}) \stackrel{\text{def}}{=} \sup_{\boldsymbol{u}: \|\mathsf{D}(\boldsymbol{v})\boldsymbol{u}\| \leq \mathbf{r}} \sup_{\boldsymbol{\gamma} \in \mathbb{R}^{p}} \frac{|\langle \mathbb{F}(\boldsymbol{v}+\boldsymbol{u}) - \mathbb{F}(\boldsymbol{v}), \boldsymbol{\gamma}^{\otimes 2} \rangle|}{\|\mathsf{D}(\boldsymbol{v})\boldsymbol{\gamma}\|^{2}}.$$
 (A.4)

This definition of  $\omega^+(\boldsymbol{v})$  is, of course, stronger than the one-directional definition of  $\omega(\boldsymbol{v})$  in (A.1). However, in typical examples these quantities  $\omega(\boldsymbol{v})$  and  $\omega^+(\boldsymbol{v})$  are similar.

We also present a Fréchet version of  $(S_3)$ .

$$(\mathcal{S}_3^+)$$
  $-f(\boldsymbol{v}) = nh(\boldsymbol{v})$  with  $h(\cdot)$  strongly concave,  $\mathbf{m}^2(\boldsymbol{v}) \leq \nabla^2 h(\boldsymbol{v})$ , and

$$\sup_{\|\mathsf{m}(\boldsymbol{v})\boldsymbol{u}\| \leq \mathbf{r}/\sqrt{n}} \sup_{\boldsymbol{\gamma} \in \mathbb{R}^p} \frac{\left| \langle \nabla^3 h(\boldsymbol{v} + \boldsymbol{u}), \boldsymbol{u} \otimes \boldsymbol{\gamma}^{\otimes 2} \rangle \right|}{\|\mathsf{m}(\boldsymbol{v})\boldsymbol{u}\| \, \|\mathsf{m}(\boldsymbol{v})\boldsymbol{\gamma}\|^2} \leq \mathsf{c}_3$$

**Lemma A.3.** For  $\omega^+(\boldsymbol{v})$  from (A.4) and any  $\boldsymbol{u}$  with  $\|\mathbb{F}^{1/2}(\boldsymbol{v})\boldsymbol{u}\| \leq r$ , it holds

$$\|\mathbb{F}^{-1/2}(\boldsymbol{v})\,\mathbb{F}(\boldsymbol{v}+\boldsymbol{u})\,\mathbb{F}^{-1/2}(\boldsymbol{v})-I_p\|\leq\omega^+(\boldsymbol{v}).\tag{A.5}$$

Moreover,  $(\mathcal{S}_3^+)$  yields  $\omega^+(\upsilon) \leq c_3 \operatorname{r} n^{-1/2}$  and for any u with  $\|\mathbb{F}^{1/2}(\upsilon)u\| \leq \operatorname{r} n^{-1/2}$ 

$$\|\mathbb{F}^{-1/2}(\boldsymbol{v})\,\mathbb{F}(\boldsymbol{v}+\boldsymbol{u})\,\mathbb{F}^{-1/2}(\boldsymbol{v})-I_p\| \leq \frac{\mathsf{c}_3}{n^{1/2}}\,\|\mathbb{F}^{1/2}(\boldsymbol{v})\boldsymbol{u}\| \leq \frac{\mathsf{c}_3\,\mathsf{r}}{n^{1/2}}\,.\tag{A.6}$$

*Proof.* Denote  $\Delta(u) = \mathbb{F}(v+u) - \mathbb{F}(v)$ . Then by (A.4) for any  $\gamma \in \mathbb{R}^p$  with  $\delta = \mathbb{F}^{-1/2}(v)\gamma$ 

$$ig|ig\langle \mathbb{F}^{-1/2}(oldsymbol{v}) \, \mathbb{F}(oldsymbol{v}+oldsymbol{u}) \, \mathbb{F}^{-1/2}(oldsymbol{v}) - I_p, oldsymbol{\gamma}^{\otimes 2} ig
angle ig| = ig|\langle \Delta(oldsymbol{u}), oldsymbol{\delta}^{\otimes 2} ig
angle ig| \ \leq \omega^+(oldsymbol{v}) \, \|\mathbb{F}^{1/2}(oldsymbol{v}) \, oldsymbol{\delta} \|^2 = \omega^+(oldsymbol{v}) \, \|oldsymbol{\gamma}\|^2.$$

This yields (A.5). The arguments from Lemma A.2 yield bound (A.6).

Define now for any u

$$\overset{\circ}{\mathbb{F}}(\boldsymbol{\upsilon};\boldsymbol{u}) \stackrel{\text{def}}{=} \int_0^1 \mathbb{F}(\boldsymbol{\upsilon} + t\boldsymbol{u}) \, dt \,. \tag{A.7}$$

Lemma A.4. For any  $u \in \mathbb{R}^p$  with  $\|\mathbb{F}^{1/2}(v)u\| \leq r$ 

$$\left\| \mathbb{F}^{-1/2}(\boldsymbol{v}) \stackrel{\circ}{\mathbb{F}}(\boldsymbol{v};\boldsymbol{u}) \mathbb{F}^{-1/2}(\boldsymbol{v}) - I_p \right\| \le \omega^+(\boldsymbol{v}).$$
(A.8)

Moreover,

$$\{1 - \omega^{+}(\boldsymbol{v})\}\mathbb{F}(\boldsymbol{v}) \leq \overset{\circ}{\mathbb{F}}(\boldsymbol{v};\boldsymbol{u}) \leq \{1 + \omega^{+}(\boldsymbol{v})\}\mathbb{F}(\boldsymbol{v}).$$
(A.9)

*Proof.* For any  $\gamma \in \mathbb{R}^p$  and  $t \in [0,1]$ , the definition (A.4) implies

$$\left|\left\langle \mathbb{F}(\boldsymbol{v}+t\boldsymbol{u})-\mathbb{F}(\boldsymbol{v}),\boldsymbol{\gamma}^{\otimes 2}\right
angle \right| \leq \omega^{+}(\boldsymbol{v}) \,\|\mathbb{F}^{1/2}(\boldsymbol{v})\,\boldsymbol{\gamma}\|^{2}$$

This obviously yields under  $(\mathcal{S}_3^+)$ 

$$\left|\left\langle \mathring{\mathbb{F}}(\boldsymbol{\upsilon};\boldsymbol{u}) - \mathbb{F}(\boldsymbol{\upsilon}), \boldsymbol{\gamma}^{\otimes 2} \right\rangle\right| \leq \frac{\mathsf{c}_3\,\mathsf{r}}{n^{1/2}}\,\|\mathbb{F}^{1/2}(\boldsymbol{\upsilon})\,\boldsymbol{\gamma}\|^2 \int_0^1 t\,dt = \frac{\mathsf{c}_3\,\mathsf{r}}{2n^{1/2}}\,\|\mathbb{F}^{1/2}(\boldsymbol{\upsilon})\,\boldsymbol{\gamma}\|^2$$

and (A.8) follows as in Lemma A.3.

If  $f(\boldsymbol{v})$  is quadratic, then  $\nabla f(\boldsymbol{v})$  is linear while  $\mathbb{F} \equiv -\nabla^2 f(\boldsymbol{v})$  is constant and we obtain the identity

$$\mathbb{F}^{-1}\big\{\nabla f(\boldsymbol{\upsilon}+\boldsymbol{u})-\nabla f(\boldsymbol{\upsilon})\big\}=-\boldsymbol{u}.$$

Now we consider the case of a smooth  $f(\cdot)$  satisfying (A.4) or  $(\mathcal{S}_3^+)$ .

**Lemma A.5.** Suppose the conditions of Lemma A.3. For any u with  $\|\mathbb{F}^{1/2}(v)u\| \leq r$ 

$$\nabla f(\boldsymbol{v} + \boldsymbol{u}) - \nabla f(\boldsymbol{v}) = - \check{\mathbb{F}}(\boldsymbol{v}; \boldsymbol{u}) \boldsymbol{u}.$$
(A.10)

Moreover, for any positive definite symmetric operator  $Q \colon \mathbb{R}^p \to \mathbb{R}^p$ , it holds

$$egin{aligned} & \left\|Q\left\{
abla f(oldsymbol{v}+oldsymbol{u})-
abla f(oldsymbol{v})
ight\}
ight\|&\leq \left\{1+\omega^+(oldsymbol{v})
ight\}\|Q\operatorname{ extsf{F}}(oldsymbol{v})oldsymbol{u}\|, \ & \left\|Q\operatorname{ extsf{F}}(oldsymbol{v})oldsymbol{u}
ight\|&\leq rac{1}{1-\omega^+(oldsymbol{v})}\left\|Q\left\{
abla f(oldsymbol{v}+oldsymbol{u})-
abla f(oldsymbol{v})
ight\}
ight\|, \end{aligned}$$

and

$$\left\|Q\left\{\nabla f(\boldsymbol{\upsilon}+\boldsymbol{u})-\nabla f(\boldsymbol{\upsilon})+\mathbb{F}(\boldsymbol{\upsilon})\,\boldsymbol{u}\right\}\right\| \leq \omega^{+}(\boldsymbol{\upsilon})\,\|Q\,\mathbb{F}(\boldsymbol{\upsilon})\,\boldsymbol{u}\|.$$
 (A.11)

*Proof.* First we check (A.10). Indeed, for any  $\gamma \in \mathbb{R}^p$ , consider the univariate function  $h(t) = \langle \nabla f(\boldsymbol{v} + t\boldsymbol{u}) - \nabla f(\boldsymbol{v}), \boldsymbol{\gamma} \rangle$ . The the statement follows from definition (A.7) and the identity  $h(1) - h(0) = \int_0^1 h'(t) dt$ . Further, it holds by (A.10) and (A.9)

$$\begin{split} \left\| Q\left\{ \nabla f(\boldsymbol{v} + \boldsymbol{u}) - \nabla f(\boldsymbol{v}) \right\} \right\| &= \| Q \,\mathring{\mathbb{F}}(\boldsymbol{v}; \boldsymbol{u}) \, \boldsymbol{u}\| = \left\| Q \,\mathring{\mathbb{F}}(\boldsymbol{v}; \boldsymbol{u}) \mathbb{F}^{-1}(\boldsymbol{v}) \, Q^{-1} \, Q \, \mathbb{F}(\boldsymbol{v}) \, \boldsymbol{u} \right\| \\ &\leq \left\| Q \,\mathring{\mathbb{F}}(\boldsymbol{v}; \boldsymbol{u}) \mathbb{F}^{-1}(\boldsymbol{v}) \, Q^{-1} \right\| \, \| Q \, \mathbb{F}(\boldsymbol{v}) \, \boldsymbol{u}\| \leq \left\{ 1 + \omega^{+}(\boldsymbol{v}) \right\} \| Q \, \mathbb{F}(\boldsymbol{v}) \, \boldsymbol{u}\| \end{split}$$

and

$$\begin{split} \|Q\boldsymbol{u}\| &= \left\| Q \,\mathring{\mathbb{F}}^{-1}(\boldsymbol{v};\boldsymbol{u}) \left\{ \nabla f(\boldsymbol{v}+\boldsymbol{u}) - \nabla f(\boldsymbol{v}) \right\} \right\| \\ &= \left\| Q \,\mathring{\mathbb{F}}^{-1}(\boldsymbol{v};\boldsymbol{u}) \,\mathbb{F}(\boldsymbol{v}) \,Q^{-1} \,Q \,\mathbb{F}^{-1}(\boldsymbol{v}) \left\{ \nabla f(\boldsymbol{v}+\boldsymbol{u}) - \nabla f(\boldsymbol{v}) \right\} \right\| \\ &\leq \left\| Q \,\mathring{\mathbb{F}}^{-1}(\boldsymbol{v};\boldsymbol{u}) \,\mathbb{F}(\boldsymbol{v}) \,Q^{-1} \right\| \,\left\| Q \,\mathbb{F}^{-1}(\boldsymbol{v}) \left\{ \nabla f(\boldsymbol{v}+\boldsymbol{u}) - \nabla f(\boldsymbol{v}) \right\} \right\| \\ &\leq \frac{1}{1 - \omega^{+}(\boldsymbol{v})} \,\left\| Q \,\mathbb{F}^{-1}(\boldsymbol{v}) \left\{ \nabla f(\boldsymbol{v}+\boldsymbol{u}) - \nabla f(\boldsymbol{v}) \right\} \right\| \end{split}$$

as required. Similarly

$$\left\|Q\left\{\nabla f(\boldsymbol{\upsilon}+\boldsymbol{u})-\nabla f(\boldsymbol{\upsilon})+\mathbb{F}(\boldsymbol{\upsilon})\,\boldsymbol{u}\right\}\right\|=\left\|Q\left\{\mathring{\mathbb{F}}(\boldsymbol{\upsilon};\boldsymbol{u})-\mathbb{F}(\boldsymbol{\upsilon})\right\}\boldsymbol{u}\right\|\leq\omega^{+}(\boldsymbol{\upsilon})\,\|Q\,\mathbb{F}(\boldsymbol{\upsilon})\,\boldsymbol{u}\|$$

and (A.11) follows from (A.9).

#### A.3 Optimization after linear or quadratic perturbation

Let  $f(\boldsymbol{v})$  be a smooth concave function,

$$\boldsymbol{v}^* = \operatorname*{argmax}_{\boldsymbol{v}} f(\boldsymbol{v}),$$

and  $\mathbb{F} = \mathsf{D}^2 = -\nabla^2 f(\boldsymbol{v}^*)$ . Later we study the question how the point of maximum and the value of maximum of f change if we add a linear or quadratic component to f.

#### A.3.1 A linear perturbation

This section studies the case of a linear change of f. More precisely, let another function  $g(\boldsymbol{v})$  satisfy for some vector  $\boldsymbol{A}$ 

$$g(\boldsymbol{v}) - g(\boldsymbol{v}^*) = \langle \boldsymbol{v} - \boldsymbol{v}^*, \boldsymbol{A} \rangle + f(\boldsymbol{v}) - f(\boldsymbol{v}^*).$$
(A.12)

A typical example corresponds to  $f(\boldsymbol{v}) = \boldsymbol{E}L(\boldsymbol{v})$  and  $g(\boldsymbol{v}) = L(\boldsymbol{v})$  for a random function  $L(\boldsymbol{v})$  with a linear stochastic component  $\zeta(\boldsymbol{v}) = L(\boldsymbol{v}) - \boldsymbol{E}L(\boldsymbol{v})$ . Then (A.12)

is satisfied with

$$\boldsymbol{A}=\nabla\zeta.$$

The aim of the analysis is evaluate the values

$$\boldsymbol{v}^{\circ} \stackrel{\text{def}}{=} \operatorname*{argmax}_{\boldsymbol{v}} g(\boldsymbol{v}), \qquad g(\boldsymbol{v}^{\circ}) = \max_{\boldsymbol{v}} g(\boldsymbol{v}).$$
 (A.13)

The results will be stated mainly in terms of the quantity  $\|\mathbf{F}^{-1/2}\mathbf{A}\|$ . First we consider the case of a quadratic function f.

**Lemma A.6.** Let  $f(\boldsymbol{v})$  be quadratic with  $\nabla^2 f(\boldsymbol{v}) \equiv -\mathbb{F}$ . If  $g(\boldsymbol{v})$  satisfy (A.12), then

$$\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*} = \mathbb{F}^{-1}\boldsymbol{A}, \qquad g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^{*}) = \frac{1}{2} \|\mathbb{F}^{-1/2}\boldsymbol{A}\|^{2}.$$
 (A.14)

*Proof.* If  $f(\boldsymbol{v})$  is quadratic, then, of course, under (A.12),  $g(\boldsymbol{v})$  is quadratic as well with  $-\nabla^2 g(\boldsymbol{v}) \equiv -\mathbb{F}$ . This implies

$$\nabla g(\boldsymbol{v}^*) - \nabla g(\boldsymbol{v}^\circ) = \mathbb{F}(\boldsymbol{v}^\circ - \boldsymbol{v}^*).$$

Further, (A.12) and  $\nabla f(\boldsymbol{v}^*) = 0$  yield  $\nabla g(\boldsymbol{v}^*) = \boldsymbol{A}$ . Together with  $\nabla g(\boldsymbol{v}^\circ) = 0$ , this implies  $\boldsymbol{v}^\circ - \boldsymbol{v}^* = \mathbb{F}^{-1}\boldsymbol{A}$ . The Taylor expansion of g at  $\boldsymbol{v}^\circ$  yields by  $\nabla g(\boldsymbol{v}^\circ) = 0$ 

$$g(v^*) - g(v^\circ) = -\frac{1}{2} \|\mathbf{F}^{1/2}(v^\circ - v^*)\|^2 = -\frac{1}{2} \|\mathbf{F}^{-1/2} \mathbf{A}\|^2$$

and the assertion follows.

The next result describes the concentration properties of  $v^{\circ}$  from (A.13) in a local elliptic set of the form

$$\mathcal{A}(\mathbf{r}) \stackrel{\text{def}}{=} \{ \boldsymbol{v} \colon \| \mathbb{F}^{1/2}(\boldsymbol{v} - \boldsymbol{v}^*) \| \le \mathbf{r} \},$$
(A.15)

where **r** is slightly larger than  $\|\mathbf{F}^{-1/2}\mathbf{A}\|$ .

**Proposition A.7.** Let  $f(\boldsymbol{v})$  be a strongly concave function with  $f(\boldsymbol{v}^*) = \max_{\boldsymbol{v}} f(\boldsymbol{v})$ and  $\mathbb{F} = -\nabla^2 f(\boldsymbol{v}^*)$ . Let further  $g(\boldsymbol{v})$  and  $f(\boldsymbol{v})$  be related by (A.12) with some vector  $\boldsymbol{A}$ . Fix  $\boldsymbol{v} \leq 2/3$  and  $\mathbf{r}$  such that  $\|\mathbb{F}^{-1/2}\boldsymbol{A}\| \leq \boldsymbol{v}\mathbf{r}$ . Suppose now that  $f(\boldsymbol{v})$  satisfy (A.1) for  $\boldsymbol{v} = \boldsymbol{v}^*$ ,  $\mathsf{D}(\boldsymbol{v}^*) = \mathbb{F}^{1/2} = \mathsf{D}$ , and  $\omega'$  such that

$$1 - \nu - \omega' \ge 0. \tag{A.16}$$

Then for  $\boldsymbol{v}^{\circ}$  from (A.13), it holds

$$\|\mathbb{F}^{1/2}(\boldsymbol{v}^{\circ}-\boldsymbol{v}^{*})\|\leq ext{r}$$
 .
*Proof.* With  $D = \mathbb{F}^{1/2}$ , the bound  $\|D^{-1}A\| \leq \nu r$  implies for any u

$$|\langle \boldsymbol{A}, \boldsymbol{u} \rangle| = |\langle \mathsf{D}^{-1} \boldsymbol{A}, \mathsf{D} \boldsymbol{u} \rangle| \leq \nu \, \mathsf{r} \|\mathsf{D} \boldsymbol{u}\|.$$

If  $\|\mathsf{D}\boldsymbol{u}\| > r$ , then  $r\|\mathsf{D}\boldsymbol{u}\| \le \|\mathsf{D}\boldsymbol{u}\|^2$ . Therefore,

$$\left|\langle \boldsymbol{A}, \boldsymbol{u} 
angle 
ight| \leq 
u \| \mathsf{D} \boldsymbol{u} \|^2, \qquad \| \mathsf{D} \boldsymbol{u} \| > \mathtt{r}.$$

Let  $\boldsymbol{v}$  be a point on the boundary of the set  $\mathcal{A}(\mathbf{r})$  from (A.15). We also write  $\boldsymbol{u} = \boldsymbol{v} - \boldsymbol{v}^*$ . The idea is to show that the derivative  $\frac{d}{dt}g(\boldsymbol{v}^* + t\boldsymbol{u}) < 0$  is negative for t > 1. Then all the extreme points of  $g(\boldsymbol{v})$  are within  $\mathcal{A}(\mathbf{r})$ . We use the decomposition

$$g(\boldsymbol{v}^* + t\boldsymbol{u}) - g(\boldsymbol{v}^*) = \langle \boldsymbol{A}, \boldsymbol{u} \rangle t + f(\boldsymbol{v}^* + t\boldsymbol{u}) - f(\boldsymbol{v}^*).$$

With  $h(t) = f(\boldsymbol{v}^* + t\boldsymbol{u})$ , it holds

$$\frac{d}{dt}h(\boldsymbol{v}^* + t\boldsymbol{u}) = \langle \boldsymbol{A}, \boldsymbol{u} \rangle + h'(t).$$
(A.17)

By definition of  $v^*$ , it also holds h'(0) = 0. The identity  $\nabla^2 f(v^*) = -\mathsf{D}^2$  yields  $h''(0) = -\|\mathsf{D}u\|^2$ . Bound (A.2) implies for  $|t| \le 1$ 

$$\left|h'(t) - th''(0)\right| = \left|h'(t) - h'(0) - th''(0)\right| \le t^2 \left|h''(0)\right| \omega'.$$

For t = 1, we obtain by (A.16)

$$h'(1) \le h''(0) - h''(0) \omega' = -|h''(0)|(1 - \omega') < 0$$

Moreover, concavity of h(t) and h'(0) = 0 imply that h'(t) decreases in t for t > 1. Further, summing up the above derivation yields

$$\frac{d}{dt}h(\boldsymbol{v}^* + t\boldsymbol{u})\Big|_{t=1} \le -\|\mathsf{D}\boldsymbol{u}\|^2(1-\nu-\omega') < 0.$$

As  $\frac{d}{dt}h(v^* + tu)$  decreases with  $t \ge 1$  together with h'(t) due to (A.17), the same applies to all such t. This implies the assertion.

The result of Proposition A.7 allows to localize the point  $\boldsymbol{v}^{\circ} = \operatorname{argmax}_{\boldsymbol{v}} g(\boldsymbol{v})$  in the local vicinity  $\mathcal{A}(\mathbf{r})$  of  $\boldsymbol{v}^*$ . The use of smoothness properties of g or, equivalently, of f, in this vicinity helps to obtain rather sharp expansions for  $\boldsymbol{v}^{\circ} - \boldsymbol{v}^*$  and for  $g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^*)$ ; cf. (A.14).

**Proposition A.8.** Under the conditions of Proposition A.7

$$-\frac{\omega}{1+\omega} \|\mathsf{D}^{-1}\boldsymbol{A}\|^2 \le 2g(\boldsymbol{v}^\circ) - 2g(\boldsymbol{v}^*) - \|\mathsf{D}^{-1}\boldsymbol{A}\|^2 \le \frac{\omega}{1-\omega} \|\mathsf{D}^{-1}\boldsymbol{A}\|^2.$$
(A.18)

Also

$$\|\mathsf{D}(\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*}) - \mathsf{D}^{-1}\boldsymbol{A}\|^{2} \leq \frac{3\omega}{(1-\omega)^{2}} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2},$$
  
$$\|\mathsf{D}(\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*})\| \leq \frac{1+\sqrt{2\omega}}{1-\omega} \|\mathsf{D}^{-1}\boldsymbol{A}\|.$$
 (A.19)

*Proof.* By (A.1), for any  $\boldsymbol{v} \in \mathcal{A}(\mathbf{r})$ 

$$\left|f(\boldsymbol{\upsilon}^*) - f(\boldsymbol{\upsilon}) - \frac{1}{2} \|\mathsf{D}(\boldsymbol{\upsilon} - \boldsymbol{\upsilon}^*)\|^2\right| \le \frac{\omega}{2} \|\mathsf{D}(\boldsymbol{\upsilon} - \boldsymbol{\upsilon}^*)\|^2.$$
(A.20)

Further,

$$g(\boldsymbol{v}) - g(\boldsymbol{v}^*) - \frac{1}{2} \| \mathsf{D}^{-1} \boldsymbol{A} \|^2$$
  
=  $\langle \boldsymbol{v} - \boldsymbol{v}^*, \boldsymbol{A} \rangle + f(\boldsymbol{v}) - f(\boldsymbol{v}^*) - \frac{1}{2} \| \mathsf{D}^{-1} \boldsymbol{A} \|^2$   
=  $-\frac{1}{2} \| \mathsf{D}(\boldsymbol{v} - \boldsymbol{v}^*) - \mathsf{D}^{-1} \boldsymbol{A} \|^2 + f(\boldsymbol{v}) - f(\boldsymbol{v}^*) + \frac{1}{2} \| \mathsf{D}(\boldsymbol{v} - \boldsymbol{v}^*) \|^2.$  (A.21)

As  $\boldsymbol{v}^{\circ} \in \mathcal{A}(\mathbf{r})$  and it maximizes  $g(\boldsymbol{v})$ , we derive by (A.20)

$$g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^{*}) - \frac{1}{2} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2} = \max_{\boldsymbol{v}\in\mathcal{A}(\mathbf{r})} \Big\{ g(\boldsymbol{v}) - g(\boldsymbol{v}^{*}) - \frac{1}{2} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2} \Big\}$$
  
$$\leq \max_{\boldsymbol{v}\in\mathcal{A}(\mathbf{r})} \Big\{ -\frac{1}{2} \|\mathsf{D}(\boldsymbol{v}-\boldsymbol{v}^{*}) - \mathsf{D}^{-1}\boldsymbol{A}\|^{2} + \frac{\omega}{2} \|\mathsf{D}(\boldsymbol{v}-\boldsymbol{v}^{*})\|^{2} \Big\}.$$

Further,  $\max_{\boldsymbol{u}} \left\{ \omega \| \boldsymbol{u} \|^2 - \| \boldsymbol{u} - \boldsymbol{\xi} \|^2 \right\} = \frac{\omega}{1-\omega} \| \boldsymbol{\xi} \|^2$  for  $\omega \in [0,1)$  and  $\boldsymbol{\xi} \in \mathbb{R}^p$ , yielding

$$g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^{*}) - \frac{1}{2} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2} \leq \frac{\omega}{2(1-\omega)} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2}.$$

Similarly

$$g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^{*}) - \frac{1}{2} \| \mathsf{D}^{-1}\boldsymbol{A} \|^{2} \ge \max_{\boldsymbol{v} \in \mathcal{A}(\mathbf{r})} \left\{ -\frac{1}{2} \| \mathsf{D}(\boldsymbol{v} - \boldsymbol{v}^{*}) - \mathsf{D}^{-1}\boldsymbol{A} \|^{2} - \frac{\omega}{2} \| \mathsf{D}(\boldsymbol{v} - \boldsymbol{v}^{*}) \|^{2} \right\}$$
  
$$= -\frac{\omega}{2(1+\omega)} \| \mathsf{D}^{-1}\boldsymbol{A} \|^{2}.$$
(A.22)

These bounds imply (A.18).

Now we derive similarly to (A.21) that for  $v \in \mathcal{A}(r)$ 

$$g(\boldsymbol{v}) - g(\boldsymbol{v}^*) \le \langle \boldsymbol{v} - \boldsymbol{v}^*, \boldsymbol{A} \rangle - \frac{1-\omega}{2} \|\mathsf{D}(\boldsymbol{v} - \boldsymbol{v}^*)\|^2.$$

A particular choice  $\boldsymbol{v} = \boldsymbol{v}^{\circ}$  yields

$$g(\boldsymbol{v}^{\circ}) - g(\boldsymbol{v}^{*}) \leq \langle \boldsymbol{v}^{\circ} - \boldsymbol{v}^{*}, \boldsymbol{A} \rangle - \frac{1-\omega}{2} \|\mathsf{D}(\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*})\|^{2}$$

Combining with (A.22) allows to bound

$$\langle \boldsymbol{v}^{\circ} - \boldsymbol{v}^{*}, \boldsymbol{A} \rangle - \frac{1-\omega}{2} \|\mathsf{D}(\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*})\|^{2} - \frac{1}{2} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2} \ge -\frac{\omega}{2(1+\omega)} \|\mathsf{D}^{-1}\boldsymbol{A}\|^{2}.$$

Further, for  $\boldsymbol{\xi} = \mathsf{D}^{-1}\boldsymbol{A}$ ,  $\boldsymbol{u} = \mathsf{D}(\boldsymbol{v}^{\circ} - \boldsymbol{v}^{*})$ , and  $\omega \in [0, 1/3]$ , the inequality

$$2\langle \boldsymbol{u}, \boldsymbol{\xi} \rangle - (1-\omega) \|\boldsymbol{u}\|^2 - \|\boldsymbol{\xi}\|^2 \ge -\frac{\omega}{1+\omega} \|\boldsymbol{\xi}\|^2$$

implies

$$\left\| \boldsymbol{u} - \frac{1}{1-\omega} \boldsymbol{\xi} \right\|^2 \le \frac{2\omega}{(1+\omega)(1-\omega)^2} \| \boldsymbol{\xi} \|^2$$

yielding for  $\omega \leq 1/3$ 

$$\begin{aligned} \|\boldsymbol{u} - \boldsymbol{\xi}\| &\leq \left(\omega + \sqrt{\frac{2\omega}{1+\omega}}\right) \frac{\|\boldsymbol{\xi}\|}{1-\omega} \leq \frac{\sqrt{3\omega}\|\boldsymbol{\xi}\|}{1-\omega} \,, \\ \|\boldsymbol{u}\| &\leq \left(1 + \sqrt{\frac{2\omega}{1+\omega}}\right) \frac{\|\boldsymbol{\xi}\|}{1-\omega} \leq \frac{1 + \sqrt{2\omega}\|\boldsymbol{\xi}\|}{1-\omega} \end{aligned}$$

and (A.19) follows.

#### A.3.2 Quadratic penalization

Here we discuss the case when g(v) - f(v) is quadratic. The general case can be reduced to the situation with  $g(v) = f(v) - ||Gv||^2/2$ . To make the dependence of Gmore explicit, denote

$$f_G(\boldsymbol{v}) = f(\boldsymbol{v}) - \|G\boldsymbol{v}\|^2/2.$$

With  $\boldsymbol{v}^* = \operatorname{argmax}_{\boldsymbol{v}} f(\boldsymbol{v})$  and  $\boldsymbol{v}_G^* = \operatorname{argmax}_{\boldsymbol{v}} f_G(\boldsymbol{v})$ , we study the bias  $\boldsymbol{v}_G^* - \boldsymbol{v}^*$  induced by this penalization under Fréchet-type smoothness conditions. To get some intuition, consider first the case of a quadratic function  $f(\boldsymbol{v})$ .

**Lemma A.9.** Let  $f(\boldsymbol{v})$  be quadratic with  $\mathbb{F} \equiv -\nabla^2 f(\boldsymbol{v})$  and  $A_G \equiv -G^2 \boldsymbol{v}^*$ . Then it holds with  $\mathbb{F}_G = \mathbb{F} + G^2$ 

$$oldsymbol{v}_G^* - oldsymbol{v}^* = \mathbb{F}_G^{-1} oldsymbol{A}_G = -\mathbb{F}_G^{-1} G^2 oldsymbol{v}^*,$$
  
 $f_G(oldsymbol{v}_G^*) - f_G(oldsymbol{v}^*) = rac{1}{2} \|\mathbb{F}_G^{-1/2} oldsymbol{A}_G\|^2 = rac{1}{2} \|\mathbb{F}_G^{-1/2} G^2 oldsymbol{v}^*\|^2.$ 

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*Proof.* Quadraticity of  $f(\boldsymbol{v})$  implies quadraticity of  $f_G(\boldsymbol{v})$  with  $\nabla^2 f_G(\boldsymbol{v}) \equiv -\mathbb{F}_G$ . This implies

$$\nabla f_G(\boldsymbol{v}^*) - \nabla f_G(\boldsymbol{v}^*_G) = \mathbb{F}_G(\boldsymbol{v}^*_G - \boldsymbol{v}^*).$$

Further,  $\nabla f(\boldsymbol{v}^*) = 0$  yielding  $\nabla f_G(\boldsymbol{v}^*) = \boldsymbol{A}_G = -G^2 \boldsymbol{v}^*$ . Together with  $\nabla f_G(\boldsymbol{v}_G^*) = 0$ , this implies  $\boldsymbol{v}_G^* - \boldsymbol{v}^* = \mathbb{F}_G^{-1} \boldsymbol{A}_G$ . The Taylor expansion of  $f_G$  at  $\boldsymbol{v}_G^*$  yields with  $\mathsf{D}_G = \mathbb{F}_G^{1/2}$ 

$$f_G(\boldsymbol{v}^*) - f_G(\boldsymbol{v}_G^*) = -\frac{1}{2} \|\mathsf{D}_G(\boldsymbol{v}_G^* - \boldsymbol{v}^*)\|^2 = -\frac{1}{2} \|\mathsf{D}_G^{-1}\boldsymbol{A}_G\|^2$$

and the assertion follows.

Now we turn to the general case with f smooth in Fréchet sense. Let  $\mathbb{F}(v) = -\nabla^2 f(v)$ . For  $v \in \Upsilon$  and  $u \in \mathbb{R}^p$ , define

$$\overset{\circ}{\mathbb{F}}(\boldsymbol{\upsilon};\boldsymbol{u}) \stackrel{\text{def}}{=} \int_0^1 \mathbb{F}(\boldsymbol{\upsilon} + t\boldsymbol{u}) \, dt \,; \tag{A.23}$$

cf. (A.7). Similarly define  $\mathbb{F}_G(v) = -\nabla^2 f_G(v) = \mathbb{F}(v) + G^2$  and

$$\mathring{\mathbb{F}}_{G}(\boldsymbol{v};\boldsymbol{u}) \stackrel{\text{def}}{=} \int_{0}^{1} \mathbb{F}_{G}(\boldsymbol{v}+t\boldsymbol{u}) dt = \mathring{\mathbb{F}}(\boldsymbol{v};\boldsymbol{u}) + G^{2}.$$
(A.24)

**Lemma A.10.** For the vector  $\mathbf{b}_G \stackrel{\text{def}}{=} \mathbf{v}_G^* - \mathbf{v}^*$ , define  $\mathring{\mathbb{F}}_G = \mathring{\mathbb{F}}_G(\mathbf{v}^*; \mathbf{b}_G)$ . Then

$$\boldsymbol{v}_G^* - \boldsymbol{v}^* = \mathring{\mathbb{F}}_G^{-1} \boldsymbol{A}_G.$$
 (A.25)

*Proof.* First we show for any  $\boldsymbol{v} \in \boldsymbol{\Upsilon}$  and  $\boldsymbol{u} \in \mathbb{R}^p$  that

$$\nabla f_G(\boldsymbol{v} + \boldsymbol{u}) - \nabla f_G(\boldsymbol{v}) = -\mathring{\mathbb{F}}_G(\boldsymbol{v}; \boldsymbol{u}) \, \boldsymbol{u}. \tag{A.26}$$

Indeed, for any  $\gamma \in \mathbb{R}^p$ , consider the univariate function  $h(t) = \langle \nabla f_G(\boldsymbol{v} + t\boldsymbol{u}) - \nabla f_G(\boldsymbol{v}), \boldsymbol{\gamma} \rangle$ . Statement (A.26) follows from definitions (A.23), (A.24), and the identity  $h(1) - h(0) = \int_0^1 h'(t) dt$ .

Further, the definition  $v^* = \operatorname{argmax}_{v} f(v)$  yields  $\nabla f(v^*) = 0$  and

$$\nabla f_G(\boldsymbol{v}^*) = \nabla f(\boldsymbol{v}^*) - G^2 \boldsymbol{v}^* = \boldsymbol{A}_G.$$

In view of  $\nabla f_G(\boldsymbol{v}_G^*) = 0$ , we derive

$$\nabla f_G(\boldsymbol{v}_G^*) - \nabla f_G(\boldsymbol{v}^*) = -\boldsymbol{A}_G$$

Representation (A.26) with  $\boldsymbol{v} = \boldsymbol{v}^*$  and  $\boldsymbol{u} = \boldsymbol{b}_G$  yields (A.25).

Representation (A.25) is very useful to bound from above the bias  $\boldsymbol{v}_G^* - \boldsymbol{v}^*$ . Indeed, assuming that  $\boldsymbol{v}_G^*$  is in a local vicinity of  $\boldsymbol{v}^*$  we may use Fréchet smoothness of f in terms of the value  $\omega^+(\boldsymbol{v}^*)$  from (A.4) to approximate  $\mathring{\mathbb{F}}_G \approx \mathbb{F}_G(\boldsymbol{v}^*)$  and  $\boldsymbol{v}_G^* - \boldsymbol{v}^* \approx$  $-\mathbb{F}_G^{-1}(\boldsymbol{v}^*) G^2 \boldsymbol{v}^*$ .

**Proposition A.11.** Define  $\mathbb{D}_G$  by

$$\mathbb{D}_G^2 = \mathbb{F}_G(\boldsymbol{v}^*),$$

and let Q be a positive definite symmetric operator in  $\mathbb{R}^p$  with  $Q \leq \mathbb{D}_G$ . Fix

$$\mathbf{b}_G = \|Q \, \mathbb{D}_G^{-2} \, G^2 \boldsymbol{v}^*\| = \|Q \, \mathbb{D}_G^{-2} \, \boldsymbol{A}_G\|.$$

With  $\nu = 2/3$ , assume

$$\omega_G^* \stackrel{\text{def}}{=} \sup_{\boldsymbol{u}: \|Q\boldsymbol{u}\| \le \nu^{-1} \mathsf{b}_G} \|\mathbb{D}_G^{-1} \mathbb{F}_G(\boldsymbol{v}^* + \boldsymbol{u}) \mathbb{D}_G^{-1} - I_p\| \le \frac{1}{3};$$
(A.27)

cf. (A.5). Then  $||Q(\boldsymbol{v}_G^* - \boldsymbol{v}^*)|| \leq \nu^{-1} \mathbf{b}_G$  or, equivalently,

$$\boldsymbol{v}_G^* \in \mathcal{A}_G \stackrel{\text{def}}{=} \{ \boldsymbol{v} \colon \| Q(\boldsymbol{v} - \boldsymbol{v}^*) \| \le \nu^{-1} \mathsf{b}_G \}.$$
(A.28)

Moreover,

$$\|Q(\boldsymbol{v}_G^* - \boldsymbol{v}^* - \mathbb{D}_G^{-2}\boldsymbol{A}_G)\| \le \omega_G^* \nu^{-1} \mathsf{b}_G.$$
(A.29)

Proof. First we check that  $\boldsymbol{v}_G^*$  concentrates in the local vicinity  $\mathcal{A}_G$  from (A.28). Strong concavity of  $f_G$  implies that the solution  $\boldsymbol{v}_G^*$  exists and unique. Let us fix any vector  $\boldsymbol{u} \in \mathbb{R}^p$  with  $\|Q\boldsymbol{u}\| = \nu^{-1} \mathbf{b}_G$ . Due to (A.25), we are looking at the solution  $\mathring{\mathbb{F}}_G(\boldsymbol{v}^*; s\boldsymbol{u}) s\boldsymbol{u} = \mathcal{A}_G$  in s. It suffices to ensure that

$$s Q \boldsymbol{u} = Q \mathring{\mathbb{F}}_G(\boldsymbol{v}^*; s \boldsymbol{u})^{-1} \boldsymbol{A}_G$$
 (A.30)

is impossible for  $s \ge 1$ . For s = 1, we can use that  $\mathring{\mathbb{F}}_{G}(\boldsymbol{v}^{*};\boldsymbol{u}) \ge (1-\omega_{G}^{*})\mathbb{D}_{G}^{2}$ ; see (A.9) of Lemma A.4. Therefore,

$$\begin{split} \|Q\,\mathring{\mathbb{F}}_{G}^{-1}(\boldsymbol{v}^{*};\boldsymbol{u})\boldsymbol{A}_{G}\| &\leq \|Q\,\mathring{\mathbb{F}}_{G}^{-1}(\boldsymbol{v}^{*};\boldsymbol{u})\mathbb{D}_{G}^{2}Q^{-1}\|\,\|Q\,\mathbb{D}_{G}^{-2}\,\boldsymbol{A}_{G}\| \\ &\leq (1-\omega_{G}^{*})^{-1}\mathsf{b}_{G} < \nu^{-1}\mathsf{b}_{G} \end{split}$$

and (A.30) with s = 1 is impossible because  $||Q\boldsymbol{u}|| = \nu^{-1} \mathsf{b}_G$ . It remains to note that the matrix  $s \mathring{\mathsf{F}}_G(\boldsymbol{v}^*; s\boldsymbol{u})$  grows with s as

$$s \overset{\circ}{\mathbb{F}}_{G}(\boldsymbol{v}^{*}; s\boldsymbol{u}) = s \int_{0}^{1} \mathbb{F}_{G}(\boldsymbol{v}^{*} + t s \boldsymbol{u}) dt = \int_{0}^{s} \mathbb{F}_{G}(\boldsymbol{v}^{*} + t \boldsymbol{u}) dt.$$

Now we bound  $\|Q \mathbf{b}_G\|$  assuming that  $\|Q(\mathbf{v}_G^* - \mathbf{v}^*)\| \leq \nu^{-1} \mathbf{b}_G$  and (A.27) applies. Statement (A.9) of Lemma A.4 implies  $\mathring{\mathbb{F}}_G^{-1} \leq (1 - \omega_G^*)^{-1} \mathbb{D}_G^2$  and

$$\begin{split} \|Q \, \mathbf{b}_G\| &= \|Q \,\mathring{\mathbb{F}}_G^{-1} \, \mathbb{D}_G^2 \, Q^{-1} \, Q \, \mathbb{D}_G^{-2} \, \mathbf{A}_G\| \le \|Q \,\mathring{\mathbb{F}}_G^{-1} \, \mathbb{D}_G^2 \, Q^{-1}\| \, \|Q \, \mathbb{D}_G^{-2} \mathbf{A}_G\| \\ &\le \frac{1}{1 - \omega_G^*} \, \|Q \, \mathbb{D}_G^{-2} \mathbf{A}_G\| = \frac{\mathbf{b}_G}{1 - \omega_G^*} \,. \end{split}$$

In the same way we derive

$$\|Q(\boldsymbol{b}_{G} - \mathbb{D}_{G}^{-2}\boldsymbol{A}_{G})\| = \|Q(\mathring{\mathbb{F}}_{G}^{-1} - \mathbb{D}_{G}^{-2})\boldsymbol{A}_{G}\| \leq \frac{\omega_{G}^{*}}{1 - \omega_{G}^{*}} \|Q\mathbb{D}_{G}^{-2}\boldsymbol{A}_{G}\|,$$

and (A.29) follows as well.

**Remark A.1.** Inspection of the proofs of Proposition A.11 indicates that the results (A.28) through (A.29) can be restated with  $\mathsf{D}_G^2 = \mathbb{F}_G(\boldsymbol{v}_G^*)$  in place of  $\mathbb{D}_G^2 = \mathbb{F}_G(\boldsymbol{v}^*)$ .

### A.4 Conditional and marginal optimization

This section describes the problem of sequential and marginal optimization. Consider a function  $f(\boldsymbol{v})$  of a parameter  $\boldsymbol{v} \in \mathbb{R}^{p^*}$  which can be represented as  $\boldsymbol{v} = (\boldsymbol{x}, \boldsymbol{a})$ , where  $\boldsymbol{x} \in \mathbb{R}^p$  is the target subvector while  $\boldsymbol{a} \in \mathbb{R}^q$  is a nuisance variable.

#### A.4.1 Partial optimization and local partial smoothness

For any fixed value of the nuisance variable  $a \in A$ , consider  $f_a(x) = f(x, a)$  as a function of x only. Below we assume that  $f_a(x)$  is concave in x for any  $a \in A$ . Define

$$\begin{aligned} \boldsymbol{x_a} &\stackrel{\text{def}}{=} \operatorname*{argmax}_{\boldsymbol{x}} f_{\boldsymbol{a}}(\boldsymbol{x}), \\ \phi_{\boldsymbol{a}} &\stackrel{\text{def}}{=} \operatorname*{max}_{\boldsymbol{x}} f_{\boldsymbol{a}}(\boldsymbol{x}) - f(\boldsymbol{v}^*) = f_{\boldsymbol{a}}(\boldsymbol{x_a}) - f(\boldsymbol{v}^*) \end{aligned}$$

Also define

$$\mathbb{F}_{\boldsymbol{a}} \stackrel{\text{def}}{=} -\nabla^2 f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}) = -\nabla^2_{\boldsymbol{x}\boldsymbol{x}} f(\boldsymbol{x}_{\boldsymbol{a}}, \boldsymbol{a}).$$

Local smoothness of each function  $f_{a}(\cdot)$  around  $x_{a}$  can be well described under the self-concordance property. Let some radius  $\mathbf{r}$  be fixed. In general it may depend on a or on the effective dimension  $\mathbf{p}_{a}$  for  $a \in A$ . We also assume that for each  $a \in A$ , a local metric on  $\mathbb{R}^{p}$  for the target variable x is defined by a matrix  $\mathsf{m}_{a} \in \mathfrak{M}_{p}$ .

 $(S_{3|a})$  For any  $a \in A$ , it holds  $f_a(x) = -nh_a(x)$  with a strongly convex function  $h_a(x)$  such that  $m_a^2 \leq \nabla^2 h_a(x_a)$ , and

$$\sup_{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\| \leq \mathbf{r}/\sqrt{n}} \sup_{t \in [0,1]} \frac{\left| \langle \nabla^3 h_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}} + t\boldsymbol{u}), \boldsymbol{u}^{\otimes 3} \rangle \right|}{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\|^3} \leq \mathsf{c}_3 \, .$$

 $(\mathcal{S}_{4|a})$  For any  $a \in \mathsf{A}$ , the function  $h_a(\cdot)$  satisfies  $(\mathcal{S}_{3|a})$  and

$$\sup_{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\| \leq \mathbf{r}/\sqrt{n}} \sup_{t \in [0,1]} \frac{\left| \langle \nabla^4 h_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}} + t\boldsymbol{u}), \boldsymbol{u}^{\otimes 4} \rangle \right|}{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\|^4} \leq \mathsf{c}_4 \,.$$

Under  $(S_{3|a})$  it holds for all u with  $||m_a(x)u|| \le r/\sqrt{n}$  for the corresponding errors of the Taylor expansion

$$\begin{split} \delta_{3,\boldsymbol{a}}(\boldsymbol{u}) &\stackrel{\text{def}}{=} f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}) - f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}) - \left\langle f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}), \boldsymbol{u} \right\rangle + \|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2/2 \\ &\leq \frac{1}{6} c_3 n \|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\|^3 \leq \frac{c_3 \mathbf{r}}{6n^{1/2}} \|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2, \end{split}$$

and

$$\begin{split} \delta_{4,\boldsymbol{a}}(\boldsymbol{u}) &\stackrel{\text{def}}{=} f_{\boldsymbol{a}}(\boldsymbol{x}) - f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}) - \left\langle f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}), \boldsymbol{u} \right\rangle + \|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2/2 - \left\langle \nabla^3 f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}), \boldsymbol{u}^{\otimes 3} \right\rangle/6 \\ &\leq \frac{1}{24} \operatorname{c}_4 n \|\mathsf{m}_{\boldsymbol{a}}\boldsymbol{u}\|^4 \leq \frac{\operatorname{c}_4 \operatorname{r}^2}{24n} \|\mathbb{F}_{\boldsymbol{a}}^{1/2}\boldsymbol{u}\|^2; \end{split}$$

see Lemma A.2.

Condition  $(\mathcal{S}_3^+)$  can also be extended to the *a*-conditional framework.

 $(\mathcal{S}_{3|a}^+)$   $f_a(\mathbf{x}) = -nh_a(\mathbf{x})$  with  $h_a(\mathbf{x})$  strongly concave.  $m_a^2 \leq \nabla^2 h_a(\mathbf{x}_a)$ , and

$$\sup_{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\| \leq \mathbf{r}/\sqrt{n}} \sup_{\boldsymbol{\gamma} \in \mathbb{R}^{p}} \frac{\left| \langle \nabla^{3} h_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}} + \boldsymbol{u}), \boldsymbol{u} \otimes \boldsymbol{\gamma}^{\otimes 2} \rangle \right|}{\|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{u}\| \|\mathbf{m}_{\boldsymbol{a}}\boldsymbol{\gamma}\|^{2}} \leq c_{3}.$$
(A.31)

To pull together the results of partial optimization w.r.t. x conditioned on a, we also need a condition on the cross derivative of f(x, a).

 $(\mathcal{S}_{3,a}^+)$  It holds f(v) = -nh(v) with a strongly convex function h(v) = h(x, a) satisfying  $(\mathcal{S}_{3|a})$  for each  $a \in A$ . Moreover, it holds

$$\sup_{\boldsymbol{\gamma}\in\mathbb{R}^{p}} \sup_{\|\mathbf{m}\,\boldsymbol{w}\|\leq\mathbf{r}_{\circ}/\sqrt{n}} \sup_{t\in[0,1]} \frac{|\langle\nabla_{\boldsymbol{x}}\nabla^{2}h(\boldsymbol{v}^{*}+t\boldsymbol{w}),\boldsymbol{\gamma}\otimes\boldsymbol{w}^{\otimes2}\rangle|}{\|\mathbf{m}_{\boldsymbol{a}^{*}}\boldsymbol{\gamma}\|\|\mathbf{m}\,\boldsymbol{w}\|^{2}} \leq c_{3},$$

$$\sup_{\boldsymbol{\gamma}\in\mathbb{R}^{p}} \sup_{\|\mathbf{m}\,\boldsymbol{w}\|\leq\mathbf{r}_{\circ}/\sqrt{n}} \sup_{t\in[0,1]} \frac{|\langle\nabla_{\boldsymbol{x}\boldsymbol{x}}^{2}\nabla h(\boldsymbol{v}^{*}+t\boldsymbol{w}),\boldsymbol{\gamma}^{\otimes2}\otimes\boldsymbol{w}\rangle|}{\|\mathbf{m}_{\boldsymbol{a}^{*}}\boldsymbol{\gamma}\|^{2}\|\mathbf{m}\,\boldsymbol{w}\|} \leq c_{3}. \quad (A.32)$$

This condition bounds the third order cross derivative in x and a. Of course, it suffices to bound the third full derivative of h(v); see  $(S_3^+)$ .

#### A.4.2 Conditional optimization and a bound on the bias

Here we study variability of the value  $x_a = \operatorname{argmax}_{x} f(x, a)$  w.r.t. the nuisance parameter a. It appears that local quadratic approximation of the function f in a vicinity of the extreme point  $v^*$  yields a nearly linear dependence of  $x_a$  on a. We illustrate this fact on the case of a quadratic function  $f(\cdot)$ . Consider the negative Hessian  $\mathscr{F} = -\nabla^2 f(v^*)$  in the block form:

$$\mathscr{F} \stackrel{\text{def}}{=} -\nabla^2 f(\boldsymbol{v}^*) = \begin{pmatrix} \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} & \mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} \\ \mathscr{F}_{\boldsymbol{a}\boldsymbol{x}} & \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}} \end{pmatrix}$$
(A.33)

with  $\mathscr{F}_{ax} = \mathscr{F}_{xa}^{\top}$ . If f(v) is quadratic then  $\mathscr{F}$  and its blocks do not depend on v.

**Lemma A.12.** Let f(v) be quadratic, strongly concave, and  $\nabla f(v^*) = 0$ . Then

$$\boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^* = -\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1} \,\mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} \, (\boldsymbol{a} - \boldsymbol{a}^*). \tag{A.34}$$

Proof. The condition  $\nabla f(\boldsymbol{v}^*) = 0$  implies  $f(\boldsymbol{v}) = f(\boldsymbol{v}^*) - (\boldsymbol{v} - \boldsymbol{v}^*)^\top \mathscr{F} (\boldsymbol{v} - \boldsymbol{v}^*)/2$  with  $\mathscr{F} = -\nabla^2 f(\boldsymbol{v}^*)$ . For  $\boldsymbol{a}$  fixed, the point  $\boldsymbol{x}_{\boldsymbol{a}}$  maximizes  $-(\boldsymbol{x} - \boldsymbol{x}^*)^\top \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} (\boldsymbol{x} - \boldsymbol{x}^*)/2 - (\boldsymbol{x} - \boldsymbol{x}^*)^\top \mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} (\boldsymbol{a} - \boldsymbol{a}^*)$  and thus,  $\boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^* = -\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1} \mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} (\boldsymbol{a} - \boldsymbol{a}^*)$ .

This observation (A.34) is in fact discouraging because the bias  $x_a - x^*$  has the same magnitude as the nuisance parameter  $a - a^*$ . However, the condition  $\mathscr{F}_{xa} = 0$  yields  $x_a \equiv x^*$  and the bias vanishes. If f(v) is not quadratic, the *orthogonality* condition  $\nabla_a \nabla_x f(x, a) \equiv 0$  for all  $(x, a) \in \mathcal{W}$  still ensures a vanishing bias.

**Lemma A.13.** Let  $f(\mathbf{x}, \mathbf{a})$  be a continuously differentiable and  $\nabla_{\mathbf{a}} \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{a}) \equiv 0$ . Then the point  $\mathbf{x}_{\mathbf{a}} = \operatorname{argmax}_{\mathbf{x}} f(\mathbf{x}, \mathbf{a})$  does not depend on  $\mathbf{a}$ .

*Proof.* The condition  $\nabla_{a}\nabla_{x} f(x, a) \equiv 0$  implies the decomposition  $f(x, a) = f_{1}(x) + f_{2}(a)$  for some functions  $f_{1}$  and  $f_{2}$ . This in turn yields  $x_{a} \equiv x^{*}$ .

As a corollary, the maximizer  $\boldsymbol{x}_{\boldsymbol{a}}$  and the corresponding negative Hessian  $\mathbb{F}_{\boldsymbol{a}} = \mathsf{D}_{\boldsymbol{a}}^2$ do not depend on  $\boldsymbol{a}$ . Unfortunately, the orthogonality condition  $\nabla_{\boldsymbol{a}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{a}) \equiv 0$  is too restrictive and fulfilled only in the special additive case  $f(\boldsymbol{x}, \boldsymbol{a}) = f_1(\boldsymbol{x}) + f_2(\boldsymbol{a})$ .

In some cases, one can check *semi-orthogonality* condition

$$\nabla_{\boldsymbol{a}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{a}) = 0, \qquad \forall \boldsymbol{a} \in \mathsf{A}.$$
(A.35)

Lemma A.14. Assume (A.35). Then

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{a}) \equiv 0, \qquad \nabla_{\boldsymbol{x}\boldsymbol{x}}^2 f(\boldsymbol{x}^*, \boldsymbol{a}) \equiv \nabla_{\boldsymbol{x}\boldsymbol{x}}^2 f(\boldsymbol{x}^*, \boldsymbol{a}^*), \qquad \boldsymbol{a} \in \mathsf{A}.$$
(A.36)

Moreover, if f(x, a) is concave in x given a then

$$\boldsymbol{x_a} \stackrel{\text{def}}{=} \operatorname*{argmax}_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{a}) \equiv \boldsymbol{x}^*, \qquad \forall \boldsymbol{a} \in \mathsf{A} \,.$$
 (A.37)

*Proof.* Consider the vector

$$\boldsymbol{A_a} \stackrel{\text{def}}{=} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{a})$$

Obviously  $A_{a^*} = 0$ . Moreover, (A.35) implies that  $A_a$  does not depend on a and thus, vanishes everywhere. As f is concave in x, this implies  $f(x^*, a) = \max_x f(x, a)$  and  $x_a = \operatorname{argmax}_x f(x, a) \equiv x^*$ . Similarly, (A.35) implies  $\nabla_a \nabla_{xx} f(x^*, a) \equiv 0$  and (A.36) follows. Concavity of f(x, a) in x for a fixed and (A.36) imply (A.37).

Unfortunately, semi-orthogonality (A.35) condition is also rather restrictive and fulfilled only in special situations. A weaker condition of *one-point orthogonality* means  $\nabla_{\boldsymbol{a}}\nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{a}^*) = 0$ . This condition is not restrictive and can always be enforced by a linear transform of the nuisance variable  $\boldsymbol{a}$ ; see Section A.4.3. Here we evaluate variability of  $\mathbb{F}_{\boldsymbol{a}} = -\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 f(\boldsymbol{x}^*, \boldsymbol{a})$  and of the norm of  $\boldsymbol{b}_{\boldsymbol{a}} = \boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^*$  under this condition. Similarly to Lemma A.3, we derive the following bound.

**Lemma A.15.** Assume (A.32) from  $(\mathcal{S}_{3,a}^+)$  and let

$$\omega^+ = c_3 r_0 n^{-1/2} \le 1/3. \tag{A.38}$$

Then for any  $\boldsymbol{\upsilon} = (\boldsymbol{x}^*, \boldsymbol{a})$  with  $\|\mathsf{m}(\boldsymbol{\upsilon} - \boldsymbol{\upsilon}^*)\| \leq \mathtt{r}_{\circ}/\sqrt{n}$ , it holds

$$(1 - \omega^+) \mathbb{F}_{a^*} \le \mathbb{F}_a \le (1 + \omega^+) \mathbb{F}_{a^*}.$$
(A.39)

**Proposition A.16.** Assume one-point orthogonality  $\nabla_a \nabla_x f(x^*, a^*) = 0$ . Let also conditions  $(\mathcal{S}_{3|a}^+)$ ,  $(\mathcal{S}_{3,a}^+)$  hold and the involved radii  $\mathbf{r}$  and  $\mathbf{r}_{\circ}$  satisfy

$$c_3 r_o n^{-1/2} \le 1/3, \qquad r \ge c_3 n^{-1/2} r_o^2.$$
 (A.40)

Then for any  $\boldsymbol{v} = (\boldsymbol{x}^*, \boldsymbol{a})$  with  $\|\mathbf{m}(\boldsymbol{v} - \boldsymbol{v}^*)\| \leq \mathbf{r}_{\circ}/\sqrt{n}$  and any linear mapping  $Q \colon \mathbb{R}^p \to \mathbb{R}^q$ , the bias  $\boldsymbol{b}_{\boldsymbol{a}} = \boldsymbol{x}_{\boldsymbol{a}} - \boldsymbol{x}^*$  satisfies with  $\mathbb{F} = \mathbb{F}_{\boldsymbol{a}^*}$ 

$$\|Q \boldsymbol{b}_{\boldsymbol{a}}\| \leq \frac{\mathsf{c}_{3} \, \mathsf{r}_{\circ}^{2}}{\sqrt{n}} \|Q \, \mathbb{F}^{-1} Q^{\top}\|^{1/2} \,.$$
 (A.41)

In particular, with  $Q = \mathbb{F}^{1/2}$ 

$$\|\mathbb{F}^{1/2} \boldsymbol{b}_{\boldsymbol{a}}\| \leq \frac{\mathsf{c}_3\,\mathsf{r}_\circ^2}{\sqrt{n}}.$$

**Remark A.2.** Condition  $(\mathcal{S}_3^+)$  with  $\mathbf{r} = \mathbf{r}_\circ$  satisfying  $\mathbf{c}_3 \mathbf{r}_\circ n^{-1/2} \le 1/3$  obviously implies  $(\mathcal{S}_{3|a}^+)$ ,  $(\mathcal{S}_{3,a}^+)$  with the same  $\mathbf{r} = \mathbf{r}_\circ$  and (A.40) is fulfilled as well.

*Proof.* Fix  $\boldsymbol{v} = (\boldsymbol{x}^*, \boldsymbol{a})$  with  $\|\mathbf{m}(\boldsymbol{v} - \boldsymbol{v}^*)\| \leq \mathbf{r}_{\circ}/\sqrt{n}$ . Define the vector  $\boldsymbol{A}_{\boldsymbol{a}} \in \mathbb{R}^p$  by

$$\boldsymbol{A_a} \stackrel{\text{def}}{=} \nabla f_{\boldsymbol{a}}(\boldsymbol{x}^*) = \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{a}).$$

Define  $w = v - v^*$ ,  $\eta = a - a^*$ . For bounding the vector  $A_a$ , use  $A_{a^*} = 0$  and one-point orthogonality  $\nabla_a A_{a^*} = \nabla_a \nabla_x f(v^*) = 0$ . This implies for  $B_a(t) = A_{a^*+t\eta}$ 

$$\boldsymbol{A}_{\boldsymbol{a}} = \boldsymbol{B}_{\boldsymbol{a}}(1) - \boldsymbol{B}_{\boldsymbol{a}}(0) - \boldsymbol{B}'_{\boldsymbol{a}}(0) = \int_{0}^{1} (\boldsymbol{B}'_{\boldsymbol{a}}(t) - \boldsymbol{B}'_{\boldsymbol{a}}(0)) \, dt = \int_{0}^{1} (1-s) \, \boldsymbol{B}''_{\boldsymbol{a}}(s) \, ds \,,$$

where  $B'_{a}(t) = \frac{d}{dt}B_{a}(t)$ ,  $B''_{a}(t) = \frac{d^{2}}{dt^{2}}B_{a}(t)$ . Condition  $(\mathcal{S}_{3,a}^{+})$  ensures

$$\begin{split} \left| \langle \boldsymbol{B}_{\boldsymbol{a}}^{\prime\prime}(s), \boldsymbol{\gamma} \rangle \right| &= \left| \left\langle \nabla_{\boldsymbol{x} \boldsymbol{a} \boldsymbol{a}}^{3} h(\boldsymbol{x}^{*}, \boldsymbol{a}^{*} + t\boldsymbol{\eta}), \boldsymbol{\gamma} \otimes \boldsymbol{\eta}^{\otimes 2} \right\rangle \right| \\ &\leq \mathsf{c}_{3} \, n \, \|\mathsf{m}_{\boldsymbol{a}^{*}} \boldsymbol{\gamma}\| \, \|\mathsf{m} \, \boldsymbol{w}\|^{2} \leq \mathsf{c}_{3} \, n^{1/2} \, \|\mathbb{F}^{1/2} \boldsymbol{\gamma}\| \, \|\mathsf{m} \, \boldsymbol{w}\|^{2}. \end{split}$$

Now we use that

$$\begin{split} \|\mathbb{F}^{-1/2}\boldsymbol{B}_{\boldsymbol{a}}^{\prime\prime}(s)\| &= \sup_{\boldsymbol{\gamma}: \|\mathbb{F}^{1/2}\boldsymbol{\gamma}\| \leq 1} \left| \langle \mathbb{F}^{-1/2}\boldsymbol{B}_{\boldsymbol{a}}^{\prime\prime}(s), \mathbb{F}^{1/2}\boldsymbol{\gamma} \rangle \right| = \sup_{\boldsymbol{\gamma}: \|\mathbb{F}^{1/2}\boldsymbol{\gamma}\| \leq 1} \left| \langle \boldsymbol{B}_{\boldsymbol{a}}^{\prime\prime}(s), \boldsymbol{\gamma} \rangle \right| \\ &\leq \mathsf{c}_{3} \, n^{1/2} \, \sup_{\boldsymbol{\gamma}: \|\mathbb{F}^{1/2}\boldsymbol{\gamma}\| \leq 1} \|\mathbb{F}^{1/2}\boldsymbol{\gamma}\| \, \|\mathbf{m} \, \boldsymbol{w}\|^{2} \leq \mathsf{c}_{3} \, n^{1/2} \, \|\mathbf{m} \, \boldsymbol{w}\|^{2} \end{split}$$

yielding

$$\|\mathbf{F}^{-1/2} \mathbf{A}_{\mathbf{a}}\| \le c_3 n^{1/2} \|\mathbf{m} \, \mathbf{w}\|^2 \int_0^1 (1-s) \, ds \le \frac{c_3 \, \mathbf{r}_{\circ}^2}{2\sqrt{n}}$$

Now we bound the norm of  $b_a$ . We use that  $c_3 n^{-1/2} r_o^2 \leq r$  and (A.31) of  $(\mathcal{S}_{3|a}^+)$  holds for this r. As  $\nabla f_a(x_a) = 0$ , we derive with  $b_a = x_a - x^*$ 

$$\boldsymbol{A}_{\boldsymbol{a}} = \nabla f_{\boldsymbol{a}}(\boldsymbol{x}^*) - \nabla f_{\boldsymbol{a}}(\boldsymbol{x}_{\boldsymbol{a}}) = -\left(\int_0^1 \nabla^2 f_{\boldsymbol{a}}(\boldsymbol{x}^* + t\boldsymbol{b}_{\boldsymbol{a}}) \, dt\right) \boldsymbol{b}_{\boldsymbol{a}} = \mathring{\mathbb{F}}_{\boldsymbol{a}} \, \boldsymbol{b}_{\boldsymbol{a}};$$

see Lemma A.5. This yields  $\boldsymbol{b}_{\boldsymbol{a}} = \overset{\circ}{\mathbb{F}}_{\boldsymbol{a}}^{-1}\boldsymbol{A}_{\boldsymbol{a}}$ . Moreover, for  $\mathbf{r}_{\boldsymbol{a}} = \mathbf{c}_3 n^{-1/2} \mathbf{r}_{\circ}^2$ , it holds  $\omega_{\boldsymbol{a}}^+ \stackrel{\text{def}}{=} \mathbf{c}_3 n^{-1/2} \mathbf{r}_{\boldsymbol{a}} \leq \omega_3^{+2}$  for  $\omega^+ \stackrel{\text{def}}{=} \mathbf{c}_3 \mathbf{r}_{\circ} n^{-1/2}$  implying  $(1 - \omega_{\boldsymbol{a}}^+)(1 - \omega^+) \geq 1/2$  and

by (A.9) of Lemma A.4 and (A.39)

$$\begin{split} \|Q \, \boldsymbol{b}_{\boldsymbol{a}}\| &= \|Q \, \mathring{\mathbb{F}}_{\boldsymbol{a}}^{-1} \boldsymbol{A}_{\boldsymbol{a}}\| \leq \frac{1}{1 - \omega_{\boldsymbol{a}}^{+}} \|Q \, \mathbb{F}^{-1}(\boldsymbol{a}) \boldsymbol{A}_{\boldsymbol{a}}\| \leq \frac{1}{(1 - \omega_{\boldsymbol{a}}^{+})(1 - \omega^{+})} \|Q \, \mathbb{F}^{-1} \boldsymbol{A}_{\boldsymbol{a}}\| \\ &\leq \frac{1}{(1 - \omega_{\boldsymbol{a}}^{+})(1 - \omega^{+})} \|Q \, \mathbb{F}^{-1} Q^{\top}\|^{1/2} \, \|\mathbb{F}^{-1/2} \boldsymbol{A}_{\boldsymbol{a}}\| \leq \frac{\mathsf{c}_{3} \, \mathsf{r}_{\circ}^{2}}{\sqrt{n}} \|Q \, \mathbb{F}^{-1} Q^{\top}\|^{1/2} \, . \end{split}$$

This yields the assertion.

#### A.4.3 One-point orthogonality by a linear transform

One-point orthogonality condition means  $\nabla_a \nabla_x f(v^*) = 0$ . This section explains how this condition can be enforced for a general function f by a linear transform of the nuisance parameter. We only need a mild separability condition which assumes that the full dimensional information matrix  $\mathscr{F}(v) = -\nabla^2 f(v)$  is well posed for  $v = v^*$ .

(
$$\mathscr{F}$$
) The matrix  $\mathscr{F} = \mathscr{F}(\boldsymbol{v}^*)$  is positive definite and for some constant  $\rho = \rho(\mathscr{F}) < 1$ 

$$\|\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\mathscr{F}_{\boldsymbol{x}\boldsymbol{a}}\,\mathscr{F}_{\boldsymbol{a}\boldsymbol{a}}^{-1}\,\mathscr{F}_{\boldsymbol{a}\boldsymbol{x}}\,\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\| \le \rho < 1.$$
(A.42)

Lemma A.17. Suppose  $(\mathcal{F})$ . Then

$$(1-\rho)$$
 block  $\{\mathscr{F}_{xx}, \mathscr{F}_{aa}\} \leq \mathscr{F} \leq (1+\rho)$  block  $\{\mathscr{F}_{xx}, \mathscr{F}_{aa}\}$ 

and the matrices

$$\breve{\mathscr{F}}_{xx} \stackrel{\text{def}}{=} \mathscr{F}_{xx} - \mathscr{F}_{xa} \, \mathscr{F}_{aa}^{-1} \, \mathscr{F}_{ax}, \qquad \breve{\mathscr{F}}_{aa} \stackrel{\text{def}}{=} \mathscr{F}_{aa} - \mathscr{F}_{ax} \, \mathscr{F}_{xx}^{-1} \, \mathscr{F}_{xa},$$

satisfy

$$(1-\rho) \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} \leq \breve{\mathscr{F}}_{\boldsymbol{x}\boldsymbol{x}} \leq \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}, \qquad (1-\rho) \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}} \leq \breve{\mathscr{F}}_{\boldsymbol{a}\boldsymbol{a}} \leq \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}},$$

*Proof.* Define  $D^2 = \mathscr{F}_{xx}$ ,  $H^2 = \mathscr{F}_{aa}$ ,  $\mathbb{F} = \text{block}\{D^2, H^2\}$ ,  $j = D^{-1}\mathscr{F}_{xa}H^{-1}$ , and consider the matrix

$$\mathbb{F}^{-1/2}\mathscr{F} \mathbb{F}^{-1/2} = \begin{pmatrix} I_p & \mathsf{D}^{-1}\mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} \mathsf{H}^{-1} \\ \mathsf{H}^{-1}\mathscr{F}_{\boldsymbol{a}\boldsymbol{x}} \mathsf{D}^{-1} & I_q \end{pmatrix} = \begin{pmatrix} I_p & \mathsf{j} \\ \mathsf{j}^\top & I_q \end{pmatrix}.$$

Condition (A.42) implies  $\|\mathbf{j}\mathbf{j}^{\top}\| \leq \rho$  and hence,

$$1-\rho \le \|\mathbb{F}^{-1/2}\mathscr{F}\mathbb{F}^{-1/2}\| \ge 1+\rho.$$

Moreover,

$$\breve{\mathscr{F}}_{\boldsymbol{x}\boldsymbol{x}} = \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} - \mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} \, \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}}^{-1} \, \mathscr{F}_{\boldsymbol{a}\boldsymbol{x}} = \mathsf{D}(I_p - jj^{\top})\mathsf{D} \ge (1-\rho)\mathsf{D}^2\,,$$

and similarly for  $\check{\mathscr{F}}_{aa}$ .

Note that  $D^2 = \mathscr{F}_{xx}$  is the xx-block of  $\mathscr{F} = -\nabla^2 f(v^*)$ , while  $\check{D}^{-2} = \check{\mathscr{F}}_{xx}^{-1}$  is the xx-block of  $\mathscr{F}^{-1}$  by the formula of block-inversion. The matrices  $D^2$  and  $\check{D}^2$  only coincide if the matrix  $\mathscr{F}$  is of block-diagonal structure.

**Lemma A.18.** With block representation (A.33), define  $\mathscr{C} = \mathscr{F}_{aa}^{-1} \mathscr{F}_{ax}$  and

$$\tau = \mathbf{a} + \mathscr{F}_{aa}^{-1} \mathscr{F}_{ax} \left( \mathbf{x} - \mathbf{x}^* \right) = \mathbf{a} + \mathscr{C} \left( \mathbf{x} - \mathbf{x}^* \right),$$
  
$$\breve{f}(\mathbf{x}, \tau) = f(\mathbf{x}, \mathbf{a}) = f(\mathbf{x}, \tau - \mathscr{C} \left( \mathbf{x} - \mathbf{x}^* \right)).$$
 (A.43)

Then

$$\nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \, \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}) \Big|_{\substack{\boldsymbol{x}=\boldsymbol{x}^*\\\boldsymbol{\tau}=\boldsymbol{a}^*}} = 0$$

$$\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \, \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}) \Big|_{\substack{\boldsymbol{x}=\boldsymbol{x}^*\\\boldsymbol{\tau}=\boldsymbol{a}^*}} = \breve{\mathsf{D}}^2 \,.$$
(A.44)

*Proof.* By definition  $f(x, a) = f(x, \tau - \mathscr{C} x)$ , and it is straightforward to check that

$$\nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \, \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}) \Big|_{\substack{\boldsymbol{x} = \boldsymbol{x}^* \\ \boldsymbol{\tau} = \boldsymbol{a}^*}} = \nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \, f(\boldsymbol{x}, \boldsymbol{\tau} - \mathscr{C} \, (\boldsymbol{x} - \boldsymbol{x}^*)) \Big|_{\substack{\boldsymbol{x} = \boldsymbol{x}^* \\ \boldsymbol{\tau} = \boldsymbol{a}^*}} = 0.$$

Similarly

$$\nabla_{\boldsymbol{x}\boldsymbol{x}}^{2} \, \breve{f}(\boldsymbol{v}^{*}) = \nabla_{\boldsymbol{x}\boldsymbol{x}}^{2} \, f(\boldsymbol{x}, \boldsymbol{\tau} - \mathscr{C} \, (\boldsymbol{x} - \boldsymbol{x}^{*})) \Big|_{\substack{\boldsymbol{x} = \boldsymbol{x}^{*} \\ \boldsymbol{\tau} = \boldsymbol{a}^{*}}} = \mathscr{F}_{\boldsymbol{x}\boldsymbol{x}} - \mathscr{F}_{\boldsymbol{x}\boldsymbol{a}} \, \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}}^{-1} \, \mathscr{F}_{\boldsymbol{a}\boldsymbol{x}} = \breve{\mathsf{D}}^{2}$$

as required.

We can summarize that the linear transform (A.43) ensures the one-point orthogonality condition  $\nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{v}^*) = 0$  for the function  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau}) = f(\boldsymbol{x}, \boldsymbol{\tau} - \mathscr{C}(\boldsymbol{x} - \boldsymbol{x}^*))$  with  $-\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \check{f}(\boldsymbol{v}^*) = \check{\mathsf{D}}^2$ . For this function, one can redefine all the characteristics including

$$\begin{split} \breve{\phi}_{\tau} &\stackrel{\text{def}}{=} \max_{\boldsymbol{x}} \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}), \\ \breve{\boldsymbol{x}}_{\tau} &\stackrel{\text{def}}{=} \arg_{\boldsymbol{x}} \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}), \\ \breve{\mathsf{D}}_{\tau}^2 &\stackrel{\text{def}}{=} -\nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \breve{f}(\breve{\boldsymbol{x}}_{\tau}, \boldsymbol{\tau}). \end{split}$$

48

If  $f(\boldsymbol{x}, \boldsymbol{a})$  is quadratic, then orthogonality can be achieved by a linear transform of the nuisance parameter  $\boldsymbol{a}$ . In particular, for  $f(\boldsymbol{v}) = f(\boldsymbol{v}^*) - (\boldsymbol{v} - \boldsymbol{v}^*)^\top \mathscr{F} (\boldsymbol{v} - \boldsymbol{v}^*)/2$  quadratic, it holds with  $\mathsf{H}^2 = \mathscr{F}_{\boldsymbol{a}\boldsymbol{a}}$ 

$$\check{f}(x, \tau) = f(v^*) - \frac{\|\check{\mathsf{D}}(x - x^*)\|^2}{2} - \frac{\|\mathsf{H}(\tau - a^*)\|^2}{2},$$

and hence

$$raket{x}_{m{ au}}\equiv m{x}^*, \qquad raket{\mathsf{D}}_{m{ au}}^2\equivraket{\mathsf{D}}^2, \qquad raket{\phi}_{m{ au}}=-rac{\|\mathsf{H}(m{ au}-m{a}^*)\|^2}{2}.$$

Next we discuss another special case when the mixed derivative of f(x, a) only depends on x:

$$\nabla_{\boldsymbol{a}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{a}) \equiv -\mathcal{G}(\boldsymbol{x}), \qquad \nabla_{\boldsymbol{a}}^2 f(\boldsymbol{x}, \boldsymbol{a}) \equiv -\mathcal{H}^2(\boldsymbol{x}), \tag{A.45}$$

for a  $q \times p$ -matrix function  $\mathcal{G}(\boldsymbol{x})$  and a positive  $q \times q$ -matrix function  $\mathcal{H}^2(\boldsymbol{x})$ . We also write  $\mathcal{G}$  and  $\mathcal{H}^2$  in place of  $\mathcal{G}(\boldsymbol{x}^*)$  and  $\mathcal{H}^2(\boldsymbol{x}^*)$ . Due to the next result, this condition yields a semi-orthogonality of the transformed function  $\check{f}(\cdot)$ .

**Lemma A.19.** Assume (A.45). Then the function  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau})$  from (A.43) satisfies the semi-orthogonality condition

$$abla_{oldsymbol{ au}}
abla_{oldsymbol{x}}oldsymbol{ar{f}}(oldsymbol{x}^*,oldsymbol{ au})\equiv 0.$$

Moreover, for any  $\boldsymbol{\tau}$  with  $(\boldsymbol{x}^*, \boldsymbol{\tau}) \in \check{\boldsymbol{\Upsilon}}$ , it holds

$$\nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{x}^*, \boldsymbol{\tau}) \equiv 0, \qquad \nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \check{f}(\boldsymbol{x}^*, \boldsymbol{\tau}) \equiv \nabla_{\boldsymbol{x}\boldsymbol{x}}^2 \check{f}(\boldsymbol{x}^*, \boldsymbol{a}^*). \tag{A.46}$$

If  $f(\boldsymbol{v})$  is concave in  $\boldsymbol{v}$  then

$$\breve{\boldsymbol{x}}_{\boldsymbol{\tau}} \stackrel{\text{def}}{=} \operatorname*{argmax}_{\boldsymbol{x}} \breve{f}(\boldsymbol{x}, \boldsymbol{\tau}) \equiv \boldsymbol{x}^* \,. \tag{A.47}$$

*Proof.* Let  $\check{f}(\boldsymbol{x}, \boldsymbol{\tau})$  be defined by (A.43). Lemma A.18 ensures one-point orthogonality  $\nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{v}^*) = \nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{x}^*, \boldsymbol{a}^*) = 0$ . Moreover, (A.45) yields  $\mathscr{C} = \mathcal{H}^{-2} \mathcal{G}$ . Now consider  $\nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{x}^*, \boldsymbol{\tau})$ . It holds by (A.45) and definition (A.43)

$$\begin{aligned} \nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} \check{f}(\boldsymbol{x}^*, \boldsymbol{\tau}) &= \left. \nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{\tau} - \mathscr{C} \left( \boldsymbol{x} - \boldsymbol{x}^* \right) \right) \right|_{\boldsymbol{x} = \boldsymbol{x}^*} \\ &= \left. \nabla_{\boldsymbol{\tau}} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^*, \boldsymbol{\tau}) - \nabla_{\boldsymbol{\tau}}^2 f(\boldsymbol{x}^*, \boldsymbol{\tau}) \mathscr{C} = -\mathcal{G} + \mathcal{H}^2 \mathscr{C} = 0 \end{aligned}$$

yielding semi-orthogonality of  $\check{f}$ . Now (A.46) and (A.47) follow from Lemma A.14.

For a general smooth function f(x, a) satisfying  $(S_3^+)$ , we expect that these identities are fulfilled in a local vicinity of  $v^*$  up to the error of quadratic approximation. The next lemma quantifies this guess.

**Proposition A.20.** Let f(v) satisfy  $(\mathscr{F})$ ,  $(\mathscr{S}_3^+)$  with  $r = r_\circ$ , and

$$\omega^+ = \mathbb{C}_{\mathscr{F}} \, \mathbb{c}_3 \, \mathbb{r}_0 n^{-1/2} \le 1/3. \tag{A.48}$$

Then the result (A.41) of Proposition A.16 continues to apply.

*Proof.* The linear transform (A.43) reduces the statement to the case with one-point orthogonality. Condition (A.48) ensures (A.38) after this transform. Conditions  $(\mathcal{S}_{3|a})$ ,  $(\mathcal{S}_{4|a})$ ,  $(\mathcal{S}_{3|a}^+)$ , and  $(\mathcal{S}_{3,a}^+)$  follow from  $(\mathcal{S}_3^+)$ .

#### A.4.4 Composite nuisance variable

For some situations, the nuisance variable a is by itself a composition of few other subvectors. Checking condition ( $\mathscr{F}$ ) in the scope of variables can be involved. However, it can be reduced to a check for each subvectors. We only consider the case of two variables  $a = (z, \tau)$ , that is,

$$f(\boldsymbol{v}) = f(\boldsymbol{x}, \boldsymbol{a}) = f(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{\tau}).$$

Denote by  $\mathscr{F}_{x,x}$ ,  $\mathscr{F}_{x,z}$ ,  $\mathscr{F}_{x,\tau}$ ,  $\mathscr{F}_{z,z}$ ,  $\mathscr{F}_{\tau,\tau}$  the corresponding blocks of  $\mathscr{F}$ .

**Lemma A.21.** For the matrix  $\mathscr{F} = -\nabla^2 f(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{\tau})$ , suppose that

$$\|\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\mathscr{F}_{\boldsymbol{x}\boldsymbol{z}}\,\mathscr{F}_{\boldsymbol{z}\boldsymbol{z}}^{-1}\,\mathscr{F}_{\boldsymbol{z}\boldsymbol{x}}\,\mathscr{F}_{\boldsymbol{x}\boldsymbol{x}}^{-1/2}\| \le \rho_{\boldsymbol{z}} < 1,\tag{A.49}$$

$$\|\mathscr{F}_{xx}^{-1/2}\mathscr{F}_{x\tau}\mathscr{F}_{\tau\tau}^{-1}\mathscr{F}_{\tau x}\mathscr{F}_{xx}^{-1/2}\| \le \rho_{\tau} < 1.$$
(A.50)

Then (F) is fulfilled for  $\mathbf{a} = (\mathbf{z}, \mathbf{\tau})$  with  $\rho = \rho_{\mathbf{z}} + \rho_{\mathbf{\tau}}$ .

*Proof.* Define the scalar product

$$\langle \boldsymbol{v}_1, \boldsymbol{v}_2 
angle = \boldsymbol{v}_1^\top \mathscr{F} \boldsymbol{v}_2.$$

Let us fix any vectors x, z, au with the natural embedding in the v -space and define

$$oldsymbol{x}_1 \stackrel{ ext{def}}{=} oldsymbol{x} - rac{\langle oldsymbol{x}, oldsymbol{z} 
angle}{\langle oldsymbol{z}, oldsymbol{z} 
angle} oldsymbol{z}, \qquad oldsymbol{ au}_1 \stackrel{ ext{def}}{=} oldsymbol{ au} - rac{\langle oldsymbol{ au}, oldsymbol{z} 
angle}{\langle oldsymbol{z}, oldsymbol{z} 
angle} oldsymbol{z},$$

Then  $\langle \boldsymbol{x}_1, \boldsymbol{z} \rangle = 0$ ,  $\langle \boldsymbol{\tau}_1, \boldsymbol{z} \rangle = 0$ . Condition (A.49) yields

$$||x_1|| \ge (1 - \rho_z) ||x||.$$

Similarly define

$$oldsymbol{x}_2 \stackrel{ ext{def}}{=} oldsymbol{x}_1 - rac{\langle oldsymbol{x}_1, oldsymbol{ au}_1 
angle}{\langle oldsymbol{ au}_1, oldsymbol{ au}_1 
angle} oldsymbol{ au}_1$$

Then  $\langle \boldsymbol{x}_2, \boldsymbol{z} \rangle = 0$  and  $\langle \boldsymbol{x}_2, \boldsymbol{\tau} \rangle = 0$  and by (A.50)

$$\|\boldsymbol{x}_2\| \ge (1 - \rho_{\tau}) \|\boldsymbol{x}_1\| \ge (1 - \rho_{z})(1 - \rho_{\tau}) \|\boldsymbol{x}\| \ge (1 - \rho_{z} - \rho_{\tau}) \|\boldsymbol{x}\|$$

and  $(\mathcal{F})$  follows.

# **B** Dimension free bounds for Laplace approximation

Here we present several issues related to Laplace approximation. Section B.2 states general results about the accuracy of Laplace approximation for finite samples. Technical assertions and proofs are collected in Section B.3.

### **B.1** Setup and conditions

Let  $f(\boldsymbol{x})$  be a function in a high-dimensional Euclidean space  $\mathbb{R}^p$  such that  $\int e^{f(\boldsymbol{x})} d\boldsymbol{x} = C < \infty$ , where the integral sign  $\int$  without limits means the integral over the whole space  $\mathbb{R}^p$ . Then f determines a distribution  $\mathbb{P}_f$  with the density  $C^{-1}e^{f(\boldsymbol{x})}$ . Let  $\boldsymbol{x}^*$  be a point of maximum:

$$f(\boldsymbol{x}^*) = \sup_{\boldsymbol{u} \in \mathbb{R}^p} f(\boldsymbol{x}^* + \boldsymbol{u}).$$

We also assume that  $f(\cdot)$  is at least three time differentiable. Introduce the negative Hessian  $\mathbb{F} = -\nabla^2 f(\boldsymbol{x}^*)$  and assume  $\mathbb{F}$  strictly positive definite. We aim at approximating the measure  $\mathbb{P}_f$  by a Gaussian measure  $\mathcal{N}(\boldsymbol{x}^*, \mathbb{F}^{-1})$ . Given a function  $g(\cdot)$ , define its expectation w.r.t.  $\mathbb{P}_f$  after centering at  $\boldsymbol{x}^*$ :

$$\mathcal{I}(g) \stackrel{\text{def}}{=} \frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x}^* + \boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x}^* + \boldsymbol{u})} d\boldsymbol{u}}.$$
 (B.1)

A Gaussian approximation  $\mathcal{I}_{\mathbb{F}}(g)$  for  $\mathcal{I}(g)$  is defined as

$$\mathcal{I}_{\mathbb{F}}(g) \stackrel{\text{def}}{=} \frac{\int g(\boldsymbol{u}) \,\mathrm{e}^{-\|\mathbb{F}^{1/2}\boldsymbol{u}\|^2/2} \,d\boldsymbol{u}}{\int \mathrm{e}^{-\|\mathbb{F}^{1/2}\boldsymbol{u}\|^2/2} \,d\boldsymbol{u}} = I\!\!E g(\boldsymbol{\gamma}_{\mathbb{F}}), \qquad \boldsymbol{\gamma}_{\mathbb{F}} \sim \mathcal{N}(0, \mathbb{F}^{-1}) \,.$$

The choice of the distance between  $\mathbb{P}_f$  and  $\mathcal{N}(x^*, \mathbb{F}^{-1})$  specifies the considered class of functions g. The most strong total variation distance can be obtained as the supremum

of  $|\mathcal{I}(g) - \mathcal{I}_{\mathbb{F}}(g)|$  over all measurable functions  $g(\cdot)$  with  $|g(u)| \leq 1$ :

$$\operatorname{TV}(\mathbb{P}_f, \mathcal{N}(\boldsymbol{x}^*, \mathbb{F}^{-1})) = \sup_{\|g\|_{\infty} \leq 1} |\mathcal{I}(g) - \mathcal{I}_{\mathbb{F}}(g)|.$$

The results can be substantially improved if only centrally symmetric functions  $g(\cdot)$  with  $g(\mathbf{x}) = g(-\mathbf{x})$  are considered. Obviously, for any  $g(\cdot)$ 

$$\mathcal{I}(g) = \frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x}^* + \boldsymbol{u}) - f(\boldsymbol{x}^*)} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x}^* + \boldsymbol{u}) - f(\boldsymbol{x}^*)} d\boldsymbol{u}}$$

Moreover, as  $\boldsymbol{x}^* = \operatorname{argmax}_{\boldsymbol{x}} f(\boldsymbol{x})$ , it holds  $\nabla f(\boldsymbol{x}^*) = 0$  and

$$\mathcal{I}(g) = \frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x}^*;\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x}^*;\boldsymbol{u})} d\boldsymbol{u}},$$
(B.2)

where  $f(\boldsymbol{x}; \boldsymbol{u})$  is the Bregman divergence

$$f(\boldsymbol{x};\boldsymbol{u}) = f(\boldsymbol{x}+\boldsymbol{u}) - f(\boldsymbol{x}) - \langle \nabla f(\boldsymbol{x}), \boldsymbol{u} \rangle.$$
(B.3)

Implicitly we assume that the negative Hessian  $\mathbb{F} = -\nabla^2 f(\boldsymbol{x}^*)$  is sufficiently large in the sense that the Gaussian measure  $\mathcal{N}(0, \mathbb{F}^{-1})$  concentrates on a small local set  $\mathcal{U}$ . This allows to use a local Taylor expansion for  $f(\boldsymbol{x}^*; \boldsymbol{u}) \approx -\|\mathbb{F}^{1/2}\boldsymbol{u}\|^2/2$  in  $\boldsymbol{u}$  on  $\mathcal{U}$ . If  $f(\cdot)$  is also strongly concave, then the  $\mathbb{P}_f$ -mass of the complement of  $\mathcal{U}$  is exponentially small yielding the desirable Laplace approximation.

Our setup is motivated by Bayesian inference. Assume for a moment that

$$f(\mathbf{x}) = \ell(\mathbf{x}) - \|G(\mathbf{x} - \mathbf{x}_0)\|^2 / 2$$
(B.4)

for some  $\boldsymbol{x}_0$  and a symmetric p-matrix  $G^2 \geq 0$ . Here  $\ell(\cdot)$  stands for a log-likelihood function while the quadratic penalty  $\|G(\boldsymbol{x} - \boldsymbol{x}_0)\|^2/2$  corresponds to a Gaussian prior  $\mathcal{N}(\boldsymbol{x}_0, G^{-2})$ . Let also  $\ell(\cdot)$  be concave with  $\mathsf{D}^2 \stackrel{\text{def}}{=} -\nabla^2 \ell(\boldsymbol{x}^*) > 0$ . Then

$$-\nabla^2 f(\boldsymbol{x}^*) = -\nabla^2 \ell(\boldsymbol{x}^*) + G^2 = \mathsf{D}^2 + G^2.$$

In typical asymptotic setups, the log-likelihood function  $\ell(\mathbf{x})$  scales with the sample size n or inverse noise variance while the prior is kept fixed; see, e.g. Schillings et al. (2020); Helin and Kretschmann (2022). We allow  $G^2$  depend on n as well, this is important for obtaining the dimension free results and to obtain optimal contraction rate; see Section C.1.

#### B.1.1 Concavity

Below we implicitly assume decomposition (B.4) with a *weakly concave* function  $\ell(\cdot)$ . More specifically, we assume the following condition.

 $(\mathcal{C}_0)$  There exists an operator  $G^2 \geq 0$  in  $\mathbb{R}^p$  such that  $G^2 \leq -\nabla^2 f(\boldsymbol{x}^*)$  and

$$\ell(\boldsymbol{x}^* + \boldsymbol{u}) \stackrel{\text{def}}{=} f(\boldsymbol{x}^* + \boldsymbol{u}) + \|G\boldsymbol{u}\|^2/2$$

is a concave function.

If  $\ell(\cdot)$  in decomposition (B.4) is concave then this condition is obviously fulfilled. More generally, if  $\ell(\cdot)$  in (B.4) is weakly concave, so that  $\ell(\boldsymbol{x}^* + \boldsymbol{u}) - ||G_0\boldsymbol{u}||^2/2$  is concave in  $\boldsymbol{u}$  with  $G_0^2 \leq G^2$ , then  $(\mathcal{C}_0)$  is fulfilled with  $G^2 - G_0^2$  in place of  $G^2$ .

The operator  $D^2$  plays an important role in our conditions and results:

$$\mathsf{D}^{2} = -\nabla^{2} f(\boldsymbol{x}^{*}) - G^{2} \quad \left(= -\nabla^{2} \ell(\boldsymbol{x}^{*}) \text{ under (B.4)}\right). \tag{B.5}$$

**Remark B.1.** The condition of strong concavity of f on the whole space  $\mathbb{R}^p$  can be too restrictive. This condition can be replaced by its local version: f is concave on a set  $\mathcal{X}_0$  such that the Gaussian prior  $\mathcal{N}(\mathbf{x}_0, G^{-2})$  concentrates on  $\mathcal{X}_0$  and the maximizer  $\mathbf{x}_G^*$  belongs to  $\mathcal{X}_0$ . In all the results, the integral over  $\mathbb{R}^p$  has to be replaced by the integral over  $\mathcal{X}_0$ .

#### **B.1.2** Laplace effective dimension

With decomposition (B.5) in mind, we use a decomposition for  $\mathbb{F} = -\nabla^2 f(\boldsymbol{x}^*)$ :

$$\mathbb{F} = -\nabla^2 f(\boldsymbol{x}^*) = \mathsf{D}^2 + G^2.$$

The Laplace effective dimension  $\mathbf{p}(\mathbf{x}^*)$  is given by

$$\mathbf{p}(\boldsymbol{x}^*) \stackrel{\text{def}}{=} \operatorname{tr} \left( \mathsf{D}^2 \, \mathbb{F}^{-1} \right) = \operatorname{tr} \left\{ \mathsf{D}^2 \, (\mathsf{D}^2 + G^2)^{-1} \right\}. \tag{B.6}$$

Of course,  $p(\boldsymbol{x}^*) \leq p$  but a proper choice of the penalty  $G^2$  in (B.4) allows to avoid the "curse of dimensionality" issue and ensure a small effective dimension  $p(\boldsymbol{x}^*)$  even for p large or infinite; see Spokoiny and Panov (2021) for more rigorous discussion.

Later we write p instead of  $p(x^*)$  without risk of confusion because the parameter dimension p does not show up anymore. The value p helps to describe a local vicinity  $\mathcal{U}$  around  $x^*$  such that the most of mass of  $\mathbb{P}_f$  concentrates on  $\mathcal{U}$ ; see Section B.3.5. Namely, let us fix some  $\nu < 1$ , e.g.  $\nu = 2/3$ , and some x > 0 ensuring that  $e^{-x}$  is our significance level. Define

$$\mathbf{r} = 2\sqrt{\mathbf{p}} + \sqrt{2\mathbf{x}}, \qquad \mathcal{U} = \left\{ \boldsymbol{u} \colon \|\mathsf{D}\boldsymbol{u}\| \le \nu^{-1}\mathbf{r} \right\}.$$
(B.7)

#### **B.1.3** Local smoothness conditions

Let  $p \leq \infty$  and let  $f(\cdot)$  be a three times continuously differentiable function on  $\mathbb{R}^p$ . We fix a reference point x and local region around x given by the local set  $\mathcal{U} \subset \mathbb{R}^p$ from (B.7). Consider the remainder of the second and third order Taylor approximation

$$egin{aligned} &\delta_3(m{x},m{u})=f(m{x};m{u})-ig\langle 
abla^2 f(m{x}),m{u}^{\otimes 2}ig
angle/2,\ &\delta_4(m{x},m{u})=f(m{x};m{u})-ig\langle 
abla^2 f(m{x}),m{u}^{\otimes 2}ig
angle/2-ig\langle 
abla^3 f(m{x}),m{u}^{\otimes 3}ig
angle/6 \end{aligned}$$

with  $f(\boldsymbol{x}; \boldsymbol{u})$  from (B.3). The use of the Taylor formula allows to bound

$$\left|\delta_k(\boldsymbol{x}, \boldsymbol{u})\right| \leq \sup_{t \in [0,1]} \frac{1}{k!} \left| \left\langle \nabla^k f(\boldsymbol{x} + t\boldsymbol{u}), \boldsymbol{u}^{\otimes k} \right\rangle \right|, \quad k \geq 3.$$

Note that the quadratic penalty  $-\|G(\boldsymbol{x}-\boldsymbol{x}_0)\|^2/2$  in f does not affect the remainders  $\delta_3(\boldsymbol{x}, \boldsymbol{u})$  and  $\delta_4(\boldsymbol{x}, \boldsymbol{u})$ . Indeed, with  $f(\boldsymbol{x}) = \ell(\boldsymbol{x}) - \|G(\boldsymbol{x}-\boldsymbol{x}_0)\|^2/2$ , it holds

$$f(\boldsymbol{x};\boldsymbol{u}) \stackrel{\text{def}}{=} f(\boldsymbol{x}+\boldsymbol{u}) - f(\boldsymbol{x}) - \left\langle \nabla f(\boldsymbol{x}), \boldsymbol{u} \right\rangle = \ell(\boldsymbol{x};\boldsymbol{u}) - \|G\boldsymbol{u}\|^2/2$$

and the quadratic term in definition of the values  $\delta_k(\boldsymbol{x}, \boldsymbol{u})$  cancels,  $k \geq 3$ . Local smoothness of  $f(\cdot)$  or, equivalently, of  $\ell(\cdot)$ , at  $\boldsymbol{x}$  will be measured by the value  $\omega(\boldsymbol{x})$ :

$$\omega(\boldsymbol{x}) \stackrel{\text{def}}{=} \sup_{\boldsymbol{u} \in \mathcal{U}} \frac{1}{\|\mathsf{D}\boldsymbol{u}\|^2/2} |\delta_3(\boldsymbol{x}, \boldsymbol{u})|; \tag{B.8}$$

cf. (A.1). We also denote  $\omega \stackrel{\text{def}}{=} \omega(\boldsymbol{x}^*)$ . Our results apply if  $\omega \ll 1$ . Local concentration of the measure  $\mathbb{P}_f$  requires  $\omega \leq 1/3$ ; see Proposition B.16. The results about Gaussian approximation are valid under a stronger condition  $\omega p \leq 2/3$  with p from (B.6).

## B.2 Error bounds for Laplace approximation

Our first result describes the quality of approximation of the measure  $\mathbb{P}_f$  by the Gaussian measure  $\mathcal{N}(\boldsymbol{x}^*, \mathbb{F}^{-1})$  with mean  $\boldsymbol{x}^*$  and the covariance  $\mathbb{F}^{-1}$  in total variation distance. In all our result, the value  $\mathbf{x}$  is fixed to ensure that  $e^{-\mathbf{x}}$  is negligible. First we present the general results which will be specified later under the self-concordance condition. **Theorem B.1.** Suppose  $(C_0)$ . Let also p be defined by (B.6) and r and U by (B.7). If  $\omega$  from (B.8) satisfies  $\omega \leq 1/3$ , then

$$\mathbb{P}_f(\mathbf{X} - \mathbf{x}^* \notin \mathcal{U}) \le e^{-\mathbf{x}}.$$
(B.9)

If  $\omega p \leq 2/3$ , then for any  $g(\cdot)$  with  $|g(u)| \leq 1$ , it holds for  $\mathcal{I}(g)$  from (B.1)

$$\left|\mathcal{I}(g) - \mathcal{I}_G(g)\right| \le \frac{2(\diamondsuit + e^{-\mathbf{x}})}{1 - \diamondsuit - e^{-\mathbf{x}}} \le 4(\diamondsuit + e^{-\mathbf{x}})$$
(B.10)

with

$$\diamondsuit = \diamondsuit_2 = \frac{0.75\,\omega\,\mathsf{p}}{1-\omega}\,.\tag{B.11}$$

This section presents more advanced bounds on the error of Laplace approximation under conditions  $(\mathcal{T}_3)$  and  $(\mathcal{T}_4)$  with  $v = x^*$  or  $(\mathcal{S}_3)$  and  $(\mathcal{S}_4)$  with  $v = x^*$  and  $\mathsf{m}(x^*) = n^{-1/2}\mathsf{D}$ ; see Section A.

**Theorem B.2.** Suppose ( $C_0$ ) and ( $T_3$ ) and let  $\tau_3 \nu^{-1} \mathbf{r} \leq 3/4$  for  $\mathbf{r}$  from (B.7). Then the concentration bound (B.9) holds. Moreover, if

$$\tau_3 \nu^{-1} \mathbf{r} \, \mathbf{p} \le 2, \tag{B.12}$$

then the accuracy bound (B.10) applies with  $\alpha = \|\mathbf{D} \mathbf{F}^{-1} \mathbf{D}\| \leq 1$ 

$$\diamondsuit = \diamondsuit_3 \stackrel{\text{def}}{=} \frac{\tau_3(\mathbf{p} + \alpha)^{3/2}}{4(1 - \omega)^{3/2}} \le \frac{\tau_3(\mathbf{p} + \alpha)^{3/2}}{2}, \tag{B.13}$$

where  $\omega \stackrel{\text{def}}{=} \tau_3 \nu^{-1} \mathbf{r}/3 \leq 1/4$ . Furthermore, under  $(\mathcal{T}_4)$ , for any symmetric function  $g(\mathbf{u}) = g(-\mathbf{u})$ ,  $|g(\mathbf{u})| \leq 1$ , the accuracy bound (B.10) applies with

$$\diamondsuit = \diamondsuit_4 = \frac{\tau_3^2 \,(\mathbf{p} + 2\alpha)^3 + 2\tau_4 (\mathbf{p} + \alpha)^2}{16(1 - \omega)^2} \le \frac{\tau_3^2 \,(\mathbf{p} + 2\alpha)^3 + 2\tau_4 (\mathbf{p} + \alpha)^2}{8}$$

Under  $(S_3)$  and  $(S_4)$  instead of  $(T_3)$  and  $(T_4)$ , the results apply with  $\tau_3 = c_3 n^{-1/2}$ and  $\tau_4 = c_4 n^{-1}$ .

Let  $\mathscr{B}(\mathbb{R}^p)$  be the  $\sigma$ -field of all Borel sets in  $\mathbb{R}^p$ , while  $\mathscr{B}_s(\mathbb{R}^p)$  stands for all centrally symmetric sets from  $\mathscr{B}(\mathbb{R}^p)$ . By X we denote a random element with the distribution  $\mathbb{P}_f$ , while  $\gamma_{\mathbb{F}} \sim \mathcal{N}(0, \mathbb{F}^{-1})$ .

**Corollary B.3.** Under the conditions of Theorem B.2, it holds for  $X \sim \mathbb{P}_f$ 

$$\sup_{A \in \mathscr{B}(\mathbb{R}^p)} \left| \mathcal{P}_f(X - x^* \in A) - \mathcal{P}(\gamma_{\mathbb{F}} \in A) \right| \le 4(\diamondsuit_3 + e^{-x}),$$
$$\sup_{A \in \mathscr{B}_s(\mathbb{R}^p)} \left| \mathcal{P}_f(X - x^* \in A) - \mathcal{P}(\gamma_{\mathbb{F}} \in A) \right| \le 4(\diamondsuit_4 + e^{-x}).$$

#### B.2.1 Critical dimension

Here we briefly discuss the important issue of *critical dimension* meaning a relation between **p** and *n* sufficient for our results. Theorem B.2 states concentration of  $\mathbb{P}_f$ under the condition  $\tau_3 \mathbf{r} \leq 1$ . Under  $(S_3)$ , we can use  $\tau_3 = c_3 n^{-1/2}$ . Together with  $\mathbf{r} \approx \sqrt{\mathbf{p}}$ , this yields the condition  $\mathbf{p} \ll n$ . Gaussian approximation applies under  $c_3 \nu^{-1} \mathbf{r} \mathbf{p} n^{-1/2} \leq 2$ ; see (B.12), yielding  $\mathbf{p}^3 \ll n$ . We see that there is a gap between these conditions. We guess that in the region  $n^{1/3} \leq \mathbf{p} \leq n$ , non-Gaussian approximation of the posterior is possible; cf. Bochkina and Green (2014).

#### B.3 Tools and proofs

Here we collect the proofs of the main results and some useful technical statements about the error of Laplace approximation. Below we write  $\boldsymbol{x}$  instead of  $\boldsymbol{x}^*$ . After passing to representation (B.2), many results below apply to any  $\boldsymbol{x}$ , not necessarily for  $\boldsymbol{x} = \boldsymbol{x}^*$ . We only use  $\mathsf{D}_G^2 = \mathbb{F} = -\nabla^2 f(\boldsymbol{x})$  and  $\boldsymbol{\omega}$  instead of  $\boldsymbol{\omega}(\boldsymbol{x})$ . Everywhere we assume the local set  $\mathcal{U}$  to be fixed by (B.7). We separately study the integrals over  $\mathcal{U}$  and over its complement. The local error of approximation is measured by

$$\diamondsuit = \diamondsuit(\mathcal{U}) \stackrel{\text{def}}{=} \left| \frac{\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} g(\boldsymbol{u}) d\boldsymbol{u} - \int_{\mathcal{U}} e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} g(\boldsymbol{u}) d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \right|.$$
(B.14)

As a special case with  $g(u) \equiv 1$  we obtain an approximation of the denominator in (B.2). In addition, we have to bound the tail integrals

$$\rho = \rho(\mathcal{U}) \stackrel{\text{def}}{=} \frac{\int \mathbf{I}(\boldsymbol{u} \notin \mathcal{U}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}},$$

$$\rho_{G} = \rho_{G}(\mathcal{U}) \stackrel{\text{def}}{=} \frac{\int \mathbf{I}(\boldsymbol{u} \notin \mathcal{U}) e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}.$$
(B.15)

Everywhere later  $\gamma_G \sim \mathcal{N}(0, \mathsf{D}_G^{-2})$  is a Gaussian element in  $\mathbb{R}^p$ . The analysis will be split into several steps.

#### **B.3.1** Overall error of Laplace approximation

First we show how to seam together the error  $\diamondsuit$  of local approximation and the bounds for the tail integrals  $\rho$  and  $\rho_G$ ; see (B.15). **Proposition B.4.** Suppose that for a function  $g(u) \in [0,1]$  and some  $\diamondsuit, \diamondsuit_g$ 

$$\left|\frac{\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} - \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \diamondsuit,$$
(B.16)

$$\left|\frac{\int_{\mathcal{U}} g(\boldsymbol{u}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} - \int_{\mathcal{U}} g(\boldsymbol{u}) e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \diamondsuit_{g}.$$
 (B.17)

Then with  $\rho$  and  $\rho_G$  from (B.15)

$$\frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}} \leq \frac{1}{1-\rho_G - \Diamond} \frac{\int g(\boldsymbol{u}) e^{-\|\mathbf{D}_G \boldsymbol{u}\|^2/2} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_G \boldsymbol{u}\|^2/2} d\boldsymbol{u}} + \frac{\rho + \Diamond_g}{1-\rho_G - \Diamond}, 
\frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}} \geq \frac{1}{1+\rho + \Diamond} \frac{\int g(\boldsymbol{u}) e^{-\|\mathbf{D}_G \boldsymbol{u}\|^2/2} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_G \boldsymbol{u}\|^2/2} d\boldsymbol{u}} - \frac{\rho_G + \Diamond_g}{1+\rho + \Diamond}.$$
(B.18)

*Proof.* It follows from (B.16)

$$\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} \geq \int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} \geq \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u} - \diamondsuit \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}$$

$$\geq (1 - \diamondsuit - \rho_{G}) \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}, \qquad (B.19)$$

$$\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} \leq \int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} + \rho \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}$$

$$\leq (1 + \diamondsuit + \rho) \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}. \qquad (B.20)$$

Similarly for  $g(\boldsymbol{u}) \geq 0$ 

$$\begin{split} \int g(\boldsymbol{u}) e^{f(\boldsymbol{x};\boldsymbol{u})} \, d\boldsymbol{u} &\geq \int_{\mathcal{U}} g(\boldsymbol{u}) e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} - \diamondsuit_{g} \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} \\ &\geq \int g(\boldsymbol{u}) e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} - (\rho_{G} + \diamondsuit_{g}) \int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u}, \end{split}$$

$$\begin{split} \int g(\boldsymbol{u}) \, \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \, d\boldsymbol{u} &\leq \int_{\mathcal{U}} g(\boldsymbol{u}) \, \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \, d\boldsymbol{u} + \rho \int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} \\ &\leq \int g(\boldsymbol{u}) \, \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} + (\rho + \diamondsuit_{g}) \int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u} \, . \end{split}$$

Putting together all these bounds yields (B.18).

The next corollary is straightforward.

**Corollary B.5.** Let  $\rho_G \leq \rho^*$ ,  $\rho \leq \rho^*$ ; see (B.15). Let also for a function  $g(\boldsymbol{u})$  with  $|g(\boldsymbol{u})| \leq 1$ , (B.16), (B.17) hold with  $\Diamond_g \leq \Diamond$ . If  $\Diamond + \rho^* \leq 1/2$  then

$$\left|\frac{\int g(\boldsymbol{u}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}} - \frac{\int g(\boldsymbol{u}) e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \frac{2(\rho^{*} + \diamondsuit)}{1 - \rho^{*} - \diamondsuit} \leq 4(\rho^{*} + \diamondsuit).$$

#### B.3.2 Lower and upper Gaussian measures

This section introduces the lower and upper Gaussian measure which locally sandwich the measure  $\mathbb{P}_f$  using the decomposition from condition  $(\mathcal{C}_0)$ . Denote  $-\nabla^2 f(\boldsymbol{x}) = \mathsf{D}_G^2$ . Definition (B.8) enables us to bound with  $\omega = \omega(\boldsymbol{x})$ 

$$\frac{1}{2}(\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}-\omega\|\mathsf{D}\boldsymbol{u}\|^{2}) \leq f(\boldsymbol{x};\boldsymbol{u}) \leq \frac{1}{2}(\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}+\omega\|\mathsf{D}\boldsymbol{u}\|^{2})$$

yielding two Gaussian measures which bounds  $\mathbb{P}_f$  locally from above and from below. The next technical result provides sufficient conditions for their contiguity.

**Proposition B.6.** Let  $\omega$  from (B.8) satisfy  $\omega \leq 1/3$ . Then with p from (B.6)

$$\det\left(I + \omega \mathsf{D}_{G}^{-1} \mathsf{D}^{2} \,\mathsf{D}_{G}^{-1}\right) \le \exp(\omega \,\mathsf{p})\,,\tag{B.21}$$

$$\det \left( I - \omega \mathsf{D}_{G}^{-1} \mathsf{D}^{2} \, \mathsf{D}_{G}^{-1} \right)^{-1/2} \le \exp \left\{ 3/2 \log(3/2) \, \omega \, \mathsf{p} \right\}.$$
(B.22)

*Proof.* W.l.o.g. assume that  $\mathsf{D}_G^{-1}\mathsf{D}^2\mathsf{D}_G^{-1}$  is diagonal with eigenvalues  $\lambda_j \in [0,1]$ . As  $-x^{-1}\log(1-x) \leq 3\log(3/2)$  for  $x \in [0,1/3]$ , it holds by (B.8)

$$\log \det \left( I - \omega \, \mathsf{D}_G^{-1} \mathsf{D}^2 \, \mathsf{D}_G^{-1} \right)^{-1} = -\sum_{j=1}^p \log \left( 1 - \omega \lambda_j \right) \le 3 \log(3/2) \sum_{j=1}^p \omega \lambda_j$$
$$= 3 \log(3/2) \, \omega \, \operatorname{tr} \left( \mathsf{D}_G^{-1} \mathsf{D}^2 \, \mathsf{D}_G^{-1} \right) = 3 \log(3/2) \, \omega \, \mathsf{p}$$

yielding (B.22). The proof of (B.21) is similar using  $\log(1+x) \le x$  for  $x \ge 0$ .

# B.3.3 Gaussian moments

The presented bounds involve the Gaussian moments  $\mathbb{E} \| \mathsf{D} \gamma_G \|^k$  for k = 3, 4, 6 and  $\gamma_G \sim \mathcal{N}(0, \mathsf{D}_G^{-2})$ . We make use of the following lemma.

**Lemma B.7.** It holds for  $\gamma_G \sim \mathcal{N}(0, \mathsf{D}_G^{-2})$  and  $\alpha = \|\mathsf{D} \, \mathsf{D}_G^{-2} \mathsf{D}\|$ 

$$\begin{split} & \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^3 \leq (\mathsf{p} + \alpha)^{3/2} \,, \\ & \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^4 \leq (\mathsf{p} + \alpha)^2 \,, \\ & \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^6 \leq (\mathsf{p} + 2\alpha)^3 \,, \\ & \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^8 \leq (\mathsf{p} + 3\alpha)^4 \,. \end{split}$$

*Proof.* Represent  $\|\mathsf{D}\,\boldsymbol{\gamma}_G\|^2 = \|\mathsf{D}\,\mathsf{D}_G^{-1}\boldsymbol{\gamma}\|^2 = \langle \mathbb{B}_G\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle$  with  $\mathbb{B}_G = \mathsf{D}\,\mathsf{D}_G^{-2}\mathsf{D} \leq I_p$  and  $\boldsymbol{\gamma} \sim \mathcal{N}(0, I_p)$ . By Lemma D.1, for m = 1, 2, 3

$$\begin{split} \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^{2m+2} &= \mathbb{E} \big\langle \mathbb{B}_G \boldsymbol{\gamma}, \boldsymbol{\gamma} \big\rangle^{m+1} \le \big\{ \operatorname{tr}(\mathbb{B}_G) + m \, \alpha \big\}^{m+1} = (\mathsf{p} + m \, \alpha)^{m+1}, \\ \mathbb{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^3 \le \mathbb{E}^{3/4} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^4 \le (\mathsf{p} + \alpha)^{3/2} \,. \end{split}$$

and  $\mathbb{E} \| \mathsf{D} \boldsymbol{\gamma}_G \|^3 \leq \mathbb{E}^{3/4} \| \mathsf{D} \boldsymbol{\gamma}_G \|^4 \leq (\mathsf{p} + \alpha)^{3/2}$ .

#### B.3.4Local approximation

This section presents the bounds on the error  $\diamond$  of local approximation (B.14). The first result only uses  $\omega p \leq 2/3$ . More advanced bounds also assume  $(\mathcal{T}_3)$  and  $(\mathcal{T}_4)$  with  $\boldsymbol{\upsilon}=\boldsymbol{x}\,.$  We also present some extensions for the moments of  $\, I\!\!P_f\,.$ 

**Proposition B.8.** Let  $\omega = \omega(\mathbf{x})$  from (B.8) and p from (B.6) satisfy

$$\omega \, \mathbf{p} \le 2/3 \,. \tag{B.23}$$

Then for any function  $g(\mathbf{u})$  with  $|g(\mathbf{u})| \leq 1$ 

$$\left|\frac{\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} g(\boldsymbol{u}) d\boldsymbol{u} - \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} g(\boldsymbol{u}) d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \diamondsuit$$
(B.24)

with

$$\diamondsuit = \diamondsuit_2 = \frac{0.75\,\omega\,\mathsf{p}}{1-\omega}$$

*Proof.* The condition  $\omega \mathbf{p} \leq 2/3$  from (B.23) and bound (B.22) imply

$$\det \left( I - \omega \mathsf{D}_{G}^{-1} \mathsf{D}^{2} \, \mathsf{D}_{G}^{-1} \right)^{-1/2} \le \exp \left\{ 3/2 \log(3/2) \, \omega \, \mathsf{p} \right\} \le 3/2 \,. \tag{B.25}$$

Define for  $t \ge 0$ 

$$\mathcal{R}(t) = \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 + t\delta_{3}(\boldsymbol{x},\boldsymbol{u})} g(\boldsymbol{u}) d\boldsymbol{u}.$$
 (B.26)

Then for  $t \in [0, 1]$  by (B.8)

$$\begin{aligned} \left| \mathcal{R}'(t) \right| &= \left| \int_{\mathcal{U}} \delta_3(\boldsymbol{x}, \boldsymbol{u}) \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2 / 2 + t \delta_3(\boldsymbol{x}, \boldsymbol{u})} g(\boldsymbol{u}) \, d\boldsymbol{u} \right| \\ &\leq \int_{\mathcal{U}} \left| \delta_3(\boldsymbol{x}, \boldsymbol{u}) \right| \mathrm{e}^{-(\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega \|\mathsf{D} \boldsymbol{u}\|^2) / 2} \, d\boldsymbol{u}. \end{aligned} \tag{B.27}$$

Now we make change of variable  $\Gamma \boldsymbol{u}$  to  $\boldsymbol{u}$  with  $\Gamma^2 = \boldsymbol{I} - \omega \mathsf{D}_G^{-1} \mathsf{D}^2 \mathsf{D}_G^{-1}$ . By (B.25) det  $\Gamma^{-1} \leq 3/2$  and also  $\|\Gamma^{-1}\| \leq (1-\omega)^{-1/2}$ . By (B.8) and (B.27)

$$\begin{aligned} \left| \mathcal{R}(1) - \mathcal{R}(0) \right| &\leq \sup_{t \in [0,1]} \left| \mathcal{R}'(t) \right| \leq \frac{\omega}{2} \int_{\mathcal{U}} \| \mathsf{D} \boldsymbol{u} \|^2 \mathrm{e}^{-(\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega \|\mathsf{D} \boldsymbol{u}\|^2)/2} \, d\boldsymbol{u} \\ &\leq \frac{3\omega}{4} \int \| \mathsf{D} \boldsymbol{\Gamma}^{-1} \boldsymbol{u} \|^2 \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \leq \frac{3\omega}{4(1-\omega)} \int \| \mathsf{D} \boldsymbol{u} \|^2 \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \end{aligned}$$

In view of  $\mathbb{E} \| \mathsf{D} \gamma_G \|^2 = \operatorname{tr} \left( \mathsf{D}^2 \, \mathsf{D}_G^{-2} \right)$  for a standard normal  $\gamma$ , we derive

$$\frac{\left|\mathcal{R}(1) - \mathcal{R}(0)\right|}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2}d\boldsymbol{u}} \leq \frac{3\omega}{4(1-\omega)} \frac{\int \|\mathsf{D}\boldsymbol{u}\|^{2} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2}d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2}d\boldsymbol{u}} \leq \frac{3\omega\,\mathsf{p}}{4(1-\omega)}$$

and (B.24) follows.

**Proposition B.9.** Assume  $(\mathcal{T}_3)$  with  $\boldsymbol{v} = \boldsymbol{x}$  and let  $\tau_3 \nu^{-1} r p \leq 2$ . Define  $\omega \stackrel{\text{def}}{=} \tau_3 \nu^{-1} r/3$ . Then bound (B.24) applies with

$$\diamondsuit = \diamondsuit_3 \stackrel{\text{def}}{=} \frac{\tau_3 \mathbb{E} \|\mathsf{D}\boldsymbol{\gamma}_G\|^3}{4(1-\omega)^{3/2}} \le \frac{\tau_3 \,(\mathsf{p}+\alpha)^{3/2}}{4(1-\omega)^{3/2}} \,.$$

*Proof.* The proof follows the same line as for Proposition B.8. Under  $(\mathcal{T}_3)$ , it holds  $|\delta_3(\boldsymbol{x}, \boldsymbol{u})| \leq \tau_3 \|\mathsf{D}\boldsymbol{u}\|^3/6$  for  $\boldsymbol{u} \in \mathcal{U}$  and

$$\begin{aligned} \left| \mathcal{R}(1) - \mathcal{R}(0) \right| &\leq \frac{\tau_3 \det(\Gamma^{-1})}{6} \int \| \mathsf{D} \, \Gamma^{-1} \boldsymbol{u} \|^3 \, \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \\ &\leq \frac{\tau_3}{4(1-\omega)^{3/2}} \int \| \mathsf{D} \boldsymbol{u} \|^3 \, \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \end{aligned} \tag{B.28}$$

yielding the statement in view of  $\mathbb{E} \| \mathsf{D} \gamma_G \|^3 \leq (\mathsf{p} + \alpha)^{3/2}$ ; see Lemma B.7. It remains to note that by Lemma A.1  $\omega \leq \tau_3 \nu^{-1} \mathsf{r} / 3$ . Hence,  $\tau_3 \nu^{-1} \mathsf{r} \, \mathsf{p} \leq 2$  implies  $\omega \mathsf{p} \leq 2/3$ .

The result can be extended to the case of a m-homogeneous function g(u).

**Proposition B.10.** Suppose the conditions of Proposition B.8 and  $(\mathcal{T}_3)$ . Then for  $m \geq 1$  and any *m*-homogeneous function  $g(\cdot)$  with  $g(t\boldsymbol{u}) = t^m g(\boldsymbol{u})$ 

$$\left|\frac{\int_{\mathcal{U}} \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} g(\boldsymbol{u}) \, d\boldsymbol{u} - \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} g(\boldsymbol{u}) \, d\boldsymbol{u}}{\int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \frac{\tau_{3} \mathbb{E}\left\{|g(\boldsymbol{\gamma}_{G})| \|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{3}\right\}}{4(1-\omega)^{(m+3)/2}}.$$
 (B.29)

*Proof.* As in the proof of Proposition B.8, under  $(\mathcal{T}_3)$ , it holds for  $\mathcal{R}(t)$  from (B.26)

$$\begin{aligned} \left| \mathcal{R}(1) - \mathcal{R}(0) \right| &\leq \frac{\tau_3 \det(\Gamma^{-1})}{6} \int \|\mathsf{D} \, \Gamma^{-1} \boldsymbol{u}\|^3 \left| g(\Gamma^{-1} \boldsymbol{u}) \right| \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \\ &\leq \frac{\tau_3}{4(1-\omega)^{(m+3)/2}} \int \|\mathsf{D} \boldsymbol{u}\|^3 \left| g(\boldsymbol{u}) \right| \mathrm{e}^{-\|\mathsf{D}_G \boldsymbol{u}\|^2/2} \, d\boldsymbol{u} \end{aligned}$$

yielding similarly to (B.28)

$$\frac{\left|\mathcal{R}(1) - \mathcal{R}(0)\right|}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2}d\boldsymbol{u}} \leq \frac{\tau_{3}}{4(1-\omega)^{(m+3)/2}} \frac{\int \|\mathsf{D}\boldsymbol{u}\|^{3} \left|g(\boldsymbol{u})\right| e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}.$$

This yields (B.29).

Important special cases correspond to m = 1.

**Proposition B.11.** Suppose the conditions of Proposition B.10. Then it holds for any linear mapping  $Q: \mathbb{R}^p \to \mathbb{R}^q$  and any unit vector  $\mathbf{a} \in \mathbb{R}^q$ 

$$\frac{\left|\int_{\mathcal{U}} \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle \, d\boldsymbol{u} - \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle \, d\boldsymbol{u}\right|}{\int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \, d\boldsymbol{u}} \leq 0.6 \, \tau_{3} \, (\mathsf{p} + \alpha)^{3/2} \, \|Q \, \mathsf{D}_{G}^{-2} Q^{\top}\|^{1/2}. \tag{B.30}$$

Proof. Proposition B.10 yields

$$\frac{\left|\int_{\mathcal{U}} \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \left\langle Q\boldsymbol{u}, \boldsymbol{a} \right\rangle d\boldsymbol{u} - \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \left\langle Q\boldsymbol{u}, \boldsymbol{a} \right\rangle d\boldsymbol{u}\right|}{\int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \leq \frac{\tau_{3} \operatorname{I\!\!E}\left\{\left|\left\langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \right\rangle\right| \|D\boldsymbol{\gamma}_{G}\|^{3}\right\}}{4(1-\omega)^{2}}.$$

By Lemma B.7

$$\begin{split} \mathbf{E} \left\{ |\langle Q \, \boldsymbol{\gamma}_G, \boldsymbol{a} \rangle| \, \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^3 \right\} \\ & \leq \left( \mathbf{E} \| \mathsf{D} \, \boldsymbol{\gamma}_G \|^4 \right)^{3/4} \, \left( \mathbf{E} \langle Q \boldsymbol{\gamma}_G, \boldsymbol{a} \rangle^4 \right)^{1/4} \leq 3^{1/4} \, (\mathsf{p} + \alpha)^{3/2} \sqrt{\boldsymbol{a}^\top Q \, \mathsf{D}_G^{-2} Q^\top \boldsymbol{a}}. \end{split}$$

Here we used that  $\mathbb{E}\langle Q\gamma_G, a\rangle^4 = \mathbb{E}\langle \gamma, \mathsf{D}_G^{-1}Q^{\top}a\rangle^4 = 3(a^{\top}Q \,\mathsf{D}_G^{-2}Q^{\top}a)^2$ . Now (B.30) follows from

$$\sup_{\boldsymbol{a}\in\mathbb{R}^q:\,\|\boldsymbol{a}\|=1}\boldsymbol{a}^\top Q\,\mathsf{D}_G^{-2}Q^\top\boldsymbol{a}=\|Q\,\mathsf{D}_G^{-2}Q^\top\|.$$

and  $3^{1/4}(1-\omega)^{-2} \le 2.4$ .

Now we state a sharper result based on  $(\mathcal{T}_4)$ .

	-	-	

**Proposition B.12.** Suppose the conditions of Proposition B.8 and  $(\mathcal{T}_4)$ . Then for any function  $g(\mathbf{u})$  with  $|g(\mathbf{u})| \leq 1$  and  $g(\mathbf{u}) = g(-\mathbf{u})$ 

$$\left|\frac{\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} g(\boldsymbol{u}) d\boldsymbol{u} - \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} g(\boldsymbol{u}) d\boldsymbol{u}}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}\right| \leq \Diamond_{4}$$
(B.31)

with

$$\begin{split} \diamondsuit_4 \stackrel{\text{def}}{=} \frac{1}{16(1-\omega)^2} \Big\{ \boldsymbol{\mathbb{E}} \langle \nabla^3 f(\boldsymbol{x}), \boldsymbol{\gamma}_G^{\otimes 3} \rangle^2 + 2\tau_4 \boldsymbol{\mathbb{E}} \| \mathsf{D} \boldsymbol{\gamma}_G \|^4 \Big\} \\ &\leq \frac{1}{16(1-\omega)^2} \Big\{ \tau_3^2 \, (\mathsf{p}+2\alpha)^3 + 2\tau_4 (\mathsf{p}+\alpha)^2 \Big\} \,. \end{split} \tag{B.32}$$

If the function  $g(\cdot)$  is not bounded by one but it is symmetric and 2m-homogeneous, i.e.  $g(t\mathbf{u}) = t^{2m}g(\mathbf{u})$ , then (B.31) still applies with

$$\diamond_4 \stackrel{\text{def}}{=} \frac{1}{16(1-\omega)^{2+m}} \mathbb{E}\left\{ \left\langle \nabla^3 f(\boldsymbol{x}), \boldsymbol{\gamma}_G^{\otimes 3} \right\rangle^2 g(\boldsymbol{\gamma}_G) + 2\tau_4 \left\| \mathsf{D}\boldsymbol{\gamma}_G \right\|^4 g(\boldsymbol{\gamma}_G) \right\}.$$
(B.33)

*Proof.* We write  $f^{(3)}$  and  $\delta_k(\boldsymbol{u})$  in place of  $\nabla^3 f(\boldsymbol{x})$  and  $\delta_k(\boldsymbol{x}, \boldsymbol{u})$ , k = 3, 4. It holds

$$\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} g(\boldsymbol{u}) \, d\boldsymbol{u} = \int_{\mathcal{U}} \exp\left\{-\frac{\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}}{2} + \delta_{3}(\boldsymbol{u})\right\} g(\boldsymbol{u}) \, d\boldsymbol{u}.$$

Define for  $t \in [0, 1]$ 

$$\mathcal{R}(t) \stackrel{\text{def}}{=} \int_{\mathcal{U}} \exp\left\{-\frac{\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}}{2} + t\delta_{3}(\boldsymbol{u})\right\} g(\boldsymbol{u}) \, d\boldsymbol{u}.$$

Symmetricity of  $\mathcal{U}$  and  $g(\boldsymbol{u}) = g(-\boldsymbol{u})$  implies that

$$\mathcal{R}'(0) = \frac{1}{2} \int_{\mathcal{U}} \exp\left(-\frac{\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}}{2}\right) \left\{\delta_{3}(\boldsymbol{u}) + \delta_{3}(-\boldsymbol{u})\right\} g(\boldsymbol{u}) \, d\boldsymbol{u}$$
$$= \int_{\mathcal{U}} \exp\left(-\frac{\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}}{2}\right) \overline{\delta}_{4}(\boldsymbol{u}) \, g(\boldsymbol{u}) \, d\boldsymbol{u}$$
(B.34)

with  $\overline{\delta}_4(\boldsymbol{u}) = \{\delta_4(\boldsymbol{u}) + \delta_4(-\boldsymbol{u})\}/2$ . Moreover, as  $|\delta_3(\boldsymbol{u})| \leq \omega \|\mathsf{D}\boldsymbol{u}\|^2/2$ , it holds for  $t \in [0, 1]$ 

$$egin{aligned} |\mathcal{R}''(t)| &\leq \int_{\mathcal{U}} \delta_3^2(oldsymbol{u}) \expigg\{ -rac{\|\mathsf{D}_Goldsymbol{u}\|^2}{2} + t\delta_3(oldsymbol{u})igg\} |g(oldsymbol{u})| \,doldsymbol{u} \ &\leq \int_{\mathcal{U}} \delta_3^2(oldsymbol{u}) \expigg( -rac{\|\mathsf{D}_Goldsymbol{u}\|^2}{2} - \omega\|\mathsf{D}oldsymbol{u}\|^2}{2}igg) \,doldsymbol{u} \,. \end{aligned}$$

As 
$$\delta_3(\boldsymbol{u}) = \langle f^{(3)}, \boldsymbol{u}^{\otimes 3} \rangle / 6 + \delta_4(\boldsymbol{u}) \text{ and } |\delta_4(\boldsymbol{u})| \leq 1$$
, one can bound for  $t \in [0, 1]$   
 $|\mathcal{R}''(t)| \leq 2 \int_{\mathcal{U}} \{\overline{\delta}_4^2(\boldsymbol{u}) + |\langle f^{(3)}, \boldsymbol{u}^{\otimes 3} \rangle / 6|^2\} \exp\left(-\frac{\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega\|\mathsf{D} \boldsymbol{u}\|^2}{2}\right) d\boldsymbol{u}$   
 $\leq 2 \int_{\mathcal{U}} \{|\overline{\delta}_4(\boldsymbol{u})| + \langle f^{(3)}, \boldsymbol{u}^{\otimes 3} \rangle^2 / 36\} \exp\left(-\frac{\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega\|\mathsf{D} \boldsymbol{u}\|^2}{2}\right) d\boldsymbol{u}.$ 

This and (B.34) yield

$$\begin{aligned} \left| \mathcal{R}(1) - \mathcal{R}(0) \right| &\leq \left| \mathcal{R}'(0) \right| + \frac{1}{2} \sup_{t \in [0,1]} \left| \mathcal{R}''(t) \right| \leq 2 \int_{\mathcal{U}} \left| \overline{\delta}_4(\boldsymbol{u}) \right| e^{-(\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega \|\mathsf{D} \boldsymbol{u}\|^2)/2} \, d\boldsymbol{u} \\ &+ \frac{1}{36} \int_{\mathcal{U}} \left\langle f^{(3)}, \boldsymbol{u}^{\otimes 3} \right\rangle^2 e^{-(\|\mathsf{D}_G \boldsymbol{u}\|^2 - \omega \|\mathsf{D} \boldsymbol{u}\|^2)/2} \, d\boldsymbol{u}. \end{aligned}$$

Change of variable  $(I - \omega \mathsf{D}_G^{-1} \mathsf{D}^2 \mathsf{D}_G^{-1})^{1/2} u$  to w yields by (B.25) in view of  $\omega \leq 1/3$ 

$$\begin{split} &\frac{1}{36}\int_{\mathcal{U}} \langle f^{(3)}, \boldsymbol{u}^{\otimes 3} \rangle^2 \exp\Bigl(-\frac{\|\mathsf{D}_{G}\boldsymbol{u}\|^2 - \omega\|\mathsf{D}\boldsymbol{u}\|^2}{2}\Bigr) \, d\boldsymbol{u} \\ &\leq \frac{3/2}{36(1-\omega)^3} \int \langle f^{(3)}, \boldsymbol{w}^{\otimes 3} \rangle^2 \exp\Bigl(-\frac{\|\mathsf{D}_{G}\boldsymbol{w}\|^2}{2}\Bigr) \, d\boldsymbol{w}. \end{split}$$

Similarly by  $(\mathcal{T}_4)$ 

$$\int_{\mathcal{U}} |\overline{\delta}_4(\boldsymbol{u})| \exp\left(-\frac{\|\mathsf{D}_G\boldsymbol{u}\|^2 - \omega\|\mathsf{D}\boldsymbol{u}\|^2}{2}\right) d\boldsymbol{u} \le \frac{3/2}{24(1-\omega)^2} \int \tau_4 \|\mathsf{D}\boldsymbol{w}\|^4 \exp\left(-\frac{\|\mathsf{D}_G\boldsymbol{w}\|^2}{2}\right) d\boldsymbol{w}.$$

The use of  $\omega \leq 1/3$  implies that

$$\frac{\left|\mathcal{R}(1) - \mathcal{R}(0)\right|}{\int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \leq \frac{3/2}{24(1-\omega)^{2}} \Big\{ \mathbb{E} \big\langle f^{(3)}, \boldsymbol{\gamma}_{G}^{\otimes 3} \big\rangle^{2} + 2\tau_{4} \mathbb{E} \|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{4} \Big\} \leq \Diamond_{4}$$

and (B.31) follows. Further,  $(\mathcal{T}_3)$  yields  $\langle \nabla^3 f(\boldsymbol{x}), \boldsymbol{u}^{\otimes 3} \rangle^2 \leq \tau_3^2 \|\mathsf{D}\boldsymbol{u}\|^6$ . Now (B.32) follows from Lemma B.7. The proof of (B.33) is similar.

Again, an important special cases correspond to m = 1 and Laplace covariance approximation.

**Proposition B.13.** Suppose the conditions of Proposition B.12 with  $\omega \leq 1/3$ . Then for any linear mapping  $Q: \mathbb{R}^p \to \mathbb{R}^q$  with  $QQ^{\top} \leq \mathsf{D}^2$  and any unit vector  $\mathbf{a} \in \mathbb{R}^q$ 

$$\frac{\left|\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle^{2} d\boldsymbol{u} - \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle^{2} d\boldsymbol{u}\right|}{\int e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \leq \frac{\|Q\,\mathsf{D}^{-2}Q^{\top}\|}{16(1-\omega)^{3}} \Big\{ 10.25\tau_{3}^{2}\,(\mathsf{p}+3\alpha)^{3}+3.5\tau_{4}(\mathsf{p}+3\alpha)^{2} \Big\} \\ \leq \|Q\,\mathsf{D}^{-2}Q^{\top}\| \Big\{ 3\tau_{3}^{2}\,(\mathsf{p}+3\alpha)^{3}+\tau_{4}(\mathsf{p}+3\alpha)^{2} \Big\}.$$

Proof. By Proposition B.12, it holds

$$\frac{\left|\int_{\mathcal{U}} \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle^{2} d\boldsymbol{u} - \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} \langle Q\boldsymbol{u}, \boldsymbol{a} \rangle^{2} d\boldsymbol{u}\right|}{\int \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \leq \frac{1}{16(1-\omega)^{3}} \mathbb{E}\Big\{\tau_{3}^{2} \|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{6} \langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{2} + 2\tau_{4} \|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{4} \langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{2}\Big\}$$

Now we use that for any unit vector  $\boldsymbol{a} \in \mathbb{R}^q$ , by Lemma B.7

$$\begin{split} \mathbb{E}\left\{ \|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{6} \langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{2} \right\} &\leq \left(\mathbb{E}\|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{8}\right)^{3/4} \mathbb{E}\left(\langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{8}\right)^{1/4} \\ &\leq 10.25(\mathsf{p}+3\alpha)^{3}\|\mathsf{D}_{G}^{-1}Q^{\top}\boldsymbol{a}\|^{2} \leq 10.25(\mathsf{p}+3\alpha)^{3}\|Q\,\mathsf{D}_{G}^{-2}Q^{\top}\|, \\ \mathbb{E}\left\{\|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{4} \langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{2}\right\} \leq \left\{\mathbb{E}\|\mathsf{D}\boldsymbol{\gamma}_{G}\|^{8}\right\}^{1/2} \left\{\mathbb{E}\langle Q\boldsymbol{\gamma}_{G}, \boldsymbol{a} \rangle^{4}\right\}^{1/2} \\ &\leq \sqrt{3}(\mathsf{p}+3\alpha)^{2}\|\mathsf{D}_{G}^{-1}Q^{\top}\boldsymbol{a}\|^{2} \leq \sqrt{3}\,(\mathsf{p}+3\alpha)^{2}\|Q\,\mathsf{D}_{G}^{-2}Q^{\top}\| \end{split}$$

and the result follows.

### B.3.5 Tail integrals

In this section we also write  $\boldsymbol{x}$  in place of  $\boldsymbol{x}^*$ . Below we evaluate  $\rho$  from (B.15) which bounds the integral of  $e^{f(\boldsymbol{x};\boldsymbol{u})}$  over the complement of the local set  $\mathcal{U}$  of a special form  $\mathcal{U} = \{\boldsymbol{u}: \|\mathsf{D}\boldsymbol{u}\| \leq \nu^{-1}\mathbf{r}\}$  for D from  $(\mathcal{C}_0)$ . Our results help to understand how the radius  $\mathbf{r}$  should be fixed to ensure  $\rho$  sufficiently small. The main tools for the analysis are deviation probability bounds for Gaussian quadratic forms; see Section D.2.

**Proposition B.14.** Suppose  $(C_0)$ . Given  $\nu < 1$  and  $\mathbf{x} > 0$ , let  $\mathcal{U}$  and  $\mathbf{r}$  be defined by (B.7). Let also  $\omega$  from (B.8) satisfy  $\omega \leq 1 - \nu$ . Then

$$\frac{\int \mathbf{I}(\boldsymbol{u} \notin \mathcal{U}) e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \le 4e^{-\mathbf{x}-\mathbf{p}/2}, \qquad (B.35)$$

$$\frac{\int \mathbb{I}(\boldsymbol{u} \notin \mathcal{U}) e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}}{\int e^{-\|\mathbf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}} \le e^{-\mathbf{x}-\mathbf{p}/2}.$$
(B.36)

*Proof.* Let  $\boldsymbol{u} \notin \mathcal{U}$ , i.e.  $\|\mathsf{D}\boldsymbol{u}\| > \mathsf{r}$  with  $\mathsf{r} = \nu^{-1}\mathsf{r}$ . Define  $\boldsymbol{u}^c = \mathsf{r}\|\mathsf{D}\boldsymbol{u}\|^{-1}\boldsymbol{u}$  yielding  $\|\mathsf{D}\boldsymbol{u}^c\| = \mathsf{r}$ . We also write  $\boldsymbol{u} = (1+\tau)\boldsymbol{u}^c$  for  $\tau > 0$ . By (B.8) and  $\nabla^2 \ell(0) = -\mathsf{D}^2$ 

$$\ell(\boldsymbol{u}^{c}) - \ell(0) - \left\langle \nabla \ell(0), \boldsymbol{u}^{c} \right\rangle \leq -(1-\omega) \|\mathsf{D}\boldsymbol{u}^{c}\|^{2}/2,$$
  
$$\left\langle \nabla \ell(\boldsymbol{u}^{c}) - \nabla \ell(0), \boldsymbol{u} - \boldsymbol{u}^{c} \right\rangle \leq -(1-\omega) \left\langle \mathsf{D}^{2}\boldsymbol{u}^{c}, \boldsymbol{u} - \boldsymbol{u}^{c} \right\rangle.$$
(B.37)

Concavity of  $\ell(\boldsymbol{u})$  implies for  $\boldsymbol{u} = (1+\tau)\boldsymbol{u}^c$ ,

$$\ell(oldsymbol{u}) \leq \ell(oldsymbol{u}^c) + \left\langle 
abla \ell(oldsymbol{u}^c), oldsymbol{u} - oldsymbol{u}^c 
ight
angle$$

yielding by (B.37) in view of  $\langle \mathsf{D}\boldsymbol{u}^c, \mathsf{D}\boldsymbol{u} \rangle = \|\mathsf{D}\boldsymbol{u}^c\| \|\mathsf{D}\boldsymbol{u}\|$ 

$$\begin{split} \ell(\boldsymbol{u}) - \ell(0) - \left\langle \nabla \ell(0), \boldsymbol{u} \right\rangle &= \ell(\boldsymbol{u}) - \left\langle \nabla \ell(\boldsymbol{u}^c), \boldsymbol{u} - \boldsymbol{u}^c \right\rangle \\ &+ \ell(\boldsymbol{u}^c) - \ell(0) - \left\langle \nabla \ell(0), \boldsymbol{u}^c \right\rangle + \left\langle \nabla \ell(\boldsymbol{u}^c) - \nabla \ell(0), \boldsymbol{u} - \boldsymbol{u}^c \right\rangle \\ &\leq (1 - \omega) \| \mathsf{D} \boldsymbol{u}^c \|^2 / 2 - (1 - \omega) \left\langle \mathsf{D} \boldsymbol{u}^c, \mathsf{D} \boldsymbol{u} \right\rangle \leq -(1 - \omega) \| \mathsf{D} \boldsymbol{u}^c \| \| \mathsf{D} \boldsymbol{u} \| / 2. \end{split}$$

We now use that  $\|\mathsf{D}\boldsymbol{u}^{c}\| = \mathtt{r}$ ,  $\boldsymbol{u}^{c} = \boldsymbol{u}/(1+\tau)$ , and thus,

$$f(\boldsymbol{x} + \boldsymbol{u}) - f(0) - \langle \nabla f(\boldsymbol{x}), \boldsymbol{u} \rangle = \ell(\boldsymbol{u}) - \ell(0) - \langle \nabla \ell(0), \boldsymbol{u} \rangle - \|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 + \|\mathsf{D}\boldsymbol{u}\|^{2}/2$$
  
$$\leq -(1 - \omega)\mathsf{r}\|\mathsf{D}\boldsymbol{u}\|/2 - \|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 + \|\mathsf{D}\boldsymbol{u}\|^{2}/2.$$

This yields by  $\mathbf{r} = \nu \, \mathbf{r} \leq (1 - \omega) \mathbf{r}$  with  $T = \mathsf{D}\mathsf{D}_G^{-1}$ 

$$\begin{split} \frac{\int \mathbb{I} \big( \boldsymbol{u} \notin \mathcal{U} \big) \exp \big\{ f(\boldsymbol{x} + \boldsymbol{u}) - f(\boldsymbol{x}) - \langle \nabla f(\boldsymbol{x}), \boldsymbol{u} \rangle \big\} \, d\boldsymbol{u}}{\int \exp \big( - \|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 \big) \, d\boldsymbol{u}} \\ & \leq \frac{\int \mathbb{I} \big( \|\mathsf{D}\boldsymbol{u}\| > \mathsf{r} \big) \exp \big\{ - (1 - \omega)\mathsf{r} \|\mathsf{D}\boldsymbol{u}\|/2 - \|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 + \|\mathsf{D}\boldsymbol{u}\|^{2}/2 \big\} \, d\boldsymbol{u}}{\int \exp \big( - \|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 \big) \, d\boldsymbol{u}} \\ & \leq \mathbb{E} \exp \big\{ -\mathsf{r} \|T\boldsymbol{\gamma}\|/2 + \|T\boldsymbol{\gamma}\|^{2}/2 \big\} \, \mathbb{I} \big( \|T\boldsymbol{\gamma}\| > \mathsf{r} \big) \end{split}$$

with  $\gamma$  standard normal in  $I\!\!R^p$ . Next, define

Integration by parts allows to represent the last integral as

$$\begin{aligned} \mathscr{R}_{0}(\mathbf{r}) &= -\int_{\mathbf{r}}^{\infty} \exp\left(-\mathbf{r} \, z/2 + z^{2}/2\right) d\mathbb{P}\left(\|T\boldsymbol{\gamma}\| > z\right) \\ &= \mathbb{P}\left(\|T\boldsymbol{\gamma}\| > \mathbf{r}\right) + \int_{\mathbf{r}}^{\infty} (z - \mathbf{r}/2) \exp\left(-\mathbf{r} z/2 + z^{2}/2\right) \mathbb{P}\left(\|T\boldsymbol{\gamma}\| > z\right) dz \end{aligned}$$

By Theorem D.4, for any  $z \ge \sqrt{p}$  for  $\mathbf{p} = \operatorname{tr}(T T^{\top}) = \operatorname{tr}(\mathsf{D}^2 \mathsf{D}_G^{-2})$ 

$$\mathbb{P}(\|T\boldsymbol{\gamma}\| > z) \le \exp\{-(z - \sqrt{p})^2/2\}$$

yielding for  $z \ge \mathbf{r} = 2\sqrt{\mathbf{p}} + \sqrt{2\mathbf{x}}$ 

$$\mathbb{P}(\|T\boldsymbol{\gamma}\| > z) \le \exp\{-(z-\sqrt{p})^2/2\} \le e^{-x-p/2}$$

and for  $r \geq 2\sqrt{p} + \sqrt{2x}$  and  $x \geq 2$ 

$$\begin{aligned} \mathscr{R}_{0}(\mathbf{r}) &\leq \mathrm{e}^{-\mathbf{x}-\mathbf{p}/2} + \int_{\mathbf{r}}^{\infty} (z-\mathbf{r}/2) \exp\left\{-\frac{\mathbf{r}z}{2} + \frac{z^{2}}{2} - \frac{(z-\sqrt{\mathbf{p}})^{2}}{2}\right\} dz \\ &\leq \mathrm{e}^{-\mathbf{x}-\mathbf{p}/2} + \exp\left(-\frac{(\mathbf{r}-\sqrt{\mathbf{p}})^{2}}{2}\right) \int_{0}^{\infty} \left(z+\frac{\mathbf{r}}{2}\right) \exp\left\{-\frac{(\mathbf{r}-2\sqrt{\mathbf{p}})z}{2}\right\} dz \\ &\leq 2\mathrm{e}^{-\mathbf{x}-\mathbf{p}/2}. \end{aligned}$$

This completes the proof of the result (B.35). Statement (B.36) is about Gaussian probability  $\mathbb{P}(||T\gamma|| \ge r)$  for a standard normal element  $\gamma$ , and we derive

$$\mathbb{P}(\|T\boldsymbol{\gamma}\| \ge 2\sqrt{p} + \sqrt{2x}) \le \exp\{-(\sqrt{p} + \sqrt{2x})^2/2\} \le \exp(-x - p/2)$$

and (B.36) follows.

The next result extends (B.35).

Proposition B.15. Assume the conditions of Proposition B.14 with

$$\mathtt{r} \geq 2\sqrt{\mathtt{p}} + \sqrt{2\mathtt{x}} + m$$

for some  $m \ge 0$ . Then (B.35) can be extended to

$$\frac{\int \mathbb{I}(\boldsymbol{u} \notin \mathcal{U}) \, \|\mathsf{D}\boldsymbol{u}\|^m \, \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \, d\boldsymbol{u}}{\int \mathrm{e}^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} \, d\boldsymbol{u}} \leq 4\mathrm{e}^{-\mathtt{x}-\mathtt{p}/2} \, .$$
$$\frac{\int \mathbb{I}(\boldsymbol{u} \notin \mathcal{U}) \, \|\mathsf{D}\boldsymbol{u}\|^m \, \mathrm{e}^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} \, d\boldsymbol{u}}{\int \mathrm{e}^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} \, d\boldsymbol{u}} \leq \mathrm{e}^{-\mathtt{x}-\mathtt{p}/2} \, .$$

*Proof.* The case m > 0 can be proved similarly to m = 0 using  $m \log z \le mz$ .

#### B.3.6 Local concentration

Here we show that the measure  $\mathbb{P}_f$  well concentrates on the local set  $\mathcal{U}$  from (B.7). Again we fix  $\mathbf{x} = \mathbf{x}^*$ .

**Proposition B.16.** Assume  $\omega \leq 1/3$ . Then

$$\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} \ge e^{-\omega p/2} \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}.$$
 (B.38)

Moreover,

$$\frac{\int_{\mathcal{U}^c} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}} \le 4e^{-\mathbf{x} - (1-\omega)\mathbf{p}/2} \le e^{-\mathbf{x}}.$$
(B.39)

Proof. By (B.8)

$$\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} = \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 + \delta_{3}(\boldsymbol{x},\boldsymbol{u})} d\boldsymbol{u} \ge \int_{\mathcal{U}} e^{-\|\mathsf{D}_{G}\boldsymbol{u}\|^{2}/2 - \omega\|\mathsf{D}\boldsymbol{u}\|^{2}/2} d\boldsymbol{u}$$

Change of variable  $\left(I + \omega \mathsf{D}_G^{-1} \mathsf{D}^2 \mathsf{D}_G^{-1}\right)^{1/2} u$  to w yields by (B.21)

$$\begin{split} \int_{\mathcal{U}} \mathrm{e}^{f(\boldsymbol{x};\boldsymbol{u})} \, d\boldsymbol{u} &\geq \mathrm{det} \left( I + \omega \, \mathsf{D}_{G}^{-1} \mathsf{D}^{2} \, \mathsf{D}_{G}^{-1} \right)^{-1/2} \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{w}\|^{2}/2} \, d\boldsymbol{w} \\ &\geq \mathrm{e}^{-\omega \, \mathfrak{p}/2} \int_{\mathcal{U}} \mathrm{e}^{-\|\mathsf{D}_{G}\boldsymbol{w}\|^{2}/2} \, d\boldsymbol{w}, \end{split}$$

and (B.38) follows. This and (B.35), (B.36) of Proposition B.14 imply

$$\frac{\int_{\mathcal{U}^c} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}} = \frac{\int_{\mathcal{U}^c} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}{\int_{\mathcal{U}} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u} + \int_{\mathcal{U}^c} e^{f(\boldsymbol{x};\boldsymbol{u})} d\boldsymbol{u}}$$
$$\leq \frac{4e^{-\mathbf{x}-\mathbf{p}/2} \int e^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} d\boldsymbol{u}}{e^{-\omega\,\mathsf{p}/2} \int_{\mathcal{U}} e^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} d\boldsymbol{u} + 4e^{-\mathbf{x}-\mathbf{p}/2} \int e^{-\|\mathsf{D}_G\boldsymbol{u}\|^2/2} d\boldsymbol{u}} \leq 4e^{-\mathbf{x}-(1-\omega)\mathbf{p}/2}$$

as required in (B.39).

## B.3.7 Finalizing the proof of Theorem B.1 and B.2

These results are proved by compiling the previous technical statements. Proposition B.14 provides some upper bounds for the quantities  $\rho$  and  $\rho_G$ , while Proposition B.8, Proposition B.9, and Proposition B.12 bound the local errors  $\diamondsuit$  and  $\diamondsuit_g$ . The final bound (B.10) follows from Corollary B.5.

# C Examples of priors

This section presents two typical examples of priors and some properties including the bounds for *effective dimension* and *Laplace effective dimension*.

# C.1 Truncation and smooth priors

Below we consider two non-trivial examples of Gaussian priors: truncation and smooth priors. To make the presentation clear, we impose some assumptions on the considered setup. Most of them are non-restrictive and can be extended to more general situations. We assume to be given a growing sequence of nested linear approximation subspaces  $W_1 \subset W_2 \subset \ldots \subset \mathbb{R}^p$  of dimension  $\dim(W_m) = m$ . Below  $\Pi_m$  is the projector on  $W_m$  and  $W_m^c$  is the orthogonal complement of  $W_m$ . A smooth prior is described by a

self-adjoint operator G such that  $||G\boldsymbol{u}||/||\boldsymbol{u}||$  becomes large for  $\boldsymbol{u} \in \boldsymbol{V}_m^c$  and m large. One can write this condition in the form

$$\begin{aligned} \|G\boldsymbol{u}\|^2 &\leq g_m^2 \|\boldsymbol{u}\|^2, \qquad \boldsymbol{u} \in \boldsymbol{\mathbb{V}}_m, \\ \|G\boldsymbol{u}\|^2 &\geq g_m^2 \|\boldsymbol{u}\|^2, \qquad \boldsymbol{u} \in \boldsymbol{\mathbb{V}}_m^c. \end{aligned}$$
(C.1)

Often one assumes that  $\mathbb{W}_m$  is spanned by the eigenvectors of  $G^2$  corresponding to its smallest eigenvalues  $g_1^2 \leq g_2^2 \leq \ldots \leq g_m^2$ . We only need (C.1). A typical example is given by  $G^2 = \operatorname{diag}(g_j^2)$  with  $g_j^2 = w^{-1}j^{2s}$  for s > 1/2 and some window parameter w. Below we refer to this case as (s, w)-smooth prior.

A *m*-truncation prior assumes that the prior distribution is restricted to  $W_m$ . This formally corresponds to a covariance operator  $G_m^{-2}$  with  $G_m^{-2}(I-\Pi_m) = 0$ . Equivalently, we set  $g_{m+1} = g_{m+2} = \ldots = \infty$  in (C.1).

#### C.2 Effective dimension

This section explains how the *effective dimension* and *Laplace effective dimension* can be evaluated for some typical situations.

Let  $\mathbb{F}$  be a generic information matrix while  $G^2$  a penalizing matrix. With  $\mathbb{F}_G \stackrel{\text{def}}{=} \mathbb{F} + G^2$ , define a sub-projector  $P_G$  in  $\mathbb{R}^p$  by

$$P_G \stackrel{\text{def}}{=} \mathbf{F}_G^{-1} \mathbf{F} = (\mathbf{F} + G^2)^{-1} \mathbf{F}.$$
 (C.2)

Also define the Laplace effective dimension

$$\mathbf{p}(G) \stackrel{\text{def}}{=} \operatorname{tr} P_G = \operatorname{tr} \left\{ (\mathbf{I} + G^2)^{-1} \mathbf{I} \right\}$$

The penalizing matrix  $G^2$  will be supposed diagonal,  $G^2 = \text{diag}\{g_1^2, \ldots, g_p^2\}$ . Moreover, we implicitly assume that the values  $g_j^2$  grow with j at some rate, polynomial or exponential, yielding for all  $m \ge 1$ 

$$\sum_{j>m} g_j^{-2} \le C_g \, m \, g_m^{-2} \,. \tag{C.3}$$

Our leading example is given by  $g_j^2 = w^{-1} j^{2s}$  for s > 1/2. Then (C.3) holds with  $C_g = (2s-1)^{-1}$ .

Concerning the matrix  $I\!\!F$ , we assume

$$C_{\mathbb{F}}^{-1} n \|\boldsymbol{u}\|^{2} \leq \langle \mathbb{F}\boldsymbol{u}, \boldsymbol{u} \rangle \leq C_{\mathbb{F}} n \|\boldsymbol{u}\|^{2}, \qquad \boldsymbol{u} \in \mathbb{R}^{p}, \qquad (C.4)$$

for some  $C_F \ge 1$ . It appears that the value p(G) is closely related to the index m for which  $g_m^2 \approx n$ .

$$m = m(G) \stackrel{\text{def}}{=} \min\{j \colon g_j^2 \ge n\}.$$
(C.5)

Then

$$\frac{1}{\mathsf{C}_{\mathbb{F}}+1} \le \frac{\mathsf{p}(G)}{m} \le 1 + \mathsf{C}_{\mathbb{F}}\,\mathsf{C}_g\,.$$

*Proof.* By (C.3)

$$\operatorname{tr}(P_G) \leq \sum_{j \geq 1} \frac{\mathsf{C}_{\mathbb{F}} n}{\mathsf{C}_{\mathbb{F}} n + g_j^2} \leq m + \sum_{j > m} \frac{\mathsf{C}_{\mathbb{F}} n}{\mathsf{C}_{\mathbb{F}} n + g_j^2} \leq m + \mathsf{C}_{\mathbb{F}} n \sum_{j > m} g_j^{-2}$$
$$\leq m + \mathsf{C}_{\mathbb{F}} n \operatorname{C}_g m g_m^{-2} \leq m(1 + \mathsf{C}_{\mathbb{F}} \operatorname{C}_g).$$

Similarly

$$\operatorname{tr}(P_G) \ge \sum_{j=1}^m \frac{\mathsf{C}_{\mathbb{F}}^{-1} n}{\mathsf{C}_{\mathbb{F}}^{-1} n + g_j^2} \ge m \frac{\mathsf{C}_{\mathbb{F}}^{-1} n}{\mathsf{C}_{\mathbb{F}}^{-1} n + g_m^2} \ge m \frac{\mathsf{C}_{\mathbb{F}}^{-1}}{\mathsf{C}_{\mathbb{F}}^{-1} + 1}$$

and the assertion follows.

This result yields an immediate corollary.

**Corollary C.2.** Let  $G_1^2$  and  $G_2^2$  be two different penalizing matrices satisfying (C.3) and such that  $m(G_1) = m(G_2)$ ; see (C.5). Then

$$\frac{\mathsf{p}(G_1)}{\mathsf{p}(G_2)} \le (1 + \mathsf{C}_{\mathbb{F}} \, \mathsf{C}_g)(1 + \mathsf{C}_{\mathbb{F}}).$$

Now we evaluate the effective dimension  $p_G = tr(\mathbb{F}_G^{-1}V^2)$ , where the variance matrix  $V^2$  satisfies the condition

$$\mathbf{C}_{V}^{-1} \| \mathbf{F} \boldsymbol{u} \|^{2} \leq \| V \boldsymbol{u} \|^{2} \leq \mathbf{C}_{V} \| \mathbf{F} \boldsymbol{u} \|^{2}, \qquad \boldsymbol{u} \in \mathbf{\mathbb{R}}^{p}$$
(C.6)

with some constant  $C_V \ge 1$ ; cf. (C.4).

**Lemma C.3.** Assume (C.4) for  $\mathbb{F}$  and (C.6) for  $V^2$ . Let also  $G^2 = \text{diag}\{g_1^2, \ldots, g_p^2\}$ with  $g_j^2$  satisfying (C.3) and let m be given by (C.5). Then  $\mathbf{p}_G = \text{tr}(\mathbb{F}_G^{-1}V^2)$  satisfies

$$\frac{\mathsf{C}_V^{-1}}{\mathsf{C}_F + 1} \le \frac{\mathsf{p}_G}{m} \le \mathsf{C}_V (1 + \mathsf{C}_F \, \mathsf{C}_g) \,.$$

*Proof.* It follows from (C.4) and (C.6) that

$$\operatorname{tr}(\mathbb{C}_{\mathbb{F}}I_p + G^2)^{-1}\mathbb{C}_{\mathbb{F}}\mathbb{C}_V^{-1} \leq \operatorname{tr}(\mathbb{F}_G^{-1}V^2) \leq \operatorname{tr}(\mathbb{C}_{\mathbb{F}}^{-1}I_p + G^2)^{-1}\mathbb{C}_{\mathbb{F}}^{-1}\mathbb{C}_V.$$

Further we may proceed as in the proof of Lemma C.1.

### C.3 Sobolev classes and smooth priors

This section illustrates the introduced notions and results for a typical situation of a (s, w)-smooth prior with  $g_j^2 = w j^{2s}$ .

# C.4 Properties of the sub-projector $P_G$

For the sub-projector  $P_G$  from (C.2), this section analyzes the operator  $I_p - P_G$  which naturally appears in the evaluation of the bias  $\boldsymbol{v}_G^* - \boldsymbol{v}^*$ . It turns out that the main characteristic of  $P_G$  is the index m defined by (C.5). The sub-projector  $P_G$  approximates the projector on the space  $W_m$ . The quality of approximation is controlled by the growth rate of the eigenvalues  $g_j^2$ : the faster is this rate the better is the approximation  $P_G \approx \Pi_m$ . To illustrate this point, we consider the situation with two operators  $I_n - P_G$  and  $I_n - P_{G_0}$  for two different penalizing matrices  $G^2$  and  $G_0^2$  with the same characteristic m. We slightly change the notations and assume that

$$G^2 = w^{-1} \operatorname{diag}\{g_1^2, \dots, g_p^2\}, \qquad G_0^2 = w_0^{-1} \operatorname{diag}\{g_{1,0}^2, \dots, g_{p,0}^2\},$$

with some fixed constants w and  $w_0$  and growing sequences  $(g_i^2)$  and  $(g_{i,0}^2)$  satisfying

$$w^{-1}g_m^2 \approx w_0^{-1}g_{m,0}^2 \approx n.$$
 (C.7)

To simplify the presentation we later assume that these relations in (C.7) are precisely fulfilled. We also assume that

$$g_{j,0}^2/g_{m,0}^2 \le g_j^2/g_m^2, \qquad j \le m,$$
 (C.8)

meaning that  $g_{i,0}^2$  grows faster than  $g_i^2$ .

**Lemma C.4.** Let  $\mathbb{F}$  satisfy (C.4), and let  $G^2$  and  $G_0^2$  be diagonal penalizing matrices satisfying (C.7) and (C.8) for some  $m \leq p$ . Then

$$(I_p - P_G)\Pi_m \leq \mathsf{C}_{\mathbb{F}}^2(I_p - P_{G_0})\Pi_m,$$
$$(\mathsf{C}_{\mathbb{F}} + 1)^{-1}\Pi_m^c \leq (I_p - P_G)\Pi_m^c \leq \Pi_m^c,$$

$$I_p - P_G \le C(I_p - P_{G_0}), \qquad C = C_F^2 \lor (C_F + 1).$$
(C.9)

*Proof.* The definition implies  $I_p - P_G = (I\!\!F + G^2)^{-1}G^2$  and by (C.4)

$$(\mathbb{C}_{\mathbb{F}} n I_p + G^2)^{-1} G^2 \le (\mathbb{F} + G^2)^{-1} G^2 \le (\mathbb{C}_{\mathbb{F}}^{-1} n I_p + G^2)^{-1} G^2$$

Further, for  $j \le m$ , (C.7) and  $g_j^2/g_m^2 \le g_{j,0}^2/g_{m,0}^2$  imply  $w^{-1}g_j^2 \le w_0^{-1}g_{j,0}^2$ , i.e.

$$G^2 \Pi_m \le G_0^2 \Pi_m \,.$$

Therefore,

$$(I_p - P_G)\Pi_m = \mathbb{F}_G^{-1} G^2 \Pi_m \le (\mathbb{C}_{\mathbb{F}}^{-1} n I_p + G^2)^{-1} G^2 \Pi_m$$
$$\le (\mathbb{C}_{\mathbb{F}}^{-1} n I_p + G_0^2)^{-1} G_0^2 \Pi_m \le \mathbb{C}_{\mathbb{F}}^2 (\mathbb{F} + G_0^2)^{-1} G_0^2 \Pi_m.$$

After restricting to the orthogonal complement  $\mathbb{V}_m^c$ , both operators  $I_p - P_G$  and  $I_p - P_{G_0}$ behave nearly as projectors: in view of  $g_j^2 \ge n$  for j > m

$$(\mathbf{C}_{\mathbb{F}}+1)^{-1}\Pi_m^c \le (I_p - P_G)\Pi_m^c \le \Pi_m^c$$

and similarly for  $I_p - P_{G_0}$ .

Finally we evaluate the quantity  $||Q(I - P_G)v||$  assuming  $||G_0v||$  bounded.

**Lemma C.5.** It holds for any  $Q: \mathbb{R}^p \to \mathbb{R}^q$  and any  $G^2$ 

$$\|Q(I-P_G)\boldsymbol{v}\|^2 \le \|Q\mathbb{F}_G^{-1}Q^{\top}\| \|G\boldsymbol{v}\|^2.$$

Moreover, let  $\mathbb{F}$  satisfy (C.4), and let  $G^2$  and  $G_0^2$  be diagonal penalizing matrices satisfying (C.7) and (C.8) for some  $m \leq p$ . Then

$$\|Q(I - P_G)\boldsymbol{v}\| \le C \|Q\mathbb{F}_{G_0}^{-1}Q^{\top}\|^{1/2} \|G_0\boldsymbol{v}\|$$
(C.10)

with C from (C.9).

*Proof.* It holds  $(I - P_G)\boldsymbol{v} = \boldsymbol{\mathbb{F}}_G^{-1}G^2\boldsymbol{v}$  and in view of  $G^2 \leq \boldsymbol{\mathbb{F}}_G$ 

$$\|Q(I - P_G)\boldsymbol{v}\| = \|Q\mathbb{F}_G^{-1}G^2\boldsymbol{v}\| \le \|Q\mathbb{F}_G^{-1/2}\| \|\mathbb{F}_G^{-1/2}G^2\boldsymbol{v}\| \le \|Q\mathbb{F}_G^{-1}Q^{\top}\|^{1/2} \|G\boldsymbol{v}\|.$$

For the second statement, we apply (C.9) of Lemma C.4. As  $\mathbb{F}_G^{-1} G^2 \leq \mathbb{C} \mathbb{F}_{G_0}^{-1} G_0^2$  implies  $\mathbb{F}_{G_0}^{1/2} \mathbb{F}_G^{-1} G^2 \leq \mathbb{C} \mathbb{F}_{G_0}^{-1/2} G_0^2$ , it follows in a similar way

$$\begin{split} \|Q \mathbf{F}_{G}^{-1} G^{2} \boldsymbol{v}\| &\leq \|Q \mathbf{F}_{G_{0}}^{-1/2}\| \, \|\mathbf{F}_{G_{0}}^{1/2} \, \mathbf{F}_{G}^{-1} \, G^{2} \boldsymbol{v}\| \\ &\leq \mathsf{C} \|Q \mathbf{F}_{G_{0}}^{-1/2}\| \, \|\mathbf{F}_{G_{0}}^{-1/2} \, G_{0}^{2} \boldsymbol{v}\| \leq \mathsf{C} \|Q \mathbf{F}_{G_{0}}^{-1/2}\| \, \|G_{0} \boldsymbol{v}\| \end{split}$$

as required.

For the case of  $Q = \mathbb{F}_{G_0}^{1/2}$ , we obtain a corollary of (C.10)

$$\| I\!\! I_{G_0}^{1/2} (I - P_G) v \| \le C \| G_0 v \|_{\mathcal{A}}$$

# D Some results for Gaussian quadratic forms

# D.1 Moments of a Gaussian quadratic form

Let  $\gamma$  be standard normal in  $\mathbb{R}^p$  for  $p \leq \infty$ . Given a self-adjoint trace operator B, consider a quadratic form  $\langle B\gamma, \gamma \rangle$ .

Lemma D.1. It holds

$$E\langle B\gamma, \gamma \rangle = \operatorname{tr} B,$$
  
 $\operatorname{Var}\langle B\gamma, \gamma \rangle = 2 \operatorname{tr} B^2.$ 

Moreover,

$$\begin{split} \boldsymbol{E} (\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle - \operatorname{tr} B)^2 &= 2 \operatorname{tr} B^2, \\ \boldsymbol{E} (\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle - \operatorname{tr} B)^3 &= 8 \operatorname{tr} B^3, \\ \boldsymbol{E} (\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle - \operatorname{tr} B)^4 &= 48 \operatorname{tr} B^4 + 12 (\operatorname{tr} B^2)^2, \end{split}$$

and

$$\begin{split} \mathbf{E} \langle B\gamma, \gamma \rangle^2 &= (\operatorname{tr} B)^2 + 2 \operatorname{tr} B^2, \\ \mathbf{E} \langle B\gamma, \gamma \rangle^3 &= (\operatorname{tr} B)^3 + 6 \operatorname{tr} B \operatorname{tr} B^2 + 8 \operatorname{tr} B^3, \\ \mathbf{E} \langle B\gamma, \gamma \rangle^4 &= (\operatorname{tr} B)^4 + 12 (\operatorname{tr} B)^2 \operatorname{tr} B^2 + 32 (\operatorname{tr} B) \operatorname{tr} B^3 + 48 \operatorname{tr} B^4 + 12 (\operatorname{tr} B^2)^2, \\ \operatorname{Var} \langle B\gamma, \gamma \rangle^2 &= 8 (\operatorname{tr} B)^2 \operatorname{tr} B^2 + 32 (\operatorname{tr} B) \operatorname{tr} B^3 + 48 \operatorname{tr} B^4 + 8 (\operatorname{tr} B^2)^2. \end{split}$$
Moreover, if  $B \leq I_p$  and  $\mathbf{p} = \operatorname{tr} B$ , then  $\operatorname{tr} B^m \leq \mathbf{p} \|B\|^{m-1}$  for  $m \geq 1$  and

$$\begin{split} E \langle B\gamma, \gamma \rangle^2 &\leq p^2 + 2p \|B\| &\leq (p + \|B\|)^2, \\ E \langle B\gamma, \gamma \rangle^3 &\leq p^3 + 6p^2 \|B\| + 8p \|B\|^2 &\leq (p + 2\|B\|)^3, \\ E \langle B\gamma, \gamma \rangle^4 &\leq p^4 + 12p^3 \|B\| + 44p^2 \|B\|^2 + 48p \|B\|^3 &\leq (p + 3\|B\|)^4, \\ Var \langle B\gamma, \gamma \rangle^2 &\leq 8p^3 + 40p^2 \|B\| + 48p \|B\|^2. \end{split}$$

*Proof.* Let  $\chi = \gamma^2 - 1$  for  $\gamma$  standard normal. Then  $\mathbf{E}\chi = 0$ ,  $\mathbf{E}\chi^2 = 2$ ,  $\mathbf{E}\chi^3 = 8$ ,  $\mathbf{E}\chi^4 = 60$ . Without loss of generality assume *B* diagonal:  $B = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_p)$ . Then

$$\xi \stackrel{\text{def}}{=} \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle - \operatorname{tr} B = \sum_{j=1}^{p} \lambda_j (\gamma_j^2 - 1),$$

where  $\gamma_j$  are i.i.d. standard normal. This easily yields

$$\begin{split} \mathbf{E}\xi^{2} &= \sum_{j=1}^{p} \lambda_{j}^{2} \mathbf{E}(\gamma_{j}^{2}-1)^{2} = \mathbf{E}\chi^{2} \operatorname{tr} B^{2} = 2 \operatorname{tr} B^{2}, \\ \mathbf{E}\xi^{3} &= \sum_{j=1}^{p} \lambda_{j}^{3} \mathbf{E}(\gamma_{j}^{2}-1)^{3} = \mathbf{E}\chi^{3} \operatorname{tr} B^{3} = 8 \operatorname{tr} B^{3}, \\ \mathbf{E}\xi^{4} &= \sum_{j=1}^{p} \lambda_{j}^{4}(\gamma_{j}^{2}-1)^{4} + \sum_{i \neq j} \lambda_{i}^{2}\lambda_{j}^{2} \mathbf{E}(\gamma_{i}^{2}-1)^{2} \mathbf{E}(\gamma_{j}^{2}-1)^{2} \\ &= \left(\mathbf{E}\chi^{4} - 3(\mathbf{E}\chi^{2})^{2}\right) \operatorname{tr} B^{4} + 3(\mathbf{E}\chi^{2} \operatorname{tr} B^{2})^{2} = 48 \operatorname{tr} B^{4} + 12(\operatorname{tr} B^{2})^{2}, \end{split}$$

ensuring

$$\begin{split} \mathbf{E} \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle^2 &= \left( \mathbf{E} \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle \right)^2 + \mathbf{E} \xi^2 = (\operatorname{tr} B)^2 + 2 \operatorname{tr} B^2, \\ \mathbf{E} \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle^3 &= \mathbf{E} \left( \xi + \operatorname{tr} B \right)^3 = (\operatorname{tr} B)^3 + \mathbf{E} \xi^3 + 3 \operatorname{tr} B \ \mathbf{E} \xi^2 \\ &= (\operatorname{tr} B)^3 + 6 \operatorname{tr} B \ \operatorname{tr} B^2 + 8 \operatorname{tr} B^3, \end{split}$$

and

$$\begin{aligned} \operatorname{Var} \langle B\gamma, \gamma \rangle^2 &= \mathcal{I\!\!E} \big( \xi + \operatorname{tr} B \big)^4 - \big( \mathcal{I\!\!E} \langle B\gamma, \gamma \rangle \big)^2 \\ &= \big( \operatorname{tr} B \big)^4 + 6 (\operatorname{tr} B)^2 \mathcal{I\!\!E} \xi^2 + 4 \operatorname{tr} B \, \mathcal{I\!\!E} \xi^3 + \mathcal{I\!\!E} \xi^4 - \big( (\operatorname{tr} B)^2 + 2 \operatorname{tr} B^2 \big)^2 \\ &= 8 (\operatorname{tr} B)^2 \operatorname{tr} B^2 + 32 (\operatorname{tr} B) \operatorname{tr} B^3 + 48 \operatorname{tr} B^4 + 8 (\operatorname{tr} B^2)^2. \end{aligned}$$

This implies the results of the lemma.

Now we compute the exponential moments of centered and non-centered quadratic forms.

**Lemma D.2.** Let  $||B||_{op} = \lambda$  and  $\gamma \sim \mathcal{N}(0, I_p)$ . Then for any  $\mu \in (0, \lambda^{-1})$ ,

$$\mathbb{E}\exp\left\{\frac{\mu}{2}(\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle-\boldsymbol{p})\right\} = \det(I-\mu B)^{-1/2}.$$

Moreover, with  $\mathbf{p} = \operatorname{tr} B$  and  $\mathbf{v}^2 = \operatorname{tr} B^2$ 

$$\log \mathbb{E} \exp\left\{\frac{\mu}{2} \left( \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle - \mathbf{p} \right) \right\} \le \frac{\mu^2 \mathbf{v}^2}{4(1 - \lambda \mu)} \,. \tag{D.1}$$

If B is positive semidefinite,  $\lambda_j \ge 0$ , then

$$\log \mathbb{E} \exp\left\{-\frac{\mu}{2} \left(\langle B\gamma, \gamma \rangle - p\right)\right\} \le \frac{\mu^2 \mathbf{v}^2}{4} \,. \tag{D.2}$$

*Proof.* W.l.o.g. assume  $\lambda = 1$ . Let  $\lambda_j$  be the eigenvalues of B,  $|\lambda_j| \leq 1$ . By an orthogonal transform, one can reduce the statement to the case of a diagonal matrix  $B = \operatorname{diag}(\lambda_j)$ . Then  $\langle B \boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle = \sum_{j=1}^p \lambda_j \gamma_j^2$  and by independence of the  $\gamma_j$ 's

$$\mathbb{E}\left\{\frac{\mu}{2}\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle\right\} = \prod_{j=1}^{p} \mathbb{E}\exp\left(\frac{\mu}{2}\lambda_{j}\varepsilon_{j}^{2}\right) = \prod_{j=1}^{p} \frac{1}{\sqrt{1-\mu\lambda_{j}}} = \det\left(I-\mu B\right)^{-1/2}$$

Below we use the simple bound:

$$-\log(1-u) - u = \sum_{k=2}^{\infty} \frac{u^k}{k} \le \frac{u^2}{2} \sum_{k=0}^{\infty} u^k = \frac{u^2}{2(1-u)}, \qquad u \in (0,1),$$
$$-\log(1-u) + u = \sum_{k=2}^{\infty} \frac{u^k}{k} \le \frac{u^2}{2}, \qquad u \in (-1,0).$$

Now it holds

$$\log \mathbb{E}\left\{\frac{\mu}{2}\left(\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle - \mathbf{p}\right)\right\} = \log \det(I - \mu B)^{-1/2} - \frac{\mu \mathbf{p}}{2}$$
$$= -\frac{1}{2}\sum_{j=1}^{p}\left\{\log(1 - \mu\lambda_j) + \mu\lambda_j\right\} \le \sum_{j=1}^{p}\frac{\mu^2\lambda_j^2}{4(1 - \mu)} = \frac{\mu^2\mathbf{v}^2}{4(1 - \mu)}.$$

The last statement can be proved similarly.

Now we consider the case of a non-centered quadratic form  $\langle B\gamma,\gamma\rangle/2 + \langle A,\gamma\rangle$  for a fixed vector A.

**Lemma D.3.** Let  $\lambda_{\max}(B) < 1$ . Then for any A

$$\mathbb{E}\exp\left\{\frac{1}{2}\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle+\langle \boldsymbol{A},\boldsymbol{\gamma}\rangle\right\}=\exp\left\{\frac{\|(\boldsymbol{I}-\boldsymbol{B})^{-1/2}\boldsymbol{A}\|^{2}}{2}\right\}\det(\boldsymbol{I}-\boldsymbol{B})^{-1/2}\boldsymbol{A}$$

Moreover, for any  $\mu \in (0,1)$ 

$$\log \mathbb{E} \exp\left\{\frac{\mu}{2} \left(\langle B\gamma, \gamma \rangle - \mathfrak{p}\right) + \langle A, \gamma \rangle\right\}$$
$$= \frac{\|(I - \mu B)^{-1/2} A\|^2}{2} + \log \det(I - \mu B)^{-1/2} - \mu \mathfrak{p}$$
$$\leq \frac{\|(I - \mu B)^{-1/2} A\|^2}{2} + \frac{\mu^2 \mathfrak{v}^2}{4(1 - \mu)}.$$
(D.3)

*Proof.* Denote  $a = (I - B)^{-1/2} A$ . It holds by change of variables  $(I - B)^{1/2} x = u$  for  $C_p = (2\pi)^{-p/2}$ 

$$\begin{split} \mathbb{E} \exp\left\{\frac{1}{2}\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle + \langle \boldsymbol{A},\boldsymbol{\gamma}\rangle\right\} &= \mathtt{C}_p \int \exp\left\{-\frac{1}{2}\langle (\boldsymbol{I}-\boldsymbol{B})\boldsymbol{x},\boldsymbol{x}\rangle + \langle \boldsymbol{A},\boldsymbol{x}\rangle\right\} d\boldsymbol{x} \\ &= \mathtt{C}_p \det(\boldsymbol{I}-\boldsymbol{B})^{-1/2} \int \exp\left\{-\frac{1}{2}\|\boldsymbol{u}\|^2 + \langle \boldsymbol{a},\boldsymbol{u}\rangle\right\} d\boldsymbol{u} = \det(\boldsymbol{I}-\boldsymbol{B})^{-1/2} e^{\|\boldsymbol{a}\|^2/2}. \end{split}$$

The last inequality (D.3) follows by (D.1).

## D.2 Deviation bounds for Gaussian quadratic forms

The next result explains the concentration effect of  $||Q\boldsymbol{\xi}||^2$  for a centered Gaussian vector  $\boldsymbol{\xi} \sim \mathcal{N}(0, \mathbb{V}^2)$  and a linear operator  $Q \colon \mathbb{R}^p \to \mathbb{R}^q$ ,  $p, q \leq \infty$ . We use a version from Laurent and Massart (2000). For completeness, we present a simple proof of the upper bound.

**Theorem D.4.** Let  $\boldsymbol{\xi} \sim \mathcal{N}(0, \mathbf{V}^2)$  be a Gaussian element in  $\mathbb{R}^p$  and let  $Q: \mathbb{R}^p \to \mathbb{R}^q$ be such that  $B = Q \mathbf{V}^2 Q^\top$  is a trace operator in  $\mathbb{R}^q$ . Then with  $\mathbf{p} = \operatorname{tr}(B)$ ,  $\mathbf{v}^2 = \operatorname{tr}(B^2)$ , and  $\lambda = ||B||$ , it holds for each  $\mathbf{x} \ge 0$ 

$$\mathbb{P}\left(\|Q\boldsymbol{\xi}\|^2 - \mathbf{p} > 2\mathbf{v}\sqrt{\mathbf{x}} + 2\lambda\mathbf{x}\right) \le e^{-\mathbf{x}},\tag{D.4}$$

$$\mathbb{P}\left(\|Q\boldsymbol{\xi}\|^2 - p \le -2v\sqrt{x}\right) \le e^{-x}.$$
 (D.5)

It also implies

$$\mathbb{P}\left(\left|\|Q\boldsymbol{\xi}\|^2 - p\right| > z_2(B, \mathbf{x})\right) \le 2e^{-\mathbf{x}},$$

with

$$z_2(B,\mathbf{x}) \stackrel{\text{def}}{=} 2\mathbf{v}\sqrt{\mathbf{x}} + 2\lambda\mathbf{x}$$

*Proof.* W.l.o.g. assume that  $\lambda = ||B|| = 1$ . We use the identity  $||Q\boldsymbol{\xi}||^2 = \langle B\boldsymbol{\gamma}, \boldsymbol{\gamma} \rangle$  with  $\boldsymbol{\gamma} \sim \mathcal{N}(0, I_q)$ . We apply the exponential Chebyshev inequality: with  $\mu > 0$ 

$$I\!\!P\Big(\langle Bm{\gamma},m{\gamma}
angle-{\tt p}>z_2(B,{\tt x})\Big)\leq I\!\!E\exp\Bigl(rac{\mu}{2}ig(\langle Bm{\gamma},m{\gamma}
angle-{\tt p}ig)-rac{\mu\,z_2(B,{\tt x})}{2}\Bigr)\,.$$

Given x > 0, fix  $\mu < 1$  by the equation

$$\frac{\mu}{1-\mu} = \frac{2\sqrt{\mathbf{x}}}{\mathbf{v}} \quad \text{or} \quad \mu^{-1} = 1 + \frac{\mathbf{v}}{2\sqrt{\mathbf{x}}}.$$
 (D.6)

Let  $\lambda_j$  be the eigenvalues of B,  $|\lambda_j| \leq 1$ . It holds with  $\mathbf{p} = \operatorname{tr} B$  in view of (D.1)

$$\log \mathbb{E}\Big\{\frac{\mu}{2}\big(\langle B\boldsymbol{\gamma},\boldsymbol{\gamma}\rangle-\mathtt{p}\big)\Big\} \leq \frac{\mu^2\mathtt{v}^2}{4(1-\mu)}\,.$$

For (D.4), it remains to check that the choice  $\mu$  by (D.6) yields

$$\frac{\mu^2 \mathbf{v}^2}{4(1-\mu)} - \frac{\mu \, z_2(B, \mathbf{x})}{2} = \frac{\mu^2 \mathbf{v}^2}{4(1-\mu)} - \mu \left( \mathbf{v} \sqrt{\mathbf{x}} + \mathbf{x} \right) = \mu \left( \frac{\mathbf{v} \sqrt{\mathbf{x}}}{2} - \mathbf{v} \sqrt{\mathbf{x}} - \mathbf{x} \right) = -\mathbf{x}.$$

The bound (D.5) is obtained similarly by applying the exponential Chebyshev inequality to  $-\langle B\gamma, \gamma \rangle + p$  with  $\mu = 2v^{-1}\sqrt{x}$ . The use of (D.2) yields

$$\begin{split} I\!\!P\Big(\langle B\gamma,\gamma\rangle - p < -2v\sqrt{x}\Big) &\leq I\!\!E \exp\Big\{\frac{\mu}{2}\big(-\langle B\gamma,\gamma\rangle + p\big) - \mu v\sqrt{x}\Big\} \\ &\leq \exp\Big(\frac{\mu^2 v^2}{4} - \mu v\sqrt{x}\Big) = e^{-x} \end{split}$$

as required.

**Corollary D.5.** Assume the conditions of Theorem D.4. Then for z > v

$$\mathbb{P}\left(\left|\|Q\boldsymbol{\xi}\|^{2}-\mathbf{p}\right| \geq z\right) \leq 2\exp\left\{-\frac{z^{2}}{\left(\mathbf{v}+\sqrt{\mathbf{v}^{2}+2\lambda z}\right)^{2}}\right\} \leq 2\exp\left(-\frac{z^{2}}{4\mathbf{v}^{2}+4\lambda z}\right). \tag{D.7}$$

*Proof.* Given z, define x by  $2v\sqrt{x} + 2\lambda x = z$  or  $2\lambda\sqrt{x} = \sqrt{v^2 + 2\lambda z} - v$ . Then

$$\mathbb{P}\left(\|Q\boldsymbol{\xi}\|^2 - \mathbf{p} \ge z\right) \le e^{-\mathbf{x}} = \exp\left\{-\frac{\left(\sqrt{\mathbf{v}^2 + 2\lambda z} - \mathbf{v}\right)^2}{4\lambda^2}\right\} = \exp\left\{-\frac{z^2}{\left(\mathbf{v} + \sqrt{\mathbf{v}^2 + 2\lambda z}\right)^2}\right\}.$$

This yields (D.7) by direct calculus.

**Corollary D.6.** Assume the conditions of Theorem D.4. If also  $B \ge 0$ , then

$$\mathbb{P}\Big(\|Q\boldsymbol{\xi}\|^2 \ge z^2(B,\mathbf{x})\Big) \le e^{-\mathbf{x}}$$

with

$$z^{2}(B,\mathbf{x}) \stackrel{\text{def}}{=} \mathbf{p} + 2\mathbf{v}\sqrt{\mathbf{x}} + 2\lambda\mathbf{x} \le \left(\sqrt{\mathbf{p}} + \sqrt{2\lambda\mathbf{x}}\right)^{2}$$

Also

$$\mathbb{P}\Big(\|Q\boldsymbol{\xi}\|^2 - p < -2v\sqrt{x}\Big) \le e^{-x}.$$

*Proof.* The definition implies  $v^2 \leq p\lambda$ . One can use a sub-optimal choice of the value  $\mu(\mathbf{x}) = \left\{1 + 2\sqrt{\lambda p/\mathbf{x}}\right\}^{-1}$  yielding the statement of the corollary.

As a special case, we present a bound for the chi-squared distribution corresponding to  $Q = \mathbb{V}^2 = I_p$ ,  $p < \infty$ . Then  $B = I_p$ ,  $\operatorname{tr}(B) = p$ ,  $\operatorname{tr}(B^2) = p$  and  $\lambda(B) = 1$ .

**Corollary D.7.** Let  $\gamma$  be a standard normal vector in  $\mathbb{R}^p$ . Then for any  $\mathbf{x} > 0$ 

$$\begin{split} \mathbb{P}\left(\|\boldsymbol{\gamma}\|^2 \ge p + 2\sqrt{p\,\mathbf{x}} + 2\mathbf{x}\right) &\le e^{-\mathbf{x}}, \\ \mathbb{P}\left(\|\boldsymbol{\gamma}\| \ge \sqrt{p} + \sqrt{2\mathbf{x}}\right) &\le e^{-\mathbf{x}}, \\ \mathbb{P}\left(\|\boldsymbol{\gamma}\|^2 \le p - 2\sqrt{p\,\mathbf{x}}\right) &\le e^{-\mathbf{x}}. \end{split}$$

The bound of Theorem D.4 can be represented as a usual deviation bound.

**Theorem D.8.** Assume the conditions of Theorem D.4. For y > 0, define

$$\mathbf{x}(\mathbf{y}) \stackrel{\text{def}}{=} \frac{(\sqrt{\mathbf{y} + \mathbf{p}} - \sqrt{\mathbf{p}})^2}{4\lambda}$$

Then

$$\mathbb{P}(\|Q\boldsymbol{\xi}\|^2 \ge \mathbf{p} + \mathbf{y}) \le e^{-\mathbf{x}(\mathbf{y})},\tag{D.8}$$

$$\mathbb{E}\left\{ \left( \|Q\boldsymbol{\xi}\|^2 - \mathbf{p} \right) \mathbb{I}\left( \|Q\boldsymbol{\xi}\|^2 \ge \mathbf{p} + \mathbf{y} \right) \right\} \le 2 \left( \frac{\mathbf{y} + \mathbf{p}}{\lambda \, \mathbf{x}(\mathbf{y})} \right)^{1/2} \, \mathrm{e}^{-\mathbf{x}(\mathbf{y})} \,. \tag{D.9}$$

Moreover, let  $\mu>0$  fulfill  $\epsilon=\mu\lambda+\mu\sqrt{\lambda p/x(y)}<1\,.$  Then

$$\mathbb{E}\left\{\mathrm{e}^{\mu(\|Q\boldsymbol{\xi}\|^2-\mathbf{p})/2}\,\mathbb{I}(\|Q\boldsymbol{\xi}\|^2\geq\mathbf{p}+\mathbf{y})\right\}\leq\frac{1}{1-\epsilon}\,\exp\{-(1-\epsilon)\mathbf{x}(\mathbf{y})\}\,.\tag{D.10}$$

*Proof.* Normalizing by  $\lambda$  reduces the statements to the case with  $\lambda = 1$ . Define  $\eta = \|Q\boldsymbol{\xi}\|^2 - p$  and

$$z(\mathbf{x}) = 2\sqrt{\mathbf{p}\,\mathbf{x}} + 2\mathbf{x}.\tag{D.11}$$

Then by (D.4)  $\mathbb{P}(\eta \ge z(\mathbf{x})) \le e^{-\mathbf{x}}$ . Inverting the relation (D.11) yields

$$\mathbf{x}(z) = \frac{1}{4} \big( \sqrt{z + \mathbf{p}} - \sqrt{\mathbf{p}} \big)^2$$

and (D.8) follows by applying z = y. Further,

$$\mathbb{E}\left\{\eta\,\mathrm{I\!I}(\eta\geq\mathrm{y})\right\} = \int_{\mathrm{y}}^{\infty}\mathbb{P}(\eta\geq z)\,dz \leq \int_{\mathrm{y}}^{\infty}\mathrm{e}^{-\mathrm{x}(z)}\,dz = \int_{\mathrm{x}(\mathrm{y})}^{\infty}\mathrm{e}^{-\mathrm{x}}\,z'(\mathrm{x})\,d\mathrm{x}\,.$$

As  $z'(\mathbf{x}) = 2 + \sqrt{\mathbf{p}/\mathbf{x}}$  monotonously decreases with  $\mathbf{x}$ , we derive

$$\mathbb{E}\left\{\eta\,\mathbb{I}(\eta\geq \mathtt{y})\right\} \leq z'(\mathtt{x}(\mathtt{y}))\mathrm{e}^{-\mathtt{x}(\mathtt{y})} = \frac{1}{\mathtt{x}'(\mathtt{y})}\,\mathrm{e}^{-\mathtt{x}(\mathtt{y})} = \frac{4\sqrt{\mathtt{y}+\mathtt{p}}}{\sqrt{\mathtt{y}+\mathtt{p}}-\sqrt{\mathtt{p}}}\,\mathrm{e}^{-\mathtt{x}(\mathtt{y})}$$

and (D.9) follows.

In a similar way, define z(x) from the relation  $\mu^{-1}\log z(x) = \sqrt{p x} + x$  yielding

$$\mathsf{z}(\mathsf{x}) = \exp\bigl(\mu\sqrt{\mathsf{p}\,\mathsf{x}} + \mu\,\mathsf{x}\bigr).$$

The inverse relation reads

$$\mathtt{x}_{e}(\mathtt{z}) = \big(\sqrt{\mu^{-1}\log \mathtt{z} + \mathtt{p}/4} - \sqrt{\mathtt{p}/4}\big)^{2}.$$

Then with  $x(y) = x_e(e^{\mu y/2}) = (\sqrt{y+p} - \sqrt{p})^2/4$ 

$$\begin{split} I\!\!E \big\{ \mathrm{e}^{\mu\eta/2} \ I\!\!\mathrm{I}(\eta \ge \mathbf{y}) \big\} &= \int_{\mathrm{e}^{\mu\mathbf{y}/2}}^{\infty} I\!\!P (\mathrm{e}^{\mu\eta/2} \ge \mathbf{z}) \, d\mathbf{z} = \int_{\mathrm{e}^{\mu\mathbf{y}/2}}^{\infty} I\!\!P (\eta \ge 2\mu^{-1}\log\mathbf{z}) \, d\mathbf{z} \\ &\leq \int_{\mathrm{e}^{\mu\mathbf{y}/2}}^{\infty} \mathrm{e}^{-\mathbf{x}_{\mathrm{e}}(\mathbf{z})} \, d\mathbf{z} = \int_{\mathbf{x}(\mathbf{y})}^{\infty} \mathrm{e}^{-\mathbf{x}} \, \mathbf{z}'(\mathbf{x}) \, d\mathbf{x}. \end{split}$$

Further, in view of  $\mu + 0.5 \,\mu \sqrt{p/x} < \mu + \mu \sqrt{p/x(y)} = \epsilon < 1$  for  $x \ge x(y)$ , it holds

$$\mathsf{z}'(\mathsf{x}) = \left(\mu + 0.5\,\mu\sqrt{\mathsf{p}/\mathsf{x}}\right)\exp\left(\mu\sqrt{\mathsf{p}\,\mathsf{x}} + \mu\,\mathsf{x}\right) \le \exp\left(\mu\,\mathsf{x}\sqrt{\mathsf{p}/\mathsf{x}(\mathsf{y})} + \mu\,\mathsf{x}\right) = \exp(\epsilon\,\mathsf{x})$$

and

$$\mathbb{E}\left\{\mathrm{e}^{\mu\eta/2}\,\mathbb{I}(\eta\geq \mathtt{y})\right\} \leq \int_{\mathtt{x}(\mathtt{y})}^{\infty} \mathrm{e}^{-(1-\epsilon)\mathtt{x}}\,d\mathtt{x} = \frac{1}{1-\epsilon}\,\mathrm{e}^{-(1-\epsilon)\mathtt{x}(\mathtt{y})}$$

and (D.10) follows.

## E Gaussian comparison

This section collects some recent results on Gaussian comparison from Götze et al. (2019). The reader is referred to that paper for an overview on the existing literature on this topic. Throughout this section, the following notation are used. We write  $a \leq b$  ( $a \geq b$ ) if there exists some absolute constant C such that  $a \leq Cb$  ( $a \geq Cb$  resp.). Similarly,  $a \approx b$  means that there exist c, C such that  $ca \leq b \leq Ca$ . We assume that all random variables are defined on common probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and take values in a real separable Hilbert space  $\mathscr{H}$  with a scalar product  $\langle \cdot, \cdot \rangle$  and norm  $\|\cdot\|$ . If dimension of  $\mathscr{H}$  is finite and equals p, we shall write  $\mathbb{R}^p$  instead of  $\mathscr{H}$ . We also denote by  $\mathcal{B}(\mathscr{H})$  the Borel  $\sigma$ -algebra.

For a self-adjoint operator  $\Sigma$  with eigenvalues  $\lambda_k(\Sigma)$ ,  $k \ge 1$ , define its operator norm  $\|\Sigma\|$ , nuclear (Schatten-one) norm  $\|\Sigma\|_1$ , and Frobenius norm  $\|\Sigma\|_{\text{Fr}}$  by

$$\begin{split} \|\Sigma\| \stackrel{\text{def}}{=} \sup_{\|x\|=1} \|\Sigma x\| &= \max_{k \ge 1} |\lambda_k(\Sigma)|, \\ \|\Sigma\|_1 \stackrel{\text{def}}{=} \operatorname{tr} |\Sigma| &= \sum_{k=1}^{\infty} |\lambda_k(\Sigma)|. \\ \|\Sigma\|_{\mathrm{Fr}}^2 \stackrel{\text{def}}{=} \operatorname{tr} \Sigma^2 &= \sum_{k=1}^{\infty} \lambda_k^2(\Sigma). \end{split}$$

We suppose below that  $\Sigma$  is a nuclear and  $\|\Sigma\|_1 < \infty$ .

Let  $\Sigma_{\boldsymbol{\xi}}$  be a covariance operator of an arbitrary Gaussian random element  $\boldsymbol{\xi}$  in  $\mathscr{H}$ . By  $\{\lambda_{k\boldsymbol{\xi}}\}_{k\geq 1}$  we denote the set of its eigenvalues arranged in the non-increasing order, i.e.  $\lambda_{1\boldsymbol{\xi}} \geq \lambda_{2\boldsymbol{\xi}} \geq \ldots$ , and let  $\boldsymbol{\lambda}_{\boldsymbol{\xi}} \stackrel{\text{def}}{=} \operatorname{diag}(\lambda_{j\boldsymbol{\xi}})_{j=1}^{\infty}$ . Note that  $\sum_{j=1}^{\infty} \lambda_{j\boldsymbol{\xi}} < \infty$ . Introduce the following quantities

$$\Lambda_{k\boldsymbol{\xi}}^2 \stackrel{\text{def}}{=} \sum_{j=k}^{\infty} \lambda_{j\boldsymbol{\xi}}^2, \quad k = 1, 2,$$

and

$$\varkappa(\Sigma_{\boldsymbol{\xi}}) = \begin{cases} \Lambda_{1\boldsymbol{\xi}}^{-1}, & \text{if } 3\lambda_{1,\boldsymbol{\xi}}^{2} \leq \Lambda_{1\boldsymbol{\xi}}^{2}, \\ (\lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{-1/2}, & \text{if } 3\lambda_{1\boldsymbol{\xi}}^{2} > \Lambda_{1\boldsymbol{\xi}}^{2}, \ 3\lambda_{2\boldsymbol{\xi}}^{2} \leq \Lambda_{2\boldsymbol{\xi}}^{2}, \\ (\lambda_{1\boldsymbol{\xi}}\lambda_{2\boldsymbol{\xi}})^{-1/2}, & \text{if } 3\lambda_{1\boldsymbol{\xi}}^{2} > \Lambda_{1\boldsymbol{\xi}}^{2}, \ 3\lambda_{2\boldsymbol{\xi}}^{2} > \Lambda_{2\boldsymbol{\xi}}^{2}. \end{cases}$$
(E.1)

It is easy to see that  $\|\Sigma_{\boldsymbol{\xi}}\|_{\mathrm{Fr}} = \Lambda_{1\boldsymbol{\xi}}$ . Moreover, it is straightforward to check that

$$\frac{0.9}{(\Lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{1/2}} \le \varkappa(\Sigma_{\boldsymbol{\xi}}) \le \frac{1.8}{(\Lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{1/2}}.$$
(E.2)

Hence,  $\varkappa(\Sigma_{\xi}) \asymp (\Lambda_{1\xi}\Lambda_{2\xi})^{-1/2}$  and therefore equivalent results can be formulated in terms of any of the quantities introduced. The following theorem is the main result of Götze et al. (2019).

**Theorem E.1.** Let  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$  be Gaussian elements in  $\mathscr{H}$  with zero mean and covariance operators  $\Sigma_{\boldsymbol{\xi}}$  and  $\Sigma_{\boldsymbol{\eta}}$  respectively. For any  $\boldsymbol{a} \in \mathscr{H}$ 

$$\sup_{x>0} |\mathcal{P}(\|\boldsymbol{\xi} - \boldsymbol{a}\| \le x) - \mathcal{P}(\|\boldsymbol{\eta}\| \le x)|$$
  
$$\lesssim \Big\{ \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\xi}}) + \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\eta}}) \Big\} \Big( \|\boldsymbol{\lambda}_{\boldsymbol{\xi}} - \boldsymbol{\lambda}_{\boldsymbol{\eta}}\|_{1} + \|\boldsymbol{a}\|^{2} \Big).$$
(E.3)

We see that the obtained bounds are expressed in terms of the specific characteristics of the matrices  $\Sigma_{\boldsymbol{\xi}}$  and  $\Sigma_{\boldsymbol{\eta}}$  such as their operator and the Frobenius norms rather than the dimension p. Another nice feature of the obtained bounds is that they do not involve the inverse of  $\Sigma_{\boldsymbol{\xi}}$  or  $\Sigma_{\boldsymbol{\eta}}$ . In other words, small or vanishing eigenvalues of  $\Sigma_{\boldsymbol{\xi}}$  or  $\Sigma_{\boldsymbol{\eta}}$ do not affect the obtained bounds in the contrary to the Pinsker bound. Similarly, only the squared norm  $\|\boldsymbol{a}\|^2$  of the shift  $\boldsymbol{a}$  shows up in the results, while the Pinsker bound involves  $\|\Sigma_{\boldsymbol{\xi}}^{-1/2}\boldsymbol{a}\|$  which can be very large or infinite if  $\Sigma_{\boldsymbol{\xi}}$  is not well conditioned.

Let us consider  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  in the first factor on the r.h.s of (E.3):  $\varkappa(\Sigma_{\boldsymbol{\xi}}) + \varkappa(\Sigma_{\boldsymbol{\eta}})$ . The representation (E.1) mimics well the three typical situations: in the "large-dimensional case" with three or more significant eigenvalues  $\lambda_{j\boldsymbol{\xi}}$ , one can take  $\varkappa(\Sigma_{\boldsymbol{\xi}}) = \|\Sigma_{\boldsymbol{\xi}}\|_{\mathrm{Fr}}^{-1} = \lambda_{1\boldsymbol{\xi}}^{-1}$ . In the "two dimensional" case, when the sum  $\Lambda_{k\boldsymbol{\xi}}^2$  is of the order  $\lambda_{k\boldsymbol{\xi}}^2$  for k = 1, 2, we have that  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  behaves as the product  $(\lambda_{1\boldsymbol{\xi}}\lambda_{2\boldsymbol{\xi}})^{-1/2}$ . In the intermediate case of a spike model with one large eigenvalue  $\lambda_{1\boldsymbol{\xi}}$  and many small eigenvalues  $\lambda_{j\boldsymbol{\xi}}, j \geq 2$ , we have that  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  behaves as  $(\lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{-1/2}$ .

As mentioned earlier (see (E.2)), the result of Theorem E.1 may be equivalently formulated in a "unified" way in terms of  $(\Lambda_{1\xi}\Lambda_{2\xi})^{-1/2}$  and  $(\Lambda_{1\eta}\Lambda_{2\eta})^{-1/2}$ . Moreover, we specify the bound (E.3) in the "high-dimensional" case,  $3\|\Sigma_{\xi}\|^2 \leq \|\Sigma_{\xi}\|_{\mathrm{Fr}}^2, 3\|\Sigma_{\eta}\|^2 \leq \|\Sigma_{\eta}\|_{\mathrm{Fr}}^2$ , which means at least three significantly positive eigenvalues of the matrices  $\Sigma_{\xi}$  and  $\Sigma_{\eta}$ . In this case  $\Lambda_{2\xi}^2 \geq 2\Lambda_{1\xi}^2/3, \Lambda_{2\eta}^2 \geq 2\Lambda_{1\eta}^2/3$  and we get the following corollary.

**Corollary E.2.** Let  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$  be Gaussian elements in  $\mathscr{H}$  with zero mean and covariance operators  $\Sigma_{\boldsymbol{\xi}}$  and  $\Sigma_{\boldsymbol{\eta}}$  respectively. Then for any  $\boldsymbol{a} \in \mathscr{H}$ 

$$\begin{split} \sup_{x>0} |\mathcal{P}(\|\boldsymbol{\xi} - \boldsymbol{a}\| \leq x) - \mathcal{P}(\|\boldsymbol{\eta}\| \leq x)| \\ \lesssim \bigg( \frac{1}{(\Lambda_1 \boldsymbol{\xi} \Lambda_2 \boldsymbol{\xi})^{1/2}} + \frac{1}{(\Lambda_1 \boldsymbol{\eta} \Lambda_2 \boldsymbol{\eta})^{1/2}} \bigg) \bigg( \|\boldsymbol{\lambda}_{\boldsymbol{\xi}} - \boldsymbol{\lambda}_{\boldsymbol{\eta}}\|_1 + \|\boldsymbol{a}\|^2 \bigg). \end{split}$$

By the Weilandt–Hoffman inequality,  $\|\lambda_{\xi} - \lambda_{\eta}\|_{1} \leq \|\Sigma_{\xi} - \Sigma_{\eta}\|_{1}$ , see e.g. Markus (1964). This yields the bound in terms of the nuclear norm of the difference  $\Sigma_{\xi} - \Sigma_{\eta}$ , which may be more useful in a number of applications.

**Corollary E.3.** Let  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$  be Gaussian elements in  $\mathscr{H}$  with zero mean and covariance operators  $\Sigma_{\boldsymbol{\xi}}$  and  $\Sigma_{\boldsymbol{\eta}}$  respectively. Moreover, assume that

$$3\|\Sigma_{\boldsymbol{\xi}}\|^2 \le \|\Sigma_{\boldsymbol{\xi}}\|_{\mathrm{Fr}}^2 \quad and \quad 3\|\Sigma_{\boldsymbol{\eta}}\|^2 \le \|\Sigma_{\boldsymbol{\eta}}\|_{\mathrm{Fr}}^2.$$

Then for any  $a \in \mathscr{H}$ 

$$\begin{split} \sup_{x>0} |\mathcal{P}(\|\boldsymbol{\xi} - \boldsymbol{a}\| \leq x) - \mathcal{P}(\|\boldsymbol{\eta}\| \leq x)| \\ \lesssim \left(\frac{1}{\|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}\|_{\mathrm{Fr}}} + \frac{1}{\|\boldsymbol{\Sigma}_{\boldsymbol{\eta}}\|_{\mathrm{Fr}}}\right) \left(\|\boldsymbol{\Sigma}_{\boldsymbol{\xi}} - \boldsymbol{\Sigma}_{\boldsymbol{\eta}}\|_{1} + \|\boldsymbol{a}\|^{2}\right). \end{split}$$

Since the right-hand-side of (E.3) does not change if we exchange  $\boldsymbol{\xi}$  and  $\boldsymbol{\eta}$ , Theorem E.1 and its Corollaries hold for the balls with the same shift  $\boldsymbol{a}$ . In particular, the following corollary is true.

## Corollary E.4. Under conditions of Theorem E.1 we have

$$\sup_{x>0} \left| \mathcal{P}(\|\boldsymbol{\xi} - \boldsymbol{a}\| \le x) - \mathcal{P}(\|\boldsymbol{\eta} - \boldsymbol{a}\| \le x) \right| \lesssim \left\{ \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\xi}}) + \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\eta}}) \right\} \left( \|\boldsymbol{\lambda}_{\boldsymbol{\xi}} - \boldsymbol{\lambda}_{\boldsymbol{\eta}}\|_{1} + \|\boldsymbol{a}\|^{2} \right).$$

The result of Theorem E.1 may be also rewritten in terms of the operator norm

$$\|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1/2}\boldsymbol{\Sigma}_{\boldsymbol{\eta}}\boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1/2}-\boldsymbol{I}\|.$$

Indeed, the inequality  $\|\Sigma_{\boldsymbol{\xi}}\Sigma_{\boldsymbol{\eta}}\|_1 \leq \|\Sigma_{\boldsymbol{\xi}}\|_1 \|\Sigma_{\boldsymbol{\eta}}\|$  yields the following corollary.

Corollary E.5. Under conditions of Theorem E.1 we have

$$\begin{split} \sup_{x>0} |\mathcal{P}(\|\boldsymbol{\xi} - \boldsymbol{a}\| \le x) - \mathcal{P}(\|\boldsymbol{\eta}\| \le x)| \\ \lesssim \Big\{ \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\xi}}) + \varkappa(\boldsymbol{\Sigma}_{\boldsymbol{\eta}}) \Big\} \Big( \operatorname{tr} \big(\boldsymbol{\Sigma}_{\boldsymbol{\xi}}\big) \|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1/2} \boldsymbol{\Sigma}_{\boldsymbol{\eta}} \boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1/2} - I\| + \|\boldsymbol{a}\|^2 \Big) \end{split}$$

We now discuss the origin of the value  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  which appears in the main theorem and its corollaries. Analysing the proof of Theorem E.1 one may find out that it is necessary to get an upper bound for a probability density function (p.d.f.)  $p_{\boldsymbol{\xi}}(x)$  (resp.  $p_{\boldsymbol{\eta}}(x)$ ) of  $\|\boldsymbol{\xi}\|^2$  (resp.  $\|\boldsymbol{\eta}\|^2$ ) and the more general p.d.f.  $p_{\boldsymbol{\xi}}(x, \boldsymbol{a})$  of  $\|\boldsymbol{\xi} - \boldsymbol{a}\|^2$  for all  $\boldsymbol{a} \in \mathscr{H}$ . The same arguments remain true for  $p_{\boldsymbol{\eta}}(x)$ . The following theorem provides uniform bounds. **Theorem E.6.** Let  $\boldsymbol{\xi}$  be a Gaussian element in  $\mathscr{H}$  with zero mean and covariance operator  $\Sigma_{\boldsymbol{\xi}}$ . Then it holds for any  $\boldsymbol{a}$  that

$$\sup_{x \ge 0} p_{\boldsymbol{\xi}}(x, \boldsymbol{a}) \lesssim \varkappa(\Sigma_{\boldsymbol{\xi}}) \tag{E.4}$$

with  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  from (E.1). In particular,  $\varkappa(\Sigma_{\boldsymbol{\xi}}) \lesssim (\Lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{-1/2}$ .

Since  $\boldsymbol{\xi} \stackrel{\mathrm{d}}{=} \sum_{j=1}^{\infty} \sqrt{\lambda_{j\boldsymbol{\xi}}} Z_j \boldsymbol{e}_{j\boldsymbol{\xi}}$ , we obtain that  $\|\boldsymbol{\xi}\|^2 \stackrel{\mathrm{d}}{=} \sum_{j=1}^{\infty} \lambda_{j\boldsymbol{\xi}} Z_j^2$ . Here and in what follows  $\{\boldsymbol{e}_{j\boldsymbol{\xi}}\}_{j=1}^{\infty}$  is the orthonormal basis formed by the eigenvectors of  $\Sigma_{\boldsymbol{\xi}}$  corresponding to  $\{\lambda_{j\boldsymbol{\xi}}\}_{j=1}^{\infty}$ . In the case  $\mathscr{H} = \mathbb{R}^p$ ,  $\boldsymbol{a} = 0, \Sigma_{\boldsymbol{\xi}} \asymp I$  one has that the distribution of  $\|\boldsymbol{\xi}\|^2$  is close to standard  $\chi^2$  with p degrees of freedom and

$$\sup_{x \ge 0} p_{\boldsymbol{\xi}}(x,0) \asymp p^{-1/2}$$

Hence, the bound (E.4) gives the right dependence on p because  $\varkappa(\Sigma_{\boldsymbol{\xi}}) \asymp p^{-1/2}$ . However, a lower bound for  $\sup_{x\geq 0} p_{\boldsymbol{\xi}}(x, \boldsymbol{a})$  in the general case is still an open question.

A direct corollary of Theorem E.6 is the following theorem which states for a rather general situation a dimension-free anti-concentration inequality for the squared norm of a Gaussian element  $\boldsymbol{\xi}$ . In the "high dimensional situation", this anti-concentration bound only involves the Frobenius norm of  $\Sigma_{\boldsymbol{\xi}}$ .

**Theorem E.7** ( $\varepsilon$ -band of the squared norm of a Gaussian element). Let  $\boldsymbol{\xi}$  be a Gaussian element in  $\mathscr{H}$  with zero mean and a covariance operator  $\Sigma_{\boldsymbol{\xi}}$ . Then for arbitrary  $\varepsilon > 0$ , one has

$$\sup_{x>0} \mathbb{P}(x < \|\boldsymbol{\xi} - \boldsymbol{a}\|^2 < x + \varepsilon) \lesssim \varkappa(\Sigma_{\boldsymbol{\xi}}) \varepsilon$$

with  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  from (E.1). In particular,  $\varkappa(\Sigma_{\boldsymbol{\xi}})$  can be replaced by  $(\Lambda_{1\boldsymbol{\xi}}\Lambda_{2\boldsymbol{\xi}})^{-1/2}$ .

## References

- Bartlett, P. L., Long, P. M., Lugosi, G., and Tsigler, A. (2020). Benign overfitting in linear regression. *Proceedings of the National Academy of Sciences*, 117(48):30063– 30070.
- Bickel, P. J., Klaassen, C. A., Ritov, Y., and Wellner, J. A. (1993). Efficient and adaptive estimation for semiparametric models, volume 4. Springer, New York.

- Bickel, P. J. and Kleijn, B. J. K. (2012). The semiparametric Bernstein-von Mises theorem. Ann. Statist., 40(1):206–237.
- Bochkina, N. A. and Green, P. J. (2014). The Bernstein–von Mises theorem and nonregular models. Ann. Statist., 42(5):1850–1878.
- Castillo, I. (2012). A semiparametric Bernstein–von Mises theorem for Gaussian process priors. *Probability Theory and Related Fields*, 152:53–99. 10.1007/s00440-010-0316-5.
- Castillo, I. and Rousseau, J. (2015). A Bernstein–von Mises theorem for smooth functionals in semiparametric models. Ann. Statist., 43(6):2353–2383.
- Cheng, C. and Montanari, A. (2022). Dimension free ridge regression. https://arxiv.org/abs/2210.08571.
- Ghosal, S. and van der Vaart, A. (2017). Fundamentals of nonparametric Bayesian inference, volume 44 of Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge University Press, Cambridge.
- Götze, F., Naumov, A., Spokoiny, V., and Ulyanov, V. (2019). Large ball probabilities, gaussian comparison and anti-concentration. *Bernoulli*, 25(4A):2538–2563. arXiv:1708.08663.
- Helin, T. and Kretschmann, R. (2022). Non-asymptotic error estimates for the laplace approximation in bayesian inverse problems. *Numerische Mathematik*, 150(2).
- Hoffmann, M. and Reiss, M. (2008). Nonlinear estimation for linear inverse problems with error in the operator. *Ann. Statist.*, 36(1):310–336.
- Kasprzak, M. J., Giordano, R., and Broderick, T. (2022). How good is your gaussian approximation of the posterior? finite-sample computable error bounds for a variety of useful divergences. https://arxiv.org/abs/2209.14992.
- Katsevich, A. and Rigollet, P. (2023). On the approximation accuracy of gaussian variational inference.
- Knapik, B. T., Szabó, B. T., van der Vaart, A. W., and van Zanten, J. H. (2016). Bayes procedures for adaptive inference in inverse problems for the white noise model. *Probab. Theory Related Fields*, 164(3-4):771–813.
- Knapik, B. T., van der Vaart, A. W., and van Zanten, J. H. (2011). Bayesian inverse problems with Gaussian priors. Ann. Statist., 39(5):2626–2657.

- Laurent, B. and Massart, P. (2000). Adaptive estimation of a quadratic functional by model selection. Ann. Statist., 28(5):1302–1338.
- L'Huillier, A., Travis, L., Castillo, I., and Ray, K. (2023). Semiparametric inference using fractional posteriors.
- Markus, A. S. (1964). The eigen- and singular values of the sum and product of linear operators. *Russian Mathematical Surveys*, 19(4):91–120.
- Nesterov, Y. E. (1988). Polynomial methods in the linear and quadratic programming. Sov. J. Comput. Syst. Sci., 26(5):98–101.
- Nickl, R. (2022). Bayesian non-linear statistical inverse problems. *Lecture Notes ETH Zurich*.
- Schillings, C., Sprungk, B., and Wacker, P. (2020). On the convergence of the Laplace approximation and noise-level-robustness of Laplace-based Monte Carlo methods for Bayesian inverse problems. *Numerische Mathematik*, 145:915–971.
- Spokoiny, V. (2022). Finite samples inference and critical dimension for stochastically linear models. https://arxiv.org/2201.06327.
- Spokoiny, V. (2023). Dimension free non-asymptotic bounds on the accuracy of high dimensional Laplace approximation. SIAM J. of Uncertainty Quantification. in print, https://arxiv.org/abs/2204.11038.
- Spokoiny, V. and Panov, M. (2021). Accuracy of Gaussian approximation for highdimensional posterior distributions. *Bernoulli*. in print. arXiv:1910.06028.
- Trabs, M. (2018). Bayesian inverse problems with unknown operators. *Inverse Problems*, 34(8):085001.