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**Theoretical and algorithmic advances in
multi-parametric optimization and control**

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Declaration of Originality

I herewith certify that all material in this dissertation which is not my own work has been properly acknowledged.

Richard Oberdieck

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Abstract

This thesis discusses recent advances in a variety of areas in multi-parametric programming and explicit model predictive control (MPC). First, novel theoretical and algorithmic results for multi-parametric quadratic and mixed-integer quadratic programming (mp-QP/mp-MIQP) problems extend the current state-of-the-art: for mp-QP problems, it is shown that its solution is given by a connected graph, based on which a novel solution procedure is developed. Furthermore, several computational studies investigate the performance of different mp-QP algorithms, and a new parallelization strategy is presented, together with an application of mp-QP algorithms to multi-objective optimization. For mp-MIQP problems, it is shown that it is possible to obtain the exact solution of a mp-MIQP problem without resorting to the use of envelopes of solutions, whose computational performance is compared in a computational study with different mp-MIQP algorithms. Then, the concept of robust counterparts in robust explicit MPC for discrete-time linear systems is revisited and an elegant reformulation enables the solution of closed-loop robust explicit MPC problems with a series of projection operations. This approach is extended to hybrid systems, where the same properties are proven to hold. Finally, a new approach towards unbounded and binary parameters in multi-parametric programming is introduced, and several examples highlight its potential.

Contents

1	Introduction	15
1.1	A historical perspective	15
1.2	A mathematical perspective	16
1.3	Current developments in multi-parametric programming and control	17
1.3.1	Theory and Algorithms - Where do we stand?	17
1.3.2	Applications - Where do we stand?	19
1.3.3	Software - Where do we stand?	20
1.4	Objectives and outline of this thesis	20
2	Theoretical Background	22
2.1	Notation	22
2.1.1	Nomenclature	22
2.2	Polytopes	23
2.2.1	Approaches for the removal of redundant constraints	24
2.2.2	Projections	26
2.2.3	Modelling of the union of polytopes	27
3	Contributions to multi-parametric quadratic programming	29
3.1	Introduction	29
3.2	Theoretical and algorithmic background for mp-QP problems	30
3.2.1	Theoretical Properties	31
3.2.2	Degeneracy	33
3.2.3	Solution algorithms for mp-LP and mp-QP problems	35
3.3	The connected graph approach for mp-QP problems	39
3.3.1	A motivating example	39
3.3.2	The solution of a mp-QP problem is a connected graph	40
3.3.3	Step 0: Initialization	43
3.3.4	Step 1: Feasibility	43

3.3.5	Step 2: Parametric solution	44
3.3.6	Step 3: Generation of new candidates	44
3.3.7	The example problem revisited	45
3.3.8	Comparison with the work by Ahmadi-Moshkenani <i>et al.</i>	46
3.4	Computational aspects of mp-QP problems	48
3.4.1	Computational performance of mp-QP algorithms on test sets	48
3.4.2	Computational performance of mp-QP algorithms for a combined heat and power system	50
3.4.3	Computational performance of mp-QP algorithms for a periodic chromatographic separation system	52
3.4.4	Discussion and qualitative heuristics	53
3.4.5	Parallel multi-parametric quadratic programming	56
3.5	Multi-objective optimization with convex quadratic cost functions as a new application for mp-QP problems	62
3.5.1	Multi-objective optimization <i>via</i> multi-parametric programming	64
3.5.2	Numerical Examples	67
3.5.3	Application to linear scalarization	68
3.5.4	Discussion and applicability	69

4 Contributions to multi-parametric mixed-integer quadratic programming problems 70

4.1	Introduction	70
4.2	Theoretical and algorithmic background for mp-MIQP problems	71
4.2.1	Theoretical Properties	71
4.2.2	Solution algorithms for mp-MIQP problems	72
4.2.3	The decomposition algorithm	75
4.3	On the reduction of solutions per envelope of solutions in mp-MIQP problems	77
4.4	Solution Strategy for the Exact Solution of mp-MIQP Problems	79
4.4.1	Initialization	79
4.4.2	Step 1 - Candidate Solution for Binary Variables	80
4.4.3	Step 2 - Creation of an Affine Outer Approximation	81
4.4.4	Step 3 - Solution of the mp-QP Problem	81
4.4.5	Step 4 - Comparison with Upper Bound	82
4.4.6	Step 5 - Creation of Affine Relaxations	82
4.4.7	Step 6 - Recovery of CR_i from Ξ_i	83
4.4.8	Termination	83

4.4.9	Application to the Branch-And-Bound Algorithm	83
4.5	Implementation of the algorithm	85
4.6	Numerical Examples	86
4.6.1	Example problem	86
4.6.2	The computational impact of the comparison procedure	89
4.6.3	Discussion	90
5	Robust explicit/multi-parametric model predictive control	92
5.1	Introduction	92
5.1.1	Notation	93
5.2	Background on Model Predictive Control (MPC)	93
5.2.1	Nominal Systems	94
5.2.2	Robust Systems	95
5.3	Inner approximations of robust admissible sets <i>via</i> projections	99
5.3.1	P as a polytope	99
5.3.2	P as a union of polytopes	99
5.3.3	Recursion of RAS	100
5.3.4	Robust control invariance	101
5.4	Robust Model Predictive Control	101
5.4.1	The continuous case	102
5.4.2	The hybrid case	103
5.4.3	Discussion and implications	103
5.5	Example problem	106
5.5.1	Detailed discussion	108
6	Unbounded and binary parameters in multi-parametric programming	111
6.1	Introduction	111
6.2	Theoretical Background	112
6.3	Unbounded multi-parametric programming	112
6.3.1	Motivating example	112
6.3.2	The solution of unbounded mp-LP and mp-QP problems	113
6.3.3	Numerical Example	115
6.4	Multi-parametric programming with binary parameters	116
6.4.1	The solution of problem (6.1)	117
6.4.2	Numerical Example	118
6.5	A generalized combinatorial algorithm	119
6.5.1	Numerical examples	121

7	Conclusions and Future Work	129
7.1	Conclusions	129
7.2	Future Directions	130
7.3	Publications resulting from this thesis	132
7.3.1	Full-length papers	132
7.3.2	Book chapters	133
7.3.3	Short notes	134
7.3.4	Conference papers	134
A	The POP toolbox	161
A.1	Problem solution	161
A.1.1	Solution of mp-QP problems	161
A.1.2	Solution of mp-MIQP problems	162
A.1.3	Requirements and Validation	162
A.1.4	Handling of equality constraints	162
A.2	Problem generation	163
A.3	Problem library	164
A.3.1	Merits and shortcomings of the problem library	165
A.4	Graphical User Interface (GUI)	166
B	PAROC - an Integrated Framework and Software Platform for the Opti- mization and Advanced Model-Based Control of Process Systems	168
B.1	High-Fidelity Modeling and Analysis	168
B.2	Model Approximation	169
B.3	Multi-parametric Programming	170
B.4	Multi-parametric Moving Horizon Policies	170
B.5	Software Implementation and Closed-loop Validation	171
B.5.1	Multi-parametric Programming Software	171
B.5.2	Integration of PAROC in gPROMS® ModelBuilder	171

List of Figures

- 1.1 The main developments in multi-parametric programming (mp-P). 18
- 2.1 The schematic depiction of the notions of (a) disjoint, (b) overlapping and (c) adjacent polytopes. 23
- 2.2 The schematic depiction of the notions of (a) weakly and (b) strongly redundant constraints. 25
- 3.1 Primal and dual degeneracy in linear programming. In (a), primal degeneracy occurs since there are three constraints which are active at the solution, while in (b) dual degeneracy occurs since there is more than one point (x_1, x_2) which features the optimal objective function value. 35
- 3.2 A graphical representation of the geometrical solution procedure of exploring the parameter space based on the step-size approach. Starting from an initial point $\theta_0 \in \Theta$, in (a) the first critical region CR_0 is calculated (shown with dashed lines). In (b), a facet of CR_0 is identified and a step orthogonal to that facet is taken to identify a new point $\theta_1 \notin CR_0$, while in (c) the new critical region associated with θ_1 is identified, and the remaining facet from CR_0 is identified combined with the orthogonal step from it to identify a new point. 37
- 3.3 A graphical representation of the combinatorial approach for the solution of mp-QP problems. All candidate active sets are exhaustively enumerated based on their cardinality. The computational tractability arises from the ability to discard active sets if infeasibility is detected for a candidate active set which is a subset of the currently considered candidate. 38

3.4	The solution to the example problem (3.14) from (a) a geometrical perspective and (b) from a combinatorial perspective. Note that all light gray points in (b) are checked for feasibility, and those which are crossed out did not fulfill the LICQ criterion. Additionally, note that the last layer misses the points which are fathomed based on Lemma 1, and that the black points show the optimal active set.	42
3.5	The new approach from the combinatorial perspective, where the solid lines represent connections between the nodes while the dashed lines represent attempted connections. At each iteration, all combinations are generated based on Theorem 3 and one step of the dual simplex algorithm.	46
3.6	The results of the computational study for (a) the 'POP_mpLP1' test set and (b) the 'POP_mpQP1' test set.	49
3.7	The analysis of the computational effort spent on different aspects of the algorithm for the geometrical, combinatorial and connected graph algorithm for the test set 'POP_mpLP1'.	49
3.8	The analysis of the computational effort spent on different aspects of the algorithm for the geometrical, combinatorial and connected graph algorithm for the test set 'POP_mpQP1'.	50
3.9	The computational results for the solution of the controller for the CHP system described in eq. (3.17). In (a) the performance of the different solution algorithms is shown as a function of time, while in (b) the distribution of the computational load as a function of the horizon for the case of the connected graph algorithm is shown.	51
3.10	The computational results for the optimal control of a periodic chromatographic separation system. In (a) the computational time using the combinatorial algorithm for different control and output horizons is shown while (b) presents the percentage of problems solved as a function of time required. The different problems result from the consideration of different output and control horizons.	54
3.11	The solution approach for problem (3.1) presented in [14]. Note that $\mathcal{H}(CR)$ denotes the half-spaces defining critical region CR , and that the part highlighted in gray is executed in parallel.	57
3.12	A schematic depiction of the influence of the ρ_{limit} parameter.	59
3.13	The key problem statistics for the randomly generated test set: (a) the number of variables, (b) the number of parameters and (c) the number of constraints for each test problem.	59

3.14	The numerical results for the speedup of the computation by using parallel computing. In (a), the computational benefits as a function of the number of cores is shown while in (b) the dependence on the number of iterations performed on a single thread is investigated. In (c) the computational benefits obtained when using parallel computing are shown for the multi-parametric model predictive control of a combined heat and power system.	61
3.15	The solution of the example problem. Note that the partitioning of the parameter space has been zoomed into, in order to show the details of the partitioning, which are not visible when considering the entire space with $\epsilon_2 = [-1180, 1180]$ and $\epsilon_3 = [-375, 375]$	68
4.1	A graphical representation of the decomposition algorithm. The algorithm starts with an upper bound, from where a critical region is selected. After obtaining a new candidate integer solution, the solution of the corresponding mp-QP problem yields a new solution for the given critical region. This solution is then compared with the upper bound and an updated, tighter upper bound results.	73
4.2	A graphical representation of the branch-and-bound algorithm. The algorithm starts from the root node, where all binary variables are relaxed. Subsequently, at each node a binary variable is fixed, the resulting mp-QP problem is solved and the solution is compared to a previously established upper bound to produce an updated, tighter upper bound and to fathom any part of the parameter space which is suboptimal.	74
4.3	The partitioning of the parameter space into critical regions of the example problem.	89
4.4	The computational results for the solution of a test set problems 'POP_mpMIQP1' for the different comparison procedures.	90
4.5	The computational requirements for each aspect of the algorithm for the different comparison procedures.	91
5.1	A schematic representation of a (a) polytopic and (b) box-constrained uncertainty set. The key difference lies in the ability to implicitly describe maximum of the box using a halfspace representation; this is not possible for the general polytopic case.	97

5.2	The controllability set of the nominal system \mathcal{X}_{nom} , the corresponding robust control invariant set Φ and the trajectories of 300 different simulations of 50 steps with different disturbance profiles starting from $[9.8, -5]$ is shown in (a) for the system with only continuous inputs and in (b) for the system featuring continuous and binary inputs.	107
5.3	The explicit solution of the (a) nominal and (b) robust MPC controller for the example problem.	108
5.4	The comparison of the exact robust control invariant set with the inner approximation of the same set obtained <i>via</i> robust optimization.	109
6.1	The feasible space of problem (6.2) in the (x, θ) domain.	113
6.2	A graphical visualization of the unbounded solution, as the bounds of the parameter space are increased from (a) to (b) to (c)	115
6.3	A schematic representation of a situation with one binary and one continuous variable. On the left we consider the problem where the binary variable is treated as a continuous variable $[0, 1]$ and on the right we show the equivalent binary representation.	117
6.4	A graphical visualization of the solution featuring binary parameters. In (a) we show the solution where the parameter is relaxed between 0 and 1 while (b) shows the same solution when θ_2 is treated as a binary variable.	119
6.5	Graphical representation of the lower level mp-MILP with binary parameters. Clockwise from top left the binary parameters are: $\{0, 0\}$, $\{0, 1\}$, $\{1, 0\}$, $\{1, 1\}$.124	
A.1	The problem statistics of the test sets 'POP_mpLP1' and 'POP_mpQP1'. . .	165
A.2	The problem statistics of the test sets 'POP_mpMILP1' and 'POP_mpMIQP1'.165	
A.3	The structure of the graphical user interface (GUI) of POP.	167
B.1	The PAROC framework.	169

List of Tables

3.1	The parametric solution of problem (3.14).	41
3.2	The problem class and corresponding independent element of several classes of multi-parametric programming algorithms	62
3.3	Results from the computational study in seconds of section 3.5.2, where N is the number of objective functions and m the total number of constraints. . .	68
4.1	The exact solution of the example problem.	89
6.1	The solution to problem (6.6). The notation CR_n corresponds to the n^{th} critical region or Figure 6.2.	116
6.2	The solution to problem (6.9).	118
6.3	Parametric solution of the lower level mp-MILP with binary parameters. . .	127
6.4	Reduced parametric solution of the lower level mp-MILP with binary parameters.	128

List of Abbreviations

General

LP	Linear programming
MILP	Mixed-integer linear programming
MINLP	Mixed-integer nonlinear programming
MIQP	Mixed-integer quadratic programming
MPC	Model predictive control
MHE	Moving horizon estimation
NLP	Nonlinear programming
QCQP	Quadratically constrained quadratic programming
QP	Quadratic programming
RAS	Robust admissible set

Problem classes in multi-parametric programming

mp-DO	Multi-parametric dynamic optimization
mp-DP	Multi-parametric dynamic programming
mp-LCP	Multi-parametric linear complementarity problem
mp-LP	Multi-parametric linear programming
mp-MILP	Multi-parametric mixed-integer linear programming
mp-MINLP	Multi-parametric mixed-integer nonlinear programming
mp-MIQP	Multi-parametric mixed-integer quadratic programming
mp-MOO	Multi-parametric multi-objective optimization
mp-MPC/eMPC	Multi-parametric/explicit model predictive control
mp-QCQP	Multi-parametric quadratically constrained quadratic programming
mp-NLP	Multi-parametric nonlinear programming
mp-P	Multi-parametric programming
mp-QP	Multi-parametric quadratic programming

Chapter 1

Introduction

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- Oberdieck, R.; Diangelakis, N.A.; Papathanasiou, M.M.; Nascu, I.; Pistikopoulos, E.N. (2016) POP - Parametric Optimization Toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979-8991.

1.1 A historical perspective

How does the solution of an optimization problem depend on the variation of parameters in the problem formulation? The first consideration of this question can be traced back to 1952. In an unpublished master thesis, William Orchard-Hays considered the solution of a parametric¹ linear programming problem, where he studied how the variation of the right hand side of a linear programming (LP) problem affects the change of its optimal basis [89]. In parallel, Harry Markowitz published his groundbreaking paper "Portfolio selection", where he states that a portfolio should be chosen such that it maximizes the expected return while it minimizes risk [173]. Although considered only conceptually, his problem is a parametric quadratic programming problem, as he himself discussed in 1956 [174]. These beginnings led to the first publication on parametric linear programming in 1953 by Alan Manne [171],

¹In general, the term "parametric" refers to the case where a single parameter is considered, while "multi-parametric" suggests the presence of multiple parameters.

and the development of the field of parametric programming and post-optimal analysis².

Due to computational limitations, virtually all papers published between the 1950s and the mid-1990s considered the single parameter case, i.e. how the change of a single parameter in the optimization problem impacts the optimal solution of the problem. A notable exception to this is the work by Gal and Nedoma, who in 1972 published the first general algorithm for the solution of multi-parametric linear programming (mp-LP) problems [91], i.e. LP problems featuring multiple, independent variations in the coefficients of the objective function and/or the constraints. The interested reader is referred to the excellent monographs by Gal [90] and Bank *et al.* [13] for a more in-depth treatment of these developments.

With the increased availability of computing power and commercial optimization software, the solution of multi-parametric programming problems suddenly became computationally tractable. This led to a string of publications, starting in 1997, which combined the algorithm of Gal and Nedoma with suitable integer programming techniques to develop algorithms for multi-parametric integer and mixed-integer problems [2, 3, 56–59, 72]. In 2000, this renewed interest in multi-parametric programming was brought to new heights, when it was discovered that model predictive control (MPC) problems of continuous discrete-time systems could be formulated as multi-parametric quadratic programming (mp-QP) problems [28, 29, 217]. The solution of the mp-QP problem was achieved by applying the Basic Sensitivity Theorem, developed in 1976 by Anthony Fiacco [83], in combination with a suitable geometric exploration strategy of the parameter space. This applicability led to a surge in interest, as many control problems could be solved explicitly (and thus offline) using multi-parametric programming (see [7, 213, 220] and references therein), a concept which was captured in the term "MPC-on-a-chip", i.e. the idea that MPC controllers could be delivered and implemented on a simple chip [71, 215].

1.2 A mathematical perspective

In multi-parametric programming, a constrained optimization problem is solved for a range and as a function of certain parameters. This solution is obtained based on the following statement:

Given the solution to a continuous constrained optimization problem (x^*, λ^*, μ^*) , there exists a ball of radius ϵ for which the solution features the same active constraints,

²Post-optimal analysis refers to the analysis of the solution of an optimization problem.

where x^* are the optimal values of the optimization variables (the primal solution), while λ^* and μ^* are the optimal values of the Lagrangian multipliers of the inequality and equality constraints, respectively (the dual solution). This statement is the basis of the Basic Sensitivity Theorem [83], which proves that there exists a linear approximation of the solution of the optimization problem around (x^*, λ^*, μ^*) such that the error is bounded. For the specific case of affine constraints and linear or convex quadratic cost functions, this approximation is the exact solution, i.e. the optimization variables are affine functions of the parameters [220]. However, since in different parts of the parameter space, different constraints will be active, it is intuitively clear that the solution to a multi-parametric programming problem will be given by two components:

Critical regions: A critical region CR describes the set of parameters, for which the obtained parametric solution is optimal.

Parametric solution: The parametric solution describes how the optimal solution of an optimization problem changes as a function of the parameter θ , i.e. $(x(\theta), \lambda(\theta), \mu(\theta))$. This solution often differs between critical regions.

Thus, the following general description of the solution of multi-parametric programming problems is stated:

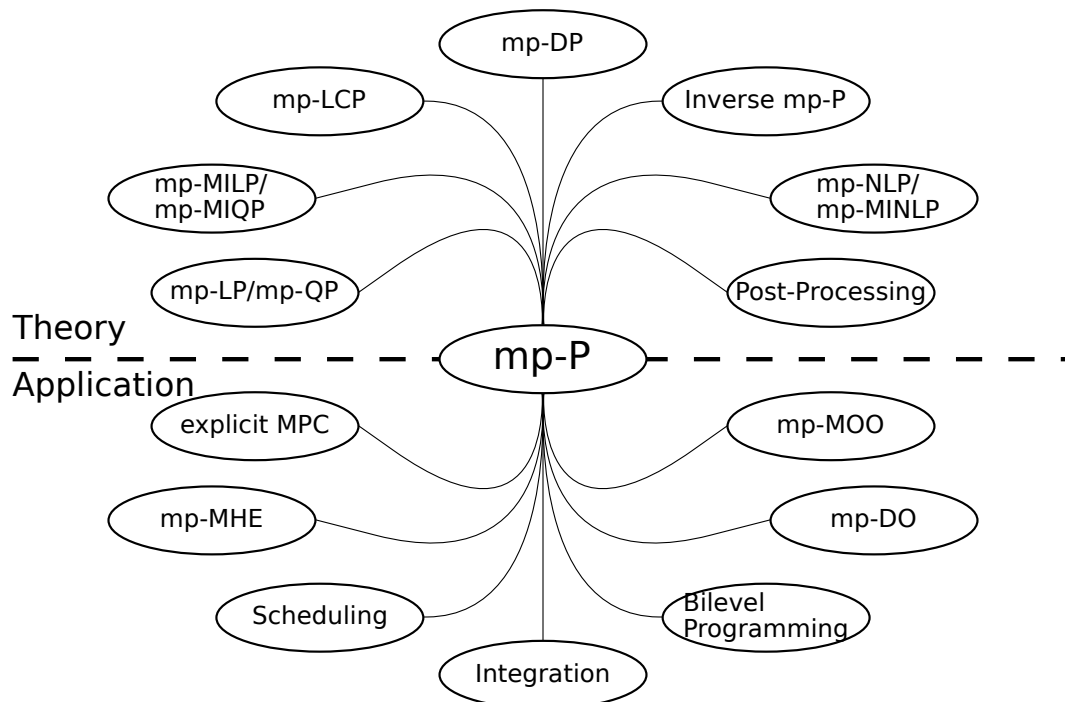
$$\theta \in CR_i \Rightarrow (x_i(\theta), \lambda_i(\theta), \mu_i(\theta)) \text{ is the optimal solution.}$$

1.3 Current developments in multi-parametric programming and control

Due to its applicability, multi-parametric programming has attracted great interest from the control and process systems engineering communities. In this section, the current state-of-the-art is highlighted in terms of theoretical/algorithmic advances and applications using multi-parametric programming are discussed (see Figure 1.1 for a summary).

1.3.1 Theory and Algorithms - Where do we stand?

Over the last 10 years, most efforts have been put into devising novel algorithms which exploit different characteristics of multi-parametric programming problems. For the case of mp-QP problems, Gupta *et al.* showed that it is possible to design a combinatorial branch-and-bound approach, based on the enumeration of active sets [110]. Similarly, Faísca *et al.* designed a new class of multi-parametric dynamic programming algorithms which avoids the



Theory		Application	
mp-LP/mp-QP	[14, 31, 74, 90, 91, 110, 244, 252]	Explicit MPC	[11, 18, 30–32, 43, 100–102, 104, 105, 127, 129, 148, 214, 217, 220, 238]
mp-MILP/mp-MIQP	[2, 11, 15, 27, 60, 73, 74, 113, 124, 163, 261, 263]	mp-MHE	[62, 151, 159, 189, 192, 256–258]
mp-LCP	[4, 53, 120, 130, 166]	Scheduling	[146, 164–166, 216, 232, 234, 242, 262, 267]
mp-DP	[15, 17, 43, 79, 229, 230]	Integration	[144, 207, 216, 220, 267]
Inverse mp-P	[12, 109, 116, 117, 135, 188, 195, 196, 198]	Bilevel programming	[67, 76–78, 138, 218, 233]
mp-NLP/mp-MINLP	[1, 50, 68, 72, 75, 85, 86, 99, 102, 106, 107, 125]	mp-DO	[236, 239, 248]
Post-Processing	[16, 19, 20, 41, 52, 61, 88, 94, 103, 119, 121, 126, 128, 132, 153, 155–157, 245, 251]	mp-MOO	[26, 51, 95, 231, 264]

Figure 1.1: The main developments in multi-parametric programming (mp-P).

comparison procedure at each stage required by previous approaches [79]. In addition, several authors considered the solution of multi-parametric nonlinear programming problems, such as Domínguez and Pistikopoulos [68], and Grancharova and co-workers [106, 107]. Other researchers also considered the question of inverse multi-parametric programming, i.e. the reconstruction of the multi-parametric optimization problem when the optimal solution is given, e.g. Hempel *et al.* [116, 117] and Olaru and co-workers [109, 197, 198].

Furthermore, the storage requirements of the parametric solution becomes prohibitive for larger problems due to the increase in the number of critical regions. Thus, strategies on how to reduce the complexity of the solution of multi-parametric programming problems have been studied, mainly by Kvasnica and co-workers [121, 122, 153, 156, 157]. In addition, the task of locating the correct critical region given a certain parameter value, called point location, has been studied, e.g. by Bayat *et al.* [19, 20] and Morari and co-workers [52, 87, 119].

1.3.2 Applications - Where do we stand?

Most of the papers that have appeared in the last 10 years in relation to multi-parametric programming problems present applications of its capabilities to other classes of problems. Although the quantity of papers has decreased, the most important area of application by far is still explicit MPC, where applications to areas such as energy systems [21, 63, 65, 114, 123, 146, 268], transportation [38, 162, 172, 204, 266], and heating, ventilating and air conditioning systems [69, 143, 210, 235], have clearly shown the capabilities of multi-parametric programming. Using an equivalent state-space representation, multi-parametric programming has also been applied to several scheduling problems [146, 164, 165, 234, 262]. In addition, many researchers have considered multi-parametric programming for robust MPC problems, such as Morari and co-workers [18, 32, 39, 222, 226] and Pistikopoulos and co-workers [49, 148, 237].

Remark 1. Note that in most cases explicit MPC has only been applied to simulated systems. However, several researchers have in fact exported their solution to real chips and proven the concept on experimental setups, e.g. [21, 114, 123, 178, 204, 235, 268]. The most impressive of these is arguably the work by Doyle and co-workers, who employed explicit MPC to design an aspect of an artificial pancreas and have recently began one of the largest ever long-term clinical trials [70].

However, there have also been developments beyond explicit MPC, which mainly exploit the fact that multi-parametric programming yields the optimal solution of an optimization problem as an explicit function over a range of parameters. This enables tasks such as

integration of design, scheduling and control, where the design and scheduling variables of the system are treated as parameters in the explicit MPC problem [216, 220]. Additionally, multi-parametric programming provides an elegant solution approach of bi-level optimization problems, as the lower level problem is solved explicitly as a function of the upper level variables [66, 67, 76, 78, 138]. Other areas of interest are multi-parametric moving horizon estimation [62, 190, 259] and multi-objective optimization *via* multi-parametric programming [25, 208, 231].

1.3.3 Software - Where do we stand?

Despite the applicability of multi-parametric programming, prior to the release of the POP toolbox (see Appendix A) only one software tool was available for the solution of multi-parametric programming problems: the Multi-Parametric Toolbox (MPT). This tool, developed jointly by groups at ETH Zurich and the Slovak University of Technology in Bratislava, enables the solution of multi-parametric linear and quadratic programming problems, performing linear algebraic geometry and set operations as well as the design of explicit MPC problems for linear discrete-time systems [118, 154, 158]. In addition, it is linked to the modelling tool YALMIP [169], which employs a tailor-made symbolic notation for dynamic systems. This link also features a solution strategy for multi-parametric mixed-integer linear and quadratic programming problems *via* dynamic programming and exhaustive enumeration.

1.4 Objectives and outline of this thesis

Despite these developments over the last 10 years, several challenges have remained and were set as the main objectives of this thesis:

- The solution of mp-LP and mp-QP problems can be obtained either *via* a geometrical or combinatorial approach. However, these two solution strategies are not linked to each other and explore fundamentally different properties of the problem formulation. Is it possible to bring these approaches together and show the link between them?
- The solution of mp-MIQP problems features so-called envelopes of solutions, where more than one parametric solution is stored in each critical region. This is necessary, as the quadratic nature of the objective function would lead to quadratically constrained critical regions, if an exact solution was considered. Is it possible to design an algorithm which solves mp-MIQP problems exactly and without resorting to envelopes of solutions?

- Is it possible to contribute towards the increased integration between robust optimization techniques in robust MPC, and can multi-parametric programming be used to do it?
- It is standard practice to assume the parameters in multi-parametric programming to be continuous and bounded. Is it possible to develop algorithms for the solution of unbounded or binary parameters?

Inspired by these open questions, this thesis discusses recent theoretical and algorithmic advances in multi-parametric programming and control. After some basic notation information and background on polytopes is provided in Chapter 2, Chapter 3 extends the results of Gal and Nedoma [91] to the case of mp-QP problems, which leads to the development of an efficient mp-QP solver. In Chapter 4, new advances for multi-parametric mixed-integer quadratic programming (mp-MIQP) problems are shown, as an algorithm is presented which enables the exact solution of such problems, resulting in quadratically constrained critical regions. In Chapter 5, the work of Kouramas *et al.* [148] on robust explicit MPC is revisited, and it is shown that it leads to a paradigm for the application of robust optimization to robust model predictive control for discrete-time linear continuous and hybrid systems. Finally, Chapter 6 presents a generalized version of the combinatorial algorithm for the solution of mp-QP problems featuring unbounded or binary parameters.

Chapter 2

Theoretical Background

This chapter sets out the recurring notation in this thesis. In addition, due to their intimate relationship with multi-parametric programming, polytopes are discussed and some definitions are given which are going to be used throughout the thesis.

2.1 Notation

The notation used in this thesis is fairly standard. The zero matrix of dimension $n \times m$ is denoted as $0_{n \times m}$. Let $a \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$, then a_k and A_k denote the vector and matrix formed from the elements and rows of a and A indexed by k^1 , A^T denotes the transpose of A , $\|a\|_2$ and $\|A\|_2$ denotes the 2-norm of a and 2-norm of each row of A respectively, and $|a|$ and $|A|$ denote the element-wise absolute value of a and A , respectively. Additionally, $\text{card}(p)$ denotes the cardinality of the set p . Let $n, k \in \mathbb{R}$ and p be a set. Then the binomial coefficient is denoted as $\binom{n}{k}$, while $\binom{p}{k}$ denotes the set of all possible sets of cardinality k which are subsets of p . Lastly, let P be a polytope, then $\text{int}(P)$ denotes the interior of P , and $\text{Co}(\cdot)$ denotes the convex hull. Furthermore, $Q \succ 0$ denotes that the matrix $Q \in \mathbb{R}^{n \times n}$ is positive definite.

2.1.1 Nomenclature

The terms 'linear' and 'affine' are used interchangeably. In addition, the term 'integer' refers to binary variables, based on which any integer variable can be modeled [229]. Furthermore, the terms 'programming' and 'optimization' (e.g. 'programming problems' and 'optimization problems') are also used interchangeably.

¹If set k is of cardinality 1, then a_k and A_k denotes the k -th element and row of a and A .

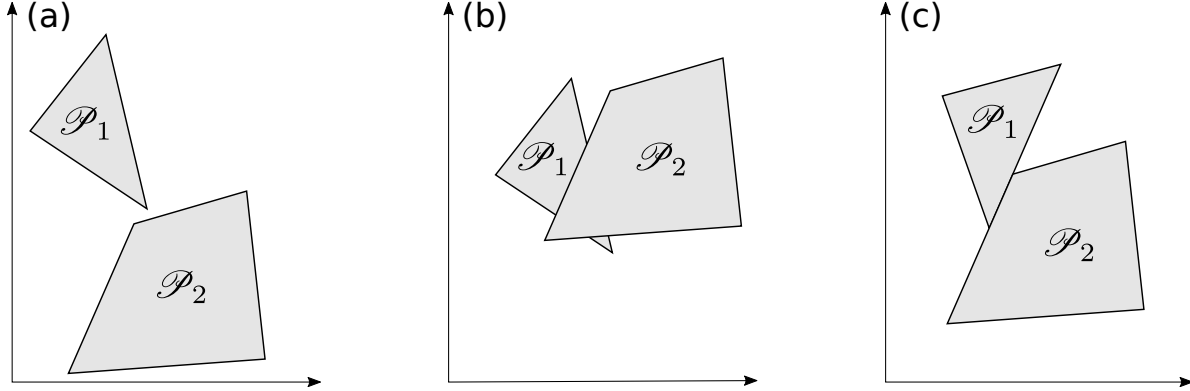


Figure 2.1: The schematic depiction of the notions of (a) disjoint, (b) overlapping and (c) adjacent polytopes.

2.2 Polytopes

In the case of mp-LP and mp-QP problems, the resulting critical regions are polytopes (see eq. (3.9)). Thus, multi-parametric programming is intimately related to the properties and operations applicable to polytopes. In the following, some basic definitions on polytopes are stated which are used throughout the thesis. For an excellent treatment on (convex) polytopes, the interested reader is referred to [108].

Definition 1. The set \mathcal{P} is called a n -dimensional polytope if and only if it satisfies:

$$\mathcal{P} := \{x \in \mathbb{R}^n \mid a_i^T x \leq b_i, i = 1, \dots, m\}, \quad (2.1)$$

where m is finite.

In addition to Definition (1) the following well-known characteristics of polytopes are considered:

- A polytope is called bounded if and only if there exists a finite $x_{\min} \in \mathbb{R}^n$ and $x_{\max} \in \mathbb{R}^n$ such $x_{\min} \leq x \leq x_{\max}$ for all $x \in \mathcal{P}$.
- A polytope which is closed and bounded is called compact. Unless stated otherwise, all polytopes considered in this thesis are assumed to be compact.
- Two polytopes \mathcal{P}_1 and \mathcal{P}_2 are called disjoint if $\mathcal{P}_1 \cap \mathcal{P}_2 = \emptyset$. Similarly, two polytopes \mathcal{P}_1 and \mathcal{P}_2 are called overlapping if $\text{int}(\mathcal{P}_1) \cap \text{int}(\mathcal{P}_2) \neq \emptyset$. Lastly, two polytopes \mathcal{P}_1 and \mathcal{P}_2 are called adjacent or neighboring if $\mathcal{P}_1 \cap \mathcal{P}_2$ is a $n - 1$ -dimensional polytope. In Figure 2.1, these definitions are depicted schematically.

- Let \mathcal{P} be an n -dimensional polytope. Then, a subset of a polytope is called a face of \mathcal{P} if it can be represented as:

$$\mathcal{F} = \mathcal{P} \cap \{x \in \mathbb{R}^n \mid a^T x = b\} \quad (2.2)$$

for some inequality $a^T x \leq b$ which holds for all $x \in \mathcal{P}$. The faces of polytopes of dimension $n - 1$, 1 and 0 are referred to as facets, edges and vertices, respectively.

- Let \mathcal{P} be an n -dimensional polytope. Then, there exists a series of k vertices $x_i \in \mathbb{R}^n$ such that:

$$\mathcal{P} := \left\{ x \in \mathbb{R}^n \mid x = \sum_{i=1}^k \lambda_i x_i, \sum_{i=1}^k \lambda_i = 1, \lambda_i \geq 0 \right\}. \quad (2.3)$$

- Eq. (2.1) is referred to the halfspace (or H) representation, while eq. (2.3) denotes the vertex (or V) representation. The process of moving from the halfspace to the vertex representation is referred to as vertex enumeration.
- The Chebyshev center of a polytope is given as the largest Euclidean ball that lies in a polytope [45]. It can be determined by solving the following linear programming problem:

$$\begin{aligned} R^* = \underset{x,r}{\text{minimize}} \quad & -r \\ \text{subject to} \quad & A_i x + r \|A_i\|_2 \leq b_i, \quad \forall i = 1, \dots, m, \end{aligned} \quad (2.4)$$

where the solution x^* and R^* denotes the location and radius of the largest Euclidean ball, respectively. Based on the solution of problem (2.4), the following conclusions can be drawn:

- Problem (2.4) is infeasible: The polytope is empty.
- $R^* = 0$: The polytope is lower-dimensional.
- $R^* > 0$: The polytope is full-dimensional.

2.2.1 Approaches for the removal of redundant constraints

A concept which is very important in multi-parametric programming is the aspect of redundancy:

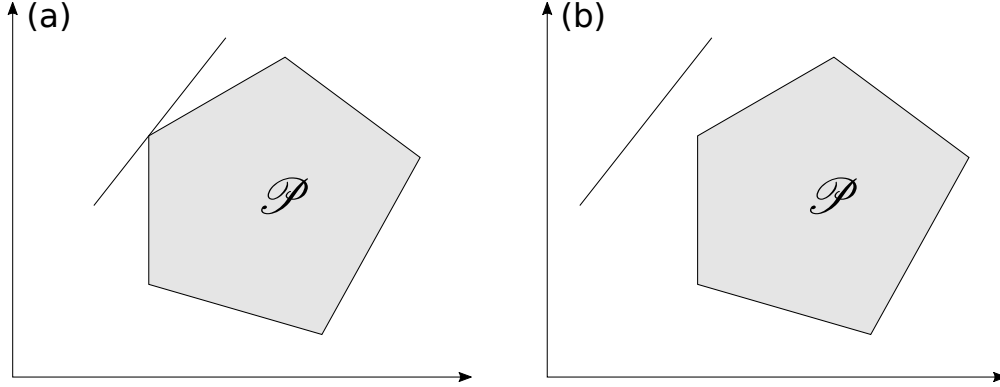


Figure 2.2: The schematic depiction of the notions of (a) weakly and (b) strongly redundant constraints.

Definition 2 ([250]). Consider a n -dimensional compact polytope \mathcal{P} in halfspace representation. A constraint $A_i^T x \leq b_i$ is called redundant if

$$\mathcal{P}_i = \{x \in \mathbb{R}^n \mid A_i x > b_i, A_k x \leq b_k, \forall k \neq i\} = \emptyset. \quad (2.5)$$

Additionally, a constraint $A_i x \leq b_i$ is called strongly redundant if

$$\mathcal{P}'_i = \{x \in \mathbb{R}^n \mid A_i x \geq b_i, A_k x \leq b_k, \forall k \neq i\} = \emptyset. \quad (2.6)$$

Remark 2. A constraint is called weakly redundant if it is redundant but not strongly redundant, i.e. eq. (2.5) but not eq. (2.6) holds. Furthermore, if a polytope \mathcal{P} does not feature any redundant constraints, it is said to be in minimal representation. A schematic representation of Definition 2 is given in Figure 2.2.

Consider an n -dimensional compact polytope $\mathcal{P} = \{x \in \mathbb{R}^n \mid Ax \leq b\}$, where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. The following strategies aim at identifying the minimal representation of \mathcal{P} :

Remark 3. Here, only the approaches used in this thesis are reported. The field of the removal of redundant constraints has been widely studied and its review is beyond the scope of this thesis. The reader is referred to [137, 250] for an interesting treatment of the matter.

Lower-Upper bound classification [46]

Given the bounds $l_j \leq x_j \leq u_j, \forall j = 1, \dots, m$, a constraint $A_i x \leq b_i$ is redundant if

$$U_i \leq b_i, \quad (2.7)$$

where

$$U_i = \sum_{j \in P_j} A_{ij} u_j + \sum_{j \in N_j} A_{ij} l_j, \quad (2.8)$$

where $P_j = \{j | A_{ij} > 0\}$ and $N_j = \{j | A_{ij} < 0\}$. This approach relies on the identification of the worst-case scenario given the lower and upper bounds. If these bounds are not available, they can be calculated by solving the following $2n$ linear programming (LP) problems [247]:

$$\begin{aligned} & \underset{x}{\text{minimize}} && \pm x_i \\ & \text{subject to} && x \in \mathcal{P}. \end{aligned} \quad (2.9)$$

Solution of linear programming problem

Consider the following constraint-specific version of problem (2.4):

$$\begin{aligned} R_i = & \underset{x, r}{\text{minimize}} && -r \\ & \text{subject to} && Ax \leq (b - \|A^i\|_2 r) \\ & && A_i x = b_i \\ & && \|A^i\|_2 = \left\| 1 - (AA_i^T)^2 \right\|_2 \\ & && x \in \mathcal{P}, r \in \mathbb{R}, \end{aligned} \quad (2.10)$$

where $(\cdot)^2$ denotes the element-wise square of (\cdot) . Note that $Ax \leq b$ is assumed to be normalized such that $\|a_i\|_2 = 1$ for all $i = 1, \dots, m$. Then the i -th constraint is redundant if and only if $R_i \leq 0$. Note that this identifies weakly and strongly redundant constraints.

Remark 4. The solution of problem (2.10) identifies the largest Euclidean ball which on the set $\mathcal{K} = \{x | x \in \mathcal{P} \cup A_i x = b_i\}$, i.e. which lies on the i -th constraint. Thus, the solution can be understood as the center of the i -th constraint with respect to \mathcal{P} .

2.2.2 Projections

One of the operations used in this thesis is the (orthogonal) projection:

Definition 3 (Projection [131]). Let $P \subset \mathbb{R}^d \times \mathbb{R}^k$ be a polytope. Then the projection $\pi_d(P)$ of P onto \mathbb{R}^d is defined as:

$$\pi_d(P) = \left\{ x \in \mathbb{R}^d \mid \exists y \in \mathbb{R}^k, (x, y) \in P \right\}. \quad (2.11)$$

Projecting polytopes is one of the fundamental operations in computational geometry

and has many applications in control theory. As its efficient calculation is paramount for this thesis, two different strategies have been implemented for this thesis:

- Solving a multi-parametric linear programming (mp-LP) problem (see e.g. [148])
- Performing a Fourier-Motzkin (FM) elimination (see e.g. [241])

In addition, the concept of a hybrid projection is introduced:

Definition 4 (Hybrid projection). Consider the set $P \subset \mathbb{R}^d \times \mathbb{R}^k \times \{0, 1\}^r$. Then, the hybrid projection $\tilde{\pi}_d(P)$ of P onto \mathbb{R}^d is defined as:

$$\tilde{\pi}_d(P) = \left\{ x \in \mathbb{R}^d \mid \exists y \in \mathbb{R}^k \times \{0, 1\}^r, (x, y) \in P \right\}. \quad (2.12)$$

By inspection it is clear that (a) $\tilde{\pi}_d(P)$ is obtained by performing at most 2^r projections, one for each combination of the binary variables and consequently (b) $\tilde{\pi}_d(P)$ is generally a union of at most 2^r possibly overlapping polytopes.

A hybrid projection can thereby be performed by solving a mp-MILP problem purely based on feasibility requirements.

2.2.3 Modelling of the union of polytopes

The aim is to represent a union of polytopes $P = \bigcup_{i=1}^p \{x \mid G^i x \leq g^i\}$ as a single set of linear inequality constraints. However, in order to address the possible non-convexity within unions of polytopes, the introduction of suitable binary variables is required. First, consider that a point $x \in P$ if and only if there exists at least one i such that $G^i x \leq g^i$. Thus, one binary variable y_i is defined such that:

$$\left[G^i x \leq g^i \right] \rightarrow [y_i = 1] \quad (2.13a)$$

$$\sum_{i=1}^p y_i \geq 1. \quad (2.13b)$$

Let G_j^i and g_j^i denote the j -th row and element of $G^i \in \mathbb{R}^{t_i \times n}$ and $g^i \in \mathbb{R}^{t_i}$, respectively. Then, the statement $G^i x \leq g^i$ holds if and only if $G_j^i x \leq g_j^i, \forall j$. Thus, one binary variable

per row of G^i , y_j^i , is defined such that:

$$\left[G_j^i x \leq g_j^i \right] \leftrightarrow \left[y_j^i = 1 \right] \quad (2.14a)$$

$$\left[\sum_{j=1}^{t_i} y_j^i = t_i \right] \rightarrow \left[y_i = 1 \right] \quad (2.14b)$$

$$\sum_{i=1}^p y_i \geq 1. \quad (2.14c)$$

Based on [23, 260], eq. (2.14a-2.14b) are reformulated as:

$$G_j^{i,T} x + M y_j^i \leq M + g_j^i \quad (2.15a)$$

$$G_j^{i,T} x - m y_j^i \geq g_j^i \quad (2.15b)$$

$$t_i y_i \leq \sum_{j=1}^{t_i} y_j^i \quad (2.15c)$$

$$y_i \geq \sum_{j=1}^{t_i} y_j^i + 1 - t_i, \quad (2.15d)$$

where $m \leq x \leq M$, $\forall x \in P$. Thus, the final formulation of the union as a set of linear inequality constraints featuring binary variables is given as:

$$P = \bigcup_{i=1}^p \{x | G^i x \leq g^i\} \rightarrow \left\{ \begin{array}{l} G_j^{i,T} x + M y_j^i \leq M + g_j^i \\ -G_j^{i,T} x + m y_j^i \leq -g_j^i \\ t_i y_i - \sum_{j=1}^{t_i} y_j^i \leq 0 \\ -y_i + \sum_{j=1}^{t_i} y_j^i \leq t_i - 1 \\ -\sum_{i=1}^p y_i \leq -1 \end{array} \right. . \quad (2.16)$$

Chapter 3

Contributions to multi-parametric quadratic programming

Portions of this chapter have published in:

- Oberdieck, R.; Diangelakis, N.A.; Papathanasiou, M.M.; Nascu, I.; Pistikopoulos, E.N. (2016) POP - Parametric Optimization Toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979 - 8991.
- Oberdieck, R.; Diangelakis, N.A.; Pistikopoulos, E.N. (2017) Explicit Model Predictive Control: A connected-graph approach. *Automatica*, 76, 103-112.
- Oberdieck, R.; Pistikopoulos, E. N. (2016) Parallel computing in multi-parametric programming. In *Computer Aided Chemical Engineering*, 38, p. 169 - 174.
- Oberdieck, R.; Pistikopoulos, E. N. (2016) Multi-objective optimization with convex quadratic cost functions: A multi-parametric programming approach. *Computers & Chemical Engineering*, 85, 36 - 39.

3.1 Introduction

Multi-parametric quadratic programming (mp-QP) problems have attracted extensive attention in recent years due to their applicability to explicit model predictive control (MPC) [31]. Despite this interest and the subsequent developments, several theoretical and algorithmic questions still remain open. The aim of this chapter is twofold: first, an overview over the current state-of-the-art from a theoretical and algorithmic perspective is given. Then, some recent advances in the area of mp-QP problems are discussed, namely:

- Development of a novel solution procedure which is based on the fact that the solution of a mp-QP problem is given by a connected graph.
- A computational analysis which shows the performance of the different solution approaches and the discussion of qualitative rules as to which algorithm is more applicable in which circumstance.
- Description of a parallelization procedure applicable to the most commonly used solution techniques for mp-QP problems.
- The approximate solution of certain multi-objective optimization problems using mp-QP problems.

3.2 Theoretical and algorithmic background for mp-QP problems

Consider the following mp-QP problem:

$$\begin{aligned}
z(\theta) = \underset{x}{\text{minimize}} \quad & (Qx + H\theta + c)^T x \\
\text{subject to} \quad & Ax \leq b + F\theta \\
& x \in \mathbb{R}^n \\
& \theta \in \Theta := \{\theta \in \mathbb{R}^q \mid CR_A\theta \leq CR_b\},
\end{aligned} \tag{3.1}$$

with $Q \in \mathbb{R}^{n \times n} \succ 0$, $H \in \mathbb{R}^{n \times q}$, $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $F \in \mathbb{R}^{m \times q}$, $CR_A \in \mathbb{R}^{r \times q}$, $CR_b \in \mathbb{R}^r$ and Θ is compact.

Remark 5. The properties discussed below are also valid for mp-LP problems of the form:

$$\begin{aligned}
z(\theta) = \underset{x}{\text{minimize}} \quad & c^T x \\
\text{subject to} \quad & Ax \leq b + F\theta \\
& x \in \mathbb{R}^n \\
& \theta \in \Theta := \{\theta \in \mathbb{R}^q \mid CR_A\theta \leq CR_b\}.
\end{aligned} \tag{3.2}$$

Note however that due to the positive semi-definite nature of problem (3.2)¹, this might lead to dual degeneracy, as discussed in section 3.2.2.

Remark 6. In order to facilitate readability, throughout this thesis equality constraints will be omitted in the problem formulations of multi-parametric programming problems as they

¹Problem (3.2) can be viewed as a special case of problem (3.1) with $Q = 0_{n \times n}$ and $H = 0_{n \times q}$, which is inherently positive semi-definite.

can be understood as inequality constraints which have to be active in the entire parameter space (i.e. they are always part of the active set).

3.2.1 Theoretical Properties

The key question when considering problem (3.1) is how to obtain the parametric solution $x(\theta)$ and $\lambda(\theta)$, where λ denotes the Lagrangian multiplier². In the open literature, two ways have been presented:

Post-optimal sensitivity analysis: Consider problem (3.1), let $f(x, \theta)$ and $g_i(x, \theta) \leq 0$ denote the objective function and the i -th constraint, respectively and let θ be fixed to θ_0 . Then the resulting quadratic programming (QP) problem can be solved using the Karush-Kuhn-Tucker (KKT) conditions, which are given by:

$$\nabla_x \mathcal{L} = \nabla_x f(x, \theta_0) + \sum_{i=1}^m \lambda_i \nabla_x g_i(x, \theta_0) = 0 \quad (3.3a)$$

$$g_i(x, \theta_0) \leq 0, \lambda_i \geq 0, \forall i = 1, \dots, m \quad (3.3b)$$

$$\lambda_i g_i(x, \theta_0) = 0, \forall i = 1, \dots, m, \quad (3.3c)$$

where the optimal solution is given by the optimizer x_0 and the Lagrangian multipliers $\lambda_0 = [\lambda_1, \lambda_2, \dots, \lambda_m]^T$. This consideration leads to the main theorem on post-optimal sensitivity analysis:

Theorem 1 (Basic Sensitivity Theorem [83]). Let θ_0 be a vector of parameter values and (x_0, λ_0) the solution derived from the KKT conditions in eq. (3.3), where λ_0 is non-negative and x_0 is feasible. Also assume that: (i) strict complementary slackness (SCS) holds; (ii) the binding constraint gradients are linearly independent (LICQ: Linear Independence Constraint Qualification); and (iii) the second-order sufficiency conditions (SOSC) hold. Then, in the neighborhood of θ_0 , there exists a unique, once differentiable function $[x(\theta), \lambda(\theta)]$ satisfying eq. (3.3) with $[x(\theta_0), \lambda(\theta_0)] = (x_0, \lambda_0)$, where $x(\theta)$ is a unique isolated minimizer for problem (3.1) and

$$\left(\frac{dx(\theta_0)}{d\theta}, \frac{d\lambda(\theta_0)}{d\theta} \right)^T = -(M_0)^{-1} N_0, \quad (3.4)$$

²For an introduction into the concept of Lagrangian multipliers and duality in general, the reader is referred to the excellent textbook by Floudas [84].

where

$$M_0 = \begin{pmatrix} \nabla^2 \mathcal{L} & \nabla g_1 & \cdots & \nabla g_m \\ -\lambda_1 \nabla^T g_1 & -g_1 & & \\ \vdots & & \ddots & \\ -\lambda_m \nabla^T g_m & & & -g_m \end{pmatrix} \quad (3.5a)$$

$$N_0 = \left(\nabla_{\theta,x}^2 \mathcal{L}, -\lambda_1 \nabla_{\theta}^T g_1, \dots, -\lambda_m \nabla_{\theta}^T g_m \right)^T \quad (3.5b)$$

$$\mathcal{L} = f(x, \theta) + \sum_{i=1}^m \lambda_i g_i(x, \theta). \quad (3.5c)$$

As a result of Theorem 1 the parametric solutions $x(\theta)$ and $\lambda(\theta)$ are affine functions of θ around θ_0 .

Parametric solution of the KKT conditions: Consider problem (3.1) and eq. (3.3) without fixing θ to θ_0 . Additionally, let k be a candidate active set, then the corresponding KKT conditions are given as³:

$$\nabla_x \mathcal{L}(x, \lambda, \theta) = \nabla_x \left((Qx + H\theta + c)^T x \right) + \nabla_x \left(\sum_{i \in k} \lambda_i (A_i x - b_i - F_i \theta) \right) \quad (3.6a)$$

$$= Qx + H\theta + c + A_k^T \lambda_k = 0 \quad (3.6b)$$

$$A_k x - b_k - F_k \theta = 0. \quad (3.6c)$$

Thus, eq. (3.6b) is reformulated such that

$$x = -Q^{-1} \left(H\theta + c + A_k^T \lambda_k \right). \quad (3.7)$$

Note that Q is invertible since it is positive definite. The substitution of eq. (3.7) into eq. (3.6c) results in:

$$\begin{aligned} & -A_k Q^{-1} \left(H^T \theta + c + A_k^T \lambda_k \right) - b_k - F_k \theta = 0 \\ \Rightarrow \lambda_k(\theta) &= - \left(A_k Q^{-1} A_k^T \right)^{-1} \left(b_k + F_k \theta + A_k Q^{-1} (H\theta + c) \right), \end{aligned} \quad (3.8)$$

which can be substituted into eq. (3.7) to obtain the full parametric solution.

³Assuming no degeneracy, in the case of mp-LP problems, the cardinality of the active set k is $\text{card}(k) = n$ and thus the parametric solution is directly given as $x(\theta) = A_k^{-1} (b_k + F_k \theta)$.

Once the parametric solution has been obtained, the set over which it is valid is defined by feasibility and optimality requirements:

$$Ax(\theta) \leq b + F\theta \quad (\text{Feasibility of } x(\theta)) \quad (3.9a)$$

$$\lambda(\theta) \geq 0 \quad (\text{Optimality of } x(\theta)) \quad (3.9b)$$

$$CR_A\theta \leq CR_b \quad (\text{Feasibility of } \theta) \quad (3.9c)$$

For mp-LP and mp-QP problems, eq. (3.9) denotes a set of linear inequalities, and thus the critical region where a parametric solution is optimal is a polytope. Since this analysis is valid for any feasible point θ_0 , the main properties of mp-LP and mp-QP solutions is given as follows:

Definition 5. A function $x(\theta) : \Theta \rightarrow \mathbb{R}^n$, where $\Theta \in \mathbb{R}^q$ is a polytope, is called piecewise affine if it is possible to partition Θ into non-overlapping polytopes, called critical regions, CR_i and

$$x(\theta) = K^i\theta + r^i, \forall \theta \in CR_i. \quad (3.10)$$

Remark 7. The definition of piecewise quadratic is analogous.

Theorem 2 (Properties of mp-QP solution [31, 74]). Consider the mp-QP problem (3.1). Then the set of feasible parameters $\Theta_f \subseteq \Theta$ is convex, the optimizer $x(\theta) : \Theta_f \mapsto \mathbb{R}^n$ is continuous and piecewise affine, and the optimal objective function $z(\theta) : \Theta_f \mapsto \mathbb{R}$ is continuous, and piecewise quadratic.

Remark 8. In the case of mp-LP problems, Theorem 2 still holds, however the optimal objective function $z(\theta) : \Theta_f \mapsto \mathbb{R}$ is continuous, convex and piecewise affine [90].

Remark 9 (Active set representation). Each critical region in a mp-LP or mp-QP problem is uniquely defined by the optimal active set associated with it, and the solution of problem (3.1) can be represented as the set of all optimal active sets.

3.2.2 Degeneracy

One of the most important issues encountered in linear and quadratic programming is degeneracy. However, since the solution to a strictly convex QP is guaranteed to be unique, some types of degeneracy do not occur in QP and consequentially in mp-QP problems. Thus, for completion consider a standard mp-LP problem, where degeneracy generally refers to the situation where the active set for a specific LP problem (e.g. problem (3.2) with $\theta = 0$)

cannot be identified uniquely⁴. Commonly, the two types of degeneracy encountered are primal and dual degeneracy (see Figure 3.1):

Primal degeneracy: In this case, the vertex of the optimal solution of the LP is overdefined, i.e. there exist multiple sets $k_1 \neq k_2 \neq \dots \neq k_{tot}$ such that:

$$x_{k_1} = x_{k_2} = \dots = x_{k_{tot}}, \quad (3.11)$$

where $x_k = A_k^{-1}b_k$.

By inspection of Figure 3.1, it is clear that primal degeneracy is caused by the presence of constraints which only coincide with the feasible space, but do not intersect it. Thus, if any of these constraints would be chosen to be part of the active set of the corresponding parametric solution, this results in a lower-dimensional critical region⁵, and only one active set k exists for which a full-dimensional critical region results, and it is constituted by those constraints which intersect with the feasible space.

Remark 10. Constraints which coincide but do not intersect with the feasible space are also referred to as weakly redundant constraints (see also Figure 2.2).

Dual degeneracy: If there exists more than one point x have the same optimal objective function value z , then the optimal solution is not unique. Thus, there exist multiple sets $k_1 \neq k_2 \neq \dots \neq k_{tot}$ with $x_{k_1} \neq x_{k_2} \neq \dots \neq x_{k_{tot}}$ such that:

$$z_{k_1} = z_{k_2} = \dots = z_{k_{tot}}, \quad (3.12)$$

where $z_k = c^T x_k$.

In general, the effect of primal degeneracy within the solution procedure of mp-LP problems is manageable, since it can be detected by substituting x_k into the constraints and if necessary solving one LP problem for each constraint⁶. However, dual degeneracy is more challenging as the different active sets might result in full-dimensional, but potentially overlapping, critical regions. In particular since the optimal solutions x_k differ, the presence of dual degeneracy might eliminate the continuous nature of the optimizer described in Theorem 2. However, three approaches have been proposed to generate continuous optimizers as well as non-overlapping critical regions [134, 205].

⁴This does not consider problems arising from scaling, round-off computational errors or the presence of identical constraints in the problem formulation.

⁵Consider Figure 3.1: if the constraint which only coincides at the single point with the feasible space is chosen as part of the active set, the corresponding parametric solution will only be valid in that point.

⁶For example, problem (2.10) can be solved for each constraint, and if $R^* = 0$, then the constraint is weakly redundant and is not part of the active set.

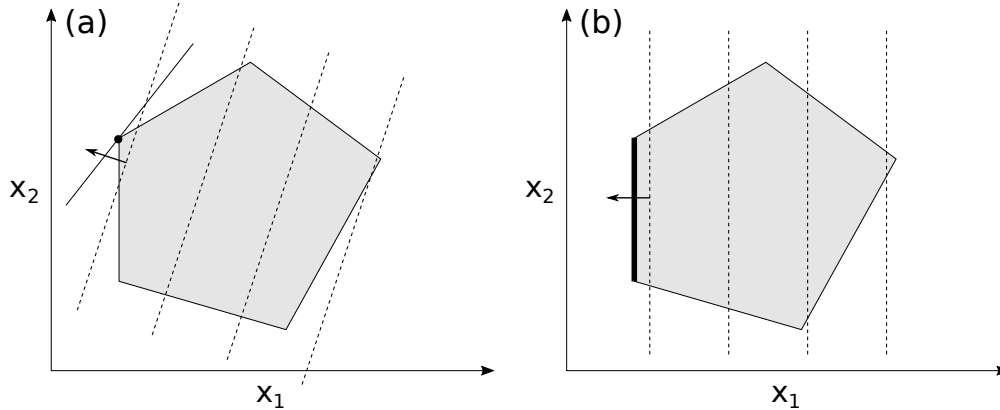


Figure 3.1: Primal and dual degeneracy in linear programming. In (a), primal degeneracy occurs since there are three constraints which are active at the solution, while in (b) dual degeneracy occurs since there is more than one point (x_1, x_2) which features the optimal objective function value.

The most promising one is thereby the application of lexicographic perturbation techniques, which is based on the idea that the problem of dual-degeneracy only arises because of the specific numerical structure of the objective function and the constraints [134]. In order to overcome the degeneracy, the right-hand side of the constraints as well as the objective function are symbolically perturbed in order to obtain a single, continuous optimizer for the solution of the mp-LP problem. Note that the problem is not actually perturbed, but only the result of a proposed perturbation is analyzed and enables the formulation of a continuous optimizer.

3.2.3 Solution algorithms for mp-LP and mp-QP problems

Based on Theorem 2 and Remark 9, it is possible to consider the solution to problem (3.1) either as a set of non-overlapping polytopes which cover the feasible parameter space Θ_f or as a set of optimal active sets, which generate the critical regions based on the parametric solution $x(\theta), \lambda(\theta)$. This has given rise to three distinct types of solution approaches: a geometrical approach, a combinatorial approach and a connected-graph approach for mp-LP problems.

Remark 11. Other approaches for the solution of problem (3.1) involve vertex enumeration [185], graphical derivatives [212] or the reformulation as a multi-parametric linear complementarity problem [53, 130, 166], which can be solved in a geometrical [118] or combinatorial [120] fashion.

The geometrical approach: Possibly the most intuitive approach to solve mp-QP prob-

lems of type (3.1) is the geometrical approach. It is based on the geometrical consideration and exploration of the parameter space Θ . The key idea is to fix a point $\theta_0 \in \Theta$, solve the resulting QP and obtain the parametric expressions $x(\theta)$ and $\lambda(\theta)$ alongside the corresponding critical region CR . Then, a new, feasible point $\theta_1 \notin CR$ is fixed and the same procedure is repeated until the entire parameter space has been explored. The different contributions differ in the way the parameter space is explored: in [31, 74], the constraints of the critical region are reversed, yielding a set of new polytopes which are considered separately. As this introduces a large number of artificial cuts [252], the step-sized approach has gained importance, as it calculates a point on the facet of each critical region and steps away from it orthogonally (see Figure 3.2) [14, 22].

However the geometrical approach presented in [14, 22] is only guaranteed to provide the full parametric map if the so-called facet-to-facet property is fulfilled [244]:

Definition 6 (Facet-to-facet property). Let CR_1 and CR_2 be two full-dimensional disjoint critical regions. Then the facet-to-facet property is said to hold if $F = CR_1 \cap CR_2$ is a facet of both CR_1 and CR_2 .

Additionally, researchers have proposed techniques to infer the active set of the adjacent critical region:

Theorem 3 (Active set of adjacent region [252]). Consider the active set of a full-dimensional critical region CR_0 in minimal representation, $k = \{i_1, i_2, \dots, i_k\}$. Additionally, let CR_i be a full-dimensional neighboring critical region to CR_0 and assume that the linear independent constraint qualification holds on their common facet $F = CR_0 \cap H$, where H is the separating hyperplane. Moreover, assume that there are no constraints which are weakly active at the optimizer $x(\theta)$ for all $\theta \in CR_0$. Then:

Type I: If H is given by $A_{i_{k+1}}x(\theta) = b_{i_{k+1}} + F_{i_{k+1}}\theta$, then the optimal active set in CR_i is $\{i_1, \dots, i_k, i_{k+1}\}$.

Type II: If H is given by $\lambda_{i_k}(\theta) = 0$, then the optimal active set in CR_i is $\{i_1, \dots, i_{k-1}\}$.

Consequently, the following corollary is stated:

Corollary 1 (Facet-to-facet conditionality [244]). The facet-to-facet property holds between CR_0 and CR_i , if the conditions of Theorem 3 are fulfilled.

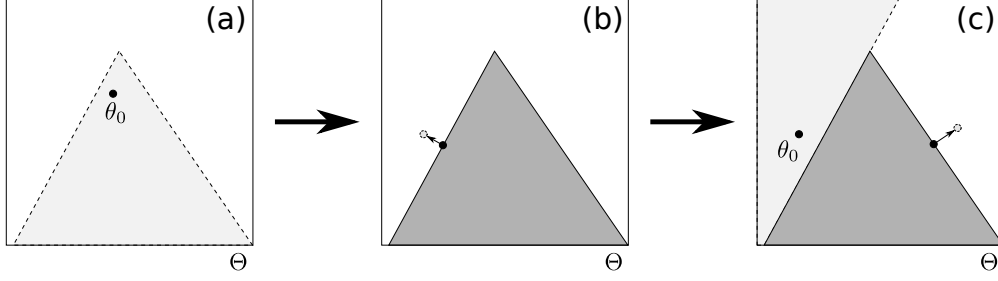


Figure 3.2: A graphical representation of the geometrical solution procedure of exploring the parameter space based on the step-size approach. Starting from an initial point $\theta_0 \in \Theta$, in (a) the first critical region CR_0 is calculated (shown with dashed lines). In (b), a facet of CR_0 is identified and a step orthogonal to that facet is taken to identify a new point $\theta_1 \notin CR_0$, while in (c) the new critical region associated with θ_1 is identified, and the remaining facet from CR_0 is identified combined with the orthogonal step from it to identify a new point.

The combinatorial approach: As stated in Remark 9, every critical region is uniquely defined by the corresponding optimal active set. Thus, a combinatorial approach has been suggested, which considers the fact that the possible number of active set is finite, and thus can be exhaustively enumerated. In order to make this approach computationally tractable, the following fathoming criteria is stated:

Lemma 1 (Fathoming of active sets [110]). Let k be an infeasible candidate active set, i.e.

$$\left\{ (x, \theta) \left| \begin{array}{l} A_k x = b_k + F_k \theta \\ A_j x \leq b_j + F_j \theta, \quad \forall j \notin k \\ \theta \in \Theta \end{array} \right. \right\} = \emptyset. \quad (3.13)$$

Then any set $k' \supset k$ is also infeasible and may be fathomed⁷.

Thus, the following branch-and-bound approach has been presented [110] (see Figure 3.3):

Step 1: Generate a tree consisting of all possible active sets.

Step 2: Select the candidate active set with the lowest cardinality of the active set and check for feasibility. If it is infeasible, fathom that node and all its child nodes.

Step 3: Obtain the parametric solution of the selected node accordingly and check whether the resulting region is non-empty.

⁷In other words: if k is infeasible, so is its powerset.

Step 4: If there are nodes to explore, go to Step 2. Otherwise terminate.

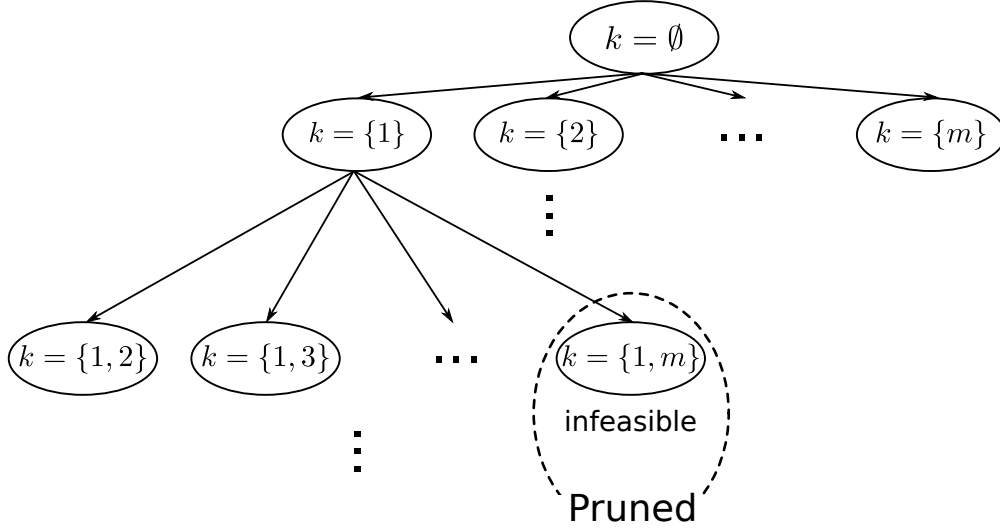


Figure 3.3: A graphical representation of the combinatorial approach for the solution of mp-QP problems. All candidate active sets are exhaustively enumerated based on their cardinality. The computational tractability arises from the ability to discard active sets if infeasibility is detected for a candidate active set which is a subset of the currently considered candidate.

This approach has been shown to be particularly efficient when symmetry is present [81, 82].

A connected graph approach for mp-LP problems: This approach was presented by Gal and Nedoma [91] for mp-LP problems:

Definition 7 (mp-LP Graph). Let each optimal active set k of a mp-LP problem be a node in the set of solutions \mathcal{S} . Then the nodes k_1 and k_2 are connected if (a) there exists $\theta^* \in \Theta_f$ such that k_1 and k_2 are both optimal active sets and (b) it is possible to pass from k_1 to k_2 by one step of the dual simplex algorithm. The resulting graph G is fully defined by the nodes \mathcal{S} as well as all connections Γ , i.e. $G = (\mathcal{S}, \Gamma)$.

Remark 12. One step of the dual simplex algorithm consists of changing one element of the active set, i.e. let $k_1 = \{i_1, \dots, i_{n-1}, i_n\}$, then the dual pivot involving the constraint i_n yields $k_2 = \{i_1, \dots, i_{n-1}, i_{n+1}\}$.

Theorem 4 (Connected graph for mp-LP problems [91]). Consider the solution to a mp-LP problem and let $\theta_1, \theta_2 \in \Theta_f$ be two arbitrary feasible parameters and $k_1 \in \mathcal{S}$ be given such that $\theta_1 \in CR_{k_1}$. Then there exists a path $\{k_1, \dots, k_j\}$ in the mp-LP graph $G = (\mathcal{S}, \Gamma)$ such that $\theta_2 \in CR_{k_j}$.

If there exists $\theta^* \in \Theta_f$ such that k_1 and k_2 are both optimal active sets, then the intersection of the corresponding critical regions is non-empty, i.e. they are neighboring in a geometrical sense. Conversely, the ability to pass from k_1 to k_2 by one step of the dual simplex algorithm means that the two optimal active sets are neighboring in a combinatorial sense. Thus, this approach bridges the division between geometrical and combinatorial considerations as it shows how they are interlinked in the case of mp-LP problems.

3.3 The connected graph approach for mp-QP problems

The most efficient solution procedures for mp-QP problems can broadly be classified into geometrical and combinatorial approaches. However, although the fact that these two algorithms solve the same type of problem, they exploit different characteristics of the mp-QP problem. This section aims at combining these two algorithms together, as it is shown that the ability to infer the optimal active set of adjacent critical regions [252] implies that the solution of mp-QP problems is given by a connected graph. This property is used to devise a novel solution algorithm, which explores the connected graph in conjunction with the powerful fathoming criterion described in Lemma 1 [110]. After highlighting the abilities of the new algorithm in a motivating example, it is contrasted with the recent and independent work by Ahmadi-Moshkenani *et al.* [5, 6].

3.3.1 A motivating example

In most mp-LP and mp-QP problems, only a small fraction of all possible combinations of active sets yields full-dimensional critical regions. To illustrate this, consider the following

example problem:

$$\begin{aligned}
& \underset{x}{\text{minimize}} \quad x^T \begin{bmatrix} 90 & 0 & 0 & 0 \\ 0 & 153 & 0 & 0 \\ 0 & 0 & 135 & 0 \\ 0 & 0 & 0 & 162 \end{bmatrix} x + 25x \\
& \text{subject to} \quad g_1 : x_1 + x_2 \leq 350 \\
& \quad \quad \quad g_2 : x_3 + x_4 \leq 600 \\
& \quad \quad \quad g_3 : -x_1 - x_3 \leq -\theta_1 \\
& \quad \quad \quad g_4 : -x_2 - x_4 \leq -\theta_2 \\
& \quad \quad \quad g_5 : -x_1 \leq 0 \\
& \quad \quad \quad g_6 : -x_2 \leq 0 \\
& \quad \quad \quad g_7 : -x_3 \leq 0 \\
& \quad \quad \quad g_8 : -x_4 \leq 0 \\
& \quad \quad \quad \theta \in \{ \theta \in \mathbb{R}^2 \mid 0 \leq \theta_i \leq 1000, i = 1, 2 \}.
\end{aligned} \tag{3.14}$$

The full solution of problem (3.14) features 4 critical regions, which are reported in Table 3.1.

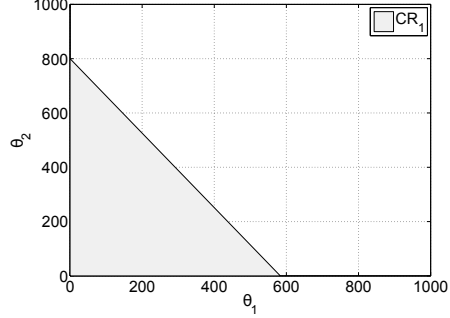
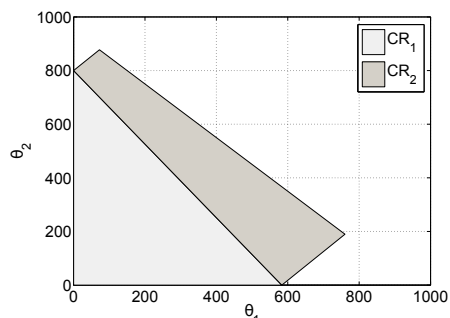
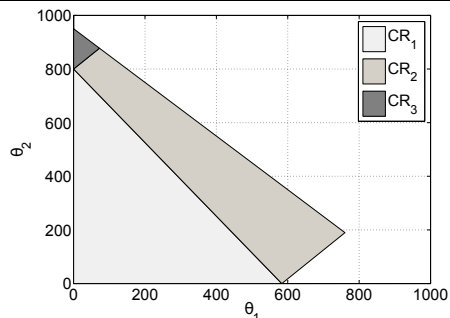
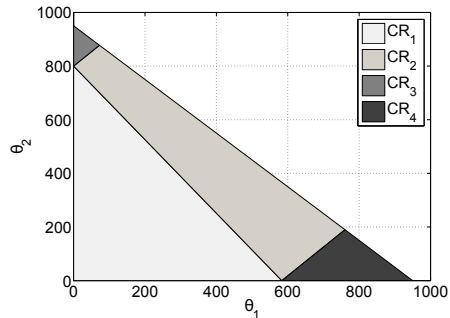
While the optimal solution only features 4 critical regions, there are a total of 163 possible combinations of active sets⁸. Even when applying Lemma 1 and removing active sets where the LICQ does not hold, the total number of combinations considered only reduces to 134. This approach is visualized in Figure 3.4, which features the optimal partitioning of the parameter space as well as the search tree resulting from the use of the combinatorial algorithm.

3.3.2 The solution of a mp-QP problem is a connected graph

Since the parametric solution of a critical region can be obtained solely based on the active set k (see eq. (3.7)), the combinatorial approach is a simple and robust solution approach to problem (3.1), as it does not feature the limitations of the geometrical approach such as the necessity of consider facet-to-facet properties and step-size determination. However, even when considering the fathoming criteria stated in Lemma 1, only $\frac{4}{134} = 3\%$ of the considered active sets in problem (3.14) result in a full-dimensional critical region. Thus, the key to a more efficient algorithm is to decrease the number of candidate active sets. In order to

⁸The total number of combinations is given as $\sum_{i=0}^4 \binom{8}{i}$.

Table 3.1: The parametric solution of problem (3.14).

$k = \{3, 4\}$	$x(\theta) = \begin{bmatrix} 0.6 & 0 \\ 0 & 0.44 \\ 0.4 & 0 \\ 0 & 0.56 \end{bmatrix} \theta$	
$k = \{1, 3, 4\}$	$x(\theta) = \begin{bmatrix} 0.26 & -0.25 \\ -0.26 & 0.25 \\ 0.74 & 0.25 \\ 0.26 & 0.75 \end{bmatrix} \theta + \begin{bmatrix} 196.5 \\ 153.51 \\ -196.49 \\ -153.51 \end{bmatrix}$	
$k = \{1, 3, 4, 5\}$	$x(\theta) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \theta + \begin{bmatrix} 0 \\ 350 \\ 0 \\ -350 \end{bmatrix}$	
$k = \{1, 3, 4, 6\}$	$x(\theta) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \theta + \begin{bmatrix} 350 \\ 0 \\ -350 \\ 0 \end{bmatrix}$	

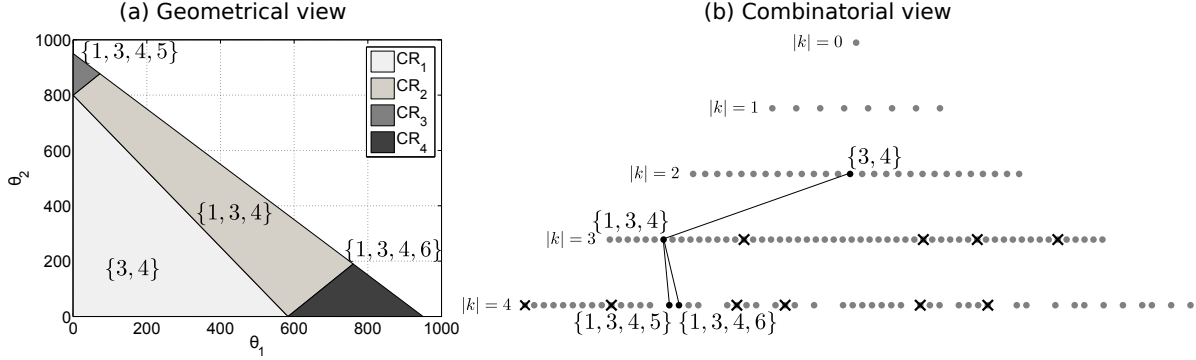


Figure 3.4: The solution to the example problem (3.14) from (a) a geometrical perspective and (b) from a combinatorial perspective. Note that all light gray points in (b) are checked for feasibility, and those which are crossed out did not fulfill the LICQ criterion. Additionally, note that the last layer misses the points which are fathomed based on Lemma 1, and that the black points show the optimal active set.

achieve this, the results on connected graphs from mp-LP problems [91] are extended to the mp-QP case:

Definition 8 (mp-QP Graph). Let each optimal active set k of a mp-QP problem be a node in \mathcal{S} . Then the nodes k_1 and k_2 are connected if (a) there exists $\theta^* \in \Theta_f$ such that k_1 and k_2 are both optimal active sets and (b) the conditions of Theorem (3) are fulfilled on the facet or it is possible to pass from k_1 to k_2 by one step of the dual simplex algorithm. The resulting graph G is fully defined by the nodes \mathcal{S} as well as all connections Γ , i.e. $G = (\mathcal{S}, \Gamma)$

Corollary 2 (Connected graph for the mp-QP solution). Consider the solution to a mp-QP problem and let $\theta_1, \theta_2 \in \Theta_f$ be two arbitrary feasible parameters and $k_1 \in \mathcal{S}$ be given such that $\theta_1 \in CR_1$. Then there exists a path $\{k_1, \dots, k_j\}$ in the mp-QP graph $G = (\mathcal{S}, \Gamma)$ such that $\theta_2 \in CR_j$.

Proof 1. If the conditions of Theorem 3 are fulfilled, then it is clear that a connected graph results. As Theorem 3 does not hold if either LICQ does not hold or weakly active constraints are present, it needs to be proven that a step of the dual simplex algorithm is enough to identify all candidates of the adjacent region. First, as strictly convex mp-QP problems do not feature weakly active constraints, only possible violations of LICQ need to be considered. The LICQ violation can only occur in Type I constraints of Theorem 3, since a constraint is added and thus the linearly independent nature of the candidate active set might change. In the case where the cardinality of the original active set is n , Theorem 4 holds directly. If the cardinality is less than n but LICQ is violated this means that an equivalent, lower-dimensional problem can be formulated where Theorem 4 holds as well, resulting in a connected graph. \square

This theorem has the following implications:

- If the conditions of Theorem 3 are fulfilled, only one candidate active set per facet of a critical region is generated.
- Let k be an active set with cardinality p . If LICQ is violated on the border of the corresponding critical region, the number of candidates is given as $\binom{p}{p-1}$.
- As stated by Gal and Nedoma [91], a disconnected graph occurs if and only if dual degeneracy occurs. Note that dual degeneracy cannot occur in strictly convex quadratic programming problems due to the uniqueness of the minimizer.

This results in the following algorithm:

3.3.3 Step 0: Initialization

The algorithm is initialized by identifying an active set that yields a full-dimensional critical region. In order to achieve this, there are two possibilities:

- Employ the standard combinatorial algorithm [110] until the first region has been found.
- Perform the first iteration of the geometrical algorithm [14].

Once the active set has been obtained, add it to the list of candidate active sets \mathcal{N} .

Remark 13. From an implementation perspective, it has proven efficient to use the first iteration of the geometrical algorithm. If this should not yield a full-dimensional region within a prescribed number of attempts, then the combinatorial algorithm is used. The reason for this is that for problems with large a large number of constraints, the combinatorial algorithm may take a long time until an initial solution is found.

3.3.4 Step 1: Feasibility

If $\mathcal{N} = \emptyset$, the algorithm terminates. Otherwise, the candidate active set k with the lowest cardinality is selected from \mathcal{N} , and the following elements are considered:

- Is $k \notin \mathcal{S}$ (where \mathcal{S} is the solution set)?
- Does $\exists j \in \mathcal{S}$ such that $k \supset j$ (where \mathcal{S} is the set of all infeasible candidate active sets according to Lemma 1)?

- Does A_k have full rank?

If these conditions are fulfilled, then the feasibility of the considered candidate active set is evaluated using Lemma 1. If it is infeasible, then k is added to \mathcal{J} , and Step 1 is started again.

3.3.5 Step 2: Parametric solution

Using the candidate active set, the corresponding parametric solution $(x(\theta), \lambda(\theta))$ is obtained, and the critical region \widehat{CR}_k is formulated according to eq. (3.9). The corresponding minimal representation CR_k is obtained by removing all redundant constraints according to section 2.2.1.

3.3.6 Step 3: Generation of new candidates

The result of the removal of all redundant constraints is the following:

$CR_k = \emptyset$: Based on the feasibility check in Lemma 1, $CR_k = \emptyset$ indicates that the parametric solution is not optimal. Thus, no critical region is formed and the algorithm returns to Step 1.

CR_k is **lower-dimensional**: This situation occurs in the case of primal degeneracy [110]. Thus, one or more of the elements of the active set k need to be removed in order to obtain a full dimensional critical region. Once that region has been obtained, any weakly redundant constraint will be removed by problem (2.10) and the full dimensional neighboring regions are identified with Theorem 3. In order to ensure the consideration of the corresponding active set, the following candidates are generated:

$$\mathcal{L} = \binom{k}{\text{card}(k) - 1}, \quad (3.15)$$

and are added to \mathcal{N} .

CR_k is **full-dimensional**: In this case, each facet of CR_k can be classified into Type I or II from Theorem 3, or as the borders of Θ . If the facet is a border of Θ , there cannot be any adjacent region. If the facet is of Type II, then it is clear that LICQ will hold, since LICQ holds for k as full rank was established in Step 1. Thus, the assumptions from Theorem 3 are fulfilled, the facet-to-facet property holds and the active set of the adjacent critical region is added to the set of candidate active sets \mathcal{N} . If the facet is of Type I, then let k_+ denote the active set obtained from Theorem 3. If A_{k_+} has full

rank, then Theorem 3 applies and the active set of the adjacent critical region is added to the set of candidate active sets \mathcal{N} . However, if full rank is not established, then similarly to the case of a lower-dimensional CR_k full rank can only be established by removing one of the elements of k_+ , i.e. to generate the following candidates:

$$\mathcal{L} = \left(\begin{array}{c} k_+ \\ \text{card}(k) \end{array} \right), \quad (3.16)$$

and to add \mathcal{L} to \mathcal{N} . Note that this corresponds to one step of the dual simplex algorithm.

Remark 14. In the case where the critical region CR features two or more identical constraints, i.e. $\exists i, j$ such that $A_i\theta - b_i = A_j\theta - b_j$ for all θ , the indices of all identical constraints corresponding to facets of the critical region are considered.

Remark 15. Note that the algorithm presented here utilizes the ordering of the candidate active sets based on their cardinality, as proposed in [110].

Thus, in summary, the following Theorem is stated:

Theorem 5. The algorithm presented in this chapter terminates in a finite number of steps and is guaranteed to explore the entire parameter space.

Proof 2. At every step of the algorithm, a candidate active set is removed from \mathcal{N} . As the number of candidate active sets is finite, and every candidate can only be considered once, the algorithm terminates in a finite number of steps. Since the union of all optimal active sets forms a connected graph (see Corollary 2), every optimal active set is found by exploring this graph. Thus, the entire parameter space is explored. \square

3.3.7 The example problem revisited

Consider the motivating example problem (3.14). After the first active set $k = \{3, 4\}$ has been obtained, the only constraint of $CR_{\{3,4\}}$ which is not part of Θ originates from constraint 1. Since the conditions of Theorem 3 are fulfilled, the only possible candidate set is $k = \{1, 3, 4\}$, which produces a full-dimensional critical region $CR_{\{1,3,4\}}$. The three sides of $CR_{\{1,3,4\}}$, which have not yet been explored, are defined by the constraints 2, 5 and 6. Thus, the candidate active sets are given as $k_1 = \{1, 2, 3, 4\}$, $k_2 = \{1, 3, 4, 5\}$ and $k_3 = \{1, 3, 4, 6\}$. However, since A_{k_1} is rank-deficient, it results in the candidates from the dual simplex step, i.e. $k_{11} = \{1, 2, 3\}$, $k_{12} = \{1, 2, 4\}$ and $k_{13} = \{2, 3, 4\}$.

For k_{11} , k_{12} and k_{13} the algorithm returns empty critical regions, and thus they are not considered further. Conversely, k_2 and k_3 result in full-dimensional critical regions. Both of

them only feature one side that has not yet been explored associated with constraint 2, which results in $k_4 = \{1, 2, 3, 4, 5\}$ and $k_5 = \{1, 2, 3, 4, 6\}$. Since A_{k_4} and A_{k_5} are rank-deficient⁹, the following candidate sets are generated: $k_{41} = \{1, 2, 3, 4\}$, $k_{42} = \{1, 2, 3, 5\}$, $k_{43} = \{1, 2, 4, 5\}$, $k_{44} = \{2, 3, 4, 5\}$ and $k_{51} = \{1, 2, 3, 4\}$, $k_{52} = \{1, 2, 3, 6\}$, $k_{53} = \{1, 2, 4, 6\}$, $k_{54} = \{2, 3, 4, 6\}$. However, all of these active sets yield empty critical regions. Thus the algorithm terminates and all four critical regions have been identified.

Note that on the contrary to the combinatorial algorithm, the graph-based algorithm only required the consideration of 13 nodes (16 if the rank-deficient ones are counted). Additionally, no considerations regarding step-size or the identification of the active set based on the solution of the QP needs to be performed as necessary in the geometrical approach. A graphical representation of the solution of the example problem is given in Figure 3.5.

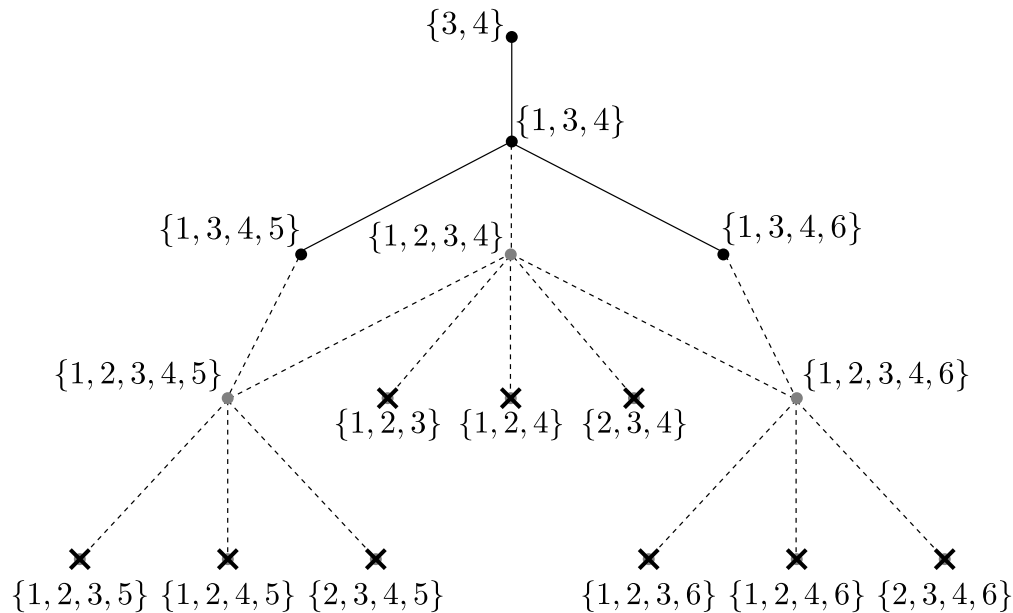


Figure 3.5: The new approach from the combinatorial perspective, where the solid lines represent connections between the nodes while the dashed lines represent attempted connections. At each iteration, all combinations are generated based on Theorem 3 and one step of the dual simplex algorithm.

3.3.8 Comparison with the work by Ahmadi-Moshkenani *et al.*

Independently of the developments presented in this thesis, a number of conference papers by Ahmadi-Moshkenani *et al.* have appeared discussing the "Exploration of Combinatorial Tree

⁹Since $n = 4$, it is obvious that any active set featuring more than 4 constraints would be rank deficient. This is the situation arising in mp-LP problems, where the conditions from [91] apply.

in Multi-Parametric Quadratic Programming” [5, 6]. The main contribution is thereby ”a method for exploring the combinatorial tree which exploits some of the underlying geometric properties of adjacent critical regions as the supplementary information in combinatorial approach to exclude a noticeable number of feasible candidate active sets from combinatorial tree” [6].

The similarity with the connected graph approach presented here is that the papers by Ahmadi-Moshkenani *et al.* use Theorem 3 in a combinatorial setting. However, the consequences and underlying properties differ from the connected graph approach, and are discussed in detail in the following. Note that for simplicity, this approach will be referred to as ”new approach” below, in order to avoid confusion.

Algorithm design: The connected graph algorithm removes all redundant constraints to identify the irredundant facets which will then, based on Theorem 3, directly yield the active set of the adjacent critical region. On the contrary, the new approach does not consider each individual facet, but the fact that Theorem 3 dictates the cardinality of the adjacent regions. For example, consider the example problem and let $k = \{1, 3, 4\}$. Then, after this has been identified as a full-dimensional critical region, the new algorithm would spawn the following new candidates:

- From Type I: $\{1, 2, 3, 4\}$, $\{1, 3, 4, 5\}$, $\{1, 3, 4, 6\}$, $\{1, 3, 4, 7\}$, $\{1, 3, 4, 8\}$
- From Type II: $\{1, 3\}$, $\{1, 4\}$, $\{3, 4\}$.

Thus, the new algorithm does not require the removal of redundant constraints, but limits the number of spawned candidate active sets by incorporating Theorem 3.

The solution is a connected graph: This statement only arises when the work by Gal and Nedoma is considered for the cases where LICQ is violated on the facets. However, this cannot be detected with the new algorithm, and thus this property is not derived.

Degeneracy handling: In the connected graph approach, degeneracy is naturally handled as it can be automatically detected when considering a specific facet. Conversely, the new algorithm initially proposed a post-processing method in [6], which effectively applies the geometrical algorithm at the end of the combinatorial algorithm to ensure the entire parameter space is explored. However, the authors stated in [5] that such post-processing ”is timeconsuming and prone to numerical errors in high-dimensional systems” [5]. Thus, a new strategy is equivalent to a step in the dual simplex algorithm, and thus identical to the work presented here.

Strict complementary slackness: The authors of the new approach consider several cases where strict complementary slackness would not be fulfilled. However, such a condition is not relevant for strictly convex mp-QP problems, as the minimizer is guaranteed to be unique.

3.4 Computational aspects of mp-QP problems

Despite its importance to the solution of explicit MPC problems, so far there has been no attempt in the open literature to contrast and compare the different solution techniques available for mp-QP problems. This section aims at providing an initial analysis of the computational aspects of mp-QP algorithms using test sets and example problems¹⁰. Unless stated otherwise, the computational experiments are performed on a 4-core machine with an Intel Core i5-4200M CPU at 2.50 GHz and 8 GB of RAM. Furthermore, MATLAB R2014a and IBM ILOG CPLEX Optimization Studio 12.6.1 was used for the computations. The mp-LP and mp-QP algorithms tested are:

- The geometrical algorithm [14]
- The combinatorial algorithm [110]¹¹
- The Multi-Parametric Toolbox (MPT) v3.1 [120], which reformulates the mp-LP and mp-QP problem into a multi-parametric linear complementarity problem (mp-LCP) which is solved using a combinatorial algorithm.
- The connected graph algorithm presented in this chapter.

In order to verify the correctness of the obtained solution, 5000 points $\hat{\theta} \in \Theta$ are randomly generated, and the corresponding LP or QP problem is solved for that parameter realization and compared to the parametric solution.

3.4.1 Computational performance of mp-QP algorithms on test sets

First, the algorithms are used to solve the test sets 'POP_mpLP1' and 'POP_mpQP1' from the POP toolbox are used, consisting of 100 mp-LP and 100 mp-QP problems, respectively. Please see Figure A.1 for the problem statistics and a discussion on the test set in section

¹⁰The example problems are explicit MPC problems, the formulation of which is considered in section 5.2.

¹¹Note that on the contrary to [110], this implementation first checks for feasibility, before performing the optimality checks.

A.3.1. The results of the computational study are shown in Figure 3.6. Additionally, a more detailed analysis of the computational aspects of the geometrical, combinatorial and the connected graph algorithm are investigated in Figure 3.7 for 'POP_mpLP1' and 3.8 for 'POP_mpQP1'. For the geometrical algorithm, the three aspects considered are (a) solution of the QP problem, (b) removal of redundant constraints and (c) identification of a new point θ_0 . For the combinatorial and the connected graph algorithm, the different aspects are (a) validation whether the selected active set was already considered or can be discarded as infeasible, (b) establishing feasibility and (c) establishing optimality.

Remark 16. Note that the computational effort of finding the first critical region is not considered. Thus, for cases where the overall solution time is relative low (i.e. a few seconds or lower), the sum of the aspects considered will not add up to 1.

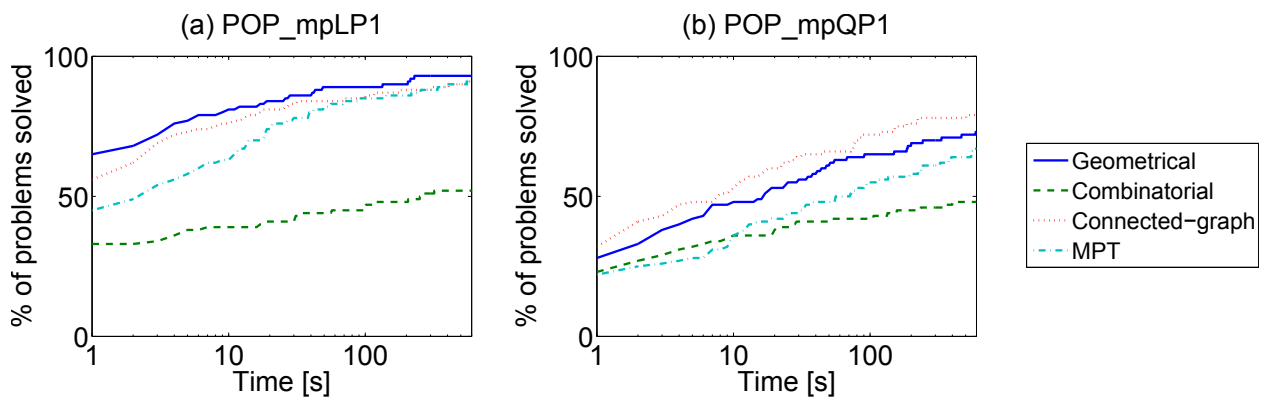


Figure 3.6: The results of the computational study for (a) the 'POP_mpLP1' test set and (b) the 'POP_mpQP1' test set.

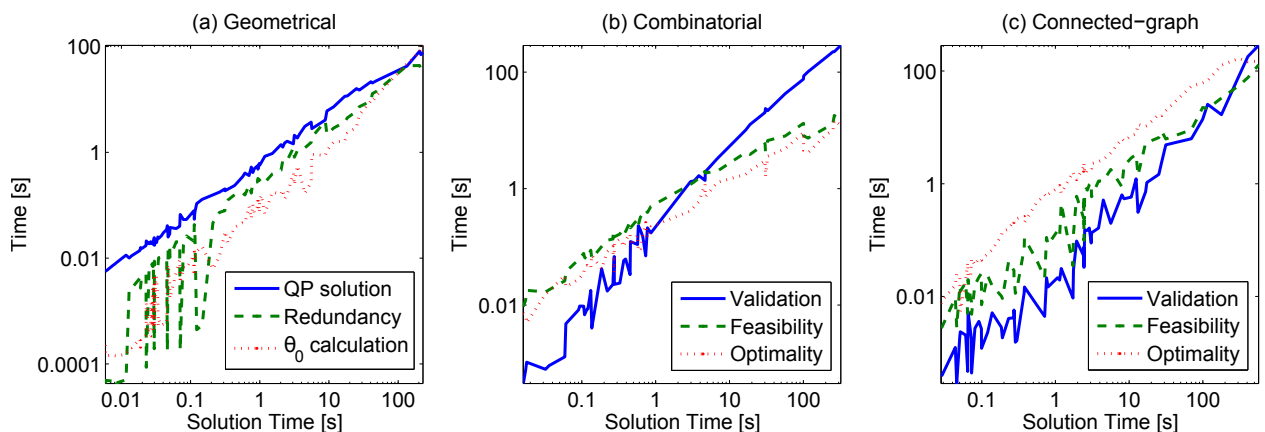


Figure 3.7: The analysis of the computational effort spent on different aspects of the algorithm for the geometrical, combinatorial and connected graph algorithm for the test set 'POP_mpLP1'.

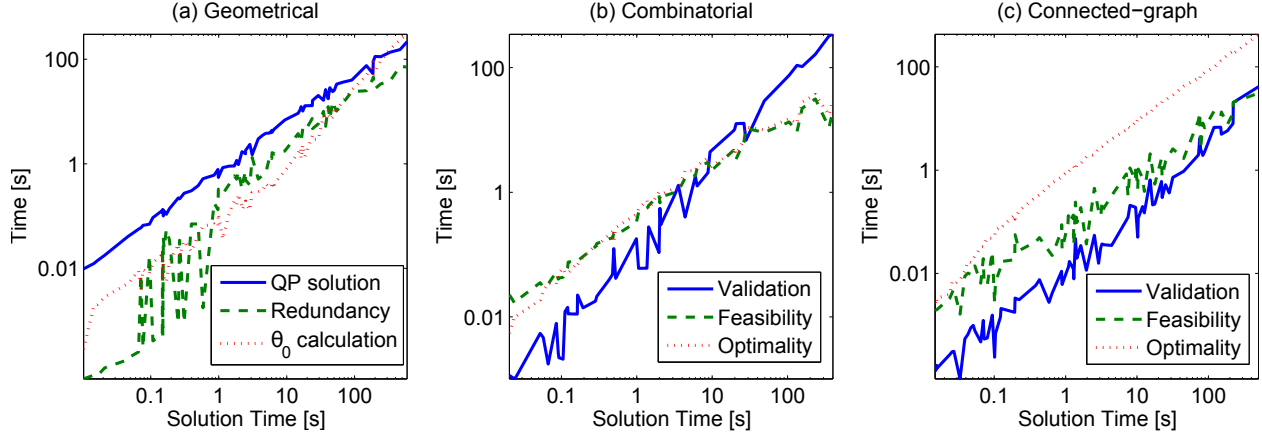


Figure 3.8: The analysis of the computational effort spent on different aspects of the algorithm for the geometrical, combinatorial and connected graph algorithm for the test set 'POP_mpQP1'.

3.4.2 Computational performance of mp-QP algorithms for a combined heat and power system

In order to analyze the capabilities of the different algorithms on real-world example, a combined heat and power (CHP) system is considered. Generally, cogeneration systems aim at increasing the system efficiency and reduce the environmental footprint by combining the production of usable heat and electrical power into a single process based on the same amount of fuel [64]. It is common practice to treat any cogeneration system as the interactions between an electrical power production subsystem and a heat generation subsystem [65]. Based on a high-fidelity CHP model, and following the PAROC framework (see Appendix B), a linear state space of the power generation subsystem capturing its dynamic behavior of the system can be developed as follows [220]:

$$x_{k+1} = 0.9913x_k + 0.00442u_k \quad (3.17a)$$

$$y_k = 3.593x_k, \quad (3.17b)$$

where $x_k \in \mathbb{R}^n$ denotes the identified system state, $u_k \in \mathbb{R}^m$ denotes the system input that determines the amount of fuel and air entering the power generation subsystem and $y_k \in \mathbb{R}^p$ denotes the amount of electrical power at time k , respectively. The approximate state space

model is thus used to formulate a MPC problem which focuses on setpoint tracking:

$$\begin{aligned}
& \underset{x}{\text{minimize}} && \sum_{k=1}^N (y_k^{SP} - y_k)^T 1000 (y_k^{SP} - y_k) + u_k^T 0.1 u_k + \Delta u_k^T 10 \Delta u_k \\
& \text{subject to} && x_{k+1} = 0.9913 x_k + 0.00442 u_k \\
& && y_k = 3.593 x_k + \hat{e} \\
& && 0 \leq x_k \leq 0.7 \\
& && 0 \leq u_k \leq 1 \\
& && -0.1 \leq \Delta u_k \leq 0.1, \forall k \in [1, N],
\end{aligned} \tag{3.18}$$

where N is the output and control horizon, which for the purposes of this computational study have been set to equal.

The MPC problem is recast as a mp-QP problem [31], considering the initial states x_0 , the control variables at the previous time step u_{k-1} , the deviation from the high-fidelity model output at the initial step $\hat{e} = y_0^{REAL} - y_0$ and the output setpoint y_k^R as uncertain but bounded parameters. The multi-parametric programming counterpart of the control problem of eq. (3.18) is solved for $N \in [2, 10]$.

In Figure 3.9, the development of the computational burden with increasing horizon length N is shown.

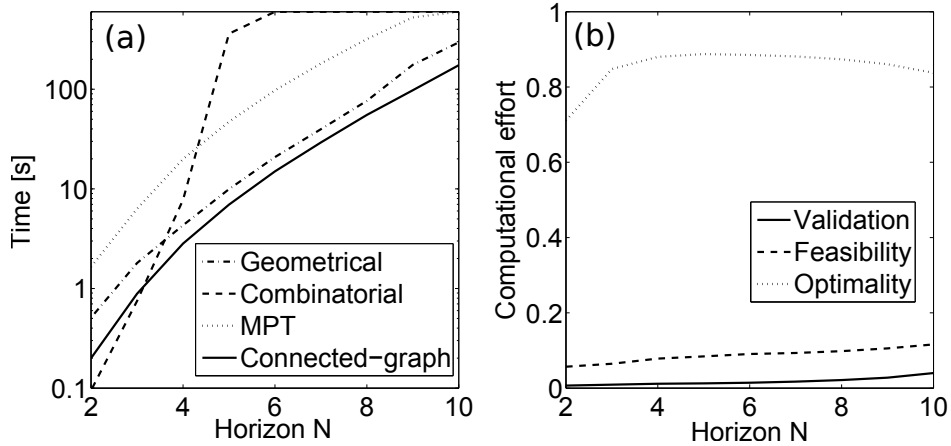


Figure 3.9: The computational results for the solution of the controller for the CHP system described in eq. (3.17). In (a) the performance of the different solution algorithms is shown as a function of time, while in (b) the distribution of the computational load as a function of the horizon for the case of the connected graph algorithm is shown.

3.4.3 Computational performance of mp-QP algorithms for a periodic chromatographic separation system

As another real-world example, the challenging problem of optimally controlling a periodic chromatographic separation system is considered [9, 186, 220]. The twin-column Multicolumn Countercurrent Solvent Gradient Purification Process (MCSGP) is an ion-exchange, semi-continuous chromatographic separation process, used for the purification of several biomolecules [150]. The setup comprises two chromatographic columns, operating in countercurrent mode and alternated between batch and interconnected state. Here, the focus is laid upon the purification of a monoclonal antibody (mAb) from a ternary mixture, composed by weak impurities (W), the product (P) and strong adsorbing impurities (S). As described in [150], at the beginning of I1 phase, column 2 starts empty and equilibrated. During this step, the outlet flow of column 1 enters column 2 mixed with an additional fraction of adsorbing eluent (E). This helps the recycling of the impure fraction of the weak impurities and the product. After the completion of I1, the two columns enter B1 phase, where the feed (F) is introduced to column 2 and the product is eluted from column 1. In I2 phase the recycling stream containing the impure fraction of product and strong impurities exits column 1 and enters column 2. By the end of I2 phase, column 2 starts eluting pure W (B2 phase). B2 phase finishes when the overlapping region of W and P reach the end of column 2. At this point the two columns switch positions. Therefore, column 1 will go through the recycling and feeding tasks as described above, while column 2 will continue with the gradient elution.

The MCSGP process is described by a PDAE model capturing the events taking place during the chromatographic separation [9, 186]. The model is based on first principles and follows a lumped-kinetic approach comprising 4119 equations with highly nonlinear terms (after spatial discretization, using 50 collocation points). For a detailed approach on the model development, the reader is referred to [187, 209].

Each chromatographic column can be approximated by a Single Input-Multiple Output (3x1 SIMO) linear state space model that is used for the formulation of the mp-QP problems [209]. The model is derived using system identification in MATLAB® and its formulation is given below:

$$x(t + T_s) = Ax(t) + Bu(t) + Dd(t) \quad (3.19a)$$

$$y(t) = Cx(t), \quad (3.19b)$$

where x , u , y are the states, inputs and outputs respectively, t corresponds to the time, T_s

is the sample time and A, B, C, D represent the matrices of the state space model, i.e.

$$A = \begin{bmatrix} 0.9998 & 0.0003667 & 0.0004885 & -9.137 \cdot 10^{-5} \\ 0.0009448 & 0.9971 & -0.003154 & -0.001599 \\ -0.001027 & 0.0003536 & 0.999 & 0.001881 \\ 0.000969 & 0.001559 & 0.0005033 & 0.9976 \end{bmatrix} \quad (3.20a)$$

$$B = \begin{bmatrix} -6.252 \cdot 10^{-6} \\ 4.514 \cdot 10^{-5} \\ 6.337 \cdot 10^{-5} \\ -3.396 \cdot 10^{-5} \end{bmatrix} \quad (3.20b)$$

$$C = \begin{bmatrix} 545.6 & 101.1 & 17.69 & 7.422 \\ 2925 & 660.2 & 102.6 & -67.49 \\ 331.9 & 78.42 & 17.12 & -11.23 \end{bmatrix} \quad (3.20c)$$

$$D = \begin{bmatrix} 1.557 \cdot 10^{-5} & 8.449 \cdot 10^{-5} & 9.616 \cdot 10^{-6} \\ -9.018 \cdot 10^{-5} & -0.0004893 & -5.57 \cdot 10^{-5} \\ -3.487 \cdot 10^{-5} & -0.0001892 & -2.154 \cdot 10^{-5} \\ 3.698 \cdot 10^{-5} & 0.0002007 & 2.284 \cdot 10^{-5} \end{bmatrix} \quad (3.20d)$$

The state space model is validated against the mathematical, process model and resulted into: 94.88%, 94.93% and 93.06% fit for the three outputs respectively.

In Figure 3.10, the computational performance is presented for different output and control horizons N_{OH} and N_{CH} , respectively. The problem size thereby varies from 13 parameters, 2 optimization variables and 20 constraints up to 62 parameters, 10 optimization variables and 240 constraints.

3.4.4 Discussion and qualitative heuristics

For mp-LP problems, the results from the test set indicate that the most efficient algorithm seems to be the geometrical algorithm (see Figure 3.6 (a)). This is due to the fact that for the combinatorial algorithm, the solution of the problem will always be found in a vertex, suggesting a smaller fathoming efficiency than for mp-QP problems. For the connected graph algorithm, it is necessary to consider all possible outcomes from the step of the dual simplex algorithm. Thus, especially for larger problems the geometrical approach avoids the resulting combinatorial problem. Note that since MPT has implemented a combinatorial version of a mp-LCP algorithm, it is assumed to suffer from the same problems as the combinatorial approach.

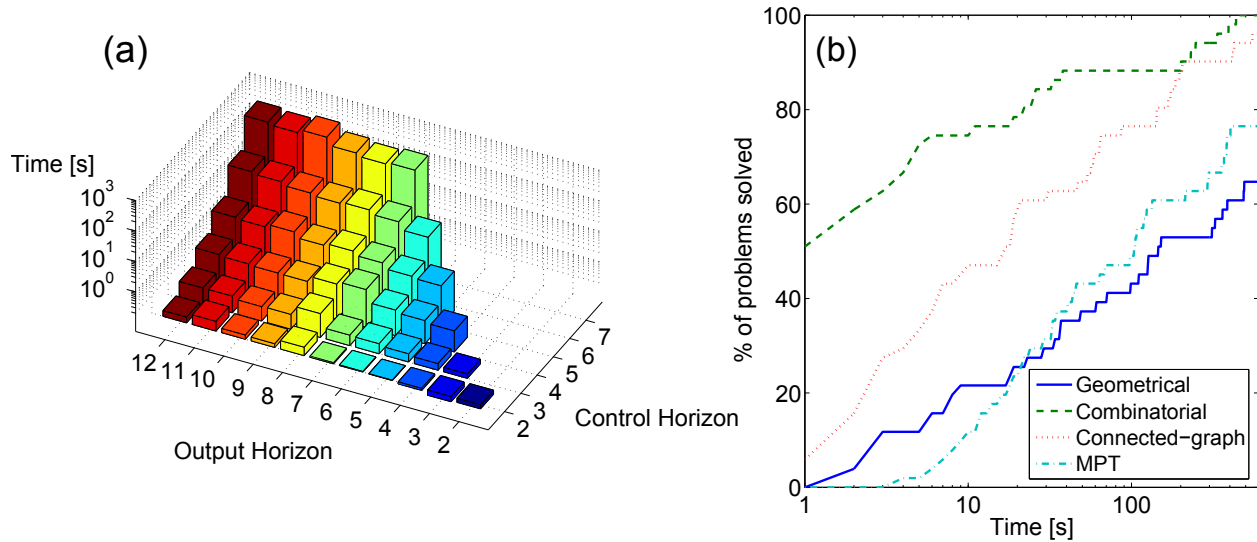


Figure 3.10: The computational results for the optimal control of a periodic chromatographic separation system. In (a) the computational time using the combinatorial algorithm for different control and output horizons is shown while (b) presents the percentage of problems solved as a function of time required. The different problems result from the consideration of different output and control horizons.

For mp-QP problems, there are three computational results: the test set, the CHP system and the MCSGP system. For the test set and the CHP system, the connected graph is the most efficient algorithm, followed by the geometrical algorithm, MPT and finally the combinatorial algorithm (see Figure 3.6 (b) and 3.9). The efficiency of the connected graph algorithm is thereby attributed to the high efficiency when finding optimal active sets. For the test set on average 68 % of the active sets considered were optimal, i.e. resulted in a full-dimensional critical region, which is significantly higher than the 36 % obtained from the combinatorial approach (for the mp-LP test set: 51 % and 19 % respectively).

However, for the MCSGP case, the combinatorial algorithm is most efficient, followed by the connected graph, MPT and geometrical algorithm. The reason for this shift is the different type of problem under consideration. The controller design presented here results in a problem with a large number of parameters (up to 62). Thus, the geometrical algorithm has to explore a 62-dimensional parameter space which seems to be computationally less favorable than the combinatorial approach. The connected graph approach initially seems to suffer from the same drawback as the geometrical algorithm, as it requires the removal of redundant constraints for a 62-dimensional polytope. However, with increased computational time, the algorithm seems to become more competitive with respect to the combinatorial algorithm.

In terms of computational effort, the geometrical algorithm does not have a clear bot-

tleneck, as the QP solution and the θ_0 calculation both demand a large part of the computational power. Conversely, the combinatorial and the connected graph seem to have a relatively clear bottleneck. The combinatorial algorithm is limited by the time required for the validation of the active set, while the connected graph is limited by the optimality requirement which is primarily associated with the removal of redundant constraints. This is an interesting perspective as this indicates that the number of candidates generated is not computationally limiting, but rather the way in which these are generated. This conclusion is supported by the computational results from the heat recovery subsystem for the CHP system (see Figure 3.9 (b)), where the connected graph approach also outperforms every other algorithm considered here.

Thus, based on these results, no algorithm is clearly superior to the others. In addition, none of the algorithms have been proven to improve on the worst-case complexity. As a result, any comparison between them highly depends on the specific problem under consideration. However, in the following several heuristics for the geometrical, combinatorial and connected graph algorithms are provided, which mirror the strengths and weaknesses of the different algorithms.

Remark 17. Note however that these are merely indicative and it is still impossible to predict prior to solving the problem which approach will be the most efficient technique.

The geometrical approach:

- In the case of well-behaved mp-QP problems, it is highly efficient.
- For pathological mp-QP problems and in general for mp-LP problems, the risk of incomplete exploration of the parameter space is significant and thus the use of a geometrical approach should be avoided.
- The algorithm tends to scale well if the number of optimization variables increases.
- For problems with large numbers of constraints, the algorithm tends to perform poorly due to the requirement of removing redundant constraints at each step.

The combinatorial approach:

- The combinatorial algorithm is ill-suited for mp-LP problems as it requires the exhaustive enumeration of all options.
- For problems with a large number of constraints but few optimization variables, the combinatorial algorithm has been proven to be effective.
- If the problem contains symmetry elements, then this can be utilized to increase the pruning efficiency as thus the overall efficiency of the algorithm.

The connected graph approach:

- As the connected graph approach is guaranteed to explore the entire parameter space, it is well suited for the solution of mp-LP problems as it does not necessarily require the exhaustive enumeration of all combinations.
- The connected graph approach is ill-suited for dual degenerate mp-LP problems, as the presence of disconnected graphs may result in incomplete parameter space exploration.
- In the case of well-behaved mp-QP problems, the connected graph approach has also been shown to be highly efficient since, if Theorem 3 is applicable, the adjacent active set can be identified unambiguously, thus dramatically reducing the number of candidate active sets to consider.
- Similarly to the geometrical approach, the connected graph approach relies on the removal of redundant constraints. Thus, problems featuring large number of constraints tend to be ill-suited for the connected graph approach.

Remark 18. Note that the worst-case computational complexity of all these algorithms is still exponential in the optimization variables.

3.4.5 Parallel multi-parametric quadratic programming

Despite the availability of different solution approaches, solving mp-QP problems is still a computationally expensive task. However, despite that, so far the use of parallel computing in multi-parametric programming (mp-P) algorithms has not been documented, and the only contribution related to mp-P considers the point location problem, a problem closely related to explicit MPC [265]. Note that while the MPT toolbox [118] explicitly considers parallel programming, neither is the exact strategy clear nor has MPT documented their procedure. Furthermore, initial tests seem to indicate that the solution using parallel computing requires more time than the sequential version. Thus, the application of parallel computing does not seem to be straightforward.

In order to investigate the applicability of parallel computing to the solution of mp-QP problems, the geometrical algorithm is considered [14]. The parallelization thereby takes place over the elements of N , i.e. the facets of the critical regions constituting the solution.

Parallelization inherently exploits independent aspects of an algorithm and distributes them on different machines, where these independent subproblems are computed in parallel. The non-overlapping nature of the critical regions thereby naturally generates independent subproblems which can be solved in parallel. Additionally, as the solution of a subproblem

```

1:  $N = 0, \mathcal{S} = \emptyset, \theta_0 \in \Theta$ 
2: Solve first iteration, get  $\mathcal{S} \leftarrow (CR_0, x_0(\theta), \lambda_0(\theta))$  and  $N = \mathcal{H}(CR)$ 
3: while  $N \neq \emptyset$  do
4:   Pop halfspace  $\omega(\theta) \leq 0$  from  $N$ 
5:   Using variable step-size, find  $\theta_0 \in \Omega := \{\theta_0 \in \Theta | \omega(\theta_0) > 0\}$ 
6:   Fix  $\theta_0$  in problem (3.1), and solve the resulting QP; identify  $x_0, \lambda_0$ 
7:   if feasible then
8:     Obtain  $x(\theta)$  and  $\lambda(\theta)$  from Basic Sensitivity Theorem
9:     Obtain  $CR = \{\theta \in \Theta | Ax(\theta) \leq b + F\theta, \lambda(\theta) \geq 0\}$  and remove redundant constraints
10:     $\mathcal{S} \leftarrow (CR, x(\theta), \lambda(\theta))$ 
11:     $N \leftarrow \mathcal{H}(CR)$ 
12:   end if
13: end while

```

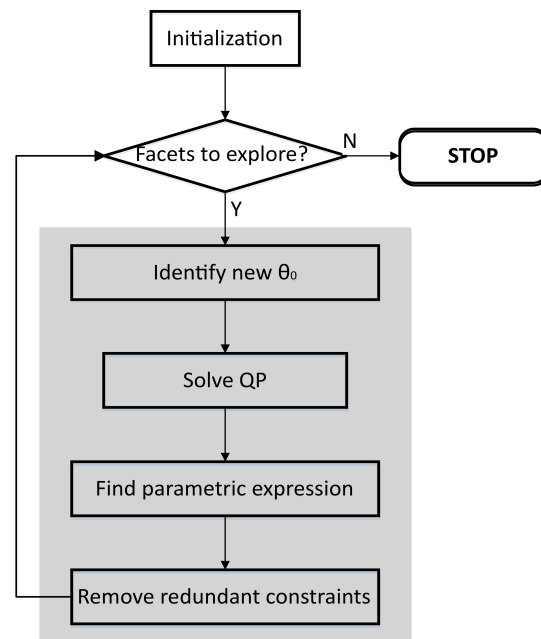


Figure 3.11: The solution approach for problem (3.1) presented in [14]. Note that $\mathcal{H}(CR)$ denotes the half-spaces defining critical region CR , and that the part highlighted in gray is executed in parallel.

might generate new subproblems due to the exploration of the parameter space, the concept of the limiting iteration number ρ_{limit} is defined:

Definition 9. The limiting iteration number ρ_{limit} is the maximum number of iterations performed on a single machine before the result is returned to the main algorithm.

Hence it is possible to choose between continuing the current computation locally or to return the results to the main algorithm and perform a re-distribution of the problems. The resulting trade-off is between an increased overhead resulting from the information transfer between the machines and the possibility of calculating possibly suboptimal or unnecessary solutions, as the re-distribution always ensures that the algorithm performs optimally.

Remark 19. Since at the end of the algorithm all results are combined together, the final solution is always optimal.

Consequently, the parallelization strategy proposed here can be summarized as follows:

Step 1: Formulation of the sequential solution algorithm

Step 2a: Identification of the most external iterative procedure

Step 2b: Identification of the independent elements computed at each iteration

Step 2c: Definition of ρ_{limit}

Step 3: Connection to different machines and equal distribution of elements

Step 4: Execution of the current computation locally until (i) the pre-defined termination criteria are met or (ii) the number of iterations has reached ρ_{limit}

A graphical representation of the use of ρ_{limit} is shown in Figure 3.4.5.

Results of the parallelization

The computations of the numerical examples were carried out on a 4-core machine with an Intel Core i7-4790 CPU at 3.60 GHz and 16 GB of RAM. Furthermore, MATLAB R2015a, IBM ILOG CPLEX Optimization Studio 12.6.2 and NAG MB24 was used for the computations. The proposed parallelization algorithm was tested on a randomly generated test set of 52 mp-QP problems, and key problem statistics are reported in Figure 3.4.5. Note that the test set has been ordered in ascending order with respect to the time needed to solve the problem sequentially.

In order to define the efficiency of the parallelization, the concept of a speedup factor is defined:

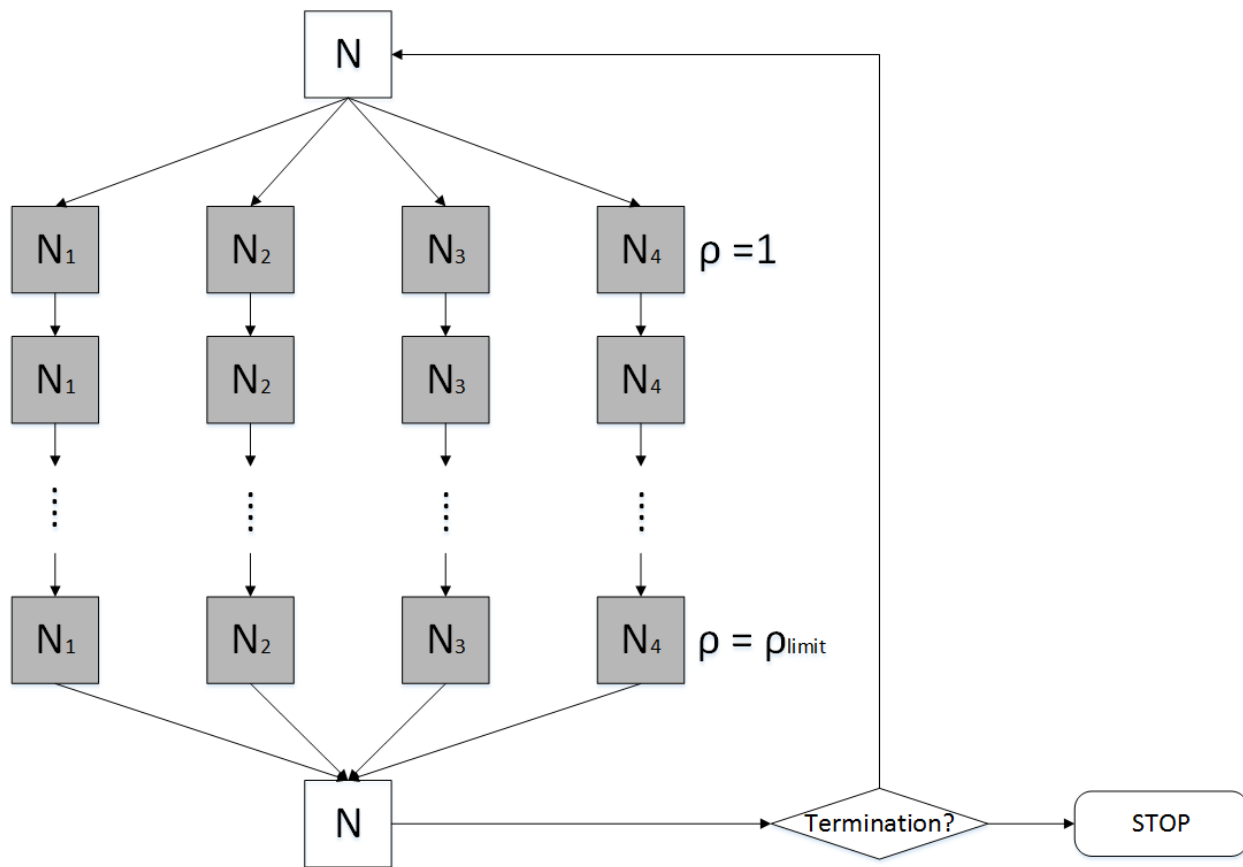


Figure 3.12: A schematic depiction of the influence of the ρ_{limit} parameter.

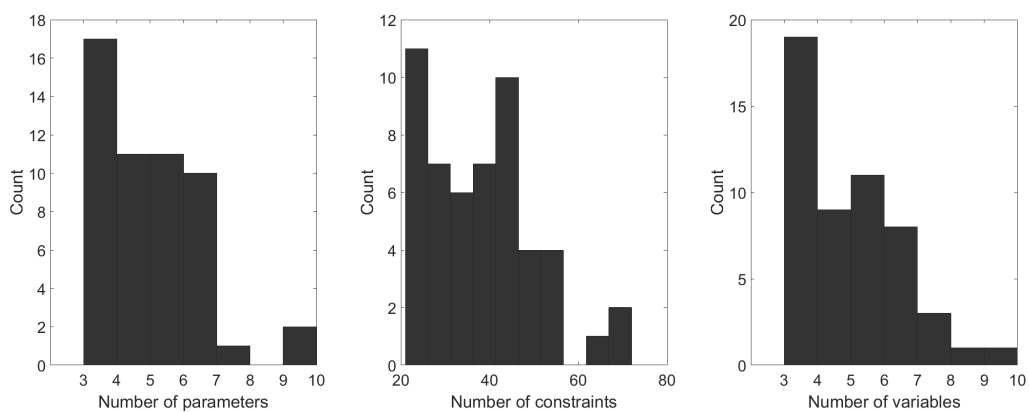


Figure 3.13: The key problem statistics for the randomly generated test set: (a) the number of variables, (b) the number of parameters and (c) the number of constraints for each test problem.

Definition 10. The speedup factor Ψ is defined as

$$\Psi = \frac{t_{Sequential}}{t_{Parallel}}, \quad (3.21)$$

where $t_{Parallel}$ and $t_{Sequential}$ are the time needed to solve the parallelized and sequential algorithm, respectively.

In Figure 3.4.5 (a) the average speedup factor is reported as a function of the number of cores with $\rho_{limit} = 1$, while in Figure 3.4.5 (b) the average speedup factor is shown as a function of ρ_{limit} , with the number of cores set to 4. In order to highlight the impact of parallel computing onto the computational efficiency, the development of a MPC controller for a residential combined heat and power (CHP) system is considered [65, 220]. The reduced-order model of the heat recovery subsystem used here is given as

$$x_{k+1} = \begin{bmatrix} 0.9712 & -0.0207 & -0.0529 \\ 0.0012 & 0.8169 & -0.0524 \\ -0.0099 & -0.0302 & 0.9551 \end{bmatrix} x_k + \begin{bmatrix} -0.0245 & -0.0079 \\ -0.1009 & 0.0593 \\ -0.02457 & 0.0125 \end{bmatrix} u_k \quad (3.22)$$

where x_k and u_k are the states and inputs of the system at time k , respectively. The corresponding MPC problem¹² is then given as

$$\begin{aligned} & \underset{x}{\text{minimize}} && x_N^T P x_N + \sum_{k=0}^{N-1} x_k^T Q x_k + u_k^T R u_k \\ & \text{subject to} && \text{Eq. (3.22)} \\ & && x_k \in [-5, 5]^2, \quad \forall k = 0, \dots, N \\ & && u_k \in [-2, 2]^2, \quad \forall k = 0, \dots, N - 1, \end{aligned} \quad (3.23)$$

where matrices have appropriate dimensions. The computational time as a function of the horizon length N is reported in Figure 3.4.5 (c), which clearly shows the computational gains possible from parallel computing.

Discussion

The results in Figure 3.4.5 indicate that the parallelization leads to a speedup of the solution time. However, investigations which are currently underway indicate that the results here cannot be generalized for the geometrical algorithm, and that in general the parallelized version is less efficient than the sequential code. The main reason for this is that the overhead

¹²In the light of brevity and conciseness, the problem formulation presented here is intentionally simplistic in the sense that it does not consider elements such as outputs, disturbances or possible differences between control and output horizons.

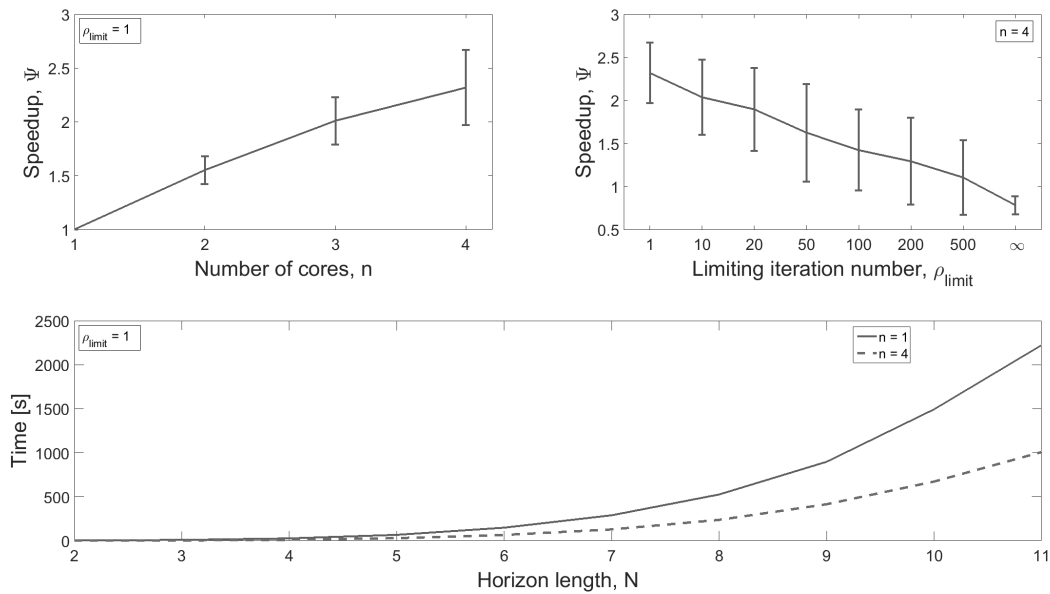


Figure 3.14: The numerical results for the speedup of the computation by using parallel computing. In (a), the computational benefits as a function of the number of cores is shown while in (b) the dependence on the number of iterations performed on a single thread is investigated. In (c) the computational benefits obtained when using parallel computing are shown for the multi-parametric model predictive control of a combined heat and power system.

is extremely high for larger problems: the point on the facet from which the parameter space has to be explored as well as all the critical regions in their explicit representation.

However, as shown in Table 3.2, the parallelization approach developed here for the geometrical algorithm can be applied to several other algorithms for the solution of multi-parametric programming problems. This is due to the fact that the presence of non-overlapping critical regions naturally lends itself to parallel computing, which bases its computational benefits on the distribution of independent elements or tasks onto different machines and the parallel execution of the required operations on these machines.

In particular, the parallelization of the combinatorial and the connected graph approach has been implemented and has yielded very good results so far. An extensive numerical investigation is currently underway, however it appears that a good value for ρ_{limit} seems to be 100. The authors is pleased to report that this approach has already been implemented in the POP toolbox and has been used on high-performance computing architectures.

Table 3.2: The problem class and corresponding independent element of several classes of multi-parametric programming algorithms

Problem class	Independent elements
Multi-parametric linear and quadratic programming - geometrical approach [14, 74]	Each facet/critical region
Multi-parametric linear and quadratic programming - combinatorial and connected graph approach [110]	Each combination of active sets
Direct multi-parametric dynamic programming [43]	Each critical region of the previous stage
Multi-parametric mixed-integer programming - Global optimization [74, 199]	Each critical region
Multi-parametric mixed-integer programming - Branch and bound and exhaustive enumeration [40, 200]	Each node/integer combination

3.5 Multi-objective optimization with convex quadratic cost functions as a new application for mp-QP problems

While the solution of mp-QP problems is mostly required for explicit MPC problems, this section shows that there are also other applications where the solution of mp-QP problems

can be applied suitably. Consider the following multi-objective optimization (MOO) problem

$$\begin{aligned} & \underset{x}{\text{minimize}} && \{f_1(x), f_2(x), \dots, f_N(x)\} \\ & \text{subject to} && Ax \leq b, \\ & && x \in \mathbb{R}^n, \end{aligned} \tag{3.24}$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and the objective functions are of the form

$$f_i(x) = x^T Q_i x + c_i^T x + d_i, \quad \forall i = 1, \dots, N, \tag{3.25}$$

where $Q_i \in \mathbb{R}^{n \times n} \succ 0$, $c_i \in \mathbb{R}^n$ and $d_i \in \mathbb{R}$, $\forall i = 1, \dots, N$. Problems of type (3.24) arise in many different applications, such as engineering, economics and biological systems [54, 182, 183]. A solution x^* of problem (3.24) is thereby called optimal if it is a Pareto point.

Definition 11 (Pareto point and Pareto front). A point x^* is called a Pareto point if there does not exist a point \hat{x} such that there exists $f_i(\hat{x}) < f_i(x^*)$ and $f_j(\hat{x}) \leq f_j(x^*)$, $j \neq i$. The set of all Pareto points is called the Pareto front \mathcal{P} .

One of the most well known strategies to obtain a Pareto point is the ϵ -constraint method¹³, i.e.

$$\begin{aligned} & \underset{x}{\text{minimize}} && f_1(x) \\ & \text{subject to} && f_j(x) \leq \epsilon_j, \quad \forall j = 2, \dots, N \\ & && Ax \leq b \\ & && x \in \mathbb{R}^n, \end{aligned} \tag{3.26}$$

where the parameter ϵ_j denotes an upper bound on the function $f_j(x)$. Another important strategy is the linear scalarization method¹⁴, i.e.

$$\begin{aligned} & \underset{x}{\text{minimize}} && \sum_{i=1}^N w_i f_i(x) \\ & \text{subject to} && Ax \leq b, \\ & && w_i \geq 0, \quad \forall i = 1, \dots, N, \\ & && \sum_{i=1}^k w_i = 1, \\ & && x \in \mathbb{R}^n, \end{aligned} \tag{3.27}$$

However in both strategies the solution of the MOO problem depends on the values of certain parameters, namely ϵ_j and w_i . Hence, while many researchers consider the iterative

¹³Note that the choice of $f_1(x)$ as the objective function is arbitrary (see [183]).

¹⁴This method is sometimes also referred to as weighting method [183].

solution of the resulting optimization problems for different parameter values [8, 48], some attention has been given to the explicit calculation of the entire Pareto front *via* parametric programming¹⁵, which solves optimization problems as a function and for a range of certain parameters. In [93, 264] the authors consider the case of linear cost functions, and in [208] the case of a mixed-integer nonlinear MOO was considered. The case of quadratic cost functions was treated in [95, 96], although either only conceptually or for the case where the quadratic part remains constant. Thus in this section, an algorithm for the approximate explicit solution of MOO problems with general convex quadratic cost functions and linear constraints *via* multi-parametric programming is proposed.

3.5.1 Multi-objective optimization *via* multi-parametric programming

By inspection, it is clear that problem (3.24) results in a quadratically constrained quadratic programming (QCQP) problem, whose explicit solution would require the solution of a multi-parametric QCQP (mp-QCQP) for which no efficient solution approach exists¹⁶. In this section an algorithm to approximate the original mp-QCQP using a multi-parametric quadratic programming (mp-QP) with a suitable set of affine overestimators is presented, which can be readily solved with existing solvers.

Reformulation of mp-QCQP

In order to convert the mp-QCQP problem (3.26) into a mp-QP, given a convex quadratic function $f(x)$, a suboptimality gap ϵ and a domain $\mathcal{X} = \{x \in \mathbb{R}^n \mid Ax \leq b\}$, the aim is to find a suitable convex piecewise affine overestimator $\mathcal{F}(x) = \max_{1 \leq k \leq M} \{\bar{f}_1(x), \bar{f}_2(x), \dots, \bar{f}_M(x)\}$, such that

$$0 \leq \mathcal{F}(x) - f(x) \leq \epsilon \quad (3.28)$$

where

$$\bar{f}_k(x) = a_k^T x + b_k, \quad \forall k = 1, \dots, M. \quad (3.29)$$

Remark 20. It is well known that $\mathcal{F}(x)$ can be described via a set of linear inequalities [45].

¹⁵In the following, this is referred to as the explicit solution of a MPP problem.

¹⁶An exact algorithm has been derived for the single parameter case in [228]. Classically, the explicit solution of the Pareto front is approximated by solving a set of global optimization problems [175].

First, consider a point x_R and define

$$f(x) \geq f(x_R) + \nabla f(x_R)(x - x_R) \quad (3.30)$$

based on the first-order Taylor expansion. Given a suboptimality gap ϵ , it is obvious that the neighbourhood around x_R for which eq. (3.30) is a sufficient approximation is given by

$$f(x) - f(x_R) - \nabla f(x_R)(x - x_R) \leq \epsilon. \quad (3.31)$$

Substitution of $f(x) = x^T Q x + c^T x + d$ and $\nabla f(x) = 2Qx + c$ then yields

$$x^T Q x - 2x_R^T Q x + x_R^T Q x_R \leq \epsilon. \quad (3.32)$$

Thus, in order to ensure that eq. (3.32) holds over the entire domain \mathcal{X} , it is necessary to find a set of points x_R^i , $1, \dots, M$ such that

$$\begin{aligned} \epsilon \geq \eta = & \underset{x}{\text{maximize}} \quad \underset{i}{\text{minimize}} \quad x^T Q x - 2x_R^{i,T} Q x + x_R^{i,T} Q x_R^i \\ & \text{subject to} \quad x \in \mathcal{X}. \end{aligned} \quad (3.33)$$

Note that problem (3.33) is can be reformulated into a classical min-max problem via

$$\underset{x}{\text{maximize}} \underset{i}{\text{minimize}} F_i(x) = -\underset{x}{\text{minimize}} \underset{i}{\text{maximize}} (-F_i(x)), \quad (3.34)$$

for which commercial solvers are readily available (e.g. in the MATLAB[®] Optimization Toolbox). Thus, it follows that

$$\mathcal{F}(x) = \max_{1 \leq k \leq M} \{\bar{f}_1(x), \bar{f}_2(x), \dots, \bar{f}_M(x)\} \quad (3.35)$$

with

$$\bar{f}_i(x) = f(x_R^i) + \nabla f(x_R^i)(x - x_R^i) + \epsilon, \quad \forall i = 1, \dots, M. \quad (3.36)$$

Remark 21. As problem (3.33) is non-convex, the convexity assumption for the objective functions in eq. (3.25) is not necessary for the application of the general strategy outlined in this section. As however eq. (3.30) only holds for convex $f(x)$, it is necessary to choose a set of affine overestimators which do not require a convex objective function such as the McCormick relaxations [180].

The algorithm on how to calculate $\mathcal{F}(x)$ is presented in Algorithm 1.

Algorithm 1 Piecewise-affine approximation on $f(x)$

Require: $f(x)$, \mathcal{X} , ϵ

Ensure: $\mathcal{F}(x)$

- 1: Set $\eta \leftarrow \infty$, $x_R^1 = \arg \min\{\text{problem (2.4)}\}$, $M = 1$
 - 2: **while** $\eta > \epsilon$ **do**
 - 3: Solve problem (3.33)
 - 4: **if** $\eta > \epsilon$ **then**
 - 5: Set $M = M + 1$, $x_R^M = \arg \min\{\text{problem (3.33)}\}$
 - 6: **end if**
 - 7: **end while**
 - 8: Set $\mathcal{F}(x) = \{f(x_R^i) + \nabla f(x_R^i)(x - x_R^i), \forall i = 1, \dots, M\}$
-

Remarks

Initial point x_R^1 : The initial point of the algorithm is the Chebyshev center of the polytope \mathcal{X} .

Choice of ϵ : Obviously, the complexity of the approximation as well as the quality of the solution of the mp-QP problem depend on the choice of ϵ . As ϵ denotes the absolute suboptimality, it cannot be fixed without considering the objective function $f(x)$. The reason relative suboptimality is not used as a measure for the quality of the approximation is that it favours very tight approximation around the origin while looser approximations further off. In order to avoid this distortion, in this approach the following relation is defined:

$$\epsilon = \epsilon^* \max_x |f(x)|, \quad (3.37)$$

where ϵ^* is a normalized suboptimality. Note that the extreme point of $f(x)$ can be obtained with limited computational effort.

Solution of the multi-parametric programming problem

Thus, $\mathcal{F}_j(x)$ is substituted for each $f_j(x)$ into problem (3.26) and thus obtain the following mp-QP problem

$$\begin{aligned} & \underset{x}{\text{minimize}} && f_1(x) \\ & \text{subject to} && \mathcal{F}_j(x) \leq \epsilon_j, \quad \forall j = 2, \dots, N \\ & && Ax \leq b, \\ & && x \in \mathbb{R}^n, \\ & && \epsilon_j \in \mathcal{E} := \left\{ \epsilon \in \mathbb{R}^{N-1} \mid \epsilon_j^{\min} \leq \epsilon_j \leq \epsilon_j^{\max}, j = 1, \dots, N-1 \right\}. \end{aligned} \quad (3.38)$$

Note that problem (3.38) is a standard mp-QP problem, which can be readily solved with existing solvers.

Remark 22. The values for ϵ_j^{min} and ϵ_j^{max} denote the lower and upper bounds of the objective function.

Generation of Pareto front

In order to retrieve the Pareto front \mathcal{P} for problem (3.24), for each polytope CR_i the solution $x(\epsilon)$ is substituted into the objective functions $f_i(x(\epsilon))$, $\forall i$, thus resulting in the description of the Pareto front in the criterion space.

Theorem 6 (Correctness of Algorithm and Convergence). Algorithm 1 solves problem (3.24) approximately up to an accuracy of ϵ in finite time.

Proof 3. It is known that problem (3.26) solves problem (3.24) [183]. Additionally, problem (3.26) is solved by solving (3.38) up to a suboptimality gap ϵ . The algorithm converges in finite time since the number of critical regions is bounded from above [110].

3.5.2 Numerical Examples

Example problem

Consider the following example problem:

$$f_1(x) = x^T \begin{bmatrix} 2.5 & 0 \\ 0 & 7.5 \end{bmatrix} x + \begin{bmatrix} 3 \\ 0 \end{bmatrix}^T x, \quad f_2(x) = x^T \begin{bmatrix} 3.3 & 0 \\ 0 & 8.5 \end{bmatrix} x + \begin{bmatrix} 1 \\ -1 \end{bmatrix}^T x - 1, \quad (3.39a)$$

$$f_3(x) = x^T \begin{bmatrix} 3.5 & 0 \\ 0 & 0.25 \end{bmatrix} x + 2, \quad A = \begin{bmatrix} 4 & -3 \\ 0 & -3 \\ -4 & 2 \\ 6 & 0 \\ -6 & -2 \\ -9 & -1 \end{bmatrix}, \quad b = \begin{bmatrix} 20 \\ 14 \\ 8 \\ 20 \\ 39 \\ 17 \end{bmatrix} \quad (3.39b)$$

where $\epsilon_2 = [-1180, 1180]$ and $\epsilon_3 = [-375, 375]$. Using $\epsilon^* = 0.001$, the optimal partitioning of the parameter space as well as the Pareto front \mathcal{P} are shown in Figure 3.15.

Computational study

In order to investigate the scaling capabilities of the presented approach, the randomly generated set $\mathcal{X} = \{x \in [-10, 10]^5 \mid Ax \leq b\}$ is considered, where $A \in \mathbb{R}^{7 \times 5}$, $b \in \mathbb{R}^7$. Using

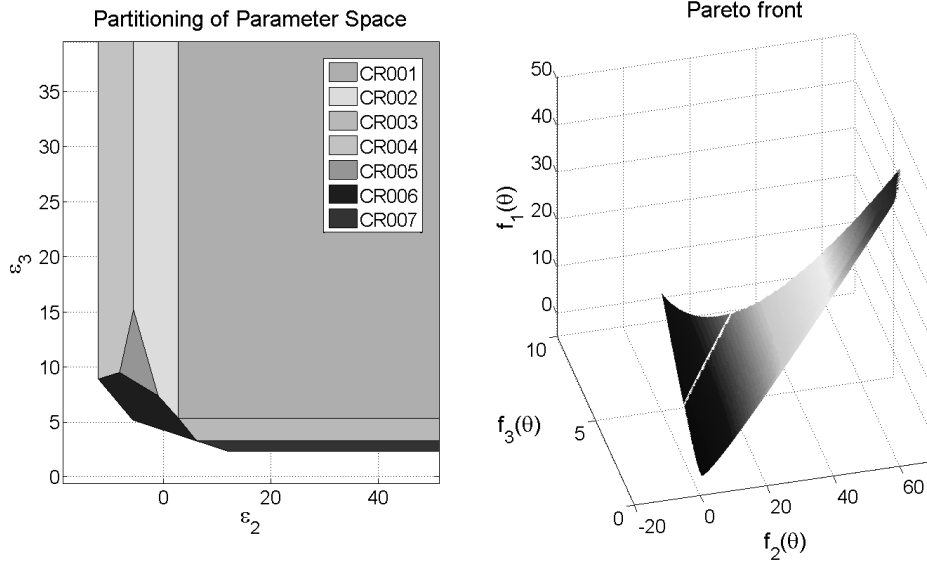


Figure 3.15: The solution of the example problem. Note that the partitioning of the parameter space has been zoomed into, in order to show the details of the partitioning, which are not visible when considering the entire space with $\epsilon_2 = [-1180, 1180]$ and $\epsilon_3 = [-375, 375]$.

$\epsilon^* = 0.1$ and starting from $N = 2$, subsequently randomly generated functions $f_i(x)$ are added to the problem and track its performance, shown in Table 3.5.2.

3.5.3 Application to linear scalarization

As mentioned in the introduction, one other key method for the formulation of multi-objective optimization problems is the the linear scalarization method. Clearly problem (3.27) can be reformulated as multi-parametric programming problem by treating the weights $w = [w_1, w_2, \dots, w_N]$ as parameters. This in turn leads to a multi-parametric non-linear

Table 3.3: Results from the computational study in seconds of section 3.5.2, where N is the number of objective functions and m the total number of constraints.

N	m	Time mp-QP [s]	Partitions
2	27	0.3	7
3	40	2.0	57
4	49	10.1	143
5	60	70.3	462
6	62	157.2	777
7	74	351.0	1317
8	88	1428.3	3313
9	100	2266.9	5470
10	112	4399.7	8309

programming (mp-NLP) problem, as the objective function features cross-terms between quadratic terms of the optimization variables and linear terms of the parameters. Thus, equivalently to problem (3.26), it is possible to reformulate problem (3.27) into a standard mp-QP by adapting the approach presented here, i.e.

$$\begin{aligned}
& \underset{x}{\text{minimize}} && \sum_{i=1}^N w_i t_i \\
& \text{subject to} && \mathcal{F}_i(x) \leq t_i, \quad \forall i = 1, \dots, N, \\
& && Ax \leq b, \\
& && w_i \geq 0, \quad \forall i = 1, \dots, N, \\
& && \sum_{i=1}^k w_i = 1, \\
& && x \in \mathbb{R}^n,
\end{aligned} \tag{3.40}$$

which follows directly from Remark 20.

3.5.4 Discussion and applicability

Based on the small computational study shown in Table 3.5.2, the applicability of the mp-MOO approach presented in this chapter seems to be promising, especially for a larger number of objective functions. Additionally, the calculation of the complete solution of the MOO problem enables similar features as with MPC, i.e. the offline solution of the problem and the online presentation of the solution for a specific parameter realization. Thus, computational elements and software are not required and enable quick and seamless application.

The main disadvantage at this point seems to be the ability to solve and store large-scale mp-QP problems, which may limit the use of this strategy to certain specific applications.

Chapter 4

Contributions to multi-parametric mixed-integer quadratic programming problems

Portions of this chapter have been published in:

- Oberdieck, R.; Pistikopoulos, E.N. (2015) Explicit hybrid model-predictive control: The exact solution. *Automatica*, 58, 152-159.
- Oberdieck, R.; Diangelakis, N.A.; Papathanasiou, M.M.; Nascu, I.; Pistikopoulos, E.N. (2016) POP - Parametric Optimization Toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979 - 8991.

4.1 Introduction

Applying MPC to hybrid systems requires the online solution of a mixed-integer quadratic programming (MIQP) problem [23]. Due to the inherently high computational burden, this has limited the use of hybrid MPC, for example by relaxing the binary variables of future time steps to continuous variables to provide a tractable problem [136]. Thus, in order to reduce this computational burden, multi-parametric programming has been used to solve the MIQP problem offline, which results in a multi-parametric MIQP (mp-MIQP) problem.

In this chapter, the current state-of-the-art of theoretical and algorithmic developments of mp-MIQP problems is described, before some recent advances are discussed, namely:

- The reduction of number of envelopes of solutions using McCormick relaxations

- An algorithm for the exact solution of mp-MIQP problems, featuring the analytical representation of the critical regions
- A computational study which provides initial insights into the computational tractability of the different algorithms

4.2 Theoretical and algorithmic background for mp-MIQP problems

Consider the following multi-parametric mixed-integer quadratic programming (mp-MIQP) problem

$$\begin{aligned}
z^*(\theta) = & \underset{x,y}{\text{minimize}} && (Q\omega + H\theta + c)^T \omega \\
& \text{subject to} && Ax + Ey \leq b + F\theta \\
& && x \in \mathbb{R}^n, \quad y \in \{0, 1\}^p, \quad \omega = \begin{bmatrix} x^T & y^T \end{bmatrix}^T \\
& && \theta \in \Theta := \{\theta \in \mathbb{R}^q \mid CR_A \theta \leq CR_b\},
\end{aligned} \tag{4.1}$$

where $Q \in \mathbb{R}^{(n+p) \times (n+p)} \succ 0$, $H \in \mathbb{R}^{(n+p) \times q}$, $c \in \mathbb{R}^{(n+p)}$, $A \in \mathbb{R}^{m \times n}$, $E \in \mathbb{R}^{m \times p}$, $b \in \mathbb{R}^m$, $F \in \mathbb{R}^{m \times q}$ and Θ is compact.

4.2.1 Theoretical Properties

The properties of the solution of mp-MIQP problems of type (4.1) are given by the following theorem, corollary and definitions.

Theorem 7 (Properties of mp-MIQP solution [43]). Consider the optimal solution of problem (4.1) with $Q \succ 0$. Then, there exists a solution in the form

$$x_i(\theta) = K_i \theta + r_i \quad \text{if } \theta \in CR_i, \tag{4.2}$$

where CR_i , $i = 1, \dots, M$ is a partition of the set Θ_f of feasible parameters θ , and the closure of the sets CR_i has the following form

$$CR_i = \left\{ \theta \in \Theta \mid \theta^T G_{i,j} \theta + h_{i,j}^T \theta \leq w_{i,j}, j = 1, \dots, t_i \right\}, \tag{4.3}$$

where t_i is the number of constraints that describe CR_i .

Corollary 3 (Quadratic boundaries [43]). Quadratic boundaries arise from the comparison of quadratic objective functions associated with the solution of mp-QP problems for different

feasible combinations of binary variables. This means that if the term $G_{i,j}$ in eq. (4.3) is non-zero, it adheres to the values given by the difference of the quadratic optimal objective functions in the critical regions featuring this quadratic boundary.

Definition 12 (Envelope of solutions [74]). In order to avoid the nonconvex critical regions described by Corollary 3, an envelope of solutions is created where more than one solution is associated with a critical region. The envelope is guaranteed to contain the optimal solution, and a point-wise comparison procedure among the envelope of solutions is performed online.

Definition 13 (The exact solution). The exact solution of a mp-MIQP problem denotes the explicit calculation of eq. (4.2) and (4.3) for every critical region, and consequently no envelopes of solutions are present.

On the notion of exactness

The notion of the exact solution for mp-MIQP problems as the explicit calculation of eq. (4.2) and (4.3) for every critical region does not imply that solutions which feature envelopes of solutions are incorrect or approximate. As stated in Definition 12, such implicit solutions are guaranteed to feature the optimal solution. Thus, the term exactness does not indicate any difference in the evaluation of the numerical value of the solution, but a difference in the solution structure itself. The merit of an exact solution, and by extension of the algorithm presented in this chapter, is the explicit availability of the critical region description in its potentially nonconvex form given in eq. (4.3). This enables the assignment of one solution to each region, and consequently an assessment of the impact and meaning of each region.

This is relevant as the solution to a multi-parametric programming problem not only yields the optimal solution for any feasible parameter realization considered, but also information regarding the structure of the underlying optimization problem. For example, the consideration of when a certain binary variable is 0 or 1 may imply when a certain decision such as a valve position is decided. This enables insights and post-optimal analysis akin to sensitivity analysis. However, such an analysis is only possible if the exact solution of the problem is obtained, and not a solution featuring envelopes of solutions, as then the critical region partitioning in itself does not have any meaning.

4.2.2 Solution algorithms for mp-MIQP problems

Literature overview

Several authors have proposed strategies for the solution of mp-MIQP problems. First, Dua *et al.* described a decomposition approach, where a candidate integer variable combination is

found by solving a mixed-integer nonlinear programming (MINLP) problem [74]. After fixing this candidate solution, the resulting mp-QP problem is solved and the solution is compared to a previously obtained upper bound, which results in a new, tighter upper bound, and a new iteration begins. The introduction of suitable integer and parametric cuts to the MINLP ensures that previously considered integer combinations as well as solutions with a worse objective function value are excluded. A schematic representation of this approach is given in Figure 4.1.

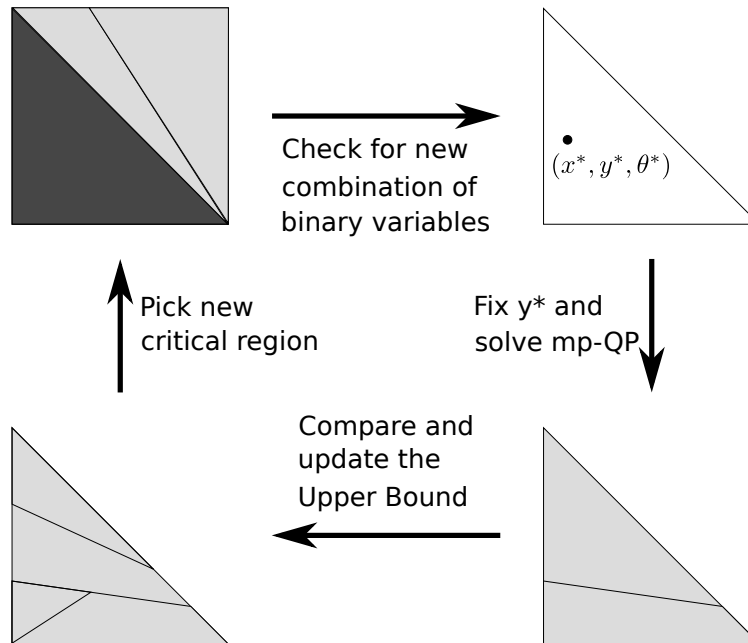


Figure 4.1: A graphical representation of the decomposition algorithm. The algorithm starts with an upper bound, from where a critical region is selected. After obtaining a new candidate integer solution, the solution of the corresponding mp-QP problem yields a new solution for the given critical region. This solution is then compared with the upper bound and an updated, tighter upper bound results.

Conversely, Borrelli *et al.* proposed an exhaustive enumeration approach instead of the solution of a MINLP [42], and the subsequent solution of all resulting mp-QP problems. Lastly, Axehill *et al.* considered a branch-and-bound approach, where at the root node the binary variables are relaxed and the resulting mp-QP problem is solved. For each subsequent node, a binary variable is fixed to a specific value and the resulting mp-QP problem is solved, followed by a suitable comparison procedure with a previously obtained upper bound in order to produce a tighter upper bound and to fathom any part of the parameter space which is guaranteed to be suboptimal. A schematic representation of this approach is given in Figure 4.2.

Remark 23. The exhaustive enumeration approach by Borrelli *et al.* may be regarded as a

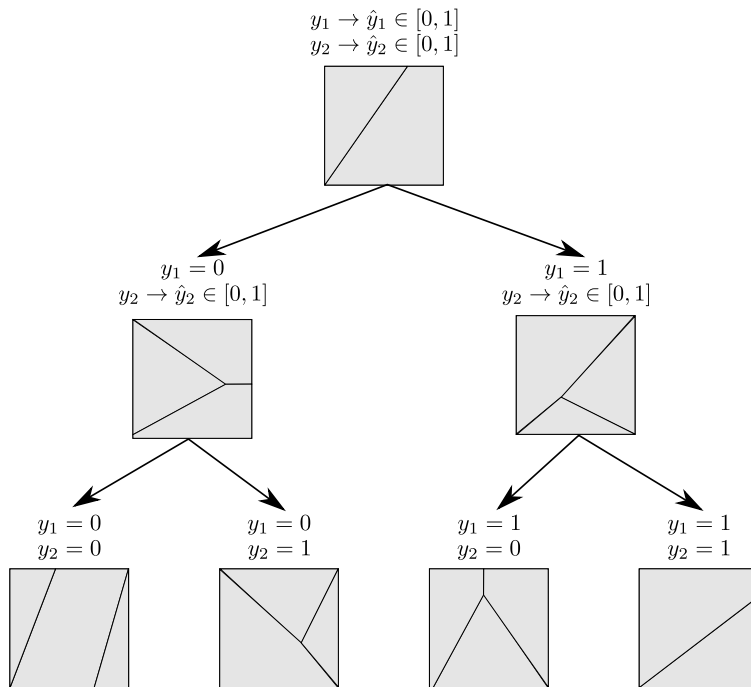


Figure 4.2: A graphical representation of the branch-and-bound algorithm. The algorithm starts from the root node, where all binary variables are relaxed. Subsequently, at each node a binary variable is fixed, the resulting mp-QP problem is solved and the solution is compared to a previously established upper bound to produce an updated, tighter upper bound and to fathom any part of the parameter space which is suboptimal.

special case of the branch-and-bound approach which only considers the leaf nodes of the tree.

As the decomposition algorithm is used in the remaining part of the chapter, it is now discussed in more detail.

4.2.3 The decomposition algorithm

The decomposition algorithm consists of three parts: calculation of a new candidate integer solution *via* the solution of a MINLP problem, solving the mp-QP problem resulting from fixing the candidate integer solution in the original mp-MIQP problem and comparing the obtained solution to a previously obtained upper bound. Note that the initial upper bound is set to ∞ .

Calculation of a new candidate integer solution

A candidate integer solution is found by solving the following global optimization problem:

$$\begin{aligned}
z_{global} = & \underset{x,y,\theta}{\text{minimize}} && (Q\omega + H\theta + c)^T \omega \\
& \text{subject to} && Ax + Ey \leq b + F\theta \\
& && (Q\omega + H\theta + c)^T \omega - \hat{z}_i(\theta) \leq 0 \\
& && \sum_{j \in J_i} y_j - \sum_{j \in T_i} y_j \leq \text{card}(J_i) - 1 \\
& && x \in \mathbb{R}^n, \quad y \in \{0, 1\}^p, \quad \omega = [x^T \ y^T]^T \\
& && \theta \in CR_i,
\end{aligned} \tag{4.4}$$

where $i = 1, \dots, v$ and v is the number of critical region that constitute the upper bound, $\hat{z}_i(\theta)$ is the objective function value of the upper bound in the critical region CR_i considered, and J_i and T_i are the sets containing the indices of the integer variables \hat{y}^i associated with the upper bound $\hat{z}_i(\theta)$ that attain the value 0 and 1 respectively, i.e.

$$J_i = \{j | \hat{y}_j^i = 1\} \tag{4.5a}$$

$$T_i = \{j | \hat{y}_j^i = 0\}. \tag{4.5b}$$

Remark 24. Without loss of generality, it is assumed that CR_i only features one upper bound $\hat{z}_i(\theta)$ in problem (4.4).

mp-QP solution

Once a candidate integer solution has been found, it is fixed in the mp-MIQP problem, thus resulting in a mp-QP problem. This problem can be solved with any mp-QP solver (see Chapter 3).

Comparison procedure

Within the algorithm, the solution obtained from the mp-QP problem is compared to a previously obtained current best upper bound $\hat{z}(\theta)$ to form a new, tighter upper bound. This can be expressed as:

$$z(\theta) = \min \{ \hat{z}(\theta), z^*(\theta) \}, \quad (4.6)$$

where $z^*(\theta)$ denotes the piecewise quadratic, optimal objective function obtained by solving the mp-QP problem resulting by fixing the candidate solution of the binary variables obtained from the solution of problem (4.4). The solution of eq. (4.6) requires in turn the comparison of the corresponding objective functions in each critical region CR_i , i.e.

$$\Delta z(\theta) = \hat{z}(\theta) - z_i^*(\theta) = 0, \quad (4.7)$$

where $z_i^*(\theta)$ denotes the objective function within the i -th critical region of the solution of the mp-QP problem. Due to the quadratic nature of the objective functions, $\Delta z(\theta)$ might be nonconvex. Within the open literature, two strategies for the solution of problem (4.6) have been presented, excluding the work presented in this thesis:

No objective function comparison: This approach, pioneered in [72] and first applied to mp-MIQP problems in [74], does not consider eq. (4.7) and stores both solutions, $\hat{z}(\theta)$ and $z_i^*(\theta)$, in CR_i , thus creating an envelope of solutions.

Objective function comparison over the entire CR: This approach was first presented for the solution of multi-parametric dynamic programming (mp-DP) problems [43], but has been applied to mp-MIQP problems in [11]. In this approach, eq. (4.7) is solved over the entire critical region CR_i , i.e. the following (possibly nonconvex) quadratic programming problem is solved:

$$\delta_{max} = \max_{\theta \in CR_i} \Delta z(\theta) \quad (4.8a)$$

$$\delta_{min} = \min_{\theta \in CR_i} \Delta z(\theta). \quad (4.8b)$$

Note that solving eq. (4.8) is not straightforward since it may be nonconvex. The results of solving eq. (4.8) allow for the following conclusions:

$$\delta_{max} \leq 0 \rightarrow z_1(\theta) \geq z_2(\theta) \quad \forall \theta \in CR_i \quad (4.9a)$$

$$\delta_{min} \geq 0 \rightarrow z_1(\theta) \leq z_2(\theta) \quad \forall \theta \in CR_i \quad (4.9b)$$

If $\delta_{min} < 0$ and $\delta_{max} > 0$, then both solutions are kept and an envelope of solutions is created.

Remark 25. Without loss of generality it was assumed in eq. (4.7) that only one objective function is associated with each critical region, and that no envelope of solutions is present (see Definition 12).

4.3 On the reduction of solutions per envelope of solutions in mp-MIQP problems

For the case of mp-MIQP problems, the optimal objective function $\bar{z}_i(\theta)$ over a critical region CR is generally quadratic. This requires the creation of envelopes of solutions is the polytopic nature of the critical regions is to be retained. However, an increased number of solutions per critical region not only requires an increased computational effort when the solution is to be evaluated, but also that the solution structure and features are not as readily available. In this section, the aim is to find a way to reduce the number of envelopes of solutions in each critical region while retaining their polytopic nature. In general, consider the critical region CR and the difference between the incumbent optimal objective value $z^*(\theta)$ and current best upper bound $\hat{z}(\theta)$, which is given by

$$\begin{aligned} \Delta z(\theta) &= \hat{z}(\theta) - z^*(\theta) \\ &= \theta^T P \theta + f^T \theta + w, \end{aligned} \quad (4.10)$$

where $P \in \mathbb{R}^{q \times q}$, $f \in \mathbb{R}^q$ and $w \in \mathbb{R}$.

Remark 26. Note that on the contrary to eq. (4.7), the index i is omitted in order to achieve a simpler representation.

If $P = 0_{q \times q}$, then $\Delta z(\theta)$ is an affine function, the critical region CR can be readily

partitioned, i.e.:

$$\begin{cases} CR^1 & = CR \cap \Delta z(\theta) \leq 0 \\ CR^2 & = CR \cap \Delta z(\theta) \geq 0, \end{cases} \quad (4.11)$$

where CR^1 and CR^2 are polytopes and in CR^1 $z^*(\theta)$ is optimal while in CR^2 $\hat{z}(\theta)$ remains optimal. However, if $P \neq 0_{q \times q}$, then a linear under- and overestimator is created, satisfying

$$g(\theta) = a_u^T \theta + b_u \quad (4.12a)$$

$$h(\theta) = a_o^T \theta + b_o \quad (4.12b)$$

with

$$\begin{aligned} g(\theta) &\leq \theta^T P \theta + f^T \theta + w \\ h(\theta) &\geq \theta^T P \theta + f^T \theta + w \\ \theta &\in CR \subseteq \Xi, \end{aligned} \quad (4.13)$$

where the subscripts u and o indicate the coefficients of the under- and overestimator, respectively. This enables the definition of the following three critical regions:

$$\begin{cases} CR^1 & = CR \cap g(\theta) \geq 0 \\ CR^2 & = CR \cap h(\theta) \leq 0 \\ CR^3 & = CR \cap g(\theta) \leq 0, h(\theta) \geq 0, \end{cases} \quad (4.14)$$

where in CR^1 $z^*(\theta)$ is optimal while in CR^2 $\hat{z}(\theta)$ remains optimal, and in CR^3 both solutions are stored in an envelope of solutions. Since $h(\theta)$ and $g(\theta)$ are affine functions, CR^1 , CR^2 and CR^3 are polytopes.

The construction of linear under- and overestimators for the comparison procedures

The task is to find

$$g(\theta) = a_u^T \theta + b_u \quad (4.15a)$$

$$h(\theta) = a_o^T \theta + b_o \quad (4.15b)$$

with

$$\begin{aligned} g(\theta) &\leq \theta^T P \theta + f^T \theta + w \\ h(\theta) &\geq \theta^T P \theta + f^T \theta + w \\ \theta &\in CR, \end{aligned} \quad (4.16)$$

where the main issue is to address the bilinearities on the right-hand side of the constraints in eq. (4.16). The number of these bilinear terms is given by the number of non-zero elements in P' . First, for every bilinear term $\theta_i\theta_j$ the McCormick under- and overestimator are created according to

$$\theta_i\theta_j \geq \max\{\theta_j^{\max}\theta_i + \theta_i^{\max}\theta_j - \theta_i^{\max}\theta_j^{\max}, \theta_j^{\min}\theta_i + \theta_i^{\min}\theta_j - \theta_i^{\min}\theta_j^{\min}\} \quad (4.17a)$$

$$\theta_i\theta_j \leq \min\{\theta_j^{\max}\theta_i + \theta_i^{\min}\theta_j - \theta_i^{\min}\theta_j^{\max}, \theta_j^{\min}\theta_i + \theta_i^{\max}\theta_j - \theta_i^{\max}\theta_j^{\min}\} \quad (4.17b)$$

Note that θ_i^{\min} and θ_i^{\max} are obtained *via* the solution of linear programming problems.

4.4 Solution Strategy for the Exact Solution of mp-MIQP Problems

The aim of this algorithm is the exact solution of mp-MIQP problem (4.1), i.e. the explicit calculation of eq. (4.2) and (4.3) for every critical region.

Remark 27. The new approach is first shown in detail in combination with the decomposition algorithm [74]. However, it can also be applied in combination with the branch-and-bound or exhaustive enumeration approach, which is shown at the end of this section.

4.4.1 Initialization

Consider mp-MIQP problem (4.1). In line with the decomposition approach presented in [74], a candidate solution for the binary variables is found by solving the following MIQP problem

$$\begin{aligned} z_{global} = \quad & \underset{x,y,\theta}{\text{minimize}} && (Q\omega + H\theta + c)^T \omega \\ & \text{subject to} && Ax + Ey \leq b + F\theta \\ & && x \in \mathbb{R}^n, \quad y \in \{0, 1\}^p, \quad \omega = \begin{bmatrix} x^T & y^T \end{bmatrix}^T \\ & && \theta \in \Theta := \{\theta \in \mathbb{R}^q \mid CR_A\theta \leq CR_b\}, \end{aligned} \quad (4.18)$$

where the parameter θ is treated as an optimization variable, and the problem is solved using available MIQP solvers. If problem (4.18) is infeasible, problem (4.1) is also infeasible. Otherwise, a binary solution y^* is obtained and subsequently fixed in (4.1), thus resulting in a mp-QP of the form (3.1). This problem can be solved using one of the approaches presented in the literature, which results in an initial partitioning of the parameter space and provides a parametric upper bound to the solution. The upper bound for the remaining part of the parameter space which has not yet been explored is set to infinity.

4.4.2 Step 1 - Candidate Solution for Binary Variables

In the first step of the algorithm, in each critical region CR_i of the current upper bound the parameter θ is treated as an optimization variable and the following optimization problem is solved

$$\begin{aligned}
 z_{global} = \quad & \underset{x,y,\theta}{\text{minimize}} && (Q\omega + H\theta + c)^T \omega \\
 & \text{subject to} && Ax + Ey \leq b + F\theta \\
 & && (Q\omega + H\theta + c)^T \omega - \hat{z}_i(\theta) \leq 0 \\
 & && \sum_{k \in J_i} y_k - \sum_{k \in T_i} y_k \leq \text{card}(J_i) - 1 \\
 & && x \in \mathbb{R}^n, \quad y \in \{0, 1\}^p, \quad \omega = [x^T \ y^T]^T \\
 & && \theta \in CR_i,
 \end{aligned} \tag{4.19}$$

where $i = 1, \dots, v$ and v is the number of critical region that constitute the upper bound, $\hat{z}_i(\theta)$ is the objective function value of the upper bound associated with the critical region CR_i and J_i and T_i are the sets containing the indices of the integer variables of the integer combination \hat{y}^i associated with the upper bound $\hat{z}_i(\theta)$ that attain the value 0 and 1 respectively, i.e.

$$J_i = \{k | \hat{y}_k^i = 1\} \tag{4.20a}$$

$$T_i = \{k | \hat{y}_k^i = 0\}. \tag{4.20b}$$

Remark 28. The two additional constraints introduced in problem (4.19) in comparison to problem (4.18) are called parametric and integer cut respectively. They ensure that the solution of problem (4.19) is better than the current upper bound, and that previously visited integer combinations are not considered again [74].

Note that in this step the general quadratic critical region CR_i of the form is considered:

$$\theta \in CR_i = \left\{ \theta \in \mathbb{R}^q \mid g_{i,j}(\theta) = \theta^T G_{i,j} \theta + h_{i,j}^T \theta + w_{i,j} \leq 0, j = 1, \dots, t_i \right\}, \tag{4.21}$$

where t_i is the total number of constraints in the i -th critical region. The constraints reported in eq. (4.21) can readily be incorporated into problem (4.19), since θ is an optimization variable and thus, from a conceptual point of view, they are as complex as the parametric cuts, which are also possibly quadratic in x , y and θ .

Problem (4.19) is a MINLP problem which is solved to global optimality using available solvers [184, 249]. If the problem is infeasible, the critical region is not considered for further evaluation, and the current upper bound is the solution of this critical region. If however a solution is found, the corresponding binary variables y^* are substituted into the original

mp-MIQP problem, which results in the following mp-QP problem:

$$\begin{aligned}
z(\theta), = \quad & \underset{x}{\text{minimize}} && (Q_x + H_x\theta + \tilde{c}_x)^T x + f(\theta) \\
& \text{subject to} && Ax \leq (b - Ey^*) + F\theta \\
& && x \in \mathbb{R}^n, \quad \theta \in CR_i.
\end{aligned} \tag{4.22}$$

where the matrices and vectors $Q_x \in \mathbb{R}^{n \times n}$, $H_x \in \mathbb{R}^{n \times q}$ and $\tilde{c}_x \in \mathbb{R}^n$ as well as the function $f(\theta)$ are obtained by fixing y^* in (4.1).

4.4.3 Step 2 - Creation of an Affine Outer Approximation

Due to the nonlinearities in CR_i , it is not possible to solve problem (4.22) using the approaches presented in the literature. Thus, in this step, a polytope Ξ_i is constructed such that

$$CR_i \subseteq \Xi_i, \tag{4.23}$$

where Ξ_i is called an affine outer approximation of CR_i . In order to create Ξ_i it is necessary to find an affine relaxation for each nonlinear constraint of CR_i , i.e. each constraint $g_{i,j}(\theta) \leq 0$ in eq. (4.21) where $G_{i,j}$ is nonzero. This is achieved by employing McCormick relaxations [180] for each bilinear or quadratic term in the constraints. Since the nonlinearities in the constraints only arise from comparison procedures (see Corollary 3), these relaxations are calculated during the comparison procedure.

4.4.4 Step 3 - Solution of the mp-QP Problem

Similarly to the Initialization step in section 4.4.1, the candidate solution of the binary variables y^* is substituted into the initial problem, thus resulting in a mp-QP. Note that Ξ_i is considered instead of CR_i , thus enabling the use of available mp-QP algorithms. This results in the following mp-QP problem

$$\begin{aligned}
z(\theta) = \quad & \underset{x}{\text{minimize}} && (Q_x + H_x\theta + \tilde{c}_x)^T x + f(\theta) \\
& \text{subject to} && Ax \leq (b - Ey^*) + F\theta \\
& && x \in \mathbb{R}^n, \quad \theta \in \Xi_i.
\end{aligned} \tag{4.24}$$

The solution of problem (4.24) is given by

$$x_{i,k}^*(\theta) = K_{i,k}\theta + r_{i,k}, \quad \forall \theta \in CR_{i,k}, \tag{4.25}$$

where $k = 1, \dots, m$ and m is the total number of critical regions created in Ξ_i .

Remark 29. The critical regions $CR_{i,k}$ in eq. (4.25) are polytopes. This directly results from Theorem 2, since Ξ_i is a polytope.

4.4.5 Step 4 - Comparison with Upper Bound

Remark 30. This and all subsequent steps have to be performed for each critical region $CR_{i,k}$ in eq. (4.25). Therefore the general (polytopic) critical region CR is considered. Furthermore, note that at this point the upper bound $\hat{z}_i(\theta)$ is assumed to be valid over Ξ_i . This will be reversed in a later stage of the algorithm.

As stated in section 4.2, the envelope of solutions is created if $\delta_{min} < 0$ and $\delta_{max} > 0$ from eq. (4.9a). However, here the explicit solution of the problem is considered and thus two new critical regions are created, namely

$$\begin{cases} CR^1 &= CR \cap \Delta z(\theta) \leq 0 \\ CR^2 &= CR \cap \Delta z(\theta) \geq 0, \end{cases} \quad (4.26)$$

where in CR^1 $z^*(\theta)$ is optimal while in CR^2 $\hat{z}(\theta)$ remains optimal, where

$$\Delta z(\theta) = \hat{z}(\theta) - z_i^*(\theta) = 0. \quad (4.27)$$

Note that as shown in eq. (4.10), $\Delta z(\theta) = \theta^T P \theta + f^T \theta + w$. Since all quadratic constraints in the critical regions stem from the comparison procedure (see Corollary 3), all non-zero elements of $G_{i,j}$ in eq. (4.3) are a result of the constraints $\Delta z(\theta) \leq 0$ or $\Delta z(\theta) \geq 0$.

4.4.6 Step 5 - Creation of Affine Relaxations

As mentioned in Step 2 in section 4.4.3, it is necessary to calculate appropriate relaxations for $\Delta z(\theta)$ in order to create the outer approximation for the next iteration. Since $\Delta z(\theta) \geq 0$ as well as $\Delta z(\theta) \leq 0$ in eq. (4.26) are considered, the McCormick under- and overestimator are created according to

$$\theta_1 \theta_2 \geq \max\{\theta_2^{\max} \theta_1 + \theta_1^{\max} \theta_2 - \theta_1^{\max} \theta_2^{\max}, \theta_2^{\min} \theta_1 + \theta_1^{\min} \theta_2 - \theta_1^{\min} \theta_2^{\min}\} \quad (4.28a)$$

$$\theta_1 \theta_2 \leq \min\{\theta_2^{\max} \theta_1 + \theta_1^{\min} \theta_2 - \theta_1^{\min} \theta_2^{\max}, \theta_2^{\min} \theta_1 + \theta_1^{\max} \theta_2 - \theta_1^{\max} \theta_2^{\min}\} \quad (4.28b)$$

Note that θ_i^{\min} and θ_i^{\max} are obtained *via* the solution of linear programming problems.

4.4.7 Step 6 - Recovery of CR_i from Ξ_i

As noted in Remark 30, the upper bound $(\hat{x}(\theta), \hat{y})$ with an optimal objective function $\hat{z}(\theta)$ was assumed to be valid for Ξ_i which is in fact incorrect. In order to account for this, the original inequalities from CR_i in eq. (4.21) are re-introduced to each newly formed critical region, while the relaxations used to create Ξ_i are removed.

However, this may lead to critical regions CR which are empty in CR_i , but not in Ξ_i , i.e.

$$CR \cap \Xi_i \neq \emptyset \wedge CR \cap CR_i = \emptyset. \quad (4.29)$$

Due to the possibly quadratic boundary of the set $CR \cap CR_i$ the problem in eq. (4.29) is equivalent to finding a feasible point in a general quadratically constrained quadratic programming problem, i.e.

$$\begin{aligned} & \underset{\theta}{\text{minimize}} && 0 \\ & \text{subject to} && \theta \in CR \cap CR_i, \end{aligned} \quad (4.30)$$

which may be challenging to solve, as it may be nonconvex. At this point, the newly formed critical regions are returned to Step 1 thus resuming the iteration.

4.4.8 Termination

Similarly to the decomposition algorithm in [74], the proposed algorithm terminates as soon as problem (4.19) is infeasible for all critical regions. Since the number of critical regions as well as the number of possible integer combinations is finite, the algorithm will terminate in a finite number of iterations. Upon termination, the parameter space will be described by a set of possibly nonconvex critical regions, and each critical region is only associated with one solution $(x(\theta), y, z(\theta))^*$. The algorithm is presented in detail in Algorithm 2.

4.4.9 Application to the Branch-And-Bound Algorithm

As suggested in Remark 27, this algorithm can be extended to branch-and-bound type algorithms. On the branching stage, the same procedure as in [200] and [11] is applied. After solving the resulting mp-QP problem at the node, the comparison between the solution at the node and the current best upper bound is performed according to Steps 4 and 5. If the currently considered node is a leaf node, then the current best upper bound is updated, if necessary. Otherwise, the node is branched and the part of the parameter space which features a smaller objective function value than the current best upper bound is passed onto the newly created nodes. If this part of the parameter space is quadratically constrained,

Algorithm 2 Exact Solution of mp-MIQP problem

Require: mp-MIQP problem, suboptimality ϵ **Ensure:** \mathcal{S}

```
1:  $(\hat{x}(\theta), \hat{y}, \hat{z}(\theta)) \leftarrow (\mathbf{void}, \mathbf{void}, \infty)$ 
2: Add  $(\Theta, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  to LIST
3: while length(LIST) > 0 do
4:   TEMP  $\leftarrow \emptyset$ 
5:   Pop element  $(CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  from LIST
6:   Solve problem (4.4) for element  $(CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$ 
7:   if problem (4.4) is infeasible then
8:     Add  $(CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  to  $\mathcal{S}$ 
9:   else
10:    Retrieve  $y^*$  from solution of problem (4.4)
11:    Generate  $\Xi$  based on eq. (4.23)
12:    Solve problem (4.24) for  $y^*$  and in  $\Xi$  and obtain  $(CR_k, x_k^*(\theta), y^*, z_k^*(\theta))$ 
13:    for each  $CR_k$  do
14:      Solve eq. (4.8)
15:      if  $\delta_{max} \leq 0$  then
16:        Add  $(CR_k \cap CR, x_k^*(\theta), y^*, z_k^*(\theta))$  to TEMP
17:      else if  $\delta_{min} \geq 0$  then
18:        Add  $(CR_k \cap CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  to TEMP
19:      else
20:        Define  $CR_k^1$  and  $CR_k^2$  according to eq. (4.26)
21:        Add  $(CR_k^1 \cap CR, x_k^*(\theta), y^*, z_k^*(\theta))$  to TEMP
22:        Add  $(CR_k^2 \cap CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  to TEMP
23:      end if
24:    end for
25:    Remove entries with redundant critical regions  $CR$  from TEMP.
26:    Remove  $(CR, \hat{x}(\theta), \hat{y}, \hat{z}(\theta))$  from LIST
27:    Add TEMP to LIST
28:  end if
29: end while
```

under- and overestimators are used to create an affine outer approximation according to eq. (4.23), in which the mp-QP problem of the new node is solved.

4.5 Implementation of the algorithm

Although the algorithm presented here was originally implemented this way, propagating quadratically constrained critical regions is an issue due to the inability of MATLAB® to handle non-linearity in a straightforward way. Thus, in order to use this algorithm beyond its conceptual value, the following changes were made so as to enable the efficient implementation¹:

- The algorithm requires the solution of the MINLP problem (4.19), where the non-linearity is given by a set of quadratic constraints featuring continuous and binary variables. Thus, the connection between MATLAB® and a MINLP solver platform (e.g. GAMS) is required, which not only is very fragile from an algorithmic standpoint, but also incurs a high overhead. Since MATLAB features a MILP solver called `intlinprog`, problem (4.19) was reformulated as:

$$\begin{aligned}
 z = & \underset{x,y,\theta,t}{\text{minimize}} && t \\
 & \text{subject to} && Ax + Ey \leq b + F\theta \\
 & && \left[(Q\omega + H\theta + c)^T \omega - \hat{z}_i(\theta) \right] \leq t \\
 & && \sum_{k \in J_i} y_k - \sum_{k \in T_i} y_k \leq |J_i| - 1 \\
 & && t \leq -\epsilon \\
 & && x \in \mathbb{R}^n, y \in \{0, 1\}^p, \omega = [x^T y^T]^T \\
 & && \theta \in [CR_i],
 \end{aligned} \tag{4.31}$$

where t is a scalar which ensures that the new solution is at least by a numerical tolerance $\epsilon > 0$ better than the upper bound², and $[\cdot]$ denote the generation of two McCormick underestimators, which linearize the constraints and convert it into a MILP. Since the left-hand side of the constraints is underestimated, it is still guaranteed that all optimal combinations of binary variables will be identified. However, also non-optimal combinations might be fixed, which will be identified in the comparison procedure.

¹These changes are purely motivated by algorithmic requirements dictated by the software used.

²This has proven to be relevant, as otherwise the combinations of binary variables of all adjacent critical regions are also needlessly considered.

- The algorithm requires the tracking of quadratically constrained regions CR_i . However, this is a difficult task in MATLAB®. Thus, the following modification was made for the implementation of the algorithm: for the iterative procedure, the algorithm uses the procedure by Dua *et al.* [74], i.e. without any comparison procedure. Once the final map featuring envelopes of solutions is obtained, problem (4.30) is solved for each stored solution using the MATLAB® function `fmincon`.
- The algorithm requires the solution of non-convex optimization problems. Thus, only an ϵ -tolerance can be given on the solution of such problems in order to guarantee a termination of the algorithm in finite time. The impact of this issue onto the algorithm will be part of future work in this research direction.

Note that the version of the algorithm featuring these modifications is implemented in POP, the Parametric OPTimization toolbox (see Appendix A).

4.6 Numerical Examples

Remark 31. The algorithm presented in this chapter has been used extensively in the application of hybrid MPC to intravenous anaesthesia. The interested reader is referred to [191–194] for further reading on this topic.

4.6.1 Example problem

Consider the following example

$$Q = \begin{bmatrix} 6 & 0 & 0 & 0 \\ -1 & 4 & 0 & 0 \\ 0 & 0 & 6 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix}, H = \begin{bmatrix} 5 & 0 \\ 0 & -8 \\ 0 & -1 \\ 3 & 0 \end{bmatrix}, c = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (4.32)$$

with

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \end{bmatrix}, E = \begin{bmatrix} 0 & 0 \\ -1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, b = \begin{bmatrix} 1.5 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, F = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (4.33)$$

and

$$\theta \in \Theta = \{\theta \in \mathbb{R}^2 \mid 0 \leq \theta_l \leq 1, l = 1, \dots, 2\}. \quad (4.34)$$

After the initialization step, the integer vector $y = [0 \ 0]^T$ is identified as the candidate combination for the binary variable and the resulting mp-QP according to eq. (4.22) is solved.

Let us consider the first critical region of the solution, namely

$$CR_1 = \{\theta \in \mathbb{R}^2 \mid 0.10417\theta_1 - \theta_2 \leq -0.5; 0 \leq \theta_1 \leq 1; \theta_2 \leq 1\} \quad (4.35)$$

with the corresponding objective function value

$$z_{(0,0)}^*(\theta) = -2.0833\theta_1^2 + 0.4167\theta_1 - 8\theta_2 + 2. \quad (4.36)$$

Since no quadratic terms are present in eq. (4.35), no outer approximation needs to be constructed. Thus, the global optimization problem (4.4) is solved in CR_1 , identifying the integer combination $y^* = [0 \ 1]^T$ as a new candidate solution. The solution of the corresponding mp-QP problem is one solution over CR_1 with the following objective function value

$$z_{(0,1)}^*(\theta) = -1.1364\theta_1^2 - 3.6364\theta_1\theta_2 - 2.9091\theta_2^2 + 6.0682\theta_1 - 7.0909\theta_2 + 2.9546, \quad (4.37)$$

The comparison of eq. (4.37) and eq. (4.36) yields

$$\begin{aligned}
\Delta z(\theta) &= z_{(0,1)}^*(\theta) - z_{(0,0)}^*(\theta) \\
&= 0.9470\theta_1^2 - 3.6364\theta_1\theta_2 - 2.9091\theta_2^2 + 5.6515\theta_1 + 0.9091\theta_2 + 0.9546 \\
&= 0.
\end{aligned} \tag{4.38}$$

In order to obtain an initial classification of optimality in CR_1 , eq. (4.8) is solved. This results in:

$$\bar{\delta}_{max} = 0.6182 \tag{4.39a}$$

$$\underline{\delta}_{min} = -1.2636, \tag{4.39b}$$

where $\bar{\delta}_{max}$ and $\underline{\delta}_{min}$ are over- and underestimators of δ_{max} and δ_{min} .

Therefore, CR_1 is divided according to eq. (4.26), thus resulting in the following critical regions

$$\begin{aligned}
CR_1^1 &= \left\{ \theta \in \mathbb{R}^2 \mid CR_1 \cap 0.9470\theta_1^2 - 3.6364\theta_1\theta_2 - \right. \\
&\quad \left. 2.9091\theta_2^2 + 5.6515\theta_1 + 0.9091\theta_2 + 0.9546 \leq 0 \right\}
\end{aligned} \tag{4.40a}$$

$$\begin{aligned}
CR_1^2 &= \left\{ \theta \in \mathbb{R}^2 \mid CR_1 \cap 0.9470\theta_1^2 - 3.6364\theta_1\theta_2 - \right. \\
&\quad \left. 2.9091\theta_2^2 + 5.6515\theta_1 + 0.9091\theta_2 + 0.9546 \geq 0 \right\}
\end{aligned} \tag{4.40b}$$

and the following affine McCormick relaxations

$$\underline{\Delta}z(\theta) = 2.9242\theta_1 - 4.1818\theta_2 + 2.9182 \tag{4.41a}$$

$$\overline{\Delta}z(\theta) = 2.4697\theta_1 - 6.6545\theta_2 + 5.6091, \tag{4.41b}$$

where $\underline{\Delta}z(\theta)$ and $\overline{\Delta}z(\theta)$ are the under- and overestimator, respectively. Note that only one linear approximator was created by only considering the first of the two possible relaxations in eq. (4.28). In CR_1^1 the solution associated with $y = [0 \ 1]^T$ is optimal, while in CR_1^2 the solution associated with $y = [0 \ 0]^T$ is. This concludes the comparison procedure, and the next iteration of the decomposition algorithm is started by considering CR_1^2 . The partitioning of the critical regions of the example problem is shown in Figure 4.3, while the corresponding numerical values are shown in Table 4.1.

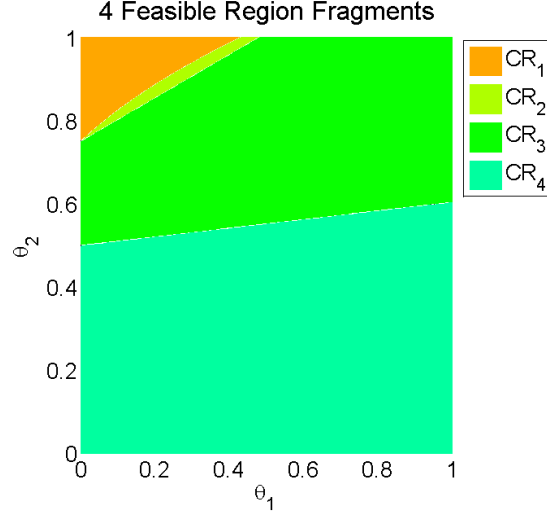


Figure 4.3: The partitioning of the parameter space into critical regions of the example problem.

Table 4.1: The exact solution of the example problem.

Critical Region	Solution
$\theta_1 \geq 0; \theta_2 \leq 0; 0.9470\theta_1^2 - 3.6364\theta_1\theta_2 - 2.9091\theta_2^2 + 5.6515\theta_1 + 0.9091\theta_2 + 0.9546 \leq 0$	$X = (-0.4546\theta_1 - 0.7273\theta_2 + 0.5455, 0.4546\theta_1 + 0.7273\theta_2 + 0.9546)$ $Y = [0 \ 1]^T$
$0.5208\theta_1 - \theta_2 \leq -0.75; \theta_2 \leq 1; 0.9470\theta_1^2 - 3.6364\theta_1\theta_2 - 2.9091\theta_2^2 + 5.6515\theta_1 + 0.9091\theta_2 + 0.9546 \geq 0$	$X = (-0.8333\theta_1, 1)$ $Y = [0 \ 0]^T$
$0.1042\theta_1 - \theta_2 \leq -0.5; -0.5208\theta_1 + \theta_1 \leq 0.75; 0 \leq \theta_1 \leq 1; \theta_2 \leq 1$	$X = (-0.8333\theta_1, 1)$ $Y = [0 \ 0]^T$
$-0.1042\theta_1 + \theta_2 \leq 0.5; 0 \leq \theta_1 \leq 1; \theta_2 \geq 0$	$X = (-0.8333\theta_1, -0.2083\theta_1 + \theta_2)$ $Y = [0 \ 0]^T$

4.6.2 The computational impact of the comparison procedure

Although different comparison procedures have been presented in the literature, no comprehensive computational study has been carried out trying to identify (a) what the impact of

the comparison procedure on the overall computational effort is and (b) how the different comparison procedures differ in their computational requirements.

Using the test set 'POP_mpMIQP1' consisting of 100 mp-MIQP problems, a first tentative answer to these questions is provided (see Chapter A for the problem statistics). In Figure 4.4 the percentage of problems in a certain time is reported for different comparison procedures, while Figure 4.5 highlights the computational requirements for each comparison procedure in the overall algorithm. The four procedures considered are:

None: No comparison procedure is carried out, as proposed in [74].

MinMax: Only optimization problem (4.8) is solved and a decision according to eq. (4.9a) is made, as proposed in [11].

Affine: McCormick relaxations [180] are used to encapsulate the nonconvexity, as shown in [200] (see section 4.3 for details).

Exact: The exact comparison between objective functions is considered, as described in this chapter.

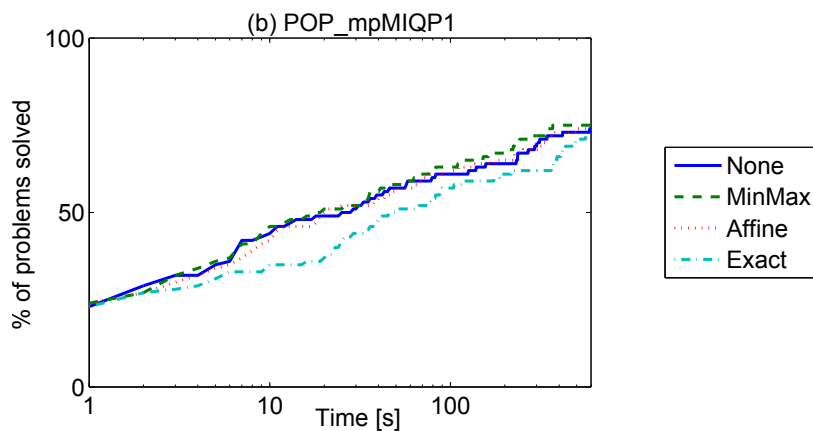


Figure 4.4: The computational results for the solution of a test set problems 'POP_mpMIQP1' for the different comparison procedures.

4.6.3 Discussion

For the mixed-integer case, the computational efficiency of using no, a min-max or an affine comparison procedure are very similar. This is due to the fact that the main computational effort is spent in the solution of the mp-QP problem. This is surprising, as eq. (4.7) is non-convex and thus its solution could be potentially limiting. However, as an approximate algorithm without strict error tolerance requirements was used, this did not cause

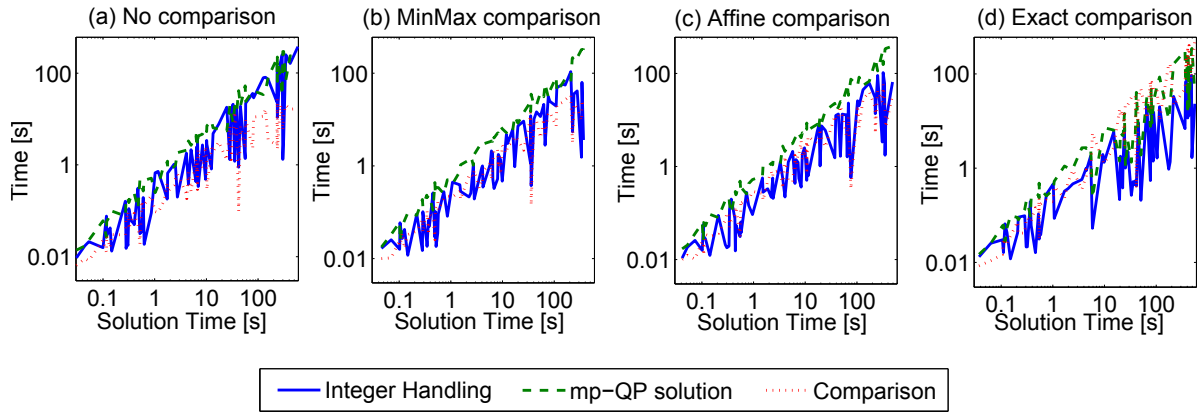


Figure 4.5: The computational requirements for each aspect of the algorithm for the different comparison procedures.

computational limitations. In addition, it appears that the increased number of partitions resulting from the use of an affine comparison procedure (see [199]) does not impact the computational performance significantly. However, the use of the exact algorithm resulted in an increased computational expense. In addition, the calculation of the exact solution for mp-MIQP problems requires the solution of a quadratically constrained feasibility problem. In numerous cases, this led to numerical tolerance issues, as the convergence of the algorithm (the MATLAB[®] in-built `fmincon`) was sometimes not guaranteed.

Chapter 5

Robust explicit/multi-parametric model predictive control

5.1 Introduction

In model predictive control (MPC), the aim is to devise an optimal, model-based control strategy able to control a multivariable, constrained system [227]. Two classes of systems considered in the open literature are discrete-time linear continuous and hybrid systems¹. In many cases, the dynamics of a system are subject to uncertainty, and thus the corresponding MPC problem needs to consider the presence of this uncertainty by devising robust MPC strategies.

The area of robust MPC has received significant attention, especially for continuous systems. Beginning with pioneering works in [47, 147], it has significantly grown, considering different types of uncertainty including parametric [32, 147, 148], unstructured [80, 170] or stochastic [221] uncertainties. The textbooks [44, 149, 227] provide an excellent overview over the current state-of-the-art in robust MPC of continuous systems. Similarly, robust hybrid MPC has also been considered for classes of hybrid systems, notably in Kerrigan and Mayne [139, 140], Raković *et al.* [223–225] and others [55, 160, 181, 255] for the case of additive disturbance.

The field of robust optimization considers the question of constraint satisfaction for a (static) set of inequality constraints subject to a given uncertainty. This field, pioneered by Soyster [243], gained significant attention with the work of Ben-Tal and Nemirowski [33–35] as well as Bertsimas and Sim [37]. The main concept is thereby the formulation of a so-called robust counterpart of the uncertain constraint set, the satisfaction of which guarantees the

¹Hybrid systems are processes which feature continuous and discrete elements such as valves, switches or logical decisions.

constraint satisfaction for all possible realizations of the uncertainty [111, 112].

Despite the similarities between robust optimization and robust MPC, only few contributions have combined these two areas of research: Löfberg discussed the use of robust counterparts for the solution of uncertain semidefinite programs [167, 168], while Goulart *et al.* expanded the notion of adjustable robust counterparts for additive disturbance [97, 98] introduced by Ben-Tal *et al.* [34]. Van Hessem and Bosgra considered a conic reformulation which utilized robust optimization principles [254]; Pistikopoulos and co-workers employed robust optimization in order to handle parametric uncertainty in combination with multi-parametric dynamic programming [148, 219].

In this chapter, a novel approach for the design of robust MPC controllers for discrete-time linear systems featuring a combination of continuous and binary inputs is described for the special case of parametric, box-constrained uncertainty. It is based on a generalization of the results in [148, 219], as it performs recursive projections of robust counterparts of the uncertain constraint sets. This enables the design of robust admissible sets, robust control invariant sets and finally robust MPC controllers. The main advance with respect to [148, 219] is twofold: first, in [148, 219] the solution of a mp-QP problem at each stage with a growing number of parameters is required. This chapter shows that it is possible to obtain the same outcome using only projection operations. Second, the approach is extended to hybrid systems, where the same principles are proven to hold.

5.1.1 Notation

The n -dimensional space of real numbers is denoted by \mathbb{R}^n , and the set of non-negative integers is denoted by \mathbb{N} . Let $a, b \in \mathbb{N}$ with $a < b$, then $\mathbb{N}_{[a,b]} = \{a, a + 1, \dots, b\}$ and $\mathbb{N}_b = \mathbb{N}_{[0,b]}$. A polytope is defined as the closed and bounded intersection of a finite number of halfspaces. Given the vector $a \in \mathbb{R}^n$ and the matrix $A \in \mathbb{R}^{m \times n}$, the element-wise absolute value is given as $|a|$ and $|A|$, respectively. The weighted 2-norm of x is given as $\|x\|_Q$, i.e. $\|x\|_Q = x^T Q x$, and the identity matrix is defined as $I_n \in \mathbb{R}^{n \times n}$. The inner approximation of a set P is denoted as \underline{P} , i.e. $\underline{P} \subseteq P$.

5.2 Background on Model Predictive Control (MPC)

Remark 32. In this thesis, only discrete-time linear systems are considered.

5.2.1 Nominal Systems

In general, nominal systems refer to the situation where the state space model is assumed to give perfect information about the dynamic development of the system, and are generally defined as:

$$x^+ = Ax + Bu, \quad (5.1)$$

where x , u and x^+ are the state, input and successor state, respectively.

Continuous Systems

In continuous systems, there are only continuously varying elements in the system. Thus, the general MPC problem for a continuous linear discrete-time system can be described as:

$$\begin{aligned} & \underset{U}{\text{minimize}} \quad x_N^T P x_N + \sum_{k=1}^{N-1} \left(x_k^T Q_k x_k + (y_k - y_k^R)^T Q R_k (y_k - y_k^R) \right) \\ & \quad + \sum_{k=0}^{M-1} \left((u_k - u_k^R)^T R_k (u_k - u_k^R) + \Delta u_k^T R_{1k} \Delta u_k \right) \\ & \text{subject to } U = [u_0, u_1, \dots, u_{M-1}]^T, \quad x_N \in \mathcal{X}_T, \quad e \in \mathcal{E} \\ & \left. \begin{aligned} x_{k+1} &= Ax_k + Bu_k + Cd_k \\ y_k &= Dx_k + Eu_k + e \\ u_k &\in \mathcal{U}, \quad x_k \in \mathcal{X}, \quad y_k \in \mathcal{Y}, \quad d_k \in \mathcal{D} \\ \Delta u_k &= u_k - u_{k-1} \in \mathcal{U}_\Delta \end{aligned} \right\} \forall k = 0, \dots, M-1 \quad (5.2) \\ & \left. \begin{aligned} x_{k+1} &= Ax_k + Bu_{M-1} + Cd_k \\ y_k &= Dx_k + Eu_{M-1} + e \\ x_k &\in \mathcal{X}, \quad y_k \in \mathcal{Y}, \quad d_k \in \mathcal{D} \end{aligned} \right\} \forall k = M, \dots, N-1 \end{aligned}$$

where u_k^R is the control variables set points, Δu_k is the difference between two consecutive control actions, y_k and y_k^R denote the outputs and their respective set points, d_k denote the measured disturbances, Q_k , R_k , R_{1k} and $Q R_k$ are the corresponding weights in the objective function, P is the stabilizing term derived from the Riccati Equation for discrete systems [179], N and M are the output horizon and control horizon respectively, k is the time step, A , B , C , D , E are the matrices of the discrete linear state space model and e denotes the mismatch between the actual system output and the predicted output at initial time. Note

that \mathcal{U} , \mathcal{X} , \mathcal{Y} , \mathcal{D} and \mathcal{U}_Δ denote compact polytopes containing the origin, and \mathcal{X}_T denotes the terminal set.

Remark 33. It is beyond the scope of this thesis to provide treatment of the intricacies of MPC, as the main focus is laid upon the explicit solution of problem (5.2) *via* multi-parametric programming. For an excellent introduction into MPC, the reader is referred to the textbook by Rawlings and Mayne [227].

Since problem (5.2) is a function of the states at the initial time (x_0), the set points (u_k^R and y_k^R), the initial output mismatch, the previous control actions in Δu_k and the disturbances (d_k), they are treated as uncertain parameters denoted by the parameter vector θ , which yields a mp-QP problem of type (3.1).

Hybrid Systems

Hybrid systems are characterized by the presence of both continuous and discrete elements. This represents a very large class of problems, such as decision processes, piecewise affine models and discrete control actions. The modelling of such systems is very complex and goes beyond the scope of this thesis. The interested reader is referred to the excellent textbook [260] and the papers [23, 115] for some of the key results. Within this thesis, hybrid systems are defined to be systems featuring discrete control actions, i.e. the state-space is given as:

$$x^+ = Ax + Bu, \tag{5.3}$$

where $u \in \mathbb{R}^{m_c} \times \{0, 1\}^{m_b}$. As a result, the hybrid MPC problem considered in this thesis is equivalent to problem (5.2), however with a changed definition of u . Note that the application of the principles of [31], as detailed above, results in a mp-MIQP problem [23, 74, 199].

5.2.2 Robust Systems

Consider the following linear discrete-time dynamics:

$$x^+ = Ax + Bu. \tag{5.4}$$

In nominal MPC, it is assumed that A and B in eq. (5.4) are exactly known and thus accurately describe the propagation of the system without any disturbance. However, due to model mismatch and unmeasured disturbances, this may not be true, as the values of state-space matrices may be uncertain, i.e. $(A, B) \in \Omega$, where Ω is called the uncertainty set. Thus, the performance of any model based strategy utilizing the predictive capability

of a system of type (5.4) with $(A, B) \in \Omega$ will need to devise methodologies to cope with the impact of the uncertainty. In the case of MPC, this has led to the development of robust MPC [10, 161, 176, 177, 203, 206]. Beginning with pioneering works in [47, 147], it has grown considerably, considering different types of uncertainty including parametric [32, 147, 148], unstructured [80, 170] or stochastic [221] uncertainties. In the following, a brief overview over the concepts used in this thesis is given. For a more in-depth treatment on robust MPC, the reader is referred to the textbooks by Kouvaritakis and Cannon [149] and Borrelli *et al.* [44].

The uncertainty set Ω

Classically², the uncertainty set Ω is considered to be a polytope of the form (see e.g. [149]):

$$\Omega = \left\{ (A, B) \left| \begin{array}{l} \sum_{i=1}^V \lambda_i A_i, 0 \leq \lambda_i \leq 1, \sum_{i=1}^V \lambda_i = 1 \\ \sum_{i=1}^V \lambda_i B_i, 0 \leq \lambda_i \leq 1, \sum_{i=1}^V \lambda_i = 1 \end{array} \right. \right\}, \quad (5.5)$$

where A_i and B_i are the i -th vertex of the uncertainty set Ω , and V denotes the total number of vertices. Clearly, eq. (5.5) defines Ω to be a polytope. However, in this thesis, the more restrictive case of box-constrained uncertainty sets is considered:

$$\Omega = \{(A, B) \mid A = A_0 + \Delta A, B = B_0 + \Delta B\}, \quad (5.6)$$

where $\Delta A \in \mathcal{A}$ and $\Delta B \in \mathcal{B}$ with:

$$\mathcal{A} = \{\Delta A \mid -\epsilon_a |A_0| \leq \Delta A \leq \epsilon_a |A_0|\} \quad (5.7a)$$

$$\mathcal{B} = \{\Delta B \mid -\epsilon_b |B_0| \leq \Delta B \leq \epsilon_b |B_0|\}, \quad (5.7b)$$

Note that (in a slight abuse of notation), ϵ_a and ϵ_b can be scalars or matrices of dimensions of A_0 and B_0 respectively, which renders the multiplication $\epsilon_a |A_0|$ also element-wise. The reason for this choice is that the extreme points of a box-constrained system can be described using the halfspace representation, and thus it is not necessary to perform a vertex enumeration to apply the robust MPC strategies discussed in this chapter. A graphical representation of the difference to the general polytopic case is shown in Figure 5.1.

Remark 34. Note that the uncertainty set Ω refers to a time-varying uncertainty.

²In the open literature, ellipsoidal uncertainty sets have also often been considered, which is however not in the focus of this chapter.

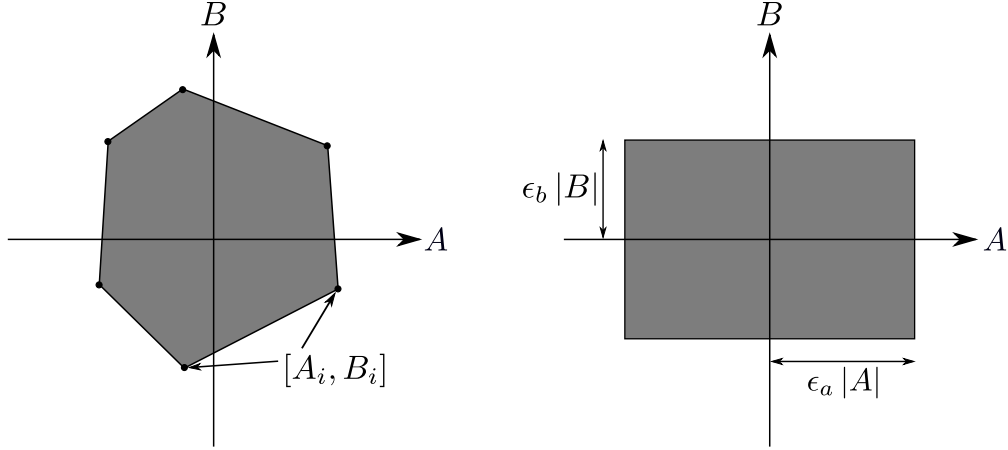


Figure 5.1: A schematic representation of a (a) polytopic and (b) box-constrained uncertainty set. The key difference lies in the ability to implicitly describe maximum of the box using a halfspace representation; this is not possible for the general polytopic case.

Robust Model Predictive Control

Consider system (5.4) with $(A, B) \in \Omega$ and eq. (5.6), $u_k \in \mathcal{U} \times \{0, 1\}^{m_b}$ and $x_k \in \mathcal{X}$, $\forall k$, where \mathcal{U} and \mathcal{X} are assumed to be compact polytopes which contain the origin³. Thus, the following sets are defined:

Definition 14 (Robust control invariant set). Given a system of type (5.4), a set $\Phi \subseteq \mathcal{X}$ is robust control invariant if $\forall x \in \Phi$, there exists an admissible control action u such that $x^+ = Ax + Bu \in \Phi$, $\forall (A, B) \in \Omega$.

Definition 15 (Robust admissible set). Given a set P , the robust admissible set (RAS) $C(P)$ is defined as:

$$C(P) = \{x \in \mathcal{X} \mid \exists u \in \mathcal{U} \times \{0, 1\}^{m_b} \text{ s.t.} \\ x^+ = Ax + Bu \in P, \forall (A, B) \in \Omega\}. \quad (5.8)$$

Remark 35. In this chapter, it is assumed that robust admissible sets and robust control invariant sets are polytopes or unions of polytopes, respectively. This is due to the fact that the projection of a polytope is a polytope, and the hybrid projection of a union of polytopes is a union of polytopes. Note that any union of polytopes can be described as a set $P = \{(x, y) \mid x \in \mathbb{R}^{n_c}, y \in \{0, 1\}^{n_b}\}$ (see section 2.2.3).

³In the case of continuous systems, $m_b = 0$.

Robust Optimization

In robust optimization, the aim is to find solutions to uncertain optimization problems which are feasible for all uncertainty realizations. In order to achieve this, the uncertain optimization problem is reformulated using an appropriate robust counterpart:

Definition 16 (Robust counterpart). A robust counterpart $\tilde{a}^T x \leq b$ of an uncertain constraint $a^T x \leq b$ with $a \in A$ is given as:

$$a^T x \leq \tilde{a}^T x \leq b, \quad \forall a \in A. \quad (5.9)$$

In this thesis, the uncertainty is present in the state-space model, and thus the robust counterpart to be formulated has to ensure the satisfaction of constraints across this state-space model, i.e. let there be a polytope $P = \{x | Gx \leq g\}$. Then given the system of type (5.4) with eq. (5.6-5.7), the constraint set to be considered is given as:

$$Gx^+ \leq g \quad (5.10a)$$

$$G(Ax + Bu) \leq g, \quad (A, B) \in \Omega \quad (5.10b)$$

$$GA_0x + \epsilon_a |G| |A_0| |x| + GB_0u + \epsilon_b |G| |B_0| |u| \leq g \quad (5.10c)$$

Eq. (5.10c) is called the robust counterpart of eq. (5.10b), and by construction it generally holds for the sets $P = \{(x, u) | \text{Eq. (5.10b)}\}$ and $Q = \{(x, u) | \text{Eq. (5.10c)}\}$ that $Q \subseteq P$.

Remark 36. In eq. (5.10c), the absolute values are relaxed using the auxiliary variables $z = |x|$ and $v = |u|$ defined by the following set of linear inequality constraints:

$$-z \leq x \leq z \quad (5.11a)$$

$$-v \leq u \leq v. \quad (5.11b)$$

Note that if $a \geq 0$, then $a = |a|$ and no auxiliary variable needs to be created. In particular, for any binary variable $\delta = \{0, 1\}$ it holds that $\delta = |\delta|$. In addition, note that eq. (5.11) is a relaxation of the absolute value terms, and only yields the exact reformulation if one of the constraints is active.

5.3 Inner approximations of robust admissible sets *via* projections

In this section, inner approximations of robust admissible sets are calculated using a series of projections. First, consider the case when the set P is a polytope, before the general case of a union of polytopes.

5.3.1 P as a polytope

Consider the set $P = \{x | Gx \leq g\}$ in conjunction with uncertain discrete-time linear system described in eq. (5.4-5.7). Then, combining the RAS definition from eq. (5.8) with eq. (5.10c) yields the following inner approximation of the RAS, $\underline{C}(P)$:

$$\underline{C}(P) = \{x | \exists (u, v, z) \text{ such that } (x, u, v, z) \in P'\}, \quad (5.12)$$

where

$$P' = \left\{ (x, u, v, z) \left| \begin{array}{l} x \in \mathcal{X}, u \in \mathcal{U} \times \{0, 1\}^{m_b} \\ GA_0x + \epsilon_a |G| |A_0| z + GB_0u + \epsilon_b |G| |B_0| v \leq g \\ -z \leq x \leq z, -v \leq u \leq v \end{array} \right. \right\}. \quad (5.13)$$

The explicit formulation of $\underline{C}(P)$ is obtained by performing the projection $\pi_n(P')$ if $m_b = 0$ or the hybrid projection $\tilde{\pi}_n(P')$ if $m_b > 0$.

5.3.2 P as a union of polytopes

In the case of hybrid systems, P may not be a polytope, however based on Definition 4, the explicit formulation of $\underline{C}(P)$ is guaranteed to be a union of polytopes (see also Remark 35). Thus, consider the set $P = \bigcup_{i=1}^p \{x | G_i x \leq g_i\}$ in conjunction with the state-space dynamics (5.4) and the uncertainty set Ω defined according to (5.6). Then, combining the RAS definition from eq. (5.8) with eq. (5.10c) yields the following inner approximation of the RAS $\underline{C}(P)$:

$$\underline{C}(P) = \{x | \exists (u, v, z) \text{ such that } (x, u, v, z) \in P'\}, \quad (5.14)$$

where

$$P' = \bigcup_{i=1}^p P'_i, \quad (5.15)$$

with

$$P'_i = \left\{ (x, u, v, z) \left| \begin{array}{l} x \in \mathcal{X}, u \in \mathcal{U} \times \{0, 1\}^{m_b} \\ G_i A_0 x + \epsilon_a |G_i| |A_0| z + G_i B_0 u + \epsilon_b |G_i| |B_0| v \leq g_i \\ -z \leq x \leq z, -v \leq u \leq v \end{array} \right. \right\}. \quad (5.16)$$

The explicit formulation of $\underline{C}(P)$ is obtained by performing p (hybrid) projections.

Theorem 8. For any $x \in \underline{C}(P)$ based on eq. (5.14), there exists a control action u such that $x^+ \in P$.

Proof 4. $\underline{C}(P)$ differs from $C(P)$ solely in the consideration of $x^+ \in P$. While eq. (5.8) utilized the description of eq. (5.10b), eq. (5.14-5.16) utilized eq. (5.10c). Thus, according to section 5.2.2, $\underline{C}(P) \subseteq C(P)$ holds, which completes the proof. \square

Remark 37. If $p = 1$, then eq. (5.15-5.16) are identical to eq. (5.13). Thus, eq. (5.12-5.13) is a special case of eq. (5.14-5.16).

Theorem 9. The calculation of $\underline{C}(P)$ based on eq. (5.14) requires at most $p2^{m_b}$ projections.

Proof 5. Consider the case of $p = 1$ as discussed in section 5.3.1. Then, the exhaustive enumeration of all possible binary variables yields 2^{m_b} combinations. If a combination is fixed in P' , then the resulting set is a polytope, and a projection yields the desired set $\underline{C}(P)$. Thus, at most 2^{m_b} projections are required in order to consider each combination of binary variables. Now consider a general p . Then for each polytope P_i , the same argument holds, i.e. at most 2^{m_b} projections are required. Thus, the number of projections is bound from above by $p2^{m_b}$. \square

Lemma 2. For the continuous case, the calculation of $\underline{C}(P)$ requires one projection.

Proof 6. This follows trivially from Theorem 9. \square

5.3.3 Recursion of RAS

In order to obtain a robust MPC formulation, the propagation of the robust admissible set beyond a single stage needs to be considered. Consider $k = N - 1$ with $P_N = \bigcup_{i=1}^p \{x | G_i x \leq g_i\}$

and the state-space dynamics in eq. (5.4) and the uncertainty set Ω defined according to eq. (5.6-5.7). Then, the k -step RAS $\underline{C}(P_{k+1})$ is given by eq. (5.14-5.16). In order to complete the recursion, set $P_k = \underline{C}(P_{k+1})$, and $k = k - 1$.

Theorem 10. If $x_0 \in P_0$ and $P_k = \underline{C}(P_{k+1})$, $\forall k \in \mathbb{N}_{N-1}$, then based on eq. (5.14-5.16) there exists an admissible control sequence u_k , $k \in \mathbb{N}_{N-1}$ such that $x_k \in P_k$, $\forall k \in \mathbb{R}_{[1,N]}$.

Proof 7. From Theorem 8, it is clear that $x_{N-1} \in P_{N-1} = \underline{C}(P_N)$ guarantees $x_N \in P_N$. By extension, it immediately follows that $x_{N-2} \in \underline{C}(P_{N-1})$ guarantees $x_{N-1} \in P_{N-1}$. Performing this computation $N - 1$ times yields the theorem and completes the proof. \square

Lemma 3. The calculation of P_0 requires at most $p \sum_{k=1}^N 2^{km_b}$ projections.

Proof 8. Based on Theorem 9, the calculation of P_{N-1} requires at most $p2^{m_b}$ projections. Thus, P_{N-1} can feature at most $p2^{m_b}$ polytopes, which by extension of Theorem 9 limits the number of projections for the calculation of P_{N-2} by:

$$p2^{m_b}2^{m_b} = p2^{2m_b}. \quad (5.17)$$

Thus, the extension of eq. (5.17) for N steps yields the desired result. \square

5.3.4 Robust control invariance

The recursion of the RAS can be used to calculate a robust control invariant set for system (5.4).

Theorem 11. Consider the set $P = \bigcup_{i=1}^p \{x | G_i x \leq g_i\}$. Then, P is robust control invariant if $P \subseteq \underline{C}(P)$.

Proof 9. According to Theorem 8, $x \in \underline{C}(P)$ guarantees $x^+ \in P$. Thus, if $P \subseteq \underline{C}(P)$, then $x \in \underline{C}(P)$ guarantees $x^+ \in \underline{C}(P)$, which completes the proof. \square

5.4 Robust Model Predictive Control

Here, a model predictive control strategy is considered robust if it results in a sequence of admissible control actions u_k , $k \in \mathbb{N}_{N-1}$ which guarantee constraint satisfaction for all future time steps in the face of the considered uncertainty for discrete-time linear systems described by eq. (5.4-5.6). Thus, the following set is defined:

$$G_k(P_{k+1}) = \left\{ (x, u) \mid \exists (v, z) \text{ s.t. } (x, u, v, z) \in P'_{k+1} \right\}. \quad (5.18)$$

As a result, for any pair $(x, u) \in G_k$ it is guaranteed that $x^+ \in P_{k+1}$. In order to obtain a robust MPC formulation, Theorem 10 and eq. (5.18) are used and the following robust MPC problem is formulated:

$$\begin{aligned}
& \underset{U}{\text{minimize}} \quad \|x_N\|_T + \sum_{i=0}^{N-1} \|x_k\|_Q + \|u_k\|_R \\
& \text{subject to } u_k \in \mathcal{U} \times \{0, 1\}^{m_b}, \quad k \in \mathbb{N}_{N-1} \\
& \quad (x_k, u_k) \in G_k(P_{k+1}), \quad k \in \mathbb{N}_{N-1} \\
& \quad P_k = \underline{C}(P_{k+1}), \quad k \in \mathbb{N}_{[1, N-1]} \\
& \quad P_N = \Phi \\
& \quad \text{Eq. (5.14-5.16, 5.18)} \\
& \quad x_{k+1} = A_0 x_k + B_0 u_k, \quad k \in \mathbb{N}_{N-1} \\
& \quad U = [u_0, u_1, \dots, u_{N-1}]^T.
\end{aligned} \tag{5.19}$$

where Φ is the robust control invariant set defined in Definition 14.

Theorem 12. If problem (5.19) is feasible for a given initial state x_0 , then the successor state $x^+ \in P_1$ for any realization of the uncertainty described by eq. (5.6-5.7).

Proof 10. Problem (5.19) is feasible if $(x_0, u_0) \in G_0(P_1)$. Thus, based on Theorem 8, the proof follows. \square

5.4.1 The continuous case

In the case of a continuous system, problem (5.19) is a convex quadratic programming problem. As a result, the robust control laws can be obtained explicitly offline *via* the solution of the corresponding multi-parametric quadratic programming problem [31]. This is very similar to the procedure presented in [148, 219], where multi-parametric programming was also used to obtain a robust MPC formulation. However, the approach presented in this chapter differs and improves upon [148, 219] in two principal ways:

The use of the projection operation: In [148, 219], the robust admissible set is calculated by solving the stage-wise control problem recursively in a multi-parametric fashion. The algorithm employed to that end in [148, 219] increases the number of parameters at each stage as it treats the future control actions as parameters. This hinders the extension of this approach to any but small enough control problems. This issue

does not occur when using the projection-based approach presented in this chapter, as the recursion can take place with constant dimensionality.

The use of the mp-QP formulation: The approach in [148, 219] solves the stage-wise control problem recursively as an mp-QP problem. Thus, the entire map of control actions is obtained for the RAS at that stage. However, this information is not required, as only the explicit of the RAS is passed onto the next stage. Note that in [148, 219] the information is also not used. The calculation of this superfluous information does not occur in the algorithm presented in this chapter.

5.4.2 The hybrid case

In the case of a hybrid system, problem (5.19) is a mixed-integer quadratic programming problem. As a result, the robust control laws can be obtained explicitly offline *via* the solution of the corresponding multi-parametric mixed-integer quadratic programming problem [220]. The main contribution of this approach is thereby twofold:

The extension of the idea in [148, 219]: The work presented in this chapter is a direct extension of the work in [148, 219] to hybrid systems. This is especially clear as the mathematical description is identical if the hybrid nature of the control action is allowed for. As a result, the conceptual understanding and implementation of this approach is straightforward.

The use of the projection operation: The approach presented in this chapter heavily relies on the execution of the projection operation. The key advantage for hybrid systems is not only given by the great amount of work done in computational geometry to design efficient algorithms for the projection operation, but also that the efficiency of the algorithm is directly linked to the ability to perform this widespread operation. Thus, the implementation, complexity analysis and convergence can be assessed in a straightforward manner based on the projection operation.

5.4.3 Discussion and implications

The formulation in eq. (5.19) is not common representation for robust MPC problems. Thus, the author would like to make the following comments:

- The objective function is given as the objective function of the nominal MPC problem (see e.g. [24, 158]). However, recently a min-max approach considering the worst-case scenario for box-constrained uncertainty has also been presented [92].

- Problem (5.19) is a closed-loop robust MPC problem, i.e. the problem formulation assumes that a measurement will be available at the next time step [32]. Thus for the time steps $k \in \mathbb{N}_{[2,N]}$, it is sufficient to ensure that $x_k \in P_k$, and the constraint $(x_0, u_0) \in G_0(P_1)$ ensures that $x_1 \in P_1$.
- The use of robust counterparts generally incurs a degree of suboptimality, i.e. the sets calculated using the approach presented here are inclusions of the exact sets, available by propagating the vertices of the uncertainty exhaustively (see e.g. [158]). However, the results presented here aim at disseminating the idea that robust counterparts can be applied efficiently to robust MPC and that this idea can directly be extended to hybrid systems.
- The set $G_k(P_{k+1})$ can be understood as a robust version of the nominal constraint set $G_k^{nom}(P_{k+1}) = \{(x, u) \mid x \in \mathcal{X}, u \in \mathcal{U}, x^+ = A_0x + B_0u \in P_{k+1}\}$, which guarantees constraint satisfaction across the uncertain state-space.
- A common representation of closed-loop robust MPC problems is the following recursion (c.f. [44]):

$$\begin{aligned}
& \underset{u_k}{\text{minimize}} && J_k(x_k, u_k) \\
& \text{subject to} && x_k \in \mathcal{X} \\
& && u_k \in \mathcal{U} \\
& && A(w_k^a)x_k + B(w_k^p)u_k \in \mathcal{X}_{k+1} \\
& && w_k^a \in \mathcal{W}^a, w_k^p \in \mathcal{W}^p,
\end{aligned} \tag{5.20}$$

where J_k is the stage-wise cost at stage k^4 , and \mathcal{W}^a and \mathcal{W}^p are the sets featuring the vertices of the uncertainty set Ω , each realization of which is shown as $A(w_k^a)$ and $B(w_k^p)$, respectively. In particular, note that \mathcal{X}_{k+1} is defined as:

$$\mathcal{X}_k = \left\{ x \in \mathcal{X} \left| \begin{array}{l} \exists u \in \mathcal{U} \text{ s.t.} \\ A(w_k^a)x + B(w_k^p)u \in \mathcal{X}_{k+1}, \\ w_k^a \in \mathcal{W}^a, w_k^p \in \mathcal{W}^p \end{array} \right. \right\} \tag{5.21}$$

where $\mathcal{X}_N = \mathcal{X}_f$ and \mathcal{X}_f is a terminal set. However, since a closed-loop control is considered, only u_0 is applied. As a consequence, the impact of the recursions

⁴Note that J_k also features the optimal cost of stage $k+1$.

$k \in \mathbb{N}_{[1, N-1]}$ is based on the propagation of the robust admissible set \mathcal{X}_k , which is equivalent to the considerations made here (see section 5.4.3).

- In this chapter, only hybrid systems which are characterized by continuous and binary inputs are considered. However, from a conceptual level the same ideas can be applied to many classes of hybrid dynamical systems such as mixed-logical dynamical systems and their equivalent representations [23, 115] by defining equivalent uncertainty sets for the state-space matrices.

A reformulation of problem (5.19) in the form of problem (5.20)

Remark 38. For ease of representation, the equivalence for uncertain discrete-time linear systems with only continuous inputs, as described in eq. (5.4-5.6) with $m_b = 0$, is shown.

The solution of problem (5.20) yields the control action of stage k , u_k , which minimizes the cost function and ensures that $x_{k+1} \in \mathcal{X}_{k+1}, \forall (A, B) \in \Omega$. The control action is thereby defined as a function of the current stage, i.e. $u_k(x_k)$. Thus, it is a closed-loop strategy as it does not consider all possible realizations of x_k for a given x_0 subject to the uncertainty but only the realization that will occur at stage k . As a result, the impact of $u_k(x_k)$ is twofold: (a) it is used to calculate \mathcal{X}_k and (b) it is substituted in the objective function $J_k^*(x_k) = J_k(x_k, u_k(x_k))$. The only exception is the last stage, i.e. $u_0(x_0)$ which is implemented at every time step.

Thus, in order to show the equivalence of problem (5.20) with problem (5.19) it is necessary to show that \mathcal{X}_k is the robust admissible set as per Definition 15 and as a consequence that any control action calculated from problem (5.19) is a feasible solution of problem (5.20).

Following Definition 15, it follows:

$$\mathcal{X}_k = \left\{ x \in \mathcal{X} \left| \begin{array}{l} \exists u \in \mathcal{U} \text{ s.t.} \\ A(w_k^a)x + B(w_k^p)u \in \mathcal{X}_{k+1}, \\ w_k^a \in \mathcal{W}^a, w_k^p \in \mathcal{W}^p \end{array} \right. \right\} \quad (5.22)$$

$$= \{x \in \mathcal{X} | \exists u \in \mathcal{U} \text{ s.t.} \\ x^+ = Ax + Bu \in \mathcal{X}_{k+1}, \forall (A, B) \in \Omega\} \quad (5.23)$$

$$= C(\mathcal{X}_{k+1}) \quad (5.24)$$

The equivalence between eq. (5.22) and eq. (5.23) is based on the fact that the uncertainty set Ω is completely characterized by the set of its vertices \mathcal{W}^a and \mathcal{W}^p . Thus, re-writing the

constraint set of (5.20) yields:

$$\mathcal{C}_k = \left\{ (x, u) \left| \begin{array}{l} x \in \mathcal{X}, u \in \mathcal{U} \\ A(w_k^a)x + B(w_k^p)u \in \mathcal{X}_{k+1}, \\ w_k^a \in \mathcal{W}^a, w_k^p \in \mathcal{W}^p \end{array} \right. \right\} \quad (5.25)$$

$$= \left\{ (x, u) \left| \begin{array}{l} x \in \mathcal{X}, u \in \mathcal{U} \\ Ax + Bu \in \mathcal{X}_{k+1}, \forall (A, B) \in \Omega \end{array} \right. \right\} \quad (5.26)$$

$$\supseteq \left\{ (x, u) \mid \exists (v, z) \text{ s.t. } (x, u, v, z) \in P'_{k+1} \right\} \quad (5.27)$$

$$= G_k(P_{k+1}), \quad (5.28)$$

which shows the equivalence.

5.5 Example problem

Remark 39. The calculations were carried out on a single-threaded machine running Microsoft Windows 7 with an Intel Core i5-4200M CPU at 2.50 GHz and 8 GB RAM. Furthermore, MATLAB R2014a, ILOG Optimization Studio 12.6.1, POP v1.62 [201] and MPT 3.1 [118] were used for the computations.

Consider the following example problem:

$$A_0 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad B_0 = \begin{bmatrix} 0 & -1 \\ 1 & 1 \end{bmatrix} \quad (5.29a)$$

$$\mathcal{X} = \left\{ x \left| \begin{array}{l} -10 \leq [1 \ 0]x \leq 10 \\ -10 \leq [0 \ 1]x \leq 10 \end{array} \right. \right\}, \quad (5.29b)$$

and $\epsilon_a = \epsilon_b = 0.1$, $Q = R = I_2$ and T the solution of the discrete-time algebraic Riccati equation of the nominal system [179]. First, consider the discrete-time linear system with

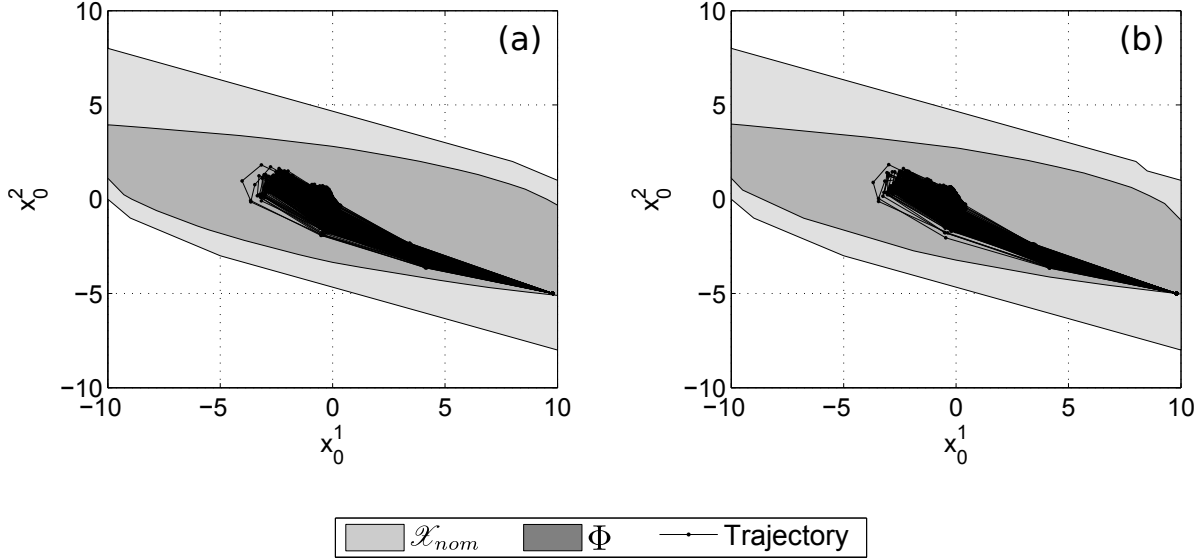


Figure 5.2: The controllability set of the nominal system \mathcal{X}_{nom} , the corresponding robust control invariant set Φ and the trajectories of 300 different simulations of 50 steps with different disturbance profiles starting from $[9.8, -5]$ is shown in (a) for the system with only continuous inputs and in (b) for the system featuring continuous and binary inputs.

only continuous inputs, i.e.:

$$\mathcal{U} = \left\{ u \left| \begin{array}{l} -1 \leq [1 \ 0] u \leq 1 \\ 0 \leq [0 \ 1] u \leq 1 \end{array} \right. \right\}, \quad (5.30)$$

and in Figure 5.2(a) the feasible space of the nominal system and the robust control invariant set Φ obtained from the application of Theorem 11 is shown. In addition, 300 simulations with 50 time steps with different disturbance signals starting from $[9.8, -5]$ are displayed. In order to consider an equivalent system featuring a combination of continuous and binary inputs, consider:

$$u \in \mathcal{U} \times \{0, 1\}, \quad (5.31)$$

where $\mathcal{U} = \{u \mid -1 \leq u \leq 1\}$, i.e. the second input has been converted from a continuous input bound between 0 and 1 to a binary variable. In Figure 5.2(b) the feasible space of the nominal system and the robust control invariant set Φ obtained from the application of Theorem 11 is shown, as well as 300 simulations with 50 time steps with different disturbance signals starting from $[9.8, -5]$. The computation of the robust control invariant set required 12.4 and 121.0 seconds for the continuous and hybrid system, respectively. For comparison,

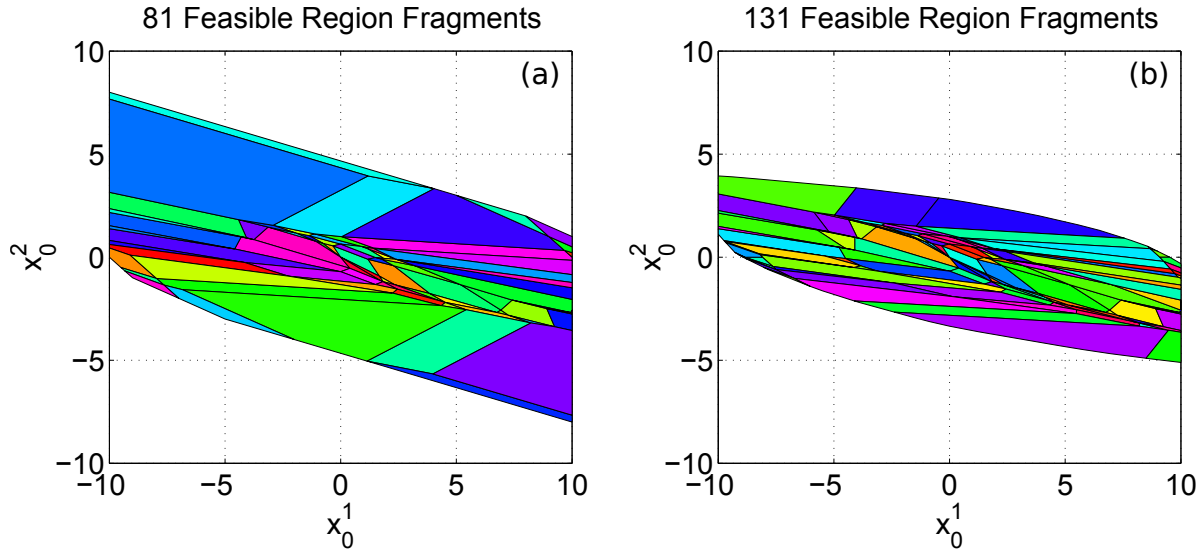


Figure 5.3: The explicit solution of the (a) nominal and (b) robust MPC controller for the example problem.

the calculation of the robust control invariant set for the continuous system was performed with MPT (see [158]) and required 23.4 seconds.

5.5.1 Detailed discussion

In this section, the example problem is used to highlight several features of the robust approach presented in this chapter.

Complexity increase from nominal to robust MPC

The calculation of a robust MPC strategy not only reduces the controllability set, but in general renders the controller more complex as the different worst-case realizations need to be considered. For the example problem, Figure 5.3 shows the explicit solution of the nominal and robust controller, respectively. In particular, it is to note that although the controllability set of the nominal controller is significantly larger, it only features 81 critical regions, as opposed to the 131 regions obtained for the robust controller. However, certain aspects of the explicit solution such as the reverse S-shaped center and the layered regions around it have been preserved, indicating the structural relationship between these controllers.

This underlying similarities are intriguing, and future research directions may focus into understanding why these features in particular have been preserved. In addition, this may lead to interesting considerations regarding the ability to infer aspects of the structure of robust controllers based on the nominal controller.

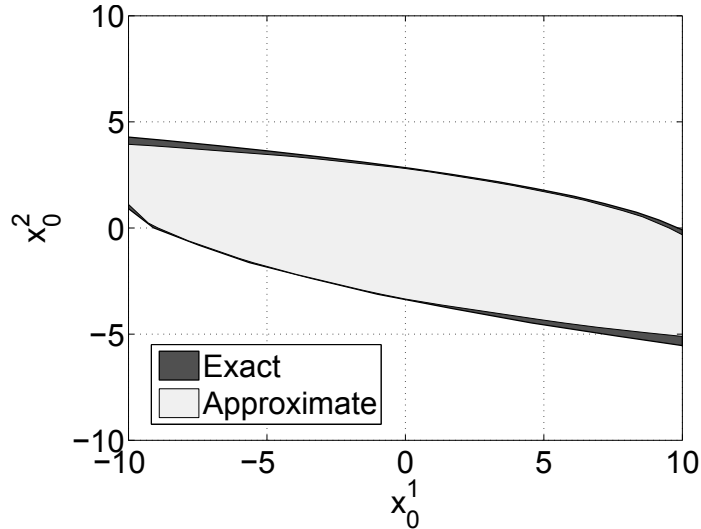


Figure 5.4: The comparison of the exact robust control invariant set with the inner approximation of the same set obtained *via* robust optimization.

Conservatism of the robust optimization approach

One of the key points in robust optimization is the introduction of overly tight constraints which decreases the feasible space beyond what would be necessary in order to ensure robustness. This aspect, brilliantly discussed in the paper "The price of robustness" by Bertsimas and Sim [37], has been a main focus for more than a decade in the area of robust optimization. In fact, it was only recently that Floudas and co-workers were able to reduce this "price" for the first time since the work of Ben-Tal and Nemirovski as well as Bertsimas and Sim [111, 112].

Consequently for the case of robust MPC *via* robust optimization, this conservatism is crucial as a robust counterpart is formed at each stage. Thus, the conservativeness is in fact compounded beyond a single stage, which leads to an increase of conservatism as the horizon length increases. For the example problem above, the conservatism is highlighted in Figure 5.4, where the exact robust control invariant set is compared to the inner approximation calculated using robust optimization. As it can be seen, for the considered example the conservatism is noticeable, however it is relatively limited.

Note however that the impact of this conservatism varies among different examples, and highly depends on the strategy used to formulate the robust counterpart. Thus, future directions will consider the incorporation of tighter robust counterparts, as well as considerations of probability bounds for the robust control invariant set in order to produce controllers with larger controllability sets.

Differences between continuous and hybrid systems

Although Figure 5.2 may suggest that the sets for the continuous and hybrid system are identical, the controllability set of the nominal system as well as the robust control invariant set of the hybrid system are subsets of the continuous system, as expected. However, the general shapes are preserved as the control actions on the extreme points are given by the maximum admissible control actions, which are still admissible for the hybrid case (i.e. 0 and 1). However, there are two important differences in terms of computation and implementation.

First, the time required for the computation of each differs by one order of magnitude. This is primarily due to two effects: (a) the number of polytopes forming the union of polytopes for the hybrid system and (b) merging polytopes whose union is convex. As these factors are in most cases bound to increase with increasing dimensionality, it is expected that the overall computation time for the hybrid system will very quickly become computationally intractable. Thus, new solutions such as parallelization, analysis of the structure of the system as well as approximate methods are expected to enable significant progress in the area of computational attractiveness of the presented approach.

Second, while there are several tools for the computation of robust controllers in general and robust control invariant sets in particular for continuous systems, to the author's knowledge such a tool does not exist for hybrid systems. Thus, comparisons in terms of conservatism and computational performance are not available. However, the author expects that such tools will be developed in the near future due to the growing interest in robust control for hybrid systems paired with the shrinking cost of computational power.

Chapter 6

Unbounded and binary parameters in multi-parametric programming

Portions of this chapter have been published in:

- Oberdieck, R.; Diangelakis, N. A.; Avraamidou, S.; Pistikopoulos, E. N. (2016) On unbounded and binary parameters in multi-parametric programming: Applications to mixed-integer bilevel optimization and duality theory. *Journal of Global Optimization, in print.*

6.1 Introduction

Commonly in multi-parametric programming, the parameters are assumed to be bounded and continuous [220]. While these conditions are met in many circumstances, there are cases where this is not true. Examples include optimal control problems where some of the states are binary variables and bilevel optimization problems featuring continuous and binary variables on both stages. In this section strategies are proposed to overcome these limitations. In particular, first conditions are derived based on which the boundedness of the parameters is not necessary. It is also shown how the concept of binary variables can be directly integrated into combinatorial approaches used for the solution of mp-LP/mp-QP problems. Then, these two strategies are combined into a new, more general version of the combinatorial algorithm which allows for the solution of multi-parametric programming problems featuring unbounded and binary parameters. Numerical examples are used to highlight the steps of the proposed strategies, along with a mixed-integer bilevel optimization example. A discussion on the parametric solution of dual problems is also presented.

6.2 Theoretical Background

We consider the following generalized version of the mp-QP problem:

$$\begin{aligned}
 z(\theta) = \underset{x}{\text{minimize}} \quad & (Qx + H\theta + c)^T x \\
 \text{subject to} \quad & Ax \leq b + F\theta \\
 & x \in \mathbb{R}^n, \theta = [\theta_c, \theta_b]^T \\
 & \theta_c \in \mathbb{R}^q, \theta_b \in \mathbb{B}^p = \{0, 1\}^p
 \end{aligned} \tag{6.1}$$

where $Q \in \mathbb{R}^{n \times n}$ is symmetric positive definite, $H \in \mathbb{R}^{n \times q+p}$, $c \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $F \in \mathbb{R}^{m \times q+p}$.

Remark 40. Commonly, the parameter θ_c are constrained to a so-called parameter space, often denoted as Θ . However, for the sake of generality, any parameter-specific constraints have been incorporated into the constraint set $Ax \leq b + F\theta$. Thus, problem (3.1) also includes the case where some or all elements of θ_c are bounded.

For the rest of the section, the following notation is defined:

Definition 17. Let $T = 1, \dots, m$ be a set of indices. Then, given the subset $\mathcal{J} \subset T$, the complement is defined as $\neg\mathcal{J}$ such that $\mathcal{J} \cup \neg\mathcal{J} = T$. Additionally, let $A \in \mathbb{R}^{m \times n}$, then $A_{\mathcal{J}}$ denotes a matrix composed of the rows of A identified by the indices in \mathcal{J} . Lastly, problem (6.1) is called unbounded if not all θ_c are bounded given the set of constraints $Ax \leq b + F\theta^1$.

6.3 Unbounded multi-parametric programming

6.3.1 Motivating example

Consider the following mp-LP problem:

$$\begin{aligned}
 \underset{x}{\text{minimize}} \quad & x \\
 \text{subject to} \quad & -4x \leq -1 + \theta \\
 & -2x \leq 2 - \theta \\
 & x \in \mathbb{R}, \theta \in \mathbb{R}
 \end{aligned} \tag{6.2}$$

¹Note that binary parameters are inherently bounded.

It is evident that problem (6.2) is unbounded (see Figure 6.1). However, by inspection it is also clear that the solution to this problem is given by

$$x_1(\theta) = -0.25\theta + 0.25, \quad \forall \theta \leq \frac{5}{3} \quad (6.3a)$$

$$x_2(\theta) = 0.5\theta - 1, \quad \forall \theta \geq \frac{5}{3} \quad (6.3b)$$

where the subscript denotes which constraint is active and the numerical values are a direct function thereof.

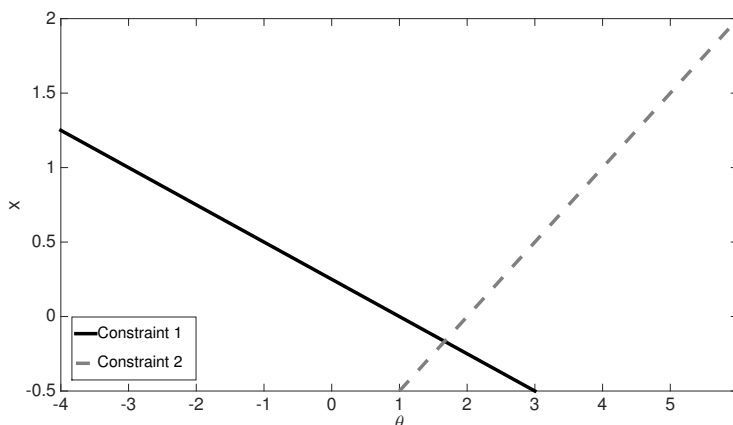


Figure 6.1: The feasible space of problem (6.2) in the (x, θ) domain.

Remark 41. Note that CPLEX 12.6.1 reports the error "unbounded or infeasible" if θ is fixed for values greater than 10^{22} , a conclusion which is avoidable by using eq. (6.3).

6.3.2 The solution of unbounded mp-LP and mp-QP problems

The key for obtaining eq. (6.3) is that we only consider the active set of the optimization problem. Thus, as soon as an initial bounded solution is found, there is no requirement for the resulting polytopic region to be bounded. This results in the following Theorem:

Theorem 13. Let there be at least one bounded solution for a parameter realization of problem (6.1), and let $p = 0$ (i.e. no binary parameters). Then, the combinatorial approach solves problem (6.1) even if any θ in the set

$$\mathcal{P} = \{(x, \theta) \in \mathbb{R}^{n \times q} \mid Ax \leq b + F\theta\} \quad (6.4)$$

are unbounded.

Proof 11. The solution $x(\theta)$ in a polytopic region only depends on the corresponding active set (see Lemma 9). Thus, if there exists a bounded solution of one parameter realization, we can initialize the tree consisting of all possible active sets. Since the active set of a region only changes if the feasibility or optimality requirements of the solution are violated, it is clear that such a violation directly results in a new active set, resulting in a new solution. Conversely, if no such violation occurs then no new active set is generated, thus allowing for the description of an unbounded solution. \square

Lemma 4. Any feasible strictly convex positive definite quadratic programming (QP) problem has a unique and bounded solution. Thus, for mp-QP problems Theorem 13 holds unconditionally.

Proof 12. Let us consider the unconstrained case. If we can prove that the solution to an unconstrained QP is bounded, then it is obvious that this extends to constrained QP problems as well. Let $f(x)$ denote the objective function. Then, due to strict convexity of $f(x)$, the necessary and sufficient condition of optimality is:

$$\nabla_x f(x) = 2Qx + c = 0, \tag{6.5}$$

where ∇_x is the Nabla-operator. Since $Q \succ 0$, the system of linear equalities in (6.5) has full rank, and thus a unique solution x^* . Since the Hessian $H > 0$ and constant, there exists a ball \mathcal{B} of radius $\epsilon > 0$ around x^* , for which all x which lie on \mathcal{B} it holds that $\nabla_x f(x) \neq 0$. This implies that there does not exist a direction d , along which x^* could become unbounded. \square

In order to apply Theorem 13, it is necessary to apply the combinatorial approach as it directly uses the active sets rather than the polytopic region description. In order to ensure that the feasibility checks do consider an unbounded problem², arbitrary bounds are put in place, which however does not impact whether the problem is recognized as feasible nor not (see section 6.5 for details).

²This was the reason for the solution reported in Remark 41.

6.3.3 Numerical Example

Consider the following mp-QP problem:

$$\begin{aligned}
 & \underset{x}{\text{minimize}} && x^T 230.08x - \theta^T \begin{bmatrix} 0 \\ 5 \end{bmatrix} \\
 & \text{subject to} && x \leq \begin{bmatrix} 4 \\ 4 \\ 9 \\ 10 \\ 2 \\ 7 \\ 13 \\ -1 \\ 8 \\ 14 \end{bmatrix} + \begin{bmatrix} 7 \\ 21 \\ 6 \\ 23 \\ 25 \\ 34 \\ 2 \\ 27 \\ 29 \\ 12 \end{bmatrix} + \begin{bmatrix} 0 & -5 \\ 0 & 0 \\ -3 & 0 \\ 0 & 0 \\ -11 & -11 \\ -3 & -6 \\ 0 & 0 \\ 0 & 0 \\ -6 & -5 \\ 0 & 0 \end{bmatrix} \theta
 \end{aligned} \tag{6.6}$$

In order to visualize the unbounded nature of problem (6.6), Figure 6.2 shows the solution of problem (6.6) for the bounded space (a) $\theta \in [-5, 5]^2$, (b) $\theta \in [-500, 200]^2$ and (c) $\theta \in [-5 \cdot 10^4, 2 \cdot 10^4]^2$. In addition, Table 6.1 presents the solution of the unbounded problem (6.6), based on section 6.3.2.

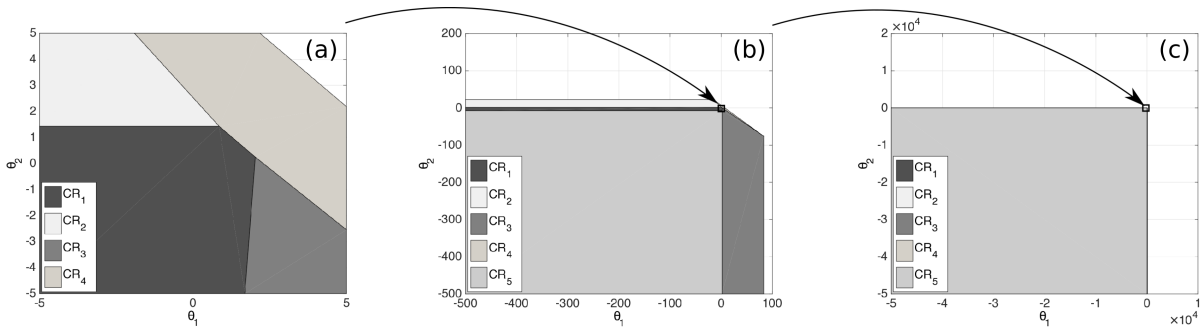


Figure 6.2: A graphical visualization of the unbounded solution, as the bounds of the parameter space are increased from (a) to (b) to (c) .

Table 6.1: The solution to problem (6.6). The notation CR_n corresponds to the n^{th} critical region or Figure 6.2.

Active Set	Critical Region	Solution
-	$CR_1: -7.28 \leq \theta_2 \leq 1.43, 0.998\theta_1 - 0.065\theta_2 \leq 2.01, 0.709\theta_1 + 0.706\theta_2 \leq 1.61$	$x(\theta) = -0.02\theta_2 - 0.004$
{1}	$CR_2: 0.791\theta_1 + 0.611\theta_2 \leq 1.55, 1.43 \leq \theta_2 \leq 23$	$x(\theta) = -1.25\theta_2 + 1.75$
{3}	$CR_3: 0.68\theta_1 + 0.73\theta_2 \leq 1.57, -0.998\theta_1 + 0.65\theta_2 \leq -2.01, 1.54 \leq \theta_1 \leq 83$	$x(\theta) = -0.333\theta_1 + 0.667$
{5}	$CR_4: -0.79\theta_1 - 0.61\theta_2 \leq -1.55, -0.69\theta_1 - 0.73\theta_2 \leq -1.57, 0.71\theta_1 + 0.71\theta_2 \leq 5.08, -0.709\theta_1 - 0.706\theta_2 \leq -1.61$	$x(\theta) = -5.5\theta_1 - 5.5\theta_2 + 12.5$
{7}	$CR_5: \theta_1 \leq 1.54, \theta_2 \leq -7.28$	$x(\theta) = 0.154$

6.4 Multi-parametric programming with binary parameters

Consider problem (6.1), featuring both continuous and binary variables. However, in the case where $\theta = [\theta_c, \theta_b]^T$, eq. (3.4) in the Basic Sensitivity Theorem has to be reconsidered for θ_b , as any function defined over $\mathbb{B}^p = \{0, 1\}^p$ from problem (6.1) is inherently non-differentiable. However, note that the right-hand side of eq. (3.4) does not depend on θ in any way, i.e. it is constant. Thus, the change of $x(\theta)$ and $\lambda(\theta)$ is constant. Consequently we can directly replace the differential with a difference equation and obtain:

$$\left(\frac{\Delta(\theta_0)}{\Delta\theta_b}, \frac{\Delta\lambda(\theta_0)}{\Delta\theta_b} \right)^T = -(M_0)^{-1} N_0, \quad (6.7)$$

where $\Delta\theta_b = 1$. Thus, the corresponding critical region is given by:

$$Ax(\theta) \leq b + F\theta \quad (\text{Feasibility of } x(\theta)) \quad (6.8a)$$

$$\lambda(\theta) \geq 0 \quad (\text{Optimality of } x(\theta)) \quad (6.8b)$$

$$\theta_b \in \mathbb{B}^p = \{0, 1\}^p \quad (\text{Integrality of } \theta_b) \quad (6.8c)$$

$$\theta = [\theta_c, \theta_b]^T \quad (6.8d)$$

As a result, the solution to a mp-QP problem featuring binary parameters is given by eq. (3.7) and eq. (3.2.1), which is optimal over the non-convex critical region described in eq. (6.8). If θ_b is fixed to any feasible combination, the resulting lower-dimensional critical region is a polytope. Thus, eq. (6.8) describes a disjoint set of polytopes, over which the same parametric solution remains optimal. This concept is graphically visualized in Figure 6.3, which highlights the transition from a parametric solution featuring only continuous parameters to a solution featuring continuous and binary parameters.

6.4.1 The solution of problem (6.1)

In order to develop solution algorithms for problem (6.1) featuring binary parameters, it is necessary to enable the handling of critical regions of type eq. (6.8). Thus, considering binary parameters in conjunction with an algorithm which requires the polytopic nature of the critical region, e.g. a geometrical approach, is challenging from a conceptual perspective. Thus, similarly to the case of unbounded parameters, we propose a modified version of the combinatorial approach for the consideration of binary parameters (see section 6.5 for details). The key idea is to incorporate the binary nature of the parameters in the feasibility and optimality checks. While this does not alter the algorithm in itself, it does require the solution of mixed-integer linear programming (MILP) problems, which might be computationally expensive.

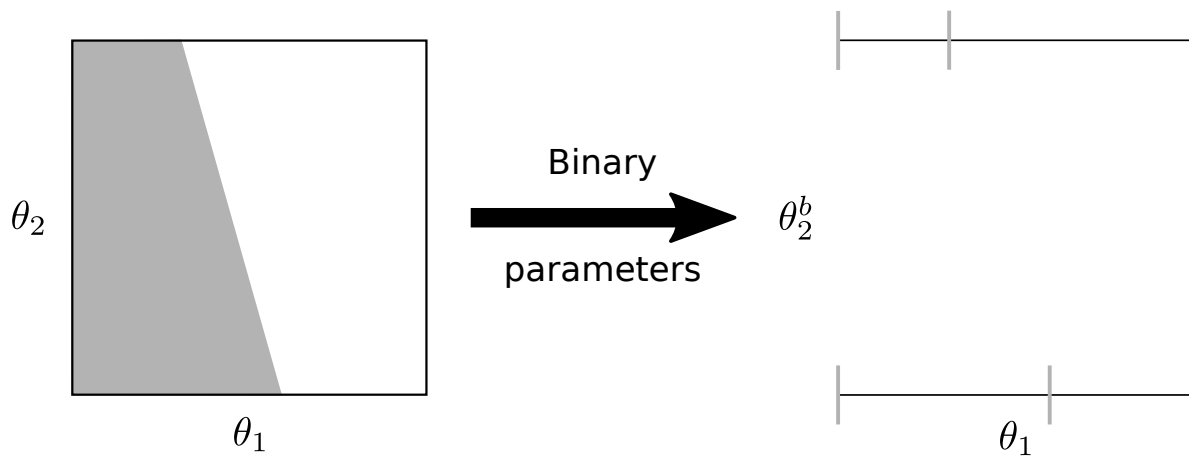


Figure 6.3: A schematic representation of a situation with one binary and one continuous variable. On the left we consider the problem where the binary variable is treated as a continuous variable $[0, 1]$ and on the right we show the equivalent binary representation.

6.4.2 Numerical Example

Consider the following mp-QP featuring binary parameters, adapted from problem (6.6):

$$\begin{aligned}
 & \underset{x}{\text{minimize}} && x^T 230.08x - \theta^T \begin{bmatrix} 0 \\ 5 \end{bmatrix} && x + x \\
 & \text{subject to} && \begin{bmatrix} 4 \\ 4 \\ 9 \\ 10 \\ 2 \\ 7 \\ 13 \\ -1 \\ 8 \\ 14 \end{bmatrix} x \leq \begin{bmatrix} 7 \\ 21 \\ 6 \\ 23 \\ 25 \\ 34 \\ 2 \\ 27 \\ 29 \\ 12 \end{bmatrix} + \begin{bmatrix} 0 & -5 \\ 0 & 0 \\ -3 & 0 \\ 0 & 0 \\ -11 & -11 \\ -3 & -6 \\ 0 & 0 \\ 0 & 0 \\ -6 & -5 \\ 0 & 0 \end{bmatrix} \theta && (6.9) \\
 & && \theta = [-5, 5] \times \{0, 1\}
 \end{aligned}$$

The solution to this problem is reported in Table (6.2) and visualized in Figure 6.4.

Table 6.2: The solution to problem (6.9).

Active Set	Critical Region	Solution
-	$\theta_1 \geq -5, \theta_2 \in \{0, 1\}, -7.28 \leq \theta_2 \leq 2.01, 0.709\theta_1 + 0.706\theta_2 \leq 1.61$	$x(\theta) = -0.02\theta_2 - 0.004$
{3}	$CR_2 : \theta_2 = 0, 2.013 \leq \theta_1 \leq 2.290$	$x(\theta) = -0.333\theta_1 + 0.667$
{5}	$CR_3 : \theta_1 \leq 5, \theta_2 = \{0, 1\}, -0.69\theta_1 - 0.73\theta_2 \leq -1.57, -0.709\theta_1 - 0.706\theta_2 \leq -1.61$	$x(\theta) = -5.5\theta_1 - 5.5\theta_2 + 12.5$

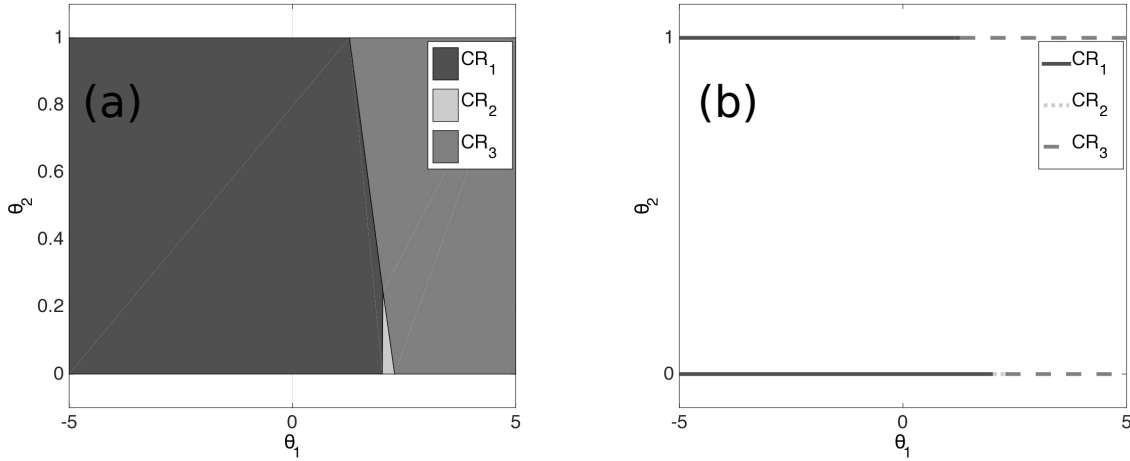


Figure 6.4: A graphical visualization of the solution featuring binary parameters. In (a) we show the solution where the parameter is relaxed between 0 and 1 while (b) shows the same solution when θ_2 is treated as a binary variable.

6.5 A generalized combinatorial algorithm

Based on the discussions in sections 6.3 and 6.4, we now combine these concepts and strategies into the description of a combinatorial algorithm which enables the solution of problem featuring unbounded and binary parameters. The pseudo-code for this approach is given in Algorithm 1.

Lemma 5 (Convergence). Algorithm 3 converges in a finite number of steps which is bounded above by

$$\phi_{\max} = \sum_{i=0}^n \binom{m}{i}, \quad (6.10)$$

where m is the number of inequality constraints.

Proof 13. Algorithm 3 represents a generalized version of the combinatorial algorithm from [110], which in its worst case relies on the exhaustive enumeration of all possible combinations of active sets, ϕ_{\max} .

Remark 42. Note that appropriate indexing avoids the repetitive consideration of active sets. In addition, note that in reality it is in most cases not necessary to evaluate ϕ_{\max} constraints due to Lemma 9.

Given a candidate active set \mathcal{S} from Algorithm 3, the first requirement is to ensure that there exists a parameter value θ for which the active set is feasible (see Lemma 9). In order

Algorithm 3 The generalized combinatorial approach enabling the solution of problems featuring unbounded and binary parameters. Note that Line 11 denotes the addition of all new candidate sets which result by adding one of the inactive constraints to the active set.

```

1:  $\mathcal{C} \leftarrow \{\emptyset\}, \mathcal{I} \leftarrow \emptyset, \mathcal{J} \leftarrow \emptyset,$ 
2: while  $\mathcal{C} \neq \emptyset$  do
3:   Pop  $\mathcal{I}$  with lowest cardinality from  $\mathcal{C}$ 
4:   if LICQ is fulfilled,  $\mathcal{I} \notin \mathcal{J}$  and problem (6.11) is feasible then
5:     Obtain  $x(\theta)$  and  $\lambda(\theta)$ 
6:     Obtain  $CR$  from eq. (6.8)
7:     if problem (6.12) is feasible then
8:        $\mathcal{I} \leftarrow (CR, x(\theta), \lambda(\theta))$ 
9:        $\mathcal{J} \leftarrow \mathcal{J} \cup \mathcal{I}$ 
10:    end if
11:     $\mathcal{C} \leftarrow \mathcal{C} \cup \left\{ \begin{pmatrix} \neg \mathcal{I} \\ 1 \end{pmatrix} \right\}$ 
12:  end if
13: end while

```

to ensure this, we solve the following Chebyshev problem:

$$\begin{aligned}
R = \underset{x, \theta, t}{\text{minimize}} \quad & -t \\
\text{subject to} \quad & A_{\neg \mathcal{I}} x - F_{\neg \mathcal{I}} \theta \leq (b_{\neg \mathcal{I}} - \|A_{\neg \mathcal{I}}\|_2 t) \\
& A_{\mathcal{I}} x - F_{\mathcal{I}} \theta = b_{\mathcal{I}} \\
& t \leq M \\
& t \in \mathbb{R}, \theta = [\theta_c, \theta_b]^T \\
& \theta_c \in \mathbb{R}^q, \theta_b \in \mathbb{B}^p = \{0, 1\}^p.
\end{aligned} \tag{6.11}$$

The constant M in the problem (6.11) represents a sufficiently large number which bounds the auxiliary variable t to an upper bound³. This boundary is required for stability, as the variable indicates the lowest distance in a 2-norm sense from the constraint. In the case of an unbounded problem, this distance will also be unbounded, which requires the introduction of the artificial bound M in order to ensure the stability of the algorithm. Note that it does not alter the outcome of the solution, as only a feasibility check is required.

If problem (6.11) is infeasible, then the active set is infeasible and together with its superset can be discarded (see Lemma 9). However, if problem (6.11) is feasible, the parametric

³Within our numerical studies, we successfully utilized $M = 10^5$.

solution can be directly calculated. Based on this, the critical region can be formulated based on eq. (6.8). However, this might lead to lower-dimensional regions due to underlying degeneracies (see [110, 133] for excellent treatments on degeneracy in multi-parametric programming). In order to identify these cases, we solve the following Chebyshev problem:

$$\begin{aligned}
R = \underset{\theta, t}{\text{minimize}} \quad & -t \\
\text{subject to} \quad & CR_A \theta \leq (CR_b - \|CR_A\|_2 t) \\
& t \leq M \\
& t \in \mathbb{R}, \theta = [\theta_c, \theta_b]^T \\
& \theta_c \in \mathbb{R}^q, \theta_b \in \mathbb{B}^p = \{0, 1\}^p.
\end{aligned} \tag{6.12}$$

If problem (6.12) is infeasible or $t \leq \epsilon$, where ϵ is a prescribed numerical tolerance, then the region is deemed lower-dimensional and the active set is discarded. Note that this however does not lead to the fathoming of its superset according to Lemma 9, since it was deemed feasible by the solution of problem (6.11). If $t > \epsilon$, then the region is considered full-dimensional and stored as a solution to problem (6.1).

Remark 43. The algorithm presented in this section requires the solution of the linear programming problems (6.11-6.12). Thus despite the generality of Theorem 13, the approach presented in this paper requires that there exists at least one point in each critical region such that the failure reported in Remark 41 does not occur. Note that it is obvious that this condition will be fulfilled for all well-posed problems, i.e. for all problems where $\theta \geq 10^{22}$ would not impact the feasibility.

6.5.1 Numerical examples

Following the examples shown in the text for the different aspects of the generalized algorithm, here we highlight two classes of problems, previously intractable with multi-parametric programming, that can now be solved using the proposed algorithm.

Case 1 - Mixed-integer bilevel optimization: In bilevel optimization, an optimization

problem is solved while subjected to a different optimization problem, i.e.

$$\begin{aligned}
& \underset{x}{\text{minimize}} && F(x, y) \\
& \text{subject to} && G(x, y) \leq 0 \\
& && x \in \mathcal{X} \\
& && y \in \underset{y}{\text{argmin}} \{f(x, y) : g(x, y) \leq 0, y \in \mathcal{Y}\},
\end{aligned} \tag{6.13}$$

where all the functions and sets have appropriate dimensions. Multi-parametric programming has been applied to bilevel and multilevel optimization ([66, 76, 78, 138]). However, the case where $F(x, y)$, $G(x, y)$, $f(x, y)$ and $g(x, y)$ are affine functions of continuous $x \in \mathcal{X}$ and binary $y \in \mathcal{Y}$ variables, with the latter appearing in both the upper and lower problem (6.14) has not been considered in the realm of multi-parametric programming.

$$\begin{aligned}
& \min_{x_i, y_j} && A^{1 \times n} [x_i, x_p]^T + B^{1 \times m} [y_j, y_q]^T + c \\
& \text{s.t.} && \min_{x_p, y_q} D^{1 \times n} [x_i, x_p]^T + E^{1 \times m} [y_j, y_q]^T + f \\
& && \text{s.t. } g^{l \times n} [x_i, x_p]^T + h^{l \times m} [y_j, y_q]^T + k \leq 0 \\
& && x_{i,p} \in \mathcal{R}^n, y_{j,p} \in \{0, 1\}^m \\
& && |i| + |p| = n, |j| + |p| = m
\end{aligned} \tag{6.14}$$

where A , B , D , E , g , h matrices of appropriate dimensions and c , f , k fixed terms.

The MILP-MILP bilevel problem is now considered:

$$\begin{aligned}
& \min_{x_3, x_4, y_3, y_4} && -x_3 - x_4 + 5y_3 + 5y_4 \\
& \text{s.t.} && \min_{x_1, x_2, y_1, y_2} && -3x_1 - 8x_2 + 4y_1 + 2y_2 \\
& && \text{s.t.} && x_1 + x_2 - x_3 \leq 13 \\
& && && 5x_1 - 4x_2 - 10y_3 \leq 10 \\
& && && -8x_1 + 22x_2 - x_4 \leq 121 \\
& && && -4x_1 - x_2 + 4y_4 \leq -4 \\
& && && 0 \leq x_i \leq 10y_i, \forall i \in \{1, 2\} \\
& && && 0 \leq x_j \leq 10, \forall j \in \{3, 4\} \\
& && && y_k \in \{0, 1\}, \forall k \in \{1, 2, 3, 4\}
\end{aligned} \tag{6.15}$$

The lower level MILP problem is reformulated as the following multi-parametric mixed integer linear programming (mp-MILP) problem featuring both continuous (θ_1, θ_2) and binary ($y_{\theta_1}, y_{\theta_2}$) parameters, i.e. x_3, x_4, y_3 and y_4 the optimal values of which are determined by the upper level problem are treated as parameters in the lower level and denoted as $\theta_1, \theta_2, y_{\theta_1}$ and y_{θ_2} , respectively:

$$\begin{aligned}
& \min_{x_1, x_2, y_1, y_2} && -3x_1 - 8x_2 + 4y_1 + 2y_2 \\
& \text{s.t.} && x_1 + x_2 \leq 13 + \theta_1 \\
& && 5x_1 - 4x_2 \leq 10 + 10y_{\theta_1} \\
& && -8x_1 + 22x_2 \leq 121 + \theta_2 \\
& && -4x_1 - x_2 \leq -4 - 4y_{\theta_2} \\
& && 0 \leq x_i \leq 10y_i \\
& && y_i \in \{0, 1\} \\
& && 0 \leq \theta_i \leq 10 \\
& && y_{\theta_i} \in \{0, 1\}, \forall i \in \{1, 2\}
\end{aligned} \tag{6.16}$$

Based on the Algorithm 1 the solution of problem 6.16 is presented in Table 6.3 and Figure 6.5.

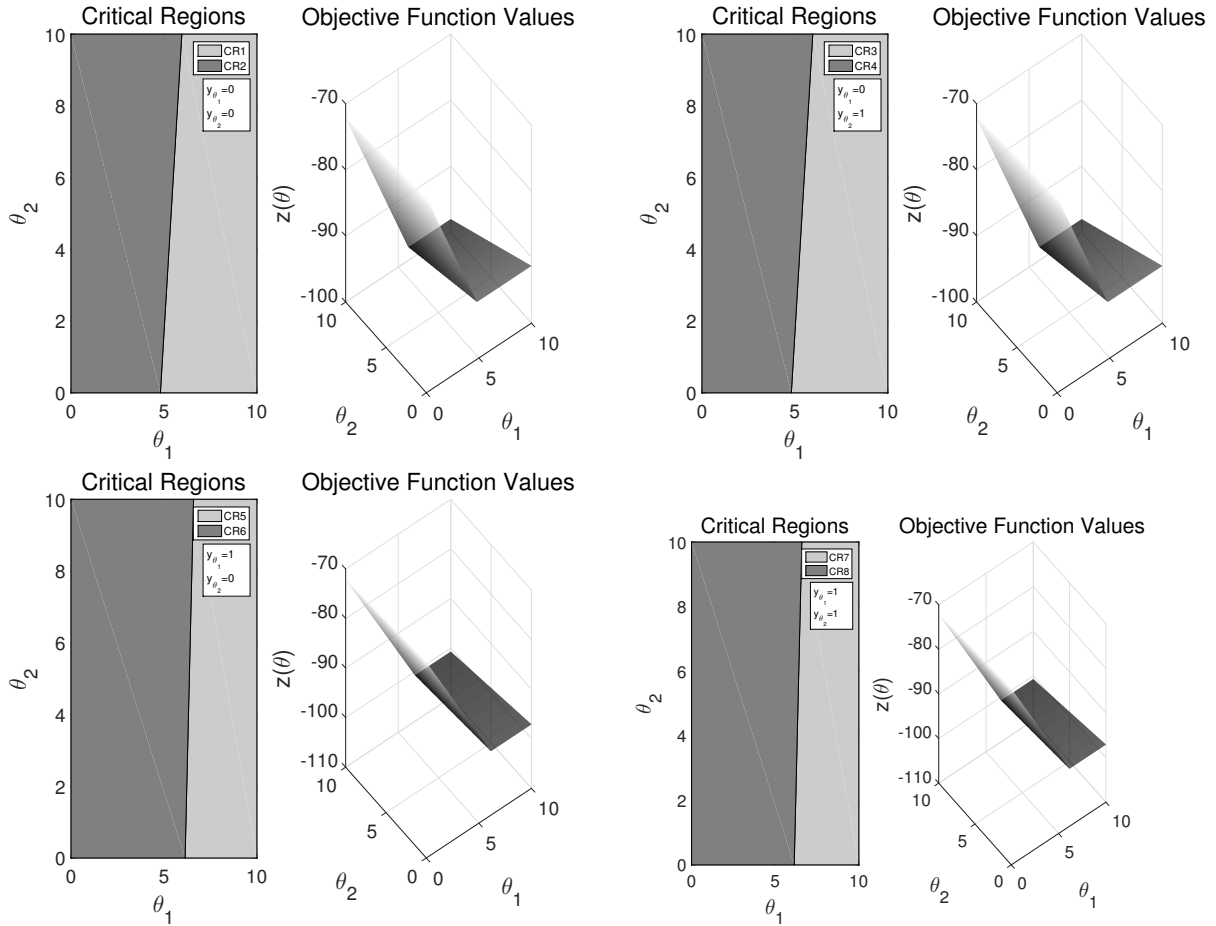


Figure 6.5: Graphical representation of the lower level mp-MILP with binary parameters. Clockwise from top left the binary parameters are: $\{0, 0\}$, $\{0, 1\}$, $\{1, 0\}$, $\{1, 1\}$.

The critical regions can be further reduced into two as shown in Table 6.4.

Note that the multi-parametric solution approach to the lower level MILP problem preserves all optimal solutions in case of multiplicity, i.e. in case the objective function value of the lower level problem is parametrically identical for more than one parametric expressions of the continuous variables, in the same parametric space, all parametric solutions are preserved in an “envelope of solutions”. Subsequently, the upper level MILP problem has to consider all possible solutions.

Case 2 - Parametrized Lagrangian multipliers: Given the optimization problem:

$$\begin{aligned}
& \underset{x}{\text{minimize}} && f(x) \\
& \text{subject to} && h(x) = 0 \\
& && g(x) \leq 0 \\
& && x \in \mathcal{X}
\end{aligned} \tag{6.17}$$

it is well known that its dual problem takes the following form (e.g. [84]):

$$\begin{aligned}
& \underset{\lambda, \mu \geq 0}{\text{maximize}} \underset{x \in \mathcal{X}}{\text{minimize}} && \mathcal{L}(x, \lambda, \mu) \\
& \text{subject to} && \mathcal{L}(x, \lambda, \mu) = f(x) + \lambda^T h(x) + \mu^T g(x).
\end{aligned} \tag{6.18}$$

Problem (6.18) is one of the cornerstones of mathematical optimization, and reviewing its rich history goes beyond the scope of this section. The interested reader is referred to the excellent textbooks [84] and [36] for an in-depth treatment of the subject. Within this section, problem (6.18) is considered through the lens of multi-parametric programming. As such, the consideration of problem (6.18) shows that the primal variables x can be expressed as a parametric function of the Lagrangian multipliers (λ, μ) . However, so far no attempt has been made to solve problem (6.18) using state-of-the-art multi-parametric programming algorithms, as the parameters should be bounded, a requirement which cannot be guaranteed for (λ, μ) . Thus, using the generalized algorithm 3, we can now consider such problems. The inner minimization problem is a mp-NLP problem the solution of which is outside the scope of this paper. It is clear though, that by considering both λ and μ as parameters then the inner minimization problem yields parametric expressions for x of the form of eq. (6.19):

$$x = pf_i(\lambda, \mu) \text{ for } \lambda, \mu \in CR_i, \forall i \in \mathcal{I} \tag{6.19}$$

where CR_i is the i^{th} critical region of the problem.

Therefore, based on this approach the outer maximization problem becomes:

$$\begin{aligned}
& \underset{\lambda, \mu}{\text{maximize}} && pf_i(\lambda, \mu) \\
& \text{subject to} && \lambda, \mu \in CR_i, \forall i \in \mathcal{I}.
\end{aligned} \tag{6.20}$$

The solution of problem (6.20) can be attractive when degeneracy is present in the primal problem and in cases where uncertainty is also considered. This is subject of currently ongoing research.

Remark 44. All computations in this paper were carried out on a Intel Core i5-4200M CPU at 2.50 GHz and 8 GB of RAM. Furthermore, MATLAB R2014a and IBM ILOG CPLEX Optimization Studio 12.6.1 were used for the computations.

$y_{\theta_1} = 0, y_{\theta_2} = 0$	
<i>CR1</i>	$-26\theta_1 + 3\theta_2 \leq -125$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{4}{78}\theta_2 + \frac{704}{78}$ $x_2 = \frac{5}{78}\theta_2 + \frac{685}{78}$
<i>CR2</i>	$26\theta_1 - 3\theta_2 \leq 125$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{22}{30}\theta_1 - \frac{1}{30}\theta_2 + \frac{165}{30}$ $x_2 = \frac{8}{30}\theta_1 + \frac{1}{30}\theta_2 + \frac{225}{30}$
$y_{\theta_1} = 0, y_{\theta_2} = 1$	
<i>CR3</i>	$-26\theta_1 + 3\theta_2 \leq -125$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{4}{78}\theta_2 + \frac{704}{78}$ $x_2 = \frac{5}{78}\theta_2 + \frac{685}{78}$
<i>CR4</i>	$26\theta_1 - 3\theta_2 \leq 125$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{22}{30}\theta_1 - \frac{1}{30}\theta_2 + \frac{165}{30}$ $x_2 = \frac{8}{30}\theta_1 + \frac{1}{30}\theta_2 + \frac{225}{30}$
$y_{\theta_1} = 1, y_{\theta_2} = 0$	
<i>CR5</i>	$-22\theta_1 + \theta_2 \leq -135$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = 10$ $x_2 = \frac{1}{22}\theta_2 + \frac{201}{22}$
<i>CR6</i>	$22\theta_1 - \theta_2 \leq 135$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{22}{30}\theta_1 - \frac{1}{30}\theta_2 + \frac{165}{30}$ $x_2 = \frac{8}{30}\theta_1 + \frac{1}{30}\theta_2 + \frac{225}{30}$
$y_{\theta_1} = 1, y_{\theta_2} = 1$	
<i>CR7</i>	$-22\theta_1 + \theta_2 \leq -135$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = 10$ $x_2 = \frac{1}{22}\theta_2 + \frac{201}{22}$
<i>CR8</i>	$22\theta_1 - \theta_2 \leq 135$ $0 \leq \theta_1 \leq 10$ $0 \leq \theta_2 \leq 10$ $y_1 = 1, y_2 = 1$ $x_1 = \frac{22}{30}\theta_1 - \frac{1}{30}\theta_2 + \frac{165}{30}$ $x_2 = \frac{8}{30}\theta_1 + \frac{1}{30}\theta_2 + \frac{225}{30}$

Table 6.3: Parametric solution of the lower-level mp-MILP with binary parameters.

$y_{\theta_1}, y_{\theta_2} \in \{0, 1\}^2$	
$-(26 - 4y_{\theta_1})\theta_1 + (3 - 2y_{\theta_1})\theta_2 \leq$ $-125 - 10y_{\theta_1}$	$-(26 - 4y_{\theta_1})\theta_1 + (3 - 2y_{\theta_1})\theta_2 \leq$ $-125 - 10y_{\theta_1}$
$0 \leq \theta_1 \leq 10$	$0 \leq \theta_1 \leq 10$
$CR1_n$ $0 \leq \theta_2 \leq 10$	$CR2_n$ $0 \leq \theta_2 \leq 10$
$y_1 = 1, y_2 = 1$	$y_1 = 1, y_2 = 1$
$x_1 = (\frac{4}{78} - \frac{4}{78}y_{\theta_1})\theta_2 + \frac{704}{78} + \frac{76}{78}y_{\theta_1}$	$x_1 = \frac{22}{30}\theta_1 - \frac{1}{30}\theta_2 + \frac{165}{30}$
$x_2 = (\frac{5}{78} - \frac{8}{429}y_{\theta_1})\theta_2 + \frac{685}{78} + \frac{152}{429}y_{\theta_1}$	$x_2 = \frac{8}{30}\theta_1 + \frac{1}{30}\theta_2 + \frac{225}{30}$

Table 6.4: Reduced parametric solution of the lower level mp-MILP with binary parameters.

Chapter 7

Conclusions and Future Work

This thesis discussed a broad range of topics in the area of multi-parametric programming and control. In this section, some conclusions from this body of work are drawn and an opinionated view on future research directions linked to this thesis is given.

7.1 Conclusions

In this thesis, some recent developments in multi-parametric programming and control are discussed. In the beginning, it is shown how the solution to a mp-QP problem is given by a connected graph, a result which enables the description of the most efficient mp-QP algorithm known to date. Then, mp-MIQP problems are considered and it is shown how the suitable use of underestimation of the critical regions leads to the first algorithm capable of solving mp-MIQP problems exactly. Additionally, the thesis considered the formulation of robust MPC problems for continuous and hybrid systems, as well as the generalization of the combinatorial algorithm for the solution of mp-QP problems featuring unbounded and binary parameters.

In summary, this thesis has presented:

- The extension of the connected-graph theorem to mp-QP problems and the design of a novel solution procedure which outperforms current state-of-the-art methods.
- The development of a solution procedure to obtain the exact solution for mp-MIQP problem.
- An approach towards the application of robust optimization in robust MPC for continuous and hybrid systems featuring parametric uncertainty.

- An algorithm for the solution of mp-QP problems featuring unbounded and binary parameters.

7.2 Future Directions

These developments have enabled the routine solution of mp-MILP and mp-MIQP problems beyond exhaustive enumeration, as well as the most efficient solution strategies for mp-LP and mp-QP problems. The topics discussed in the following build upon this ability to explore new and exciting areas of research:

Computational development and parallelization: Although it is fairly straightforward, the work presented in this thesis is the first application of parallel computing in multi-parametric programming. In particular, the parameter ρ_{limit} was introduced which provided a trade-off between overhead and efficiency of parallelization. Based on this work, parallelization options for the combinatorial and graph-based approach have been included in POP, and are currently under way for the mixed-integer solvers as well. This development enables the use of high-performance computers for the solution of multi-parametric programming problems, and will open up avenues for new problems to be considered. Specifically, the following questions are of interest:

- How many LP and QP problems are solved on average for a mp-LP or mp-QP problem?
- What is a good value for ρ_{limit} in general? Should it vary dynamically throughout the solution of the problem?
- How far can multi-parametric programming be pushed with these new software capabilities? What are the limitations at those points?
- Which architecture beyond MATLAB® is suitable for the future of multi-parametric programming? Which one is the most appropriate?

Decentralization *via* multi-parametric programming: As highlighted with its applicability to bilevel programming and multi-objective optimization problems, multi-parametric programming is very well suited to cope with vertical or horizontal decentralization of an optimization problem. If the overall problem can be decomposed into a series of smaller problems, then each of these problems can be solved using multi-parametric programming [246, 253]. This strategy was also successfully applied in [209] for periodic systems and in [65] for combined heat and power systems. These

contributions indicate that there is a huge potential for the development of techniques, specifically for the following questions:

- Is it possible to (automatically) recognize whether and how a given optimization problem can be decentralized?
- How and based on which criteria should different multi-parametric solutions be linked? Should it be direct using parameters or should there be a supervisory level?
- Can multi-parametric programming be used beyond optimization for e.g. simulation procedures where such decentralization occurs?

Robust explicit MPC: As evident from the high interest within the community, the issue of robust MPC cannot be considered solved. While some contributions were discussed in this thesis, especially the area of tube-based MPC appears to be very promising. However, regardless of the strategy which proves itself in the community, the issue of computational tractability will still remain. The author believes that multi-parametric programming offers the unique ability to overcome these challenges directly. Specifically, the following questions are of interest:

- Can the set-theoretical methods used in robust/tube-based MPC be made computationally more efficient by using special structures (such as box-constrained systems) and/or multi-parametric programming?
- Is it possible to combine the notion of decentralization (see above) with model predictive control, possibly even for the robust case?
- Can the novel robust counterparts devised by Guzman *et al.* [111, 112] be applied to robust MPC as well?

Other areas: As many topics have been discussed in this thesis, many questions have also come up which may seem peripheral but are nonetheless, at least in the authors' opinion, highly exciting questions. Note that some of these are very hard and have been considered for decades or even longer:

- Is there a (more) efficient way to perform projection operations? Although with modifications, the state-of-the-art strategy for projections is still the Fourier-Motzkin elimination. While the author is aware of the 'Equality Set Projection' approach by Jones *et al.* [131], the fact that it had been implemented in MPT v2 but is absent from v3 indicates that it may not be as promising as it initially

was conceived to be. Intuitively, it appears that there should be some approach which provides a new angle for this fundamental operation.

- What more can be understood about the structure of multi-parametric programming problems? As mentioned in the introduction of section 3, for most problems only very few of all possible combinations of active sets yield full-dimensional critical regions. While the connected-graph approach certainly reduces the number of active sets to be considered, it is still an unanswered question as to whether something can be found in the structure of the problem itself which enables an even deeper understanding of which active sets will be optimal or not.
- Is it possible to solve dual problems *via* multi-parametric programming? As mentioned in section 6, the dual of an optimization problem is inherently a multi-parametric programming problem. The author believes that solving dual problems explicitly might deliver very exciting insights into the workings of optimization problems and the role of duality beyond what is currently known.

7.3 Publications resulting from this thesis

For completion, this section lists in chronological order all publications by the author. Note that the work published in [200] was performed prior to the start of the PhD studies during a research stay. The papers are divided into full-length, book chapters, short notes and conference papers.

Remark 45. Many of the contributions presented in this thesis will be featured in a book which is currently in preparation:

Pistikopoulos, E. N.; Diangelakis, N. A.; **Oberdieck, R.** *Multi-parametric Optimization and Control*. Wiley-VCH, *in preparation*.

7.3.1 Full-length papers

- **Oberdieck, R.**; Wittmann-Hohlbein, M.; Pistikopoulos, E. N. (2014) A branch and bound method for the solution of multiparametric mixed integer linear programming problems. *Journal of Global Optimization*, 59(2-3), 527-543.
- **Oberdieck, R.**; Pistikopoulos, E. N. (2015) Explicit hybrid model-predictive control: The exact solution. *Automatica*, 58, 152-159.

- Pistikopoulos, E. N.; Diangelakis, N. A.; **Oberdieck, R.**; Papathanasiou, M. M.; Nascu, I.; Sun, I. (2015) PAROC - an Integrated Framework and Software Platform for the Optimization and Advanced Model-Based Control of Process Systems. *Chemical Engineering Science*, 136, 115-138.
- Papathanasiou, M. M.; Avraamidou, S.; Steinebach, F.; **Oberdieck, R.**; Mueller-Spaeth, T.; Morbidelli, M.; Mantalaris, A.; Pistikopoulos, E. N. (2016) Advanced Control Strategies for the Multicolumn Countercurrent Solvent Gradient Purification Process (MCSGP). *AIChE Journal*, 62(7), 2341-2357.
- **Oberdieck, R.**; Diangelakis, N. A.; Papathanasiou, M. M.; Nascu, I.; Pistikopoulos, E. N. (2016) POP - Parametric Optimization Toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979-8991.
- **Oberdieck, R.**; Diangelakis, N. A.; Avraamidou, S.; Pistikopoulos, E. N. (2016) On unbounded and binary parameters in multi-parametric programming: Applications to mixed-integer bilevel optimization and duality theory. *Journal of Global Optimization*, *in print*.
- **Oberdieck, R.**; Diangelakis, N. A.; Nascu, I.; Papathanasiou, M. M.; Sun, M.; Avraamidou, S.; Pistikopoulos, E. N. (2016) On multi-parametric programming and its applications in process systems engineering. *Chemical Engineering Research and Design*, 116, 61-82.
- **Oberdieck, R.**; Diangelakis, N. A.; Pistikopoulos, E. N. (2017) Explicit Model Predictive Control: A connected-graph approach. *Automatica*, 76, 103-112.
- Nascu, I.; **Oberdieck, R.**; Pistikopoulos, E. N. (2017) Explicit Hybrid Model Predictive Control Strategies for Intravenous Anaesthesia. *Computers & Chemical Engineering*, *in revision*.

7.3.2 Book chapters

- **Oberdieck, R.**; Nascu, I.; Pistikopoulos (2017) Explicit Hybrid Control. In Pistikopoulos, E. N.; Nascu, I.; Veillou, E. (Eds) *Modelling, Control and Optimisation of Biomedical Systems*, Wiley-VCH, *in preparation*.
- Pistikopoulos, E. N.; Diangelakis, N. A.; **Oberdieck, R.** Explicit (Offline) Optimization for MPC. In Raković, S. V.; Levine, W. S. *Handbook of Model Predictive Control (MPC)*, *in preparation*.

7.3.3 Short notes

- **Oberdieck, R.**; Pistikopoulos, E. N. (2016) Multi-objective optimization with convex quadratic cost functions: A multi-parametric programming approach. *Computers & Chemical Engineering*, 85, 36-39.
- Raković, S. V.; **Oberdieck, R.**; Pistikopoulos, E. N. (2016) Revised Simple Robust MPC. *Automatica*, *in revision*.

7.3.4 Conference papers

- Papathanasiou, M. M.; Steinebach, F.; Ströhlein, G.; Mueller-Spaeth, T.; Nascu, I.; **Oberdieck, R.**; Morbidelli, M.; Mantalaris, A.; Pistikopoulos, E. N. (2015) A control strategy for periodic systems - application to the twin-column MCSGP. Proceedings of the 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering, In *Computer Aided Chemical Engineering*, 37, 1505-1510.
- Nascu, I.; **Oberdieck, R.**; Pistikopoulos, E. N. (2015) A framework for hybrid multi-parametric model-predictive control with application to intravenous anaesthesia. Proceedings of the 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering, In *Computer Aided Chemical Engineering*, 37, 719-724.
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- Nascu, I.; **Oberdieck, R.**; Pistikopoulos, E. N. (2015) Offset-Free Explicit Hybrid Model Predictive Control of Intravenous Anaesthesia. Proceedings of the IEEE International Conference on Systems, Man, and Cybernetics, p. 2475-2480.
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- Papathanasiou, M. M.; Quiroga-Campano, A. L.; **Oberdieck, R.**; Mantalaris, A.; Pistikopoulos, E. N. (2016) Development of advanced computational tools for the intensification of monoclonal antibody production. Proceedings of the 26th European

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- Papathanasiou, M. M.; **Oberdieck, R.**; Mantalaris, A.; Pistikopoulos, E. N. (2016) Computational tools for the advanced control of periodic processes - Application to a chromatographic separation. Proceedings of the 26th European Symposium on Computer Aided Process Engineering, In *Computer Aided Chemical Engineering*, 38, 1665-1670.
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- Nascu, I.; Diangelakis, N. A.; **Oberdieck, R.**; Papathanasiou, M. M.; Pistikopoulos, E. N. (2016) Explicit MPC in real-world applications: the PAROC framework. In Proceedings of the American Control Conference, 913-918.
- Papathanasiou, M. M.; **Oberdieck, R.**; Avraamidou, S.; Nascu, I.; Mantalaris, A.; Pistikopoulos, E. N. (2016) Development of advanced control strategies for periodic systems: An application to chromatographic separation processes. In Proceedings of the American Control Conference, 4175-4180.

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Appendix A

The POP toolbox

Portions of this chapter have been submitted for publication in:

- Oberdieck, R.; Diangelakis, N. A.; Papathanasiou, M. M.; Nascu, I.; Pistikopoulos, E. N. (2016) POP - Parametric Optimization Toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979-8991.

In this section, the different aspects of POP, the Parametric OPTimization toolbox, are presented, involving three key features: problem solution, problem generation and problem library.

A.1 Problem solution

A.1.1 Solution of mp-QP problems

In POP, the geometrical [14], a variation of the combinatorial [110] and the connected-graph [202] algorithm have been implemented. These are accessible as functions in the Command Window:

```
Solution = Geometrical(problem)
Solution = Combinatorial(problem)
Solution = ConnectedGraph(problem),
```

where `problem` is the structured array containing the mp-LP/mp-QP problem to be solved. Additionally, POP provides an interface with the solver used in MPT:

```
Solution = POPviaMPT(problem).
```

Note that this requires the separate download of the MPT toolbox. Thus, POP features every major solution strategy for problems of type (3.1). These have been combined in a single wrapper:

```
Solution = mpQP(problem)
```

The interested user is referred to the User Manual available at <http://paroc.tamu.edu/Software/> and our YouTube channel 'POP Toolbox'. Additionally, each solver provides statistical information about its performance, a feature which is also explained in detail in the User Manual.

A.1.2 Solution of mp-MIQP problems

In POP, a decomposition-based algorithm based on [74] has been implemented featuring four different comparison procedures discussed below. The solver is available in the Command Window as:

```
Solution = mpMIQP(problem)
```

Additionally, the solver provides statistical information about its performance, a feature which is also explained in detail in the User Manual.

A.1.3 Requirements and Validation

It is possible to use all functionalities of POP using only the built-in functionalities of MATLAB and its toolboxes. However, for speed and stability reasons, the use of commercial tools is encouraged. In particular, POP features links to CPLEX and NAG as LP and QP solvers, as well as CPLEX for the MILP and MIQP problems.

A.1.4 Handling of equality constraints

For the case of mp-LP and mp-QP problems, equality constraints are simply considered as active constraints of the solution. Conversely, for mp-MILP and mp-MIQP problem, the global optimization problem is solved straight up, as it is expected that the chosen solver is capable of handling such issues. Once a candidate combination of binary variables has been found and fixed, the resulting equality constraints are considered in the mp-LP and mp-QP problem.

Remark 46. As CPLEX only provides MILP and MIQP solvers, in case of mp-MIQP problems the quadratic constraints in problem (4.4) are underestimated using a suitable set of

McCormick estimators. Note that this guarantees correct execution of the algorithm. However if no comparison procedure is employed, then the number of solutions per critical region might be higher than in the case where a MINLP solver is used.

In order to validate the solution obtained from problem (3.1) or (4.1), POP features the function `VerifySolution`, which randomly seeds 5000 points in the parameter space Θ and solves the corresponding deterministic problem. While this does not provide a full certificate of guarantee, it is a strong indicator that a correct solution has been obtained.

A.2 Problem generation

The aim is to generate random, feasible problems with suitably defined constraints such that different active sets become optimal in different parts of the parameter space, thus resulting in a partitioning of the parameter space into several critical regions. For the case of mp-QP problems, the development of such a generator can be decomposed into the following steps:

Step 1 - Objective Function: In order to define the objective function, Q , H and c according to problem (3.1) need to be defined. While for H and c no specific criterion apply, Q needs to be symmetric positive definite. This is achieved by randomly generating a diagonal matrix featuring positive entries.

Step 2 - Constraints: The two criteria for the generation of constraints for multi-parametric programming problems are (i) feasibility and (ii) tightness in the sense that different solutions should be optimal in different parts of the parameter space. Furthermore, any set of linear constraints can be written as a set of matrices. Thus, generating random constraints is equivalent to generating random matrices. Two of the most important things to look for in a matrix is its sparsity and its dynamic range, i.e. the scale of the weights. The algorithm used for the random generation provides random parameters for sparsity and dynamic range, and thus aims at providing structurally and numerically different constraints at each run (see in Algorithm 4).

Remark 47. Note that it is up to the user whether or not redundant constraints should be removed or not.

Remark 48. The following comments are made regarding Algorithm 4:

- Algorithm 4 also applies to multi-parametric mixed-integer programs.
- As the generator described is random, the feasibility of the generated problem cannot be guaranteed by default. Thus, in order to ensure a non-empty feasible set for any generated problem, the Chebyshev center is calculated according to eq. (2.4).

Algorithm 4 Generation of a random feasible set of inequality constraints. Note that $D_{i,k}$ represents the element of D in the i -th row and k -th column of the D -matrix, and $\lfloor \cdot \rfloor$ denotes the rounding to the closest integer below.

Require: n, q

Ensure: A, E, b, F

- 1: Define $r = \rho(\max(\lambda) - \min(\lambda))$, where $\lambda = \text{eig}(Q)$
 - 2: Define number of constraints $m = \psi(n + q)$
 - 3: **for** $k=1:m$ **do**
 - 4: Generate random $T_A \in [0, 1]^n$ and $\alpha_A = \{i | T_i \geq \alpha_A^*\}$
 - 5: Randomly generate $G_A \in [0 - G_A^*, 1 - G_A^*]^n$ and set $A_{k,\alpha_A} = \underline{r}G_A$
 - 6: Generate random $T_F \in [0, 1]^q$ and $\alpha_F = \{i | T_i \geq \alpha_F^*\}$
 - 7: Randomly generate $G_F \in [0 - G_F^*, 1 - G_F^*]^q$ and set $F_{k,\alpha_F} = \underline{r}G_F$
 - 8: **end for**
-

- The parameter space Θ is by default defined as $\Theta = \{\theta \in \mathbb{R}^q \mid -10 \leq \theta_l \leq 10, l = 1, \dots, q\}$.
- The coefficients in Algorithm 4 are randomly generated for each problem instance in order to make the generation procedure as random as possible.

Within POP, the problem generator is accessible from the Command Window as:

```
problem = ProblemGenerator(Type,Size,options)
```

where **Type** is 'mpLP', 'mpQP', 'mpMILP' or 'mpMIQP' and **Size** is a structured array featuring the desired dimensions of the optimization variables, parameters and constraints. Additionally, the **options** input specifies settings which are discussed in detail in the User Manual. In particular, it is possible to generate more than one problem directly, which enables the seamless generation of problem libraries and test sets.

A.3 Problem library

The third key feature of POP is its problem library, currently featuring the four randomly generated test sets 'POP_mpLP1', 'POP_mpQP1', 'POP_mpMILP1' and 'POP_mpMIQP1' containing 100 randomly generated mp-LP, mp-QP, mp-MILP and mp-MIQP problems respectively (see Figures A.1 and A.2). These problem libraries are used later on to analyze the performance of the different solvers and options available in POP. These test problems represent to our knowledge the first ever comprehensive library of test problems in multi-parametric programming.

Within POP, each problem is stored in the folder 'Library', which contains a folder for each test set, which in return contains all the individual problems as '.mat' files. These files

can be loaded into MATLAB and the corresponding problem can be solved. Additionally, it is possible to use the Graphical User Interface (GUI, see next section), to perform statistical analysis as well as to create customized test sets which can be exported and solved directly.

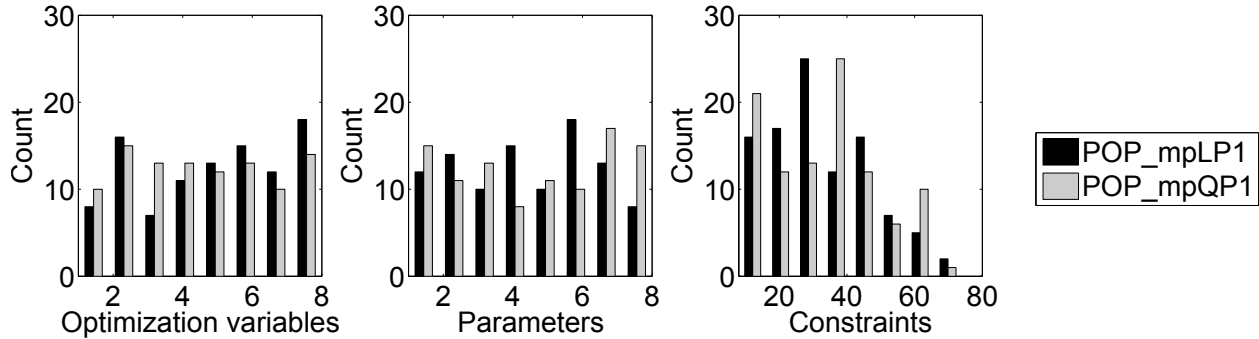


Figure A.1: The problem statistics of the test sets 'POP_mpLP1' and 'POP_mpQP1'.

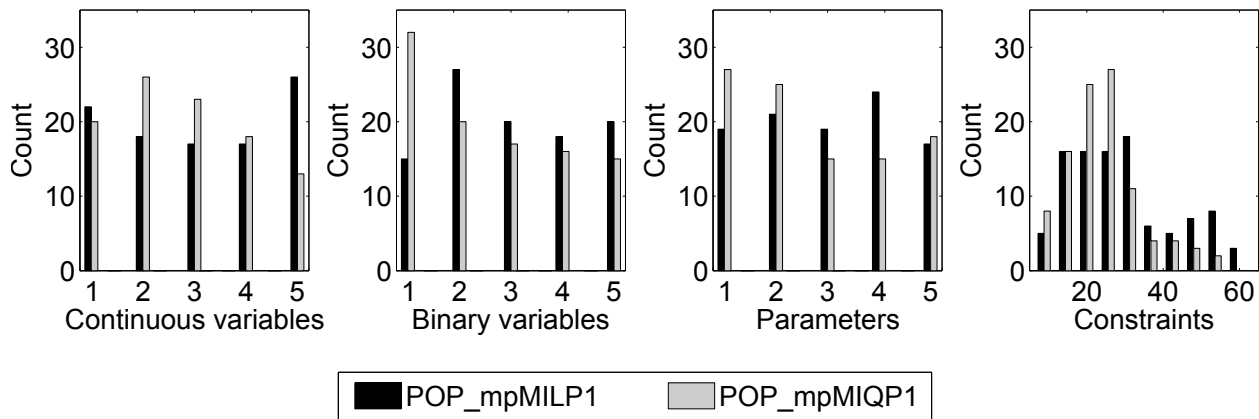


Figure A.2: The problem statistics of the test sets 'POP_mpMILP1' and 'POP_mpMIQP1'.

A.3.1 Merits and shortcomings of the problem library

The aim of the POP toolbox is not only to provide the means to solve multi-parametric programming problems, but also in general to advance the computational side of multi-parametric programming solvers beyond their description and solution of some test cases. For this purpose, it is vital to create test beds where new and old algorithms can be compared against each other. The larger this basis of test cases is, the more efficient and robust will the implementations of these algorithms be. The problem library included in POP is the first step towards this direction, as it provides 100 problems for each of the four major problem classes. It therefore enables the access to larger quantities of data for solver performance and as a result the inference of bottlenecks in algorithms and comparisons of different solvers.

However, these problems are randomly generated using the problem generator of the POP toolbox. This means that the problems themselves are not based on real-world applications. Thus, the problem library in its current form does not give any information as to what algorithm is more appropriate for a MPC or scheduling application, and therefore conclusions drawn from the results of the problem library should be taken as suggestive and not definitive. In future, the aim is to vastly expand the problem library and automate the benchmarking to an extent that enables the readily available testing of any new implementation.

A.4 Graphical User Interface (GUI)

In order to facilitate its use, POP is equipped with a GUI which can be launched from the Command Window using:

```
POP
```

It enables direct access to the different functions of POP including post-processing and exporting automatically generated code. The main screens of the interface are shown in Figure A.3, i.e. the welcome screen, and the solver, library and generator interfaces. Note that in order to maintain a user-friendly approach, some of the options available in POP are set to defaults when the interface is used. More information on the interface can be found in the User Manual.

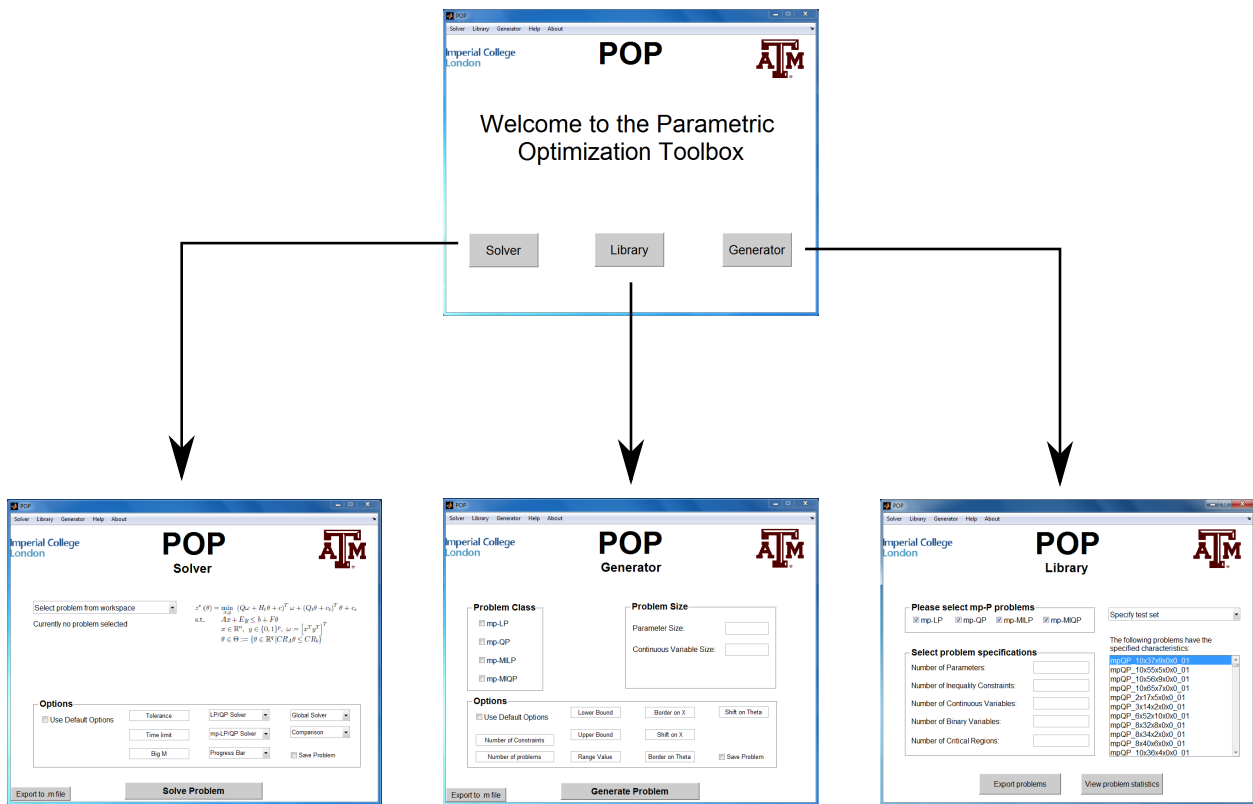


Figure A.3: The structure of the graphical user interface (GUI) of POP.

Appendix B

PAROC - an Integrated Framework and Software Platform for the Optimization and Advanced Model-Based Control of Process Systems

Portions of this chapter have been published in:

- Pistikopoulos, E.N.; Diangelakis, N.A.; Oberdieck, R.; Papathanasiou, M.M.; Nascu, I.; Sun, M. (2015) PAROC - an Integrated Framework and Software Platform for the Optimization and Advanced Model-Based Control of Process Systems. *Chemical Engineering Science*, 136, 115-138.
- Nascu, I.; Diangelakis, N. A.; Oberdieck, R.; Papathanasiou, M. M.; Pistikopoulos, E. N. (2016) Explicit MPC in real-world applications: the PAROC framework. In *Proceedings of the American Control Conference*, 913-918.

In this chapter the PAROC (PARAmetric Optimisation and Control) framework is described in detail, which is depicted in Figure B.1.

B.1 High-Fidelity Modeling and Analysis

The first step of the PAROC framework is high-fidelity modeling and analysis. In particular, the scope is to (i) develop a high-fidelity model of the process [141, 152], (ii) analyze the orig-

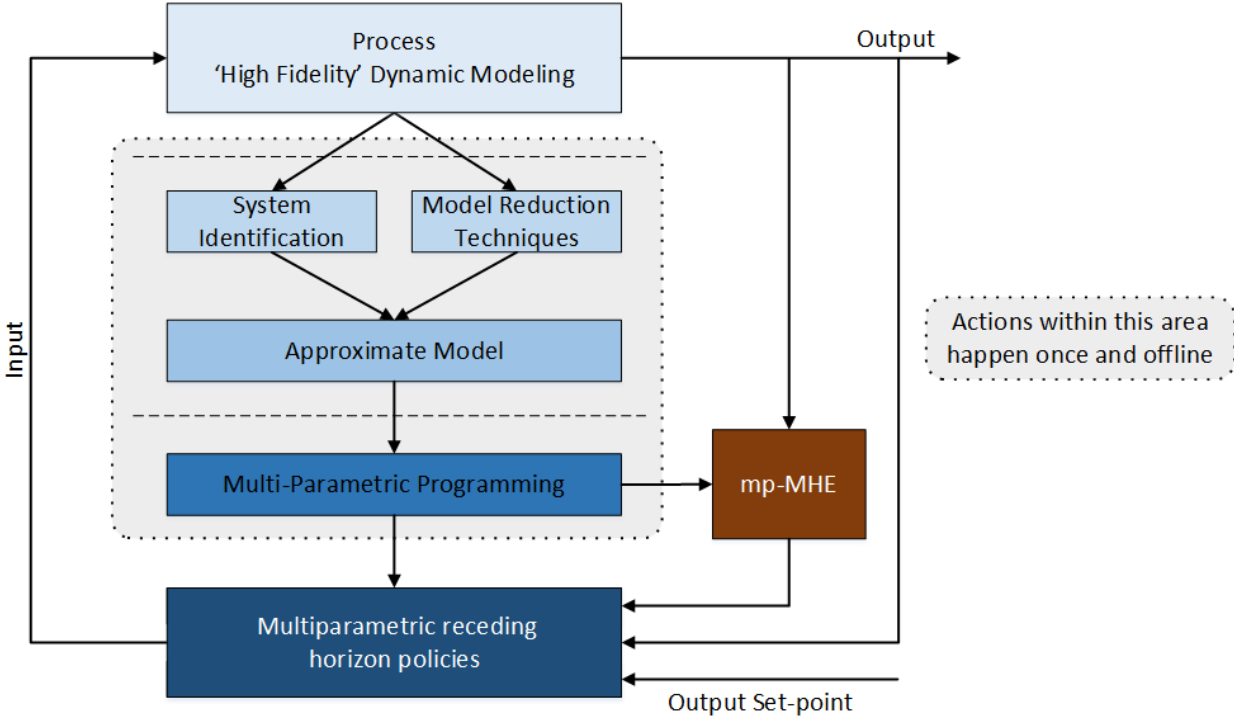


Figure B.1: The PAROC framework.

inal problem e.g. using global sensitivity analysis [142, 145, 240] and (iii) perform parameter estimation and dynamic optimization of the developed model. Within our framework, the modeling software PSE’s gPROMS® ModelBuider is used, as it provides the aforementioned tools either directly or allows for their implementation via gO:MATLAB, a connection tool between MATLAB® and gPROMS®.

B.2 Model Approximation

Although it is possible to use a high-fidelity model for optimal design decisions, its complexity may usually render its direct use for the development of model-based strategies computationally expensive. Consequently, it may be necessary to simplify the representation of the model while compromising its accuracy. In PAROC this is addressed by the following two approaches:

System Identification: A series of simulations of the high-fidelity model for different initial states is used to construct a meaningful linear state-space model of the process using statistical methods. One of the most widely applied tools within this area is the System Identification Toolbox from MATLAB®.

Model-Reduction Techniques: While system identification relies on the user in terms of interpretation of the data and processing of the results, model-reduction techniques somewhat "automate" the reduction process based on formal techniques.

B.3 Multi-parametric Programming

After the model approximation step a state-space model is obtained which is used for the development of receding horizon policies. The calculation of such policies, e.g. in the form of control laws or scheduling policies, traditionally requires the online solution of an optimisation problem, which might be computationally infeasible [214]. Therefore, the PAROC framework employs multi-parametric programming, where the optimisation problem is solved offline as a function of a set of parameters. In addition, depending on the cost function and the characteristic of the system considered, the complexity of the optimisation problem changes considerably.

B.4 Multi-parametric Moving Horizon Policies

While multi-parametric programming has been applied in a variety of areas, a key application lies in the offline calculation of moving horizon policies such as control laws and scheduling policies. The underlying idea is thereby to consider the states of the system as parameters, and thus solve the optimisation problem over a range of admissible states.

Remark 49. In addition, measured disturbances, if present, are also considered as parameters as well as state-space and model mismatch and the output set point.

In general, we consider the following optimisation problem

$$\begin{aligned}
 V_N^*(x_0) &= \min_{U \in \mathcal{U}} J(U, X) \\
 &= \min_{U \in \mathcal{U}} \|x_N\|_P^p + \sum_{k=0}^{N-1} \|x_k\|_S^p + \|u_k\|_R^p \\
 \text{s.t.} \quad &x_{k+1} = Ax_k + Bu_k + Cd_k \\
 &y_k = Dx_k + Eu_k + e \\
 &h(u_k, x_k, y_k) \leq 0 \\
 &x_{k+N} \in \mathcal{X}_T,
 \end{aligned} \tag{B.1}$$

where u , x and y are the moving horizon policies, states and outputs of the considered

system, $U = [u_0, \dots, u_{N-1}]$, $\|\cdot\|^p$ is the p -norm and P , S and R are the corresponding weights. In addition, x_0 are the initial states and the set \mathcal{X}_T is the terminal set that, if well-defined, ensures stability [227].

Remark 50. The parameter dependence of the objective function can be avoided using the Z -transformation [31], i.e.

$$z = u + H^{-1}F^T x, \tag{B.2}$$

where H is the Hessian and F is the bilinear term between u and x .

While problem (B.1) describes the general case of moving horizon policies, the remaining part of the section will focus predominately on multi-parametric model-predictive control (mp-MPC). This is due to the extensive number of contributions and advances that have been made in this field.

Remark 51. Moving horizon estimation is an estimation method based on optimization that considers a limited amount of past data. One of the main advantages of moving horizon estimation is the possibility to incorporate system knowledge as constraints in the estimation. This results in a MPC-like online optimization problem, which can be solved offline using multi-parametric programming.

B.5 Software Implementation and Closed-loop Validation

B.5.1 Multi-parametric Programming Software

In conjunction with the aforementioned theoretical developments, PAROC provides software solutions to key aspects of the framework (see paroc.tamu.edu). In particular, it offers tools for the formulation and solution of multi-parametric programming problems. Based on POP [211], it contains state-of-the-art algorithms which allow for an efficient solution of mp-LP, mp-QP, mp-MILP and mp-MIQP problems. Furthermore, its interconnection with gPROMS® ModelBuilder (see below) makes the use of the PAROC framework straightforward and allows for an intuitive approach for design, operation and control problems.

B.5.2 Integration of PAROC in gPROMS® ModelBuilder

The developed multi-parametric moving horizon policies and estimators are validated in a closed-loop fashion against the original high-fidelity model. However, within the PAROC

framework, the high-fidelity modeling and analysis is performed in gPROMS ModelBuilder® while the model reduction as well as the formulation and solution of the multi-parametric programming problem is carried out in MATLAB®. Thus currently, the closed-loop validation of the developed controller is done in MATLAB® using the gPROMS ModelBuilder® tool gO:MATLAB. While this is a valid way of performing closed-loop validation, this does not allow for the use of the tools available in gPROMS® (e.g. dynamic optimisation). In addition, this procedure is conceptually problematic, as it suggests the test of a controller given a certain system rather than the test of a mp-MPC controlled system.

Therefore, we have developed a software solution that enables the direct export of the mp-MPC controller developed in MATLAB® into gPROMS® ModelBuilder as a foreign object. This foreign object, written in C++, loads the matrix representation and provides a simple look-up table as part of the gPROMS® ModelBuilder architecture, similarly to e.g. a Proportional-Integral-Derivative (PID) controller.