SEMISMOOTH LEAST SQUARES METHODS FOR COMPLEMENTARITY PROBLEMS

Dissertation zur Erlangung des
naturwissenschaftlichen Doktorgrades
der Bayerischen Julius–Maximilians–Universität Würzburg

vorgelegt von

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aus

Cisnădie

Würzburg, 2006

Eingereicht am 23.02.2006
bei der Fakultät für Mathematik und Informatik
1. Gutachter: Prof. Dr. Christian Kanzow
2. Gutachter: Prof. Dr. Francisco Facchinei
Tag der letzten mündlichen Prüfung: 7.07.2006

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Acknowledgments

The development of this thesis during my PhD period at the University of Würzburg was a phased process, antecedently mirrored in some preprints and papers. My major source of inspiration was my supervisor Christian Kanzow, because primely his ideas led to the creation of our publications, and as a consequence, to their subsumption in the present thesis. So he is the first and foremost person to whom I want to express my gratitude. In many ways he was an excellent supervisor. I thank him for guidance, help, discussions, his many valuable insights and comments during the preparation of the thesis and the implementation of the LMMCP software and last but not least for his patience.

Of course many more people influenced the finalization process of this thesis. Without the support of my friends Oana and Daniel this process could still continue. I thank them for moral support, many helpful comments and proof-reading. Speaking of moral support I should emphasize the backing I have received from my family. I thank them for having grown me up in a happy home and having taken care of my education. Moreover, I thank Pietro for being always by my side, for always jumping in to dig me out in difficult moments by his generous encouragements and advises.

During my education, I have benefited from the dedication and work of many teachers. I am grateful to all of them, but particularly I want to thank my high school teacher Martin Bottesch who helped me to discover the beauty of mathematics, for which I will always be grateful.

Special thanks are also due to Prof. Dr. Francisco Facchinei who kindly accepted the task of reviewing the present thesis and to Prof. Dr. Manfred v. Golitschek and Dr. Daniela Kraus who served on my PhD committee.

Stefania Petra Würzburg, July 2006

Contents

Abbreviations

C^k	continuously differentiable of order k
GE	generalized equation
GMRES	generalized minimal residual method of Saad and Schultz [110]
KKT	Karush-Kuhn-Tucker
LC^1	C^1 functions with Lipschitz continuous Jacobian
LCP	linear complementarity problem
LMCP	linear mixed complementarity problem
LSQR	bidiagonalization method for least squares problems [94]
MCP	mixed complementarity problem
NCP	nonlinear complementarity problem
QP	quadratic program
PATH	algorithm for solving MCP [23] based on path search strategy
SMOOTH	algorithm for solving MCP [12] based on smoothing technique
SEMISMOOTH	semismooth algorithm for solving MCP [90]
VI	variational inequality

Notation

Spaces and Orthants

$\mathbb{R}$	the real numbers
$\mathbb{R}^n$	the n-dimensional real vector space
$\mathbb{R}^n_+$	the nonnegative orthant in $\mathbb{R}^n$
$\mathbb{R}^n_{++}$	the positive orthant in $\mathbb{R}^n$
$\mathbb{R}^{m\times n}$	the space of $m \times n$ real matrices

Sets

$\{x\}$	the set consisting of the vector x
$\operatorname{conv}\mathcal{S}$	convex hull of the set $\mathcal{S}$
$\mathcal{S}_1 \subseteq \mathcal{S}_2$	$\mathcal{S}_1$ is a subset of $\mathcal{S}_2$
$\mathcal{S}_1 \subset \mathcal{S}_2$	$\mathcal{S}_1$ is a proper subset of $\mathcal{S}_2$
$\mathcal{S}_1 \setminus \mathcal{S}_2$	the difference of two sets $\mathcal{S}_1$ and $\mathcal{S}_2$
$\mathcal{S}_1 + \mathcal{S}_2$	the vector sum of two sets $\mathcal{S}_1$ and $\mathcal{S}_2$
$\lvert\mathcal{S}\rvert$	the cardinality of a set $\mathcal{S}$
$B_\varepsilon(x)$	open ball of radius ε around x
$\mathbb{B}_\varepsilon(x)$	closed ball of radius ε around x
(a, b)	an open interval in $\mathbb{R}$
$[a, b]$	a closed interval in $\mathbb{R}$
$\operatorname*{argmax}_{x\in\mathcal{S}} f(x)$	the set of constrained maximizers of f on $\mathcal{S}$
$\operatorname*{argmin}_{x\in\mathcal{S}} f(x)$	the set of constrained minimizers of f on $\mathcal{S}$
$N_C(x)$	the normal cone of a set C at a point $x \in C$
$\mathcal{B}$	$:= [l, u]$; rectangular box in $\mathbb{R}^n$, where the lower bounds $l = (l_1, \ldots, l_n)^T$ and upper bounds $u = (u_1, \ldots, u_n)^T$ satisfy $-\infty \leq l_i < u_i \leq +\infty$ for all $i = 1, \ldots, n$.

Vectors

$x \in \mathbb{R}^n$	column vector in $\mathbb{R}^n$
x^T	$:= (x_1, \ldots, x_n)$; the transpose of a vector x with components x_i
(x, y)	column vector $(x^T, y^T)^T$
x_i	i-th component of x
x_δ	vector in $R^{\lvert\delta\rvert}$ consisting of components x_i, $i \in \delta$
$x \geq y$	componentwise comparison $x_i \geq y_i$, $i = 1, \ldots, n$
$x > y$	strict componentwise comparison $x_i > y_i$, $i = 1, \ldots, n$
$\min\{x, y\}$	the vector whose i-th component is $\min\{x_i, y_i\}$
$\max\{x, y\}$	the vector whose i-th component is $\max\{x_i, y_i\}$
$e_i \in \mathbb{R}^n$	the i-th vector of the canonical basis of $\mathbb{R}^n$
$P_C(x)$	the Euclidean projection of a vector $x \in \mathbb{R}^n$ on a convex set $C \subset \mathbb{R}^n$

Vectors (continued)

x_+	the projection of a vector $x \in \mathbb{R}^n$ onto $\mathbb{R}^n_+$
x_-	the negative of the projection onto the negative orthant
$x^T y$	the standard inner product of two vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$
$\|x\|$	the Euclidian norm of $x \in \mathbb{R}^n$, unless otherwise specified
$\|x\|_p$	$:= (\sum_{i=1}^n \|x_i\|^p)^{1/p}$; the ℓ_p-norm of $x \in \mathbb{R}^n$
$\|x\|_\infty$	$:= \max_{i \in \{1,\ldots,n\}} \|x_i\|$; the maximum norm of $x \in \mathbb{R}^n$

Matrices

A	$:= (a_{ij})$; a matrix with entries a_{ij}
$A_{\mathcal{I}\mathcal{J}}$	the $\|\mathcal{I}\| \times \|\mathcal{J}\|$ submatrix of A consisting of the elements a_{ij}, with $i \in \mathcal{I}$ and $j \in \mathcal{J}$
A^T	the transpose of a matrix A
A^{-1}	the inverse of a matrix A
M/A	the Schur complement of A in M
$\lambda_{\min}(A)$	the smallest eigenvalue of a symmetric matrix A
$\lambda_{\max}(A)$	the largest eigenvalue of a symmetric matrix A
I_n	identity matrix of order n (subscript often omitted)
$\operatorname{diag}(x)$	the diagonal matrix with diagonal elements equal to the components of the vector x

Functions

$G : \mathcal{D} \to \mathcal{R}$	a mapping with domain $\mathcal{D}$ and range $\mathcal{R}$
G_i	i-th component function of $G : \mathcal{D} \to \mathbb{R}^n$
$F \circ G$	composition of two functions F and G
$G'(\cdot, \cdot)$	directional derivative of the mapping G
G'	$:= \left(\frac{\partial G_i}{\partial x_j}\right)$; the Jacobian of a mapping $G : \mathbb{R}^n \to \mathbb{R}^m$
∇G	the transposed Jacobian
∇g	$:= (\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n})^T$; the gradient of a function $g : \mathbb{R}^n \to \mathbb{R}$
$\partial_B G$	the B-subdifferential of the locally Lipschitz continuous function $G : \mathbb{R}^n \to \mathbb{R}^m$
∂G	$:= \operatorname{conv} \partial_B G$; the Clarke subdifferential or limiting Jacobian of the locally Lipschitz continuous function $G : \mathbb{R}^n \to \mathbb{R}^m$
$\partial_C G$	$:= (\partial G_1 \times \cdots \times \partial G_n)^T$; the C-subdifferential of the locally Lipschitz continuous function $G : \mathbb{R}^n \to \mathbb{R}^m$

Landau symbols

$f(d) = o(\|d\|)$	if $\lim_{d \to 0} \frac{f(d)}{\|d\|} = 0$ for a given scalar or vector function $d \mapsto f(d)$
$f(d) = O(\|d\|)$	if $\limsup_{d \to 0} \frac{f(d)}{\|d\|} < \infty$ for a given scalar or vector function $d \mapsto f(d)$
$\alpha_k = o(\beta_k)$	if $\lim_{k \to \infty} \frac{\alpha_k}{\beta_k} = 0$ for two sequences $\{\alpha_k\}$ and $\{\beta_k\}$ converging to zero

$\alpha_k = O(\beta_k)$	if $\limsup_{k\to\infty} \frac{\alpha_k}{\beta_k} < \infty$ for two sequences $\{\alpha_k\}$ and $\{\beta_k\}$ converging to zero

Chapter 1

Introduction

This thesis is concerned with numerical methods for solving nonlinear and mixed complementarity problems. Such problems arise from a variety of applications; among the most popular ones is the Nash equilibrium, a fundamental concept introduced in noncooperative game theory by J.F. Nash. Among many practical applications of this equilibrium concept is the Nash-Cournot production/distribution problem. Already in 1838, A.A. Cournot showed how one can find what was later called the Nash equilibrium within a duopolistic market. The model by Cournot can be extended to a oligopolistic market and in this case the Nash equilibria can be found by solving a nonlinear complementarity problem.

Example 1.1 (Nash-Cournot equilibrium problem) Within a closed market, assume there are n companies producing a common product and competing for the same set of customers. If we let x_i be the quantity of the product fabricated by the i-th company, then $\xi = \sum_{i=1}^{n} x_i$ denotes the total quantity being produced. The aim of each company is to maximize its own profit, and it can achieve this goal by optimizing its production level x_i at the beginning of each period. For this purpose, the i-th company assumes that the productions of all other companies remain constant at some level $x_j^\star$. Such a setting, in which the companies do not cooperate with each other, is called a *Nash setting*. A Nash equilibrium point is a state where no company can benefit by changing its production level while the other companies keep their levels unchanged. In such a state, there will be no further change to the productions. Mathematically speaking, a *Nash equilibrium* $x^* \in \mathbb{R}^n$ with components x_i^* $(i = 1, \ldots, n)$ satisfies the optimization problem

$$\max x_i p\left(x_i + \sum_{\substack{i=1 \\ i \neq j}}^{n} x_j^*\right) - C_i(x_i) \quad \text{s.t.} \quad x_i \geq 0. \tag{1.1}$$

Here, the so called inverse demand function $p(\xi)$ gives the unit price at which the set of customers will demand and buy a quantity ξ of the product. Under generally accepted economic behavior, it is reasonable to assume that the price $p(\xi)$ will decrease with an increasing amount of available products. Similarly, we can expect the cost function C_i

to be convex in x_i and the total revenue $\xi p(\xi)$ to be concave in $\xi \geq 0$. Under these assumptions the objective function in (1.1),

$$f_i(x) = x_i p\left(x_i + \sum_{\substack{j=1 \\ i \neq j}}^{n} x_j^*\right) - C_i(x_i),$$

is concave in x_i for each $i = 1, \ldots, n$ since it is the sum of two concave functions, see also [34, 91]. Using KKT theory, the optimization problem (1.1) is equivalent to

$$\nabla f_i(x) \geq 0, \quad x_i \geq 0, \quad x_i \nabla f_i(x) = 0. \tag{1.2}$$

Problems of the form (1.2) are called *complementarity problems*. Finding Nash equilibria via (1.2) is among the simpler problems that can be addressed by the methods developed in this thesis.

Other applications of complementarity problems arise not only in other equilibria models of economics, but also from applications in engineering such as contact and structural mechanics problems, obstacle problems, and discrete-time optimal control problems. Variational inequalities with box constraints lead to (mixed) complementarity problems. Also, continuous-time optimal control problems and the Black-Scholes model for pricing American options can be turned into complementarity problems by applying an appropriate discretization. Particularly the latter applications lead to large-scale problems; a fact which represents a challenge to numerical methods and special care must be taken to obtain practicable methods. For a comprehensive overview of these and other sources of complementarity problems we refer the reader to [29, 34]. Many of these applications can be found in the collection MCPLIB [22] representing a popular benchmark for evaluating newly developed methods.

The general form of complementarity problems, which will be used throughout the rest of this thesis, is given by

$$x_i \geq 0, \;\; F_i(x) \geq 0, \;\; x_i F_i(x) = 0 \quad \forall i = 1, \ldots, n, \tag{1.3}$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ denotes a given continuously differentiable mapping. While the existence (and uniqueness) of solutions of particular instances of (1.3) is well established, see [29, 32, 51] and Chapter 2 for summaries, developing numerical methods which are reliable and efficient for a large class of complementarity problems still represents a challenging task.

In the following, we provide a brief overview of existing numerical methods for solving complementarity problems, more comprehensive accounts can be found in [30, 32, 51]. Lemke's algorithm [76, 77] was among the first general algorithms for solving linear complementarity problems. Other classes of such pivoting algorithms can be found in [18]. Scarf [111] described the first algorithm to approximate the fixed point of a continuous map, which can in turn be used to address nonlinear complementarity problems by reformulating (1.3) as a fixed point problem. Extensions of this idea led to other fixed

point schemes, see, e.g., [116]. Theoretically, these methods are rather powerful, due to their global convergence properties. However, on the practical side they suffer from slow convergence and proved to be ineffective.

Complementarity problems can be viewed as particular instances of the framework of generalized equations [104]. Josephy [54] developed Newton methods for solving such generalized equations and provided a firm theoretical basis for establishing fast convergence. Mathiesen [82, 83] successfully applied linearization techniques to solve Walrasian equilibrium models, resulting in an iterative method that requires the solution of a sequence of linear complementarity problems. The methods by Josephy and Mathiesen turned out to be theoretically equivalent. Having local quadratic convergence established, it remained unclear how to obtain global convergence of such Newton methods. A first attempt was made by Rutherford [108] using a simple line search procedure which was demonstrated to be practically powerful but had little theoretical justification. Ralph [103] proposed a theoretically sound approach using a path search algorithm.

Many algorithms for the solution of the complementarity problem are based on a suitable reformulation as a nonsmooth nonlinear system of equations. With the advent of nonsmooth Newton methods for solving semismooth systems [75, 97, 98, 100], finding such reformulations has attracted considerable attention. An early approach by Pang [95] is based on the minimum function, which belongs to the class of so called NCP functions. Combined with a line search strategy, this approach, which is based on the B-derivative of the reformulation operator, achieves global convergence under certain relatively strong regularity conditions. In contrast to the minimum approach, other NCP functions such as the popularly used Fischer-Burmeister function [36] lead to reformulations whose natural merit function is continuously differentiable. Under certain further conditions, this property facilitates the use of line search strategies for obtaining global convergence. This approach has been extensively studied, improved and extended, see e.g. [19, 11, 31, 65, 71], bringing semismooth Newton methods to a high level of reliability and efficiency.

Interestingly, equation-based methods employing smooth NCP functions only lead to a fast locally convergent method if, additionally to the nonsingularity and Lipschitz continuity conditions of the standard Newton method [93], the problem under consideration is nondegenerate. On the other hand, employing nonsmooth NCP functions can lead to fast local convergence even in the case of degenerate problems. Smoothing methods typically approximate a nonsmooth NCP function ϕ by a smooth function ϕ_μ with a smoothing parameter μ such that $\phi_\mu \to \phi$ as $\mu \to 0$. Then a standard Newton method is applied to the corresponding nonlinear system of equations while μ is driven to zero. If this is done in an appropriate manner, one can achieve favorable convergence properties under standard assumptions [8, 12, 14]. It was pointed out that smoothing methods are intimately related to interior point methods [58], which are known to have polynomial complexity [124, 125].

In this thesis we present a new formulation of nonlinear and mixed complementarity problems based on the Fischer-Burmeister function approach. Unlike traditional reformulations, our approach leads to an over-determined system of nonlinear equations. This has the advantage that certain drawbacks of the Fischer-Burmeister approach are avoided. Among other favorable properties of the new formulation, the natural merit function turns out to

be differentiable. To solve the arising over-determined system we use a nonsmooth damped Levenberg-Marquardt-type method and investigate its convergence properties. Under mild assumptions, it can be shown that the global and local fast convergence results are similar to some of the better equation-based method. Moreover, the new method turns out to be significantly more robust than the corresponding equation-based method. For the case of large complementarity problems, however, the performance of this method suffers from the need for solving the arising linear least squares problem exactly at each iteration. Therefore, we suggest a modified version which allows inexact solutions of the least squares problems by using an appropriate iterative solver. Under certain assumptions, the favorable convergence properties of the original method are preserved. As an alternative method for mixed complementarity problems, we consider a box constrained least squares formulation along with a projected Levenberg-Marquardt-type method. To globalize this method, trust region strategies are proposed. Several ingredients are used to improve this approach: affine scaling matrices and multi-dimensional filter techniques. Global convergence results as well as local superlinear/quadratic convergence are shown under appropriate assumptions. Combining the advantages of the new methods, a new software for solving mixed complementarity problems is presented.

The rest of this thesis is organized as follows. Chapter 2 summarizes some basic definitions and results of nonsmooth analysis, in particular with respect to semismooth functions. Moreover, the complementarity problem is formally introduced and we state a few existence results for nonlinear and mixed complementarity problems. In Chapter 3, we recall some existing methods for solving complementarity problems. In Chapter 4 a least squares reformulation is presented, which leads to an exact unconstrained Levenberg-Marquardt-type method. Chapter 5 is concerned with an inexact version of this method suitable for large-scale problems. A projected filter trust-region method is suggested in Chapter 6. Finally, we provide some conclusions.

Chapter 2

Theoretical Background

In this chapter we review those results of nonsmooth analysis that are required for developing and understanding our numerical methods, following the expositions given in [15, 63, 120]. Particular attention is paid to properties of semismooth functions.

2.1 Elements of Nonsmooth Analysis

In the following, we consider a function $G : \mathbb{R}^n \to \mathbb{R}^m$ and denote by $D_G \subseteq \mathbb{R}^n$ the set of all $x \in \mathbb{R}^n$ at which G admits a Fréchet-derivative $G'(x) \in \mathbb{R}^{m\times n}$. Assuming that G is locally Lipschitz continuous around $x \in \mathbb{R}^n$, there is an $\varepsilon = \varepsilon(x) > 0$ and a Lipschitz constant $L = L(x) > 0$ such that

$$\|G(x^1) - G(x^2)\| \leq L\|x^1 - x^2\| \quad \forall x^1, x^2 \in B_\varepsilon(x),$$

where $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^n$. Then according to Rademacher's theorem [102] G is almost everywhere differentiable around x, i.e., the set $B_\varepsilon(x) \setminus D_G$ has Lebesgue measure zero. As an immediate consequence there exist sequences $\{x^k\} \subset D_G$ with $x^k \to x$ for every such x. This justifies the following constructions.

Definition 2.1 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be locally Lipschitz continuous around $x \in \mathbb{R}^n$. The set*

$$\partial_B G(x) := \{H \in \mathbb{R}^{m\times n} | \exists \{x^k\} \subset D_G : x^k \to x \text{ and } G'(x^k) \to H\}$$

is called Bouligand subdifferential*, or short* B-subdifferential*, of G at x. Moreover, the convex hull*

$$\partial G(x) := \operatorname{conv} \partial_B G(x)$$

is called Clarke's generalized Jacobian *of G at x.*

When $m = 1$, in which case G is a real-valued function $g : \mathbb{R}^n \to \mathbb{R}$, $\partial g(x)$ is called the *generalized gradient* of g at x. Furthermore, in this case, consistent with the notation of the gradient of a smooth function, the elements of $\partial g(x)$ are usually viewed as column vectors.

The set

$$\partial_C G(x)^T := \partial G_1(x) \times \cdots \times \partial G_m(x),$$

denotes Qi's *C-subdifferential* of G at x [99], where the right-hand side denotes the set of matrices whose i-th column is an element of the generalized gradient of the i-th component function G_i. For $m = 1$, the generalized gradient and the C-subdifferential coincide. For notational convenience, we often refer to Clarke's generalized Jacobian simply as generalized Jacobian. Note that for $m = 1$ the generalized gradient corresponds to what would be the transposed of the generalized Jacobian.

Let us illustrate these definitions with some examples.

Example 2.2 (a) From the definition of the B-subdifferential, C-subdifferential and generalized Jacobian, it is clear that if $G : \mathbb{R}^n \to \mathbb{R}^m$ is continuously differentiable we have

$$\partial_C G(x) = \partial G(x) = \partial_B G(x) = \{G'(x)\} \quad \text{for all } x \in \mathbb{R}^n.$$

In other words, the respective differentials reduce to a singleton. On the other hand, in view of the corollary to Proposition 2.2.4 in [15], a real valued mapping G is continuously differentiable at x if G is locally Lipschitz continuous around x and the set $\partial G(x)$ consists of one element only.

(b) In some situations the generalized Jacobian can be larger than expected. For example, the generalized Jacobian does not necessarily reduce to the usual Jacobian if $G : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable but not continuously differentiable, as we can see from considering the function $G : \mathbb{R} \to \mathbb{R}$ with

$$G(x) := \begin{cases} x^2 \sin(\frac{1}{x}), & x \neq 0, \\ 0, & x = 0, \end{cases}$$

which is locally Lipschitz continuous and differentiable. While $G'(0) = 0$, we have $\partial G(0) = [-1, 1]$. Note that $G'(x) \in \partial_B G(x)$ always holds, provided that G is differentiable in x.

(c) The Euclidean norm function $g(x) = \|x\|$ on $\mathbb{R}^n$ is continuously differentiable everywhere except at the origin and globally Lipschitz continuous with Lipschitz constant $L = 1$. For $x \neq 0$ we have $g'(x) = \frac{x}{\|x\|}$, and therefore $\partial_B g(0) \subseteq \{x | \, \|x\| = 1\}$. To show that both sets are actually equal, we consider an arbitrary $x \in \mathbb{R}^n$ with $\|x\| = 1$ and define $x^k := \frac{x}{k}$. From $g'(x^k) = \frac{x}{\|x\|} \to x$ we get

$$\partial_B g(0) = \{x | \, \|x\| = 1\}, \quad \text{and} \quad \partial_C g(0) = \partial g(0) = \{x | \, \|x\| \leq 1\}.$$

(d) Given a convex function $g : \mathbb{R}^n \to \mathbb{R}$, then g is locally Lipschitz continuous around any $x \in \mathbb{R}^n$ and Proposition 2.2.7 in [15] asserts that the generalized gradient $\partial g(x)$ coincides with the subdifferential at x in the sense of convex analysis.

The following proposition summarizes some important and useful properties of the differentials introduced above.

Proposition 2.3 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be locally Lipschitz continuous. Then the following statements hold for an arbitrary $x \in \mathbb{R}^n$:*

(a) The B-subdifferential $\partial_B G(x)$ is a nonempty and compact set.

(b) The generalized Jacobian $\partial G(x)$ and the C-subdifferential $\partial_C G(x)$ are nonempty, compact and convex sets.

(c) The set-valued mappings

$$x \mapsto \partial_B G(x), \quad x \mapsto \partial G(x), \quad x \mapsto \partial_C G(x)$$

are closed, i.e., for any sequence $\{x^k\}$ converging to x, and any sequence $\{H_k\}$ with $H_k \in \partial_B G(x^k)$ for all $k \in \mathbb{N}$ converging to some element $H \in \mathbb{R}^{m\times n}$, we have $H \in \partial_B G(x)$ (and similarly for ∂G, $\partial_C G$).

(d) The set-valued mappings

$$x \mapsto \partial_B G(x), \quad x \mapsto \partial G(x), \quad x \mapsto \partial_C G(x)$$

are upper semicontinuous, i.e., for every $\varepsilon > 0$ there exists a $\delta > 0$ with

$$\partial_B G(y) \subseteq \partial_B G(x) + B_\varepsilon(0)$$

for every $y \in B_\delta(x)$ (and similarly for ∂G, $\partial_C G$).

Proof. The results for ∂G are established in [15, Prop. 2.6.2]. The statements on $\partial_C G$ are immediate consequences of the properties of $\partial_C G_i$. The assertion (d) on $\partial_B G$ can be established analogously to the upper semicontinuity of ∂G. Now it can be directly seen that part (d) implies (c), while part (c) yields that the set $\partial_B G(x)$ is closed. In view of (b), $\partial_B G(x)$ is also nonempty and bounded, since $\partial G(x) = \operatorname{conv} \partial_B G(x) \supseteq \partial_B G(x)$. Thus (a) holds. □

Remark 2.4 *(a) The inclusion $\partial G(x) \subseteq \partial_C G(x)$ holds (see Corollary 2.6) and is in general strict, as we can see from the following example:*

$$G(x) = \begin{pmatrix} G_1(x) \\ G_2(x) \end{pmatrix} \quad \text{with} \quad G_1(x) := \min\{0, x\}, \quad G_2(x) := \max\{0, x\}.$$

At the origin, this function is Lipschitz continuous and we have

$$\partial_B G(0) = \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\} \quad \text{and} \quad \partial G(0) = \left\{ \begin{pmatrix} 1-\lambda \\ \lambda \end{pmatrix} \mid \lambda \in [0,1] \right\}.$$

On the other hand, we have $\partial G_1(0) = \partial G_2(0) = [0, 1]$ and consequently $\partial_C G(0) = \{(g_1, g_2)^T \mid g_1, g_2 \in [0, 1]\}$ is a strict superset of $\partial G(0)$.

(b) Let $\{x^k\} \subset \mathbb{R}^n$ be a sequence with a subsequence $\{x^k\}_K$ converging to a vector $x \in \mathbb{R}^n$ and $\{H_k\}_K$ an associated sequence with $H_k \in \partial G(x^k)$. Then the sequence $\{H_k\}_K$ is bounded (the statement applies to $H_k \in \partial_B G(x^k)$ and $H_k \in \partial_C G(x^k)$, too), since the set $\partial G(x)$ is bounded and for a given $\varepsilon > 0$ we can find a $\tilde{k} \in K$ such that

$$H_k \in \partial G(x^k) \subseteq \partial G(x) + B_\varepsilon(0)$$

for all $k \in K$ with $k \geq \tilde{k}$.

The following chain rule holds.

Theorem 2.5 *[15, Thm. 2.6.6] Let $f := g \circ G$, where $G : \mathbb{R}^n \to \mathbb{R}^m$ is locally Lipschitz continuous at x and $g : \mathbb{R}^m \to \mathbb{R}$ is locally Lipschitz continuous at $G(x)$. Then f is locally Lipschitzian at x and*

$$\partial f(x) \subseteq \operatorname{conv}\{\partial g(G(x))\partial G(x)\} := \operatorname{conv}\{H^T\zeta \mid \zeta \in \partial g(G(x)), H \in \partial G(x)\}.$$

If, in addition to the Lipschitz conditions,

1. *g is continuously differentiable at $G(x)$, then equality holds and* conv *can be omitted, i.e., $\partial f(x) = \nabla g(G(x))\partial G(x) := \{H^T \nabla g(G(x)) \mid H \in \partial G(x)\}$;*
2. *g is convex and G is continuously differentiable at x, then equality holds too, and* conv *can be omitted, i.e., $\partial f(x) = \partial g(G(x))G'(x) := \{G'(x)^T\zeta \mid \zeta \in \partial g(G(x))\}$.*

As a special case of Theorem 2.5, by choosing $g(x) = e_i^T x = x_i$ where e_i is the i-th unit vector, we obtain the following result.

Corollary 2.6 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be locally Lipschitz continuous around x, then*

$$\partial G_i(x) = e_i^T \partial G(x) = \{h_i \mid h_i^T \text{ is the } i\text{-th row of some } H \in \partial G(x)\},$$

for $i = 1, \ldots, m$.

For the explicit application of the chain rule it is sometimes meaningful to weaken the statement of Theorem 2.5. To this end we first define the set

$$\begin{aligned}\partial g(G(x))\partial_C G(x) :=& \{H^T\zeta \mid \zeta \in \partial g(G(x)), H \in \partial_C G(x)\} \\ =& \left\{ \sum_{i=1}^m \zeta_i H_i \mid \zeta = (\zeta_1, \ldots, \zeta_m)^T \in \partial g(G(x)), H_i \in \partial G_i(x) \right\}.\end{aligned}$$

Since $\partial G(x) \subseteq \partial_C G(x)$, Theorem 2.5 yields the following result.

Corollary 2.7 *Let $f := g \circ G$, where $G : \mathbb{R}^n \to \mathbb{R}^m$ is locally Lipschitz continuous at x and $g : \mathbb{R}^m \to \mathbb{R}$ is locally Lipschitz at $G(x)$. Then f is locally Lipschitz continuous at x and*

$$\partial f(x) \subseteq \operatorname{conv}\{\partial g(G(x))\partial_C G(x)\}.$$

Appropriate variants hold under the additional assumptions of Theorem 2.5. These rules imply a number of other calculus rules, which imitate the corresponding rules for differentiable functions.

Corollary 2.8 *Let $g_i : \mathbb{R}^n \to \mathbb{R}, i = 1, \ldots, m$ be locally Lipschitz continuous functions at $x \in \mathbb{R}^n$.*

(a) For any coefficients $\alpha_i \in \mathbb{R}$, we have

$$\partial \left(\sum_{i=1}^{m} \alpha_i g_i \right)(x) \subseteq \sum_{i=1}^{m} \alpha_i \partial g_i(x),$$

with equality holding if all but at most one of the g_i are continuously differentiable at x or if all the functions are convex and each α_i is nonnegative.

(b) $\partial(g_1 g_2)(x) \subseteq g_2(x)\partial g_1(x) + g_1(x)\partial g_2(x)$, with equality holding if the functions are convex, $g_1(x) \geq 0$ and $g_1(x) \geq 0$.

(c) If $g_2(x) \neq 0$, then

$$\partial \left(\frac{g_1}{g_2} \right)(x) \subseteq \frac{g_2(x)\partial g_1(x) - g_1(x)\partial g_2(x)}{g_2^2(x)}.$$

Example 2.9 The following function, the so called *Fischer-Burmeister function*, will play an important role in our numerical methods:

$$\phi_{FB} : \mathbb{R}^2 \to \mathbb{R}, \quad \phi_{FB}(x) := \sqrt{x_1^2 + x_2^2} - x_1 - x_2.$$

This function is the difference of the Lipschitz continuous function $g(x) = \|x\|$ and the linear (and in particular differentiable) function $f(x) := x_1 + x_2$. Hence

$$\partial \phi_{FB}(0) = \partial g(0) - \nabla f(0) = \{x - (1,1)^T \mid \|x\| \leq 1\} = \mathbb{B}_1((-1,-1)^T).$$

From this relation and from

$$\partial \phi_{FB}(x) = \left\{ \frac{x}{\|x\|} - \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\}$$

for all $x \neq 0$, one can see that for all $x \in \mathbb{R}^2$ and all $h \in \partial \phi_{FB}(x)$ it holds that $h_1, h_2 \leq 0$ and

$$\sqrt{2} - 1 \leq \|h\| \leq 1 + \sqrt{2}. \tag{2.1}$$

Particularly, this shows that all generalized gradients of ϕ_{FB} are bounded above and are bounded away from zero. To see (2.1), consider $S := \bigcup_{x \in \mathbb{R}^n} \partial \phi_{FB}(x) = \mathbb{B}_1((-1,-1)^T)$, depicted in Figure 2.1. Denoting by P_1 the closest point from S to 0 and the furthest by P_2, equation (2.1) easily follows since

$$P_1 = \operatorname*{argmin}_{h \in S} \|h\| \quad \text{and} \quad P_2 = \operatorname*{argmax}_{h \in S} \|h\|.$$

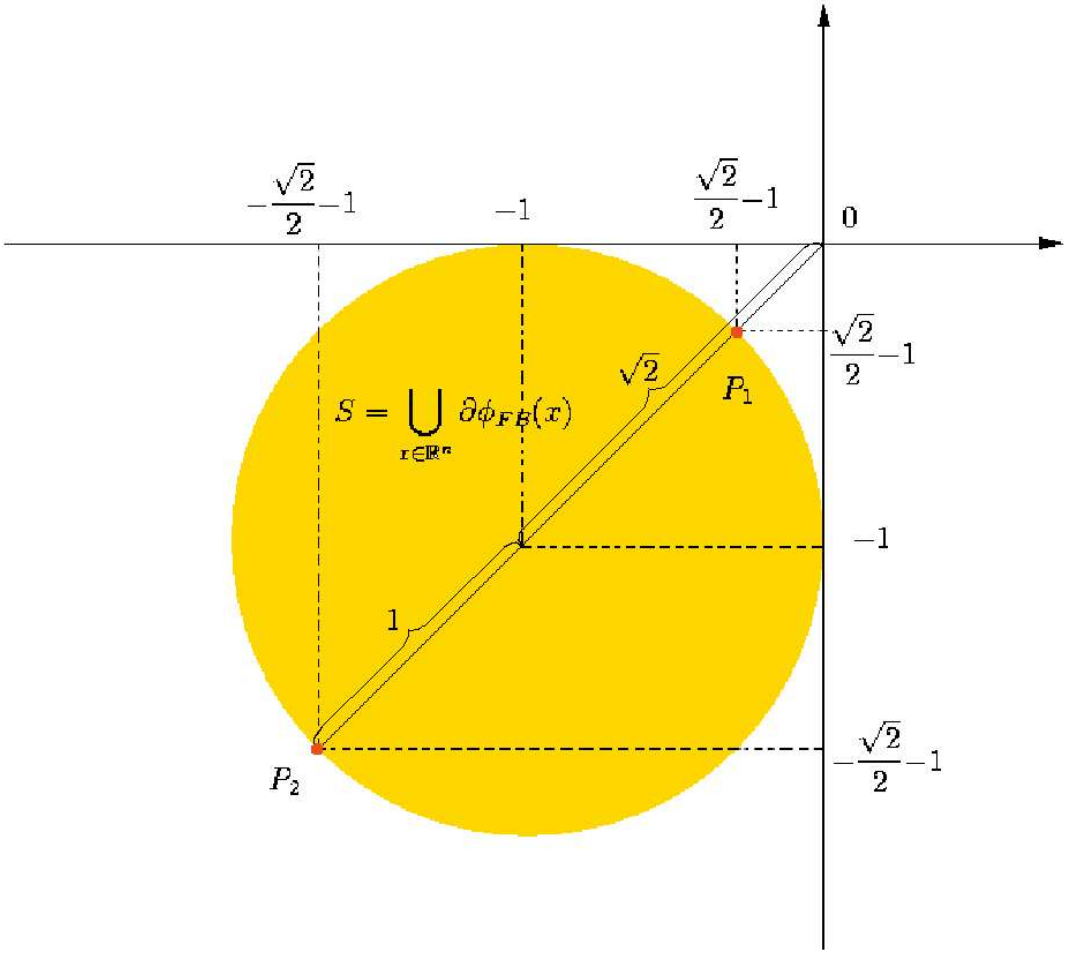

Figure 2.1: Illustration of S from Example 2.9.

2.2 Semismooth Functions

Semismooth functions represent an important subset of locally Lipschitz continuous functions. Their usefulness stems from the fact that zeros of such functions can be found by employing Newton's method, which converges locally Q-superlinearly, even for nonsmooth functions.

Extending Mifflin's definition for a scalar function [86], Qi and Sun [98, 100] introduced the following definition of semismooth functions.

Definition 2.10 *Let $X \subseteq \mathbb{R}^n$ be a nonempty and open set. The function $G : X \to \mathbb{R}^m$ is said to be* semismooth *at $x \in X$ if G is locally Lipschitz continuous around x and if additionally the limit*

$$\lim_{\substack{H\in\partial G(x+t\tilde{d})\\ \tilde{d}\to d,\, t\searrow 0}} H\tilde{d}$$

exists for all $d \in \mathbb{R}^n$. If G is semismooth at all $x \in X$, we call G semismooth (on X).

There are several equivalent ways to define semismoothness. To formulate them, we recall the notions of directional and Bouligand-differentiability (B-differentiability for short).

Definition 2.11 *Let $G : X \to \mathbb{R}^m$ with an open set $X \subseteq \mathbb{R}^n$. Then*

(a) G is called directionally differentiable *at a point $x \in X$ if the directional derivative*

$$G'(x; d) := \lim_{t \searrow 0} \frac{G(x + td) - G(x)}{t}$$

exists for all (nonzero) directions $d \in \mathbb{R}^n$;

(b) G is called B-differentiable *at a point $x \in X$ if G is directionally differentiable at x and*

$$\|G(x + d) - G(x) - G'(x; d)\| = o(\|d\|) \quad \text{as } d \to 0.$$

It is easy to see that the mapping $d \mapsto G'(x; d)$ is positive homogeneous and globally Lipschitz continuous. From Proposition 3.5 in [112] we know that directional differentiability and B-differentiability are equivalent for locally Lipschitz continuous mappings between finite-dimensional spaces, see also [52]. With a slight abuse of notation, in the following we call G to be B-differentiable at x if it is directionally differentiable at x and locally Lipschitz continuous around x. Our definition of B-differentiability follows [95].

The next proposition shows how the directional derivative at x of a B-differentiable function can be computed using a particular element $H \in \partial G(x)$.

Proposition 2.12 *[100, Lem. 2.2] Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$ be a B-differentiable function. Then for any $d \in \mathbb{R}^n$ there exists an element $H \in \partial G(x)$ such that*

$$G'(x; d) = Hd.$$

The following proposition provides alternative ways of characterizing semismoothness. We mention that version (c) is particularly well suited for the convergence analysis of Newton-type methods.

Proposition 2.13 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$. Then the following statements are equivalent:*

(a) G is semismooth at x;

(b) G is locally Lipschitz continuous around x, directionally differentiable at x and for all $d \to 0$ and $H \in \partial G(x + d)$ we have

$$\|Hd - G'(x; d)\| = o(\|d\|);$$

(c) G is locally Lipschitz continuous around x, directionally differentiable at x and

$$\|G(x+d) - G(x) - Hd\| = o(\|d\|) \tag{2.2}$$

holds for all $d \to 0$ and all $H \in \partial G(x+d)$.

Proof. The equivalence between (a) and (b) follows from Theorem 2.3 in [100]. To prove the equivalence between (b) and (c) we first note that in both cases G is locally Lipschitz continuous around x and directionally differentiable at x, implying that G is B-differentiable at x. Hence, (b) and (c) are equivalent, since for all $H \in \partial G(x+d)$ we have

$$\begin{aligned} \big|\|G(x+d) - G(x) - Hd\| - \|Hd - G'(x;d)\|\big| & \\ \leq \|G(x+d) - G(x) - G'(x;d)\| & \\ = o(\|d\|). & \end{aligned}$$

This completes the proof. □

The rate of convergence of the semismooth Newton method (see Section 3.2.1) can be improved if instead of (2.2) an estimate of higher order is available. Such a property is called p-order semismoothness according to [100].

Definition 2.14 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$ be locally Lipschitz continuous and directionally differentiable. Then for $0 < p \leq 1$ G is said to be* p-order semismooth *at x if*

$$\|Hd - G'(x;d)\| = O(\|d\|^{1+p})$$

for all $d \to 0$ and $H \in \partial G(x+d)$.

Note that 1-order semismoothness is sometimes also called *strong semismoothness*. For strong semismoothness a counterpart of Proposition 2.13 can be established under an additional assumption, which we will call *B-differentiability of degree 2*, following [98].

Definition 2.15 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$ be locally Lipschitz continuous and directionally differentiable. Then G is said to be B-differentiable of degree 2 at x if*

$$\|G(x+d) - G(x) - G'(x;d)\| = O(\|d\|^2)$$

for all $d \to 0$.

An alternative characterization of strong semismoothness is stated below.

Proposition 2.16 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$. Then the following two statements are equivalent:*

(a) G is strongly semismooth at x;

(b) G is B-differentiable of degree 2 at x and

$$\|G(x+d) - G(x) - Hd\| = O(\|d\|^2) \tag{2.3}$$

holds for all $d \to 0$ and $H \in \partial G(x+d)$.

Proof. In view of [98, Lem. 2.3], strong semismoothness at x implies B-differentiability of degree 2 at x. Now we can proceed as in the proof of Proposition 2.13. □

It is natural to ask if for a semismooth function G its component functions are semismooth and vice versa. A positive answer is given by the next proposition.

Proposition 2.17 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$ be locally Lipschitz continuous and directionally differentiable. Then the following statements hold:*

(a) G is semismooth at x if and only if each component function G_i is semismooth at x.

(b) G is strongly semismooth at x if and only if each component function G_i is strongly semismooth at x.

Proof. We will prove only part (b), since (a) follows similarly as (b). Let G be strongly semismooth at x, $d \in \mathbb{R}^n$, $i \in \{1, \ldots, m\}$ fixed and choose an arbitrary h_i with $h_i \in \partial G_i(x+d)$. Choose $H \in \partial G(x+d)$ such that its i-th row equals h_i^T (see Corollary 2.6). Then we have

$$\begin{aligned} |G_i'(x;d) - h_i^T d| &= \left|e_i^T (G'(x;d) - Hd)\right| \\ &\leq \|G'(x;d) - Hd\| \\ &= O(\|d\|^2) \quad \text{as } d \to 0, \end{aligned}$$

where e_i denotes the i-th unit vector in $\mathbb{R}^m$. On the other hand, we know that the inclusion $\partial G(x) \subseteq \partial_C G(x)$ holds. Hence if we denote by h_i the i-th row of an element $H \in \partial G(x+d)$ we obtain that $h_i^T \in \partial G_i(x+d)$ and since every G_i is strongly semismooth we also have

$$\begin{aligned} \|G'(x;d) - Hd\| &\leq \sum_{i=1}^m \left|e_i^T (G'(x;d) - Hd)\right| \\ &= \sum_{i=1}^m |G_i'(x;d) - h_i d| \\ &= O(\|d\|^2) \quad \text{as } d \to 0. \end{aligned}$$

Hence, G is strongly semismooth. □

As a consequence of Proposition 2.17 we obtain estimates of the type (2.2) and (2.3) also by choosing any element of the C-subdifferential, which in some situations may be easier to compute.

Proposition 2.18 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$. The following two statements hold:*

(a) If G is semismooth at x, then

$$\|G(x+d) - G(x) - Hd\| = o(\|d\|)$$

for all $d \to 0$ and $H \in \partial_C G(x+d)$.

(b) If G is strongly semismooth at x, then

$$\|G(x+d) - G(x) - Hd\| = O(\|d\|^2)$$

for all $d \to 0$ and $H \in \partial_C G(x+d)$.

Proof. We will prove only part (b), since (a) follows similarly as (b). Let G be strongly semismooth at x, $d \in \mathbb{R}^n$ and choose an arbitrary $H \in \partial_C G(x+d)$. Further we denote by h_i the i-th row of H and obtain that $h_i^T \in \partial G_i(x+d)$ in view of the definition of the C-subdifferential. Since every G_i is strongly semismooth by Proposition 2.17 we have

$$\begin{aligned}\|G(x+d) - G(x) - Hd\| &\leq \sum_{i=1}^{m} \left|e_i^T(G(x+d) - G(x) - Hd)\right| \\ &= \sum_{i=1}^{m} |G_i(x+d) - G_i(x) - h_i d| \\ &= O(\|d\|^2) \quad \text{as } d \to 0.\end{aligned}$$

This shows statement (b). □

The class of semismooth functions is very broad. It includes convex functions, see [86], as well as smooth functions, as shown in the following proposition.

Proposition 2.19 *Let $X \subseteq \mathbb{R}^n$ be an open set, $x \in X$ and $G : X \to \mathbb{R}^m$. The following two statements hold:*

(a) If G is continuously differentiable at x, then G is semismooth at x.

(b) If G is differentiable at x and the Jacobian map $y \mapsto G'(y)$ is locally Lipschitz continuous around x, then G is strongly semismooth at x.

Proof. We only prove (b), since the proof of (a) is rather similar. Since G is continuously differentiable, $\partial G(x+d) = \{G'(x+d)\}$ reduces to a singleton. Denoting by $L = L(x) > 0$ the local Lipschitz constant of G' around x we get for all $d \in \mathbb{R}^n$ with $d \to 0$ and all $H \in \partial G(x+d)$,

$$\|Hd - G'(x;d)\| = \|G'(x+d)d - G'(x)d\| \leq \|G'(x+d) - G'(x)\|\|d\| \leq L\|d\|^2 = O(\|d\|^2).$$

Hence, G is strongly semismooth. □

Example 2.20 (a) The Euclidean norm function $g(x) = \|x\|$ on $\mathbb{R}^n$ is an important example of a strongly semismooth function. As already mentioned it is Lipschitz continuous on $\mathbb{R}^n$ and continuously differentiable on $\mathbb{R}^n \setminus \{0\}$. We have

$$\partial g(x) = \begin{cases} \{\frac{x}{\|x\|}\} & \text{for } x \neq 0, \\ \{y \mid \|y\| \leq 1\} & \text{for } x = 0. \end{cases}$$

Hence, by Proposition 2.19 (b) g is strongly semismooth on $\mathbb{R}^n \setminus \{0\}$. On the other hand, for all $d \in \mathbb{R}^n \setminus \{0\}$ and all $h \in \partial g(d)$ we have

$$g'(0;d) - h^T d = \lim_{t \searrow 0} \frac{\|td\|}{t} - \big(\frac{d}{\|d\|}\big)^T d = \|d\| - \|d\| = 0.$$

Hence, g is also strongly semismooth at 0.

(b) The function $G : \mathbb{R}^2 \to \mathbb{R}$ defined by

$$G(x_1, x_2) := \min\{x_1, x_2\}$$

which is shown to be strongly semismooth on $\mathbb{R}^2$. At any point $x := (x_1, x_2) \in \mathbb{R}^2$ with $x_1 \neq x_2$, G is differentiable with G' being locally Lipschitz continuous around x. Hence G is strongly semismooth at x by Proposition 2.19 (b). We now consider a point $x = (x_1, x_2)$ with $x_1 = x_2$ and an arbitrary direction $d = (d_1, d_2)^T \in R^2$. It is easy to see that $G'(x;d) = \min\{d_1, d_2\}$. We distinguish three cases.

Case 1: If $d_1 < d_2$ then for any $h \in \partial G(x_1 + d_1, x_2 + d_2) = \{(1,0)^T\}$ we have

$$G'(x;d) - h^T d = \min\{d_1, d_2\} - (1,0)\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = d_1 - d_1 = 0.$$

Case 2: If $d_1 > d_2$ then for any $h \in \partial G(x_1 + d_1, x_2 + d_2) = \{(0,1)^T\}$ we have

$$G'(x;d) - h^T d = \min\{d_1, d_2\} - (0,1)\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = d_2 - d_2 = 0.$$

Case 3: If $d_1 = d_2$ we have $\partial G(x_1+d_1, x_2+d_2) = \{(\lambda,\, 1-\lambda)^T \mid \lambda \in [0,1]\}$. Therefore, for any $h \in \partial G(x_1+d_1, x_2+d_2)$, there exists $\lambda_h \in [0,1]$ such that $h = (\lambda_h, 1-\lambda_h)^T$ and

$$G'(x;d) - h^T d = \min\{d_1, d_2\} - (\lambda_h, 1-\lambda_h)\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = d_1 - \lambda_h d_1 - (1-\lambda_h)d_2 = 0.$$

The strong semismoothness of G now follows directly from the above three cases.

Replacing $G(x_1, x_2)$ by $-G(-x_1, -x_2)$ in the arguments above it follows that also the function $\max\{x_1, x_2\}$ is semismooth.

The next result, whose first part is due to Mifflin [86] and whose second part was shown by Fischer [36], states that the class of (strongly) semismooth functions is closed under composition.

Theorem 2.21 *[36, Lem. 18, Thm. 19] Let $G : \mathbb{R}^m \to \mathbb{R}^p$ and $F : \mathbb{R}^n \to \mathbb{R}^m$ be locally Lipschitzian and directionally differentiable functions, and consider the composition $H := G \circ F$. Then the following statements hold:*

(a) If F is semismooth at $x \in \mathbb{R}^n$ and G is semismooth at $F(x)$, then H is semismooth at x.

(b) If F is strongly semismooth at $x \in \mathbb{R}^n$ and G is strongly semismooth at $F(x)$, then H is strongly semismooth at x.

As a direct consequence of the above theorem we obtain that sums, products and quotients of (strongly) semismooth functions are again (strongly) semismooth.

Corollary 2.22 *Let $G_1, G_2 : \mathbb{R}^n \to \mathbb{R}$ be (strongly) semismooth at $x \in \mathbb{R}^n$. Then the following statements hold:*

(a) For any scalars $a_1, a_2 \in \mathbb{R}$ the sum $a_1 G_1 + a_2 G_2$ is (strongly) semismooth at x.

(b) The product $G_1 G_2$ is (strongly) semismooth at x.

(c) If $G_2(x) \neq 0$, then the quotient $\frac{G_1}{G_2}$ is (strongly) semismooth at x.

We conclude this section by giving two further important examples of strongly semismooth functions. The first is the Fischer-Burmeister function

$$\phi_{FB}(x) = \|x\| - x_1 - x_2, \quad x = (x_1, x_2)^T \in \mathbb{R}^2,$$

which is strongly semismooth, since it is the difference of the strongly semismooth Euclidian norm function (see Example 2.20 (a)) and the strongly semismooth part $f(x) = x_1 + x_2$.

The second example is the Euclidean projection $P_{\mathcal{B}} : \mathbb{R}^n \to \mathbb{R}^n$ of a vector $x \in \mathbb{R}^n$ on a rectangular box $\mathcal{B} = [l, u]$ with lower and upper bounds $l = (l_1, \ldots, l_n)^T$ and $u = (u_1, \ldots, u_n)^T$, with $-\infty \leq l_i < u_i \leq +\infty$ for all $i \in \{1, \ldots, n\}$. $P_{\mathcal{B}}$ can be easily computed as

$$P_{\mathcal{B}}(x)_i = \max\{l_i, \min\{x_i, u_i\}\}.$$

Since every component is strongly semismooth, being the composition of strongly semismooth functions (see Example 2.20 (b)), $P_{\mathcal{B}}$ is strongly semismooth.

2.3 P-Functions and P-Matrices

Monotone functions play a similarly important role in the area of complementarity problems as convex functions in optimization.

Definition 2.23 *Let $X \subseteq \mathbb{R}^n$ be a nonempty set. A function $F : X \to \mathbb{R}^n$ is called*

(i) monotone (on X) if, for all $x, y \in X$,

$$(F(x) - F(y))^T(x - y) \geq 0;$$

(ii) strictly monotone (on X) if, for all $x, y \in X$,

$$(F(x) - F(y))^T(x - y) > 0;$$

(iii) strongly monotone (on X) if there exists a constant $\alpha > 0$ with

$$(F(x) - F(y))^T(x - y) \geq \alpha\|x - y\|^2,$$

for all $x, y \in X$.

Conditions for the monotonicity of F can be described by properties of its Jacobian.

Proposition 2.24 *[45, Thm. 7.11] Let $X \subseteq \mathbb{R}^n$ be an open convex set and $F : X \to \mathbb{R}^n$ be continuously differentiable. Then the following statements hold:*

(a) F is monotone (on X) if and only if $F'(x)$ is positive semidefinite for all $x \in X$.

(b) F is strictly monotone (on X) if $F'(x)$ is positive definite for all $x \in X$.

(c) F is strongly monotone (on X) if and only if $F'(x)$ is uniformly positive definite on X, i.e., there exists a constant $\mu > 0$ such that

$$d^T F'(x)d \geq \mu\|d\|^2$$

holds for all $x \in X$ and all $d \in \mathbb{R}^n$.

In what follows we state some weakened concepts of monotonicity, which turn out to be very useful for stating existence and uniqueness results for (mixed) complementarity problems in the next section.

Definition 2.25 *Let $X \subseteq \mathbb{R}^n$ be a nonempty set. A function $F : X \to \mathbb{R}^n$ is called*

(i) pseudo-monotone *(on X) if, for all $x, y \in X$,*

$$F(y)^T(x - y) \geq 0 \quad \textit{implies} \quad F(x)^T(x - y) \geq 0;$$

(ii) a P_0-function (on X) if, for all $x, y \in X$ with $x \neq y$, there exists an index $i_0 := i_0(x, y) \in \{1, \ldots, n\}$ with $x_{i_0} \neq y_{i_0}$ and

$$(x_{i_0} - y_{i_0})(F_{i_0}(x) - F_{i_0}(y)) \geq 0;$$

(iii) a P-function (on X) if, for all $x, y \in X$ with $x \neq y$, there exists an index $i_0 := i_0(x, y) \in \{1, \ldots, n\}$ with

$$(x_{i_0} - y_{i_0})(F_{i_0}(x) - F_{i_0}(y)) > 0;$$

(iv) a uniform P-function (on X) if there exists a constant $\alpha > 0$ with

$$\max_{1 \leq i \leq n} (x_i - y_i)(F_i(x) - F_i(y)) \geq \alpha \|x - y\|^2,$$

for all $x, y \in X$.

Clearly, every monotone function is pseudo-monotone, and on the other hand also a P_0-function; every strictly monotone function is a P-function; and every strongly monotone function is a uniform P-function.

These function properties can be used in order to define analogous matrix properties by considering the special case of linear functions.

Definition 2.26 *A matrix $M \in \mathbb{R}^{n \times n}$ is called*

(i) a P_0-matrix, if $F(x) = Mx$ is a P_0-function on $\mathbb{R}^n$;

(ii) a P-matrix, if $F(x) = Mx$ is a P-function on $\mathbb{R}^n$.

There exist many characterizations for these classes of matrices, see, e.g., [18]. For our purpose, it is sufficient to consider the following characterization of P_0-matrices, which also holds for P-matrices by replacing $\geq$ by $>$.

Proposition 2.27 *Let $M \in \mathbb{R}^{n \times n}$. Then the following statements are equivalent:*

(a) M is a P_0-matrix;

(b) for all $x \in \mathbb{R}^n$ with $x \neq 0$ there exists an index $i_0 = i_0(x) \in \{1, \ldots, n\}$ with $x_{i_0} \neq 0$ and $x_{i_0}[Mx]_{i_0} \geq 0$.

(c) $\det(M_{JJ}) \geq 0$ for all index sets $J \subseteq \{1, \ldots, n\}$, where we made the convention $\det(M) := 1$ for a matrix $M \in \mathbb{R}^{0 \times 0}$.

The proposition above clearly shows that the class of P_0/P-matrices contains the class of symmetric positive (semi-)definite matrices. Thus, a result analogous to Proposition 2.24 for linear P_0/P-functions trivially holds, from the definition and the observations made above. A similar result for nonlinear P_0/P-functions, which is due to Moré and Rheinboldt, is stated in the next theorem.

Theorem 2.28 *[88, Thm. 5.8, Thm. 5.2, Cor. 5.3] Let $X \subseteq \mathbb{R}^n$ be a nonempty open set and $F : X \to \mathbb{R}^n$ be continuously differentiable. Then the following statements hold:*

(a) If F is a P_0-function (on X), then the Jacobian $F'(x)$ is a P_0-matrix for every $x \in X$.

(b) If F is a P-function (on X), then the Jacobian $F'(x)$ is a P-matrix for every $x \in X$.

(c) If $\mathcal{B} \subseteq X$ is a rectangle and $F'(x)$ is a P_0/P-matrix for every $x \in \mathcal{B}$, then F is a P_0/P-function on $\mathcal{B}$.

We conclude this section with a technical result which is needed in our subsequent analysis and concerns P-matrices. For a proof of this statement see [65].

Lemma 2.29 *A matrix of the form*

$$D_a + D_b M$$

is nonsingular for all positive (negative) semidefinite diagonal matrices $D_a, D_b \in \mathbb{R}^{n\times n}$ with a positive (negative) definite sum $D_a + D_b$ if and only if $M \in \mathbb{R}^{n\times n}$ is a P-matrix.

2.4 The Nonlinear Complementarity Problem

After having introduced Clarke's calculus, semismoothness, and some monotonicity concepts, we now come to complementarity problems (CPs), which are the focus of this work. Most of the literature concerning CPs handle the standard forms given by the nonlinear complementarity problem (NCP) and the linear complementarity problem (LCP).

2.4.1 Formal Definition and Related Problems

Definition 2.30 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a given function. The* complementarity problem *is to find a vector $x^* \in \mathbb{R}^n$ satisfying the following system of equations and inequalities:*

$$x \geq 0, \quad F(x) \geq 0, \quad x^T F(x) = 0$$

or, equivalently,

$$x_i \geq 0, \quad F_i(x) \geq 0, \quad x_i F_i(x) = 0 \quad \forall i = 1, \ldots, n.$$

If $F(x) = Mx + q$ is an affine function (where $M \in \mathbb{R}^{n\times n}$ and $q \in \mathbb{R}^n$), then the complementarity problem is called a linear complementarity problem *(denoted by LCP(q, M)), otherwise it is called a* nonlinear complementarity problem *(denoted by NCP(F)).*

While the standard forms are convenient from a theoretical point of view, many practical problems are more naturally formulated in the framework of mixed complementarity problems (MCPs).

Definition 2.31 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a given function, $l = (l_1, \ldots, l_n)^T$ and $u = (u_1, \ldots, u_n)^T$ be given lower and upper bounds with $-\infty \leq l_i < u_i \leq +\infty$ for all $i \in \{1, \ldots, n\}$. The* mixed complementarity problem *(denoted by MCP(F, l, u)) consists in finding a vector $x^* \in [l, u]$ such that for all $i \in \{1, \ldots, n\}$ exactly one of the following conditions holds:*

$$\begin{aligned} x_i^* = l_i \quad &and \quad F_i(x^*) > 0, \\ x_i^* = u_i \quad &and \quad F_i(x^*) < 0, \\ x_i^* \in [l_i, u_i] \quad &and \quad F_i(x^*) = 0. \end{aligned}$$

In the special case when F is an affine function we obtain the so called linear mixed complementarity problem.

Note that the assumption $l < u$ represents no loss of generality, since otherwise the variable x_i^* can be removed from the problem, for all $i \in \{1, \ldots, n\}$ with $l_i = u_i$. The above definition shows that NCP(F) is a special case of MCP(F, l, u) given by $l = 0$ and $u = \infty$.

Nonlinear complementarity problems as well as mixed complementarity problems are special cases of the finite variational inequality problem.

Definition 2.32 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a given function and let $X \subseteq \mathbb{R}^n$ be a nonempty, closed and convex set. The* variational inequality problem *(denoted by VI(F, X)) consists in finding a point $x^* \in X$ such that*

$$F(x^*)^T(x - x^*) \geq 0 \quad \forall x \in X.$$

In the following proposition we see that for $\mathcal{B} := [l, u]$ the mixed complementarity problem MCP$(F, \mathcal{B})$ is equivalent to the box-constrained variational inequality VI$(F, \mathcal{B})$, and, as a consequence, NCP(F) is equivalent to VI$(F, \mathbb{R}^n_+)$.

Proposition 2.33 *Given a rectangular set $\mathcal{B} = [l, u]$ and a function $F : \mathbb{R}^n \to \mathbb{R}^n$, then the vector x^* solves MCP$(F, \mathcal{B})$ if and only if it solves VI$(F, \mathcal{B})$.*

Proof. We first rewrite the mixed complementarity problem in the following form:

$$\begin{aligned} \text{MCP}(F, \mathcal{B}): \quad &\text{Find } x^* \in \mathcal{B} \text{ such that} \\ &(x^* - l)^T F(x^*)_+ = 0 \text{ and } (u - x^*)^T F(x^*)_- = 0. \end{aligned} \tag{2.4}$$

In the above reformulation of the MCP, note that the components of the bounds l and u may be infinite. We therefore adopt the convention $\pm\infty \cdot 0 = 0$.
($\Rightarrow$) Assume that x^* solves MCP$(F, \mathcal{B})$. Then $x^* \in \mathcal{B}$ and for all $x \in \mathcal{B}$ we have

$$\begin{aligned} F(x^*)^T(x - x^*) &= -F(x^*)_+^T(x^* - x) - F(x^*)_-^T(x - x^*) \\ &\geq -F(x^*)_+^T(x^* - l) - F(x^*)_-^T(u - x^*) \\ &= 0. \end{aligned} \tag{2.5}$$

($\Leftarrow$) If x^* solves VI$(F, \mathcal{B})$, then $l \leq x^* \leq u$. For an arbitrary index $i \in \{1, \ldots, n\}$ assume that $F_i(x^*) > 0$ and $x_i^* > l$. Since $F_i(x^*)_- = 0$ we obtain

$$F(x^*)^T(x^* + (l_i - x_i^*)e_i - x^*) = F_i(x^*)_+(l_i - x_i^*) < 0,$$

where e_i denotes the i-th unit vector of $\mathbb{R}^n$. Since $x^* + (l_i - x_i^*)e_i \in \mathcal{B}$ this contradicts our assumption that x^* solves VI$(F, \mathcal{B})$. Since i was arbitrary we get $F(x^*)_+^T(x^* - l) = 0$ as well. Similarly, $F(x^*)_-^T(u - x^*) = 0$, so that x^* solves MCP$(F, \mathcal{B})$. □

A useful reformulation of the VI involves the normal cone, which we define below.

Definition 2.34 *Let $C \subseteq \mathbb{R}^n$ be a given closed convex set. The* normal cone *at a point $x \in \mathbb{R}^n$ related to C is the set*

$$N_C(x) = \begin{cases} \{y \mid y^T(c - x) \leq 0,\ \forall c \in C\} & \text{if } x \in C, \\ \emptyset & \text{otherwise.} \end{cases}$$

It can be directly verified that $VI(F, C) \Leftrightarrow 0 \in F(x) + N_C(x)$. The latter formulation,

$$0 \in F(x) + N_C(x), \tag{2.6}$$

is a special case of a generalized equation (GE) in the sense of Robinson [104], a zero finding problem of a set-valued mapping.

2.4.2 Existence Results

Our next concern is with the existence of a solution to the box-constrained variational inequality VI$(F, \mathcal{B})$, which in turn addresses the existence of solutions of MCP$(F, \mathcal{B})$. We begin with another useful reformulation of the variational inequality problem as a classical fixed-point problem, following an early approach by Eaves [24].

Proposition 2.35 *Let $X \in \mathbb{R}^n$ be a nonempty, closed and convex set. Then $x^* \in \mathbb{R}^n$ solves the VI(F, X) problem if and only if x^* is a fixed point of the mapping $P : \mathbb{R}^n \to \mathbb{R}^n$ defined by*

$$P(x) := P_X(x - F(x)), \tag{2.7}$$

i.e., if $x^* = P(x^*)$.

The most basic result on the existence of a solution of VI(F, X) requires the set X to be compact and convex and the mapping F to be continuous. By applying Brouwer's fixed-point theorem to the mapping P defined in equation (2.7) one can state the following result.

Theorem 2.36 *[24] Let $X \subset \mathbb{R}^n$ be a nonempty, compact and convex set and let $F : X \to \mathbb{R}^n$ be continuous. Then there exists a solution to the problem VI(F, X).*

The set $\mathcal{B} = [l, u]$, to which we turn our attention, is nonempty, closed and convex but often unbounded (as in the case of the nonlinear complementarity problem). In order to give an idea of what can happen in this case, we consider the following example.

Example 2.37 In all examples the function F is defined on $\mathbb{R}$ to $\mathbb{R}$.

(a) If $F(x) := -x^2 - 1$, the corresponding NCP(F) has no solution.

(b) If $F(x) := e^{-x}$, the corresponding NCP(F) has a solution, namely $x^* = 0$.

(c) If $F(x) := x - 1$, the corresponding NCP(F) has the unique solution $x^* = 1$.

(d) For $F(x) := \sin(x)$, the NCP(F) has infinitely many isolated solutions, namely $x_k = k\pi, k \in \{0, 1, \dots\}$.

If the mapping F possesses some additional properties, such as being a P-function, then the unboundedness of X may not lead to the undesired effects observed in Example 2.37. The following result for NCPs/MCPs has been known for a long time and can be found in the survey [51].

Theorem 2.38 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a continuous mapping on the rectangular box $\mathcal{B} = [l, u]$ with lower and upper bounds $l = (l_1, \dots, l_n)^T$ and $u = (u_1, \dots, u_n)^T$, with $-\infty \leq l_i < u_i \leq +\infty$ for all $i \in \{1, \dots, n\}$. Then the following statements hold:*

(a) If F is pseudo-monotone on $\mathcal{B}$, then NCP/MCP has a convex solution set (provided it is nonempty).

(b) If F is a P-function on $\mathcal{B}$, then NCP/MCP has at most one solution.

(c) If F is a uniform P-function on $\mathcal{B}$, then NCP/MCP has a unique solution.

Considering Example 2.37, the function in (a) is not even monotone, let alone strongly monotone (uniform P- functions from $\mathbb{R}$ to $\mathbb{R}$ are strongly monotone and vice versa). Only for the problem in (c) the existence can be guaranteed using the above theorem, since the function in (c) is strongly monotone. The uniform P- property is however not a necessary condition to ensure existence. The function F in (b) is only pseudo-monotone and the underlying NCP has a solution. Fortunately, pseudo-monotonicity is sufficient to establish the existence of a solution of the NCP (where $\mathcal{B} = \mathbb{R}^n_+$ is a convex cone) under a certain Slater-type constraint qualification stated below.

Definition 2.39 *An element $\hat{x} \in \mathbb{R}^n$ is called* strictly feasible *for NCP(F) if $\hat{x} > 0$ and $F(\hat{x}) > 0$.*

The following result can be applied if F is continuous and pseudo-monotone on the cone $\mathbb{R}^n_+$. Unfortunately, it cannot be transferred to MCPs since $\mathcal{B} = [l, u]$ is usually not a cone.

Theorem 2.40 *[29, Thm. 2.4.4] Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a continuous mapping on $\mathbb{R}^n_+$. If F is pseudo-monotone on $\mathbb{R}^n_+$ and there is a strictly feasible point $\hat{x}$ for NCP, then NCP(F) has a nonempty and compact solution set.*

Theorem 2.38 (c) provides conditions under which the NCP/MCP has a unique solution. The following result provides conditions under which a given solution x^* is isolated (or locally unique), i.e., there is a neighborhood $\mathcal{U}$ of x^* such that x^* is the only solution of NCP/MCP in $\mathcal{U}$.

Proposition 2.41 *[115, Thm. 2.3] Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable and let x^* be a solution of NCP/MCP. If the Jacobian matrix $F'(x^*)$ is positive definite, then x^* is locally unique.*

Unfortunately, the above results admit no decision on the question whether the solutions $x_{2k+1} = (2k+1)\pi, k \in \{0, 1, \dots\}$ from Example 2.37 (d) are isolated. There is a different way of deriving a much weaker alternative of the above result via the local analysis of nonsmooth equations, see for instance [29] or Lemma 6.13. Under a condition which we will later call R-regularity at a solution (see Definition 3.18) the local uniqueness can be guaranteed. This condition translated to our one-dimensional example from (d) is equal to the condition $\cos(k\pi) \neq 0, k \in \{0, 1, \dots\}$, which clearly holds.

We conclude this section by mentioning that most proofs of the above results can be found in [29], although the main existence result will follow from an equivalent formulation of NCP/MCP as an optimization problem which consists in minimizing a certain merit function.

Chapter 3

Solution Methods for Complementarity Problems

The purpose of this chapter is to review existing methods for solving nonlinear and mixed complementarity problems. Here, we concentrate on Newton-type methods and will not discuss fixed points methods, which have been introduced in the pioneering years of the field of CPs but have proven to be inefficient due to their poor local convergence properties. To apply a Newton-type method, we first have to reformulate the CP into a nonlinear equation. This matter is discussed in Section 3.1. Although there exist reformulations into smooth equations, modern methods prefer nonsmooth reformulations. To address the latter class of equations, we introduce nonsmooth Newton- and Levenberg-Marquardt-like methods in Section 3.2. For achieving fast local convergence, the original CP has to satisfy certain properties, which are discussed in Section 3.3. To address the delicate matter of global convergence, several globalization techniques such as line search and trust region strategies are described in Section 3.4. While Section 3.5 is concerned with some other methods, Section 3.6 presents a summary of available software for solving complementarity problems.

3.1 Reformulation of Complementarity Problems

Various numerical algorithms have been proposed based upon reformulations of the nonlinear complementarity problem as a system of nonlinear equations $G(x) = 0$. One possibility is to use the so-called NCP-functions.

Definition 3.1 *A function $\phi : \mathbb{R}^2 \to \mathbb{R}$ having the property that*

$$\phi(a, b) = 0 \iff a \geq 0, b \geq 0, ab = 0 \tag{3.1}$$

is called an NCP-function.

Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be given, $\phi : \mathbb{R}^2 \to \mathbb{R}$ be any NCP-function and $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ be defined as follows:

$$\Phi(x) := \begin{pmatrix} \phi(x_1, F_1(x)) \\ \vdots \\ \phi(x_n, F_n(x)) \end{pmatrix}. \tag{3.2}$$

Then it can be directly seen that x^* solves the nonlinear complementarity problem NCP(F) if and only if x^* solves the nonlinear system of equations $\Phi(x) = 0$. Already in the seventies, Mangasarian [79] proved the equivalence of NCP to a system of equations choosing the NCP-function

$$\phi_M(a, b) = \theta(|a - b|) - \theta(a) - \theta(b), \tag{3.3}$$

where $\theta : \mathbb{R} \to \mathbb{R}$ is any strictly increasing function with $\theta(0) = 0$. If, in addition, θ is continuously differentiable with $\theta'(0) = 0$, then also ϕ_M is continuously differentiable. This is satisfied by choosing for example $\theta(t) = t|t|$. If F is C^1, then the resulting system $\Phi(x) = 0$ is smooth and a Newton-type method can be applied without modifications.

Nevertheless, modern algorithms prefer nondifferentiable, semismooth reformulations, because Newton's method is not applicable if strict complementarity is violated at the solution x^* [64]. Such a solution is sometimes called degenerate.

Definition 3.2 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be a given function and consider the nonlinear complementarity problem NCP(F). A solution x^* of NCP(F) is called*

(i) nondegenerate if $x_i^* + F_i(x^*) > 0$ for all $i = 1, \ldots, n$;

(ii) degenerate if it is not nondegenerate, i.e., if there exists at least one index $i_0 \in \{1, \ldots, n\}$ such that $x_{i_0}^* = 0$ and $F_{i_0}(x^*) = 0$.

In practice, degeneracy occurs quite frequently, at least numerically, since it is often difficult to decide whether a numerically obtained solution is degenerate or nondegenerate. Returning to the problems associated with degeneracy, we consider a differentiable NCP-function ϕ and see that $\nabla\phi(0, 0) = (0, 0)^T$, since $\lim_{t \searrow 0} \frac{\phi(t,0)}{t} = 0 = \lim_{t \searrow 0} \frac{\phi(0,t)}{t}$. The Jacobian of G at x^* is given by

$$\Phi'(x^*) = D_a(x^*) + D_b(x^*)F'(x^*), \tag{3.4}$$

where $D_a(x^*), D_b(x^*) \in \mathbb{R}^{n \times n}$ are diagonal matrices with

$$D_a(x^*) := \operatorname{diag}\left(\ldots, \frac{\partial \phi}{\partial a}(x_i^*, F_i(x^*)), \ldots \right),$$
$$D_b(x^*) := \operatorname{diag}\left(\ldots, \frac{\partial \phi}{\partial b}(x_i^*, F_i(x^*)), \ldots \right).$$

Hence, if the solution x^* is degenerate, there exists an index $i_0 \in \{1, \ldots, n\}$ with $x_{i_0}^* = 0 = F_{i_0}(x^*)$ and the i_0-th row of $\Phi'(x^*)$ is zero. This phenomenon can be avoided by

using semismooth NCP-functions, because they can be constructed in such a way that any element of the generalized gradient $\partial\phi(a,b)$ is bounded away from zero (see Example 2.9).

We next give some examples of semismooth NCP-functions.

Example 3.3 (a) The use of the minimum NCP-function $\phi_P(a,b) := \min\{a,b\}$ was extensively studied and propagated by Pang, see, e.g., [95]. Note that for the straightforward choice $\theta(t) = t$ in (3.3) we obtain $\phi_M(a,b) = -2\phi_P(a,b)$. Recall that ϕ_P is strongly semismooth, cf. Example 2.20 (b).

(b) The Fischer-Burmeister function $\phi_{FB}(a,b) := \sqrt{a^2+b^2} - a - b$, see also Example 2.9, first appeared in the paper [36] by Fischer, where it is attributed to Burmeister.

(c) The penalized Fischer-Burmeister function, $\phi_{CCK}(a,b) := \lambda\phi_{FB}(a,b) - (1-\lambda)a_+b_+$ with $\lambda \in (0,1)$ fixed, was introduced in [11] in order to overcome some limitations of the Fischer-Burmeister function.

It follows from Example 2.20 (b) that the plus function $z \mapsto z_+$ is strongly semismooth, thus not only the Fischer-Burmeister function but also the penalized Fischer-Burmeister function is strongly semismooth.

The reformulation via NCP-functions can be extended to the framework of mixed complementarity problems. We stress that not every NCP-function is suitable to serve this purpose. Once again, the Fischer-Burmeister function is a good choice as we will see in Section 4.4. A further important reformulation, which is due to Robinson [106], is based on the normal map.

Definition 3.4 *Let $\mathcal{B} \subseteq \mathbb{R}^n$ be a closed convex set and consider a function $F : \mathcal{B} \to \mathbb{R}^n$. Then the normal map $F_{\mathcal{B}}$ induced on F by $\mathcal{B}$ is defined as*

$$F_{\mathcal{B}}(x) := F(P_{\mathcal{B}}(x)) + (x - P_{\mathcal{B}}(x)).$$

The corresponding normal map equation is then defined as

$$F_{\mathcal{B}}(x) = 0. \tag{3.5}$$

In the case of $\mathcal{B} := [l,u]$ finding a zero of the normal map equation is equivalent to solve $\mathrm{MCP}(F,l,u)$ in the following sense.

Proposition 3.5 *Let $\mathcal{B} = [l,u]$ be a rectangular box and let $F : \mathcal{B} \to \mathbb{R}^n$ be a given function. If the vector $x \in \mathbb{R}^n$ solves the normal map equation (3.5), then $z := P_{\mathcal{B}}(x)$ solves MCP$(F,\mathcal{B})$. Conversely, if z solves MCP$(F,\mathcal{B})$, then $x := z - P_{\mathcal{B}}(z)$ solves (3.5).*

Proof. Assume that x satisfies (3.5). Then

$$P_{\mathcal{B}}(x) - F(P_{\mathcal{B}}(x)) = x.$$

If we define $z := P_{\mathcal{B}}(x)$ the above equation becomes

$$z - F(z) = x.$$

Hence, $z(= P_{\mathcal{B}}(x))$ satisfies the fixed point equation $z = P_{\mathcal{B}}(z - F(z))$, which is equivalent to solving MCP$(F, \mathcal{B})$, according to Proposition 2.35.
Conversely, if z solves MCP$(F, \mathcal{B})$, also $z = P_{\mathcal{B}}(z - F(z))$ holds. Defining $x := z - F(z)$ we get $z = P_{\mathcal{B}}(x)$. Replacing z in $F(z) + x - z = 0$ we obtain

$$F(P_{\mathcal{B}}(x)) + x - P_{\mathcal{B}}(x) = 0.$$

Thus, x satisfies the normal map equation. □

The normal map $F_{\mathcal{B}}$ is strongly semismooth, if F is strongly semismooth on $\mathcal{B}$, since the Euclidian projection $P_{\mathcal{B}}$ is strongly semismooth, as we already noticed.

3.2 Local Methods for Semismooth Equations

3.2.1 Generalized Newton Method

After having seen that the reformulation of complementarity problems leads to nonsmooth systems of equations, we now study the local behavior of nonsmooth versions of Newton's method for solving such systems. Let $G : \mathbb{R}^n \to \mathbb{R}^n$ be a given function. If G is continuously differentiable, then Newton's method for the solution of the nonlinear system of equations

$$G(x) = 0$$

generates a sequence $\{x^k\}$ according to the following rule:

$$x^{k+1} := x^k - (G'(x^k))^{-1} G(x^k), \quad k = 0, 1, \ldots,$$

where $x^0 \in \mathbb{R}^n$ is a suitable starting point. Now, if G is only locally Lipschitz continuous, one can replace this formula by

$$x^{k+1} := x^k - H_k^{-1} G(x^k), \quad k = 0, 1, \ldots,$$

where H_k is an element of some generalized Jacobian, such as the the B-subdifferential $\partial_B G(x^k)$, the generalized Jacobian $\partial G(x^k)$, or the C-subdifferential $\partial_C G(x^k)$.

We obtain the following algorithm.

Algorithm 3.6 (Nonsmooth Newton Method)

(S.0) Choose $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_B G(x^k)$ and compute a solution $d^k \in \mathbb{R}^n$ of the linear system

$$H_k d = -G(x^k). \tag{3.6}$$

(S.3) Set $x^{k+1} = x^k + d^k$, $k \leftarrow k+1$, and go to (S.1).

We note that we can obtain similar algorithms by choosing $H_k \in \partial G(x^k)$ or $H_k \in \partial_C G(x^k)$. Imitating the classical Newton method, Algorithm 3.6 needs a regularity assumption on the matrices H_k to converge locally superlinearly.

Definition 3.7 *Let $G : \mathbb{R}^n \to \mathbb{R}^n$ be locally Lipschitz continuous and let $x^* \in \mathbb{R}^n$ be a solution of $G(x) = 0$. Then*

(a) x^* is called a BD-regular *solution ("BD" for Bouligand-differential) of this system if all elements $H \in \partial_B G(x^*)$ are nonsingular.*

(b) x^* is called a CD-regular *solution ("CD" for Clarke-differential) solution of this system if all elements $H \in \partial G(x^*)$ are nonsingular.*

For example, if $G(x) = |x|$ is the absolute value function, then $x^* := 0$ is a BD-regular solution of this system of equations, but not a CD-regular solution. BD-regularity (CD-regularity) implies the following nonsingularity result, see [98, 100].

Proposition 3.8 *Let $G : \mathbb{R}^n \to \mathbb{R}^n$ be locally Lipschitz continuous and let $x^* \in \mathbb{R}^n$ be a BD-regular (alternatively CD-regular) solution of $G(x) = 0$. Then there is a neighborhood $B_\varepsilon(x^*)$ of x^* and a constant $c > 0$ such that for any $x \in B_\varepsilon(x^*)$ and for any $H \in \partial_B G(x)$ (alternatively $H \in \partial G(x)$), H is nonsingular and*

$$\|H^{-1}\| \leq c.$$

A similar nonsingularity result holds also for Qi's subdifferential $\partial_C G$ by a slight change of the corresponding proof in [100]. These nonsingularity results admit the formulation of the following local convergence properties.

Theorem 3.9 *Let $G : \mathbb{R}^n \to \mathbb{R}^n$ be locally Lipschitz continuous and denote by $x^* \in \mathbb{R}^n$ a solution of the system $G(x) = 0$. Assume that*

(A) an estimate (2.2) holds at x^* (which in particular is satisfied if G is semismooth at x^*);

(B) there is a constant $\varepsilon_1 > 0$ and a constant $c > 0$ such that, for any $x \in B_{\varepsilon_1}(x^*)$, every $H \in \partial_B G(x)$ is nonsingular and $\|H^{-1}\| \leq c$ (which in particular is satisfied if x^* is a BD-regular solution).

Then there exists an $\varepsilon > 0$ such that the following statements hold for all starting points $x^0 \in B_\varepsilon(x^*)$:

(a) Algorithm 3.6 is well-defined and generates a sequence $\{x^k\}$ converging to x^*.

(b) The rate of convergence is Q-superlinear.

(c) The rate of convergence is Q-quadratic if additionally an estimate

$$G(x^* + d) - G(x^*) - Hd = O(\|d\|^2) \tag{3.7}$$

holds for all $d \to 0$ and $H \in \partial_B G(x^* + d)$ (which in particular is satisfied if G is strongly semismooth at x^*).

Proof. Since the proof is not difficult and proliferates the understanding of later local convergence analyses we include it here. With $c > 0$ from (B), condition (A) implies that there is a constant $\varepsilon_2 > 0$ with

$$\|G(x) - G(x^*) - H(x - x^*)\| \leq \frac{1}{2c}\|x - x^*\|$$

for all $x \in B_{\varepsilon_2}(x^*)$ and all $H \in \partial_B G(x)$. Define $\varepsilon := \min\{\varepsilon_1, \varepsilon_2\}$ (with ε_1 from (A)) and choose a starting vector x^0 such that $x^0 \in B_\varepsilon(x^*)$. Then x^1 exists, and we have

$$\begin{aligned}
\|x^1 - x^*\| &= \|x^0 - x^* - H_0^{-1}G(x^0)\| \\
&\leq \|H_0^{-1}\|\|G(x^0) - G(x^*) - H_0(x^0 - x^*)\| \\
&\leq c\frac{1}{2c}\|x^0 - x^*\| \\
&= \frac{1}{2}\|x^0 - x^*\|.
\end{aligned}$$

Hence x^1 also belongs to $B_\varepsilon(x^*)$. Continuing in this manner we obtain by induction that

$$\|x^k - x^*\| \leq \left(\frac{1}{2}\right)^k \|x^0 - x^*\|$$

for all $k \in \mathbb{N}$. Hence the sequence $\{x^k\}$ generated by Algorithm 3.6 is well-defined and converges to x^*. This proves part (a). In order to verify the local superlinear rate of convergence, we exploit estimate (2.2) once again and obtain

$$\begin{aligned}
\|x^{k+1} - x^*\| &= \|x^k - x^* - H_k^{-1}G(x^k)\| \\
&\leq \|H_k^{-1}\|\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| \\
&\overset{(B)}{\leq} c\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| \\
&\overset{(2.2)}{=} o(\|x^k - x^*\|)
\end{aligned}$$

as $x^k \to x^*$. The local quadratic convergence follows similarly by using estimate (3.7). □

Various results of this type can be found in the literature, see for instance [97, 98, 100]. If in (S.2) of Algorithm 3.6 we choose an element of $H_k \in \partial G(x)$ we obtain Q-superlinear convergence towards a solution x^* of system $G(x) = 0$, provided that assumption (A) of Theorem 3.9 and the CD-regularity of x^* (see [100]) hold. In [95] the proposed search direction d^k is obtained by solving the nonlinear equation

$$G'(x^k; d) + G(x^k) = 0, \tag{3.8}$$

where G is a B-differentiable function. According to Proposition 2.12, for this solution d^k there exists an element $\tilde{H}_k \in \partial G(x^k)$ such that equation (3.8) (in general nonlinear) is identical to

$$\tilde{H}_k d^k + G(x^k) = 0.$$

However it is a nontrivial task to find this particular $\tilde{H}_k$.

In the case when G is semismooth and (3.8) has a solution, this B-derivative-based Newton method becomes a special case of Algorithm 3.6 (see [98, 100]). Hence, under the assumptions of Theorem 3.9 and the solvability of (3.8) this B-derivative-based Newton inherits the convergence properties of Algorithm 3.6.

Similar convergence properties can be established for $H_k \in \partial_C G(x)$ under an analogous regularity assumption. We conclude this section by noting that a globalization of the nonsmooth Newton method is usually a much more complicated issue than the globalization of the standard smooth Newton method.

3.2.2 Inexact Variants

Typically, the most expensive part of Algorithm 3.6 in terms of computing time and memory consists of solving the linear system of equations in step (S.2). For large n, this system becomes intractable by standard direct solvers such as Gaussian elimination. So, in order to address large-scale systems, other linear system solvers have to be employed. One possibility is to use direct sparse solvers, which can reduce the cost for sparse matrices considerably by avoiding excessive fill-in during Gaussian elimination using appropriate reordering and pivoting strategies. However, the effectiveness of direct sparse solvers heavily depends on the sparsity structure of the matrix. In contrast, iterative solvers such as LSQR [94], GMRES [110] and QMR [109] (note that the systems to be solved are in general neither symmetric nor positive definite) only require fast matrix-vector multiplications. Here, the effectiveness depends on the number of iterations; normally the iteration is stopped before the residual reaches the level of roundoff error. Consequently, using iterative solvers means that the linear system in Algorithm 3.6 is solved inexactly. To take this fact into account, we reformulate Algorithm 3.6 as follows.

Algorithm 3.10 (Nonsmooth Inexact Newton Method)

(S.0) Choose $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_B G(x^k)$ and compute a solution $d^k \in \mathbb{R}^n$ of the linear system such that

$$H_k d = -G(x^k) + r^k,$$

where the residual vector $r^k \in \mathbb{R}^n$ satisfies

$$\|r^k\| \leq \alpha_k \|G(x^k)\|$$

with α_k being a positive number.

(S.3) Set $x^{k+1} = x^k + d^k$, $k \leftarrow k+1$, and go to (S.1).

The following theorem discusses the effect of using inexact solutions on the convergence of the nonsmooth Newton method, see [26, 28, 81].

Theorem 3.11 *Let G be semismooth and let x^* be a BD-regular solution of the system $G(x) = 0$. Assume that $\{x^k\}$ is a sequence generated by Algorithm 3.10, Then the following statements hold:*

(a) Provided there is a sufficiently small number $\bar{\alpha}$ with $\alpha_k \leq \bar{\alpha}$ and $\|x^0 - x^*\|$ is sufficiently small, Algorithm 3.10 and $\{x^k\}$ converges Q-linearly to x^*.

(b) If additionally $\alpha_k \to 0$, the rate of convergence is Q-superlinear.

(c) If G is strongly semismooth, $\alpha_k = O(\|G(x^k)\|)$, and the sequence $\{x^k\}$ converges to x^* then the rate of convergence is Q-quadratic.

3.2.3 Levenberg-Marquardt Method

The Levenberg-Marquardt method is a variant of Algorithm 3.6 for solving

$$G(x) = 0. \tag{3.9}$$

Algorithm 3.12 (Nonsmooth Levenberg-Marquardt Method)

(S.0) Choose $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_B G(x^k)$ and compute a solution $d^k \in \mathbb{R}^n$ of the linear system

$$(H_k^T H_k + \nu_k I)d = -H_k^T G(x^k), \tag{3.10}$$

where $\nu_k \geq 0$ is a prescribed regularization parameter.

(S.3) Set $x^{k+1} = x^k + d^k$, $k \leftarrow k+1$, and go to (S.1).

The only notable difference between this algorithm and Algorithm 3.6 is that the linear system (3.6) is replaced by (3.10). Solving the latter system can have several advantages. First, its system matrix $H_k^T H_k + \nu_k I$ is symmetric, and positive definite if $\nu_k > 0$. Second, if the iterates are not sufficiently close to the (regular) solution, then H_k can be (close to) a singular matrix, resulting into an ill-conditioned linear system (3.6). This effect can be avoided for (3.10) by an appropriate choice of ν_k (finding such choices is discussed in [21, 93] and in the forthcoming chapters, particularly in Sections 4.5 and 5.3). Finally, and probably most importantly, Algorithm 3.12 can be used to find least squares solutions for (3.9) if $G : \mathbb{R}^n \to \mathbb{R}^m$ with $m \geq n$, i.e., to solve the nonlinear least squares problem

$$\min \frac{1}{2}\|G(x)\|^2. \tag{3.11}$$

Specifically, we have the following result for the zero residual case, which is a corollary of Theorem 3.16 below. For $m = n$, this is proven in [28].

Theorem 3.13 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be semismooth and let x^* be a solution of (3.9) such that all matrices $H_* \in \partial_B G(x^*)$ have full rank. Then the following statements hold:*

(a) Provided that $\nu_k \in (0, \hat{\nu}]$ for some sufficiently small constant $\hat{\nu} > 0$, there exists $\varepsilon > 0$ such that, for every $x^0 \in B_\varepsilon(x^*)$, Algorithm 3.12 generates a sequence $\{x^k\}$ converging at least Q-linearly to x^*.

(b) The rate of convergence is Q-superlinear if, in addition to the conditions in (a), $\nu_k \to 0$.

(c) The rate of convergence is Q-quadratic if, in addition to the conditions in (a), $\nu_k = O(\|G(x^k)\|)$ and G is strongly semismooth.

There is also an inexact version of Algorithm 3.12, much in the spirit of Algorithm 3.10. Concerning convergence results for $m = n$, the reader is referred to [28]. In Section 5.1, we deal with the case $m > n$ in a different context.

One may see that Algorithm 3.12 reduces to a *Gauss-Newton* method if for all k the regularization parameter $\nu_k = 0$. In this case, equation (3.10) represents the normal equation for the linearization of the least squares problem (3.11) around the iterate x^k, namely

$$\min \frac{1}{2}\|H_k d + G(x^k)\|^2. \tag{3.12}$$

The possible occurring unsolvability of the linear subproblems of the generalized Newton method, is avoided also by the Gauss-Newton method, although, in contrast to the Levenberg-Marquardt method, the solution of subproblem (3.12) may not be unique for a not full rank H_k.

3.2.4 Projected Levenberg-Marquardt Method

In the context of mixed complementarity problems, we will face overdetermined nonlinear equations with box constraints. It will be important that the iterates of the Levenberg-Marquardt method stay within these constraints.

To obtain such a method, let $m \geq n$ and let $G : \mathcal{O} \to \mathbb{R}^m$ be a semismooth function, which is defined on an open neighborhood $\mathcal{O} \subseteq \mathbb{R}^n$ of a box $\mathcal{B} := [l, u]$. Here and in the following, the lower bounds $l = (l_1, \ldots, l_n)^T$ and upper bounds $u = (u_1, \ldots, u_n)^T$ satisfy $-\infty \leq l_i < u_i \leq +\infty$ for all $i = 1, \ldots, n$. Let us consider the box constrained overdetermined system

$$G(x) = 0, \quad x \in \mathcal{B}, \tag{3.13}$$

which is equivalent to the box constrained least squares problem

$$\min \frac{1}{2}\|G(x)\|^2 \quad \text{s.t.} \quad x \in \mathcal{B}, \tag{3.14}$$

provided the latter problem has a zero residual at the solution. Since all bounds can be infinite, this includes the unconstrained least squares problem.

In this section, we present a local method for the box constrained overdetermined system of equations (3.13) and the related nonlinear least squares problem (3.14). To motivate our method, let us emphasize again that (3.14) is an unconstrained least squares problem if all bounds are infinite. Replacing the B-subdifferential by the C-subdifferential in Algorithm 3.12, we obtain an iterative procedure of the form

$$x^{k+1} := x^k + p_{LM}^k, \quad k = 0, 1, \ldots,$$

where p_{LM}^k is the solution of the linear system

$$\big(H_k^T H_k + \nu_k I\big) p_{LM} = -H_k^T G(x^k), \qquad H_k \in \partial_C G(x^k). \tag{3.15}$$

Now, if all or some of the bounds are finite, we consider the following projected Levenberg-Marquardt method:

$$x^{k+1} := x^k + p_{PLM}^k, \quad k = 0, 1, \ldots,$$

where

$$p_{PLM}^k := P_{\mathcal{B}}(x^k + p_{LM}^k) - x^k \tag{3.16}$$

and p_{LM}^k denotes the unconstrained Levenberg-Marquardt direction from (3.15). Formally, we therefore obtain the following method, see also [72, 118].

Algorithm 3.14 (Projected Levenberg-Marquardt Method)

(S.0) Choose $x^0 \in \mathcal{B}$, and set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_C G(x^k)$, choose a regularization parameter $\nu_k > 0$, and compute p_{LM}^k from (3.15).

(S.3) Compute p^k_{PLM} from (3.16).

(S.4) Set $x^{k+1} = x^k + p^k_{PLM}$, $k \leftarrow k+1$, and go to (S.1).

Note that Algorithm 3.14 is well-defined, and that all iterates x^k stay in the box $\mathcal{B}$. Of course, Algorithm 3.14 is a local method only. In order to state the local convergence properties of this method, we need the following result which follows from the upper semicontinuity of the generalized Jacobian.

Lemma 3.15 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be semismooth and x^* be a solution of problem (3.13) such that all elements from $\partial_C G(x^*)$ have full rank. Then there exist constants $\varepsilon > 0$ and $c > 0$ such that*

$$\|(H^T H)^{-1}\| \leq c$$

for all $H \in \partial_C G(x)$ and all $x \in \mathbb{R}^n$ with $x \in B_\varepsilon(x^*)$.

Proof. The proof is similar to the one of [98, Lem. 2.6], which states a similar result in a slightly different setting. Suppose the claim of the lemma is not true. Then there exists a sequence $\{x^k\}$ converging to x^* and a corresponding sequence of matrices $\{H_k\}$ with $H_k \in \partial_C G(x^k)$ for all $k \in \mathbb{N}$ such that either $H_k^T H_k$ is singular or $\|(H_k^T H_k)^{-1}\| \to \infty$ on a subsequence. Noting that $H_k^T H_k$ is symmetric positive semidefinite, we have $\|(H_k^T H_k)^{-1}\| = \frac{1}{\lambda_{\min}(H_k^T H_k)}$ in the nonsingular case. Hence the condition $\|(H_k^T H_k)^{-1}\| \to \infty$ is equivalent to $\lambda_{\min}(H_k^T H_k) \to 0$. Since $\{x^k\} \to x^*$ and the mapping $x \mapsto \partial_C G(x)$ is upper semicontinuous, it follows that the sequence $\{H_k\}$ is bounded (see Remark 2.4) and therefore has a convergent subsequence. Let H_* be a limiting element of such a subsequence. It then follows that $H_*^T H_*$ is singular, since $\lambda_{\min}(H_*^T H_*) = 0$ (note that the mapping $A \mapsto \lambda_{\min}(A^T A)$ is continuous), i.e., H_* is not of full rank. On the other hand, exploiting the fact that the mapping $x \mapsto \partial_C G(x)$ is closed, we have $H_* \in \partial_C G(x^*)$, so that H_* is of full rank. This contradiction completes the proof. □

We are now in the position to state the main local convergence properties of Algorithm 3.14. Later, this result will facilitate the local convergence analysis of a trust-region globalization of this method.

Theorem 3.16 *Let $G : \mathbb{R}^n \to \mathbb{R}^m$ be semismooth and let x^* be a solution of (3.13) such that all matrices $H_* \in \partial_C G(x^*)$ have full rank. Then the following statements hold:*

(a) Provided that $\nu_k \in (0, \hat{\nu}]$ for some sufficiently small constant $\hat{\nu} > 0$, there exists $\varepsilon > 0$ such that for all $x^0 \in \mathcal{B} \cap B_\varepsilon(x^*)$, Algorithm 3.14 generates a sequence $\{x^k\}$ converging at least Q-linearly to x^*.

(b) The rate of convergence is Q-superlinear if, in addition to the conditions of (a), $\nu_k \to 0$.

(c) The rate of convergence is Q-quadratic if, in addition to the conditions of (a), $\nu_k = O(\|G(x^k)\|)$ and G is strongly semismooth.

Proof. Lemma 3.15 implies that there are constants $\varepsilon_1 > 0$ and $c > 0$ such that

$$\big\|(H^T H + \nu I)^{-1}\big\| \le c \quad \forall x \in B_{\varepsilon_1}(x^*),\ \forall H \in \partial_C G(x),\ \forall \nu > 0.$$

Furthermore, from the upper semicontinuity of the generalized Jacobian, we obtain the existence of constants $\varepsilon_2 > 0$ and $\alpha > 0$ with

$$\|H^T\| \le \alpha \quad \forall x \in B_{\varepsilon_2}(x^*),\ \forall H \in \partial_C G(x).$$

Moreover, the semismoothness of G (see Proposition 2.18 (a)) implies that there is a constant $\varepsilon_3 > 0$ with

$$\big\|G(x) - G(x^*) - H(x - x^*)\big\| \le \frac{1}{4\alpha c}\|x - x^*\| \quad \forall x \in B_{\varepsilon_3}(x^*),\ \forall H \in \partial_C G(x).$$

Now take

$$\varepsilon := \min\{\varepsilon_1, \varepsilon_2, \varepsilon_3\} \quad \text{and} \quad \hat{\nu} := \frac{1}{4c}.$$

Suppose that the k-th iterate $x^k \in \mathcal{B}$ belongs to the ball $B_\varepsilon(x^*)$ (in the beginning, this is true since we choose $x^0 \in B_\varepsilon(x^*)$). Then we have the following identity:

$$\begin{aligned}
\big(H_k^T H_k + \nu_k I\big)(x^k + p_{LM}^k - x^*) &= \big(H_k^T H_k + \nu_k I\big)(x^k - x^*) + \big(H_k^T H_k + \nu_k I\big)p_{LM}^k \\
&= \big(H_k^T H_k + \nu_k I\big)(x^k - x^*) - H_k^T G(x^k) \\
&= -H_k^T\big(G(x^k) - G(x^*) - H_k(x^k - x^*)\big) + \nu_k(x^k - x^*).
\end{aligned}$$

Premultiplying with $(H_k^T H_k + \nu_k I)^{-1}$ and taking norms, we therefore obtain

$$\begin{aligned}
&\|x^k + p_{LM}^k - x^*\| \\
&\quad\le \big\|(H_k^T H_k + \nu_k I)^{-1}\big\|\big[\|H_k^T\|\,\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| + \nu_k\|x^k - x^*\|\big] \\
&\quad\le c\big[\alpha\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| + \hat{\nu}\|x^k - x^*\|\big] \\
&\quad\le c\left(\alpha\frac{1}{4\alpha c} + \frac{1}{4c}\right)\|x^k - x^*\| \\
&\quad= \frac{1}{2}\|x^k - x^*\|.
\end{aligned}$$

This implies

$$\begin{aligned}
\|x^{k+1} - x^*\| &= \|x^k + p_{PLM}^k - x^*\| \\
&= \|P_{\mathcal{B}}(x^k + p_{LM}^k) - x^*\| \\
&= \|P_{\mathcal{B}}(x^k + p_{LM}^k) - P_{\mathcal{B}}(x^*)\| \\
&\le \|x^k + p_{LM}^k - x^*\| \\
&\le \frac{1}{2}\|x^k - x^*\|
\end{aligned}$$

since the projection operator is nonexpansive. In particular, this shows that x^{k+1} also belongs to the ε-ball around x^*, and using an induction argument, it follows that

$$\|x^{k+1} - x^*\| \leq \frac{1}{2}\|x^k - x^*\| \quad \forall k \in \mathbb{N}.$$

This shows that the sequence $\{x^k\}$ converges to x^* at least Q-linearly.

The local Q-superlinear convergence can be verified by using a similar chain of inequalities. Indeed, using $\nu_k \to 0$ and the semismoothness of G, we obtain

$$\begin{aligned} \|x^{k+1} - x^*\| &= \|x^k + p^k_{PLM} - x^*\| \\ &\leq \|x^k + p^k_{LM} - x^*\| \\ &\leq c\big[\alpha\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| + \nu_k\|x^k - x^*\|\big] \\ &= o(\|x^k - x^*\|), \end{aligned}$$

using the fact that the projection operator $P_{\mathcal{B}}$ is nonexpansive. The Q-quadratic rate of convergence can be verified in a similar way using

$$\nu_k = O(\|G(x^k)\|) = O(\|G(x^k) - G(x^*)\|) = O(\|x^k - x^*\|),$$

where the last inequality follows from the local Lipschitz property of G, and by noting that the strong semismoothness of G implies

$$\|G(x^k) - G(x^*) - H_k(x^k - x^*)\| = O(\|x^k - x^*\|^2),$$

in view of Proposition 2.18 (b). This completes the proof. □

We conclude this section with the following remark.

Remark 3.17 *(a) Suppose G is continuously differentiable with a locally Lipschitzian Jacobian G', and suppose that we choose $\nu_k := \nu\|G(x^k)\|^2$ for some constant $\nu > 0$ in Algorithm 3.14. Then it was shown in [72] that the sequence $\{x^k\}$ generated by Algorithm 3.14 is locally quadratically convergent under an error bound condition. This condition is weaker than the full rank assumption made in Theorem 3.16 and might also hold in some situations where the solution set is not (locally) unique. However, in the context of this work we are mainly interested in a nonsmooth mapping G, and whether the result from [72] holds in this situation is not clear.*

(b) Similar convergence properties can be established for $H_k \in \partial_B G(x^k)$ under a weaker BD-regularity assumption. However, we will apply this local method (see Chapter 6) to a nonsmooth reformulation of the nonlinear (and mixed) complementarity problem, which admits an R-regular solution. R-regularity will imply that all elements in the C-subdifferential have full rank. Thus, choosing an element from the smaller set $\partial_B G(x^k)$ does not seem to have any significant theoretical advantage.

3.3 Regularity Conditions and Reformulations

In the previous section, we have seen that BD-regularity of the nonlinear equation at the solution is a crucial requirement for obtaining (fast) local convergence of semismooth Newton and Levenberg-Marquardt methods. We will apply these methods to reformulations of nonlinear (and mixed) complementarity problems. For this purpose, it is important to know which conditions the original complementarity problems has to satisfy such that the reformulation admits a BD-regular solution. Stating such conditions is the purpose of this section.

Let us recall that an important class of reformulations is based on the concept of NCP-functions leading to nonsmooth nonlinear equation $\Phi(x) = 0$, see Section 3.1. For the particular choice of the NCP-function $\phi \in \{\phi_P, \phi_{FB}, \phi_{CCK}\}$, we denote the resulting operator Φ by Φ_P, Φ_{FB} and Φ_{CCK}, respectively. Given the properties of $\phi_P, \phi_{FB}, \phi_{CCK}$ we stress that the resulting operators $\Phi_P, \Phi_{FB}, \Phi_{CCK}$ are semismooth if the problem function F is C^1. If, in addition, F is LC^1 then the operators are strongly semismooth. From the very definition of the operator Φ_P an element $H_k \in \partial_B \Phi(x^k)$ can be easily computed. Also for $\Phi \in \{\Phi_{FB}, \Phi_{CCK}\}$ there are simple procedures to compute an element $H_k \in \partial_B \Phi(x^k)$, see, e.g., [19, 11]. Given such an element $H_k \in \partial_B \Phi(x^k)$, a typical nonsmooth Newton method leads to the iteration

$$x^{k+1} := x^k - H_k^{-1} \Phi(x^k), \quad k = 0, 1, 2, \ldots, \tag{3.17}$$

which belongs to the framework of the local nonsmooth Newton method, Algorithm 3.6.

The structures of the B-subdifferentials of Φ_P, Φ_{FB} and Φ_{CCK} allow stating conditions which guarantee BD-regularity at a solution. This regularity concept which will be used in order to prove a nonsingularity result for an equation reformulation of the complementarity problem, can be extended to the mixed complementarity problem (see [33]). Associated with any solution $x^* \in \mathbb{R}^n$ of the complementarity problem NCP(F), we define the following three index sets:

$$\begin{aligned} \alpha &:= \{i \mid x_i^* > 0, F_i(x^*) = 0\}, \\ \beta &:= \{i \mid x_i^* = 0, F_i(x^*) = 0\}, \\ \gamma &:= \{i \mid x_i^* = 0, F_i(x^*) > 0\}. \end{aligned}$$

The set β is usually called the degenerate set for obvious reasons. Note that α, β, γ depend on the particular solution x^*, but since this dependence will always be clear from the context, it is not necessary to stress it in our notation.

The following two regularity concepts play an important role in the theoretical analysis of complementarity problems.

Definition 3.18 *Let $M := F'(x^*)$. A solution $x^* \in \mathbb{R}^n$ of NCP(F) is called*

(a) b-regular *if the principal submatrices $M_{\alpha\cup\delta,\alpha\cup\delta}$ are nonsingular for all subsets δ such that $\emptyset \subseteq \delta \subseteq \beta$;*

(b) R-regular *if $M_{\alpha\alpha}$ is nonsingular and its Schur-complement in*

$$\begin{pmatrix} M_{\alpha\alpha} & M_{\alpha\beta} \\ M_{\beta\alpha} & M_{\beta\beta} \end{pmatrix}$$

is a P-matrix.

We note that the Schur-complement used above is defined by

$$M_{\beta\beta} - M_{\beta\alpha} M_{\alpha\alpha}^{-1} M_{\alpha\beta} \in \mathbb{R}^{|\beta|\times|\beta|}. \tag{3.18}$$

The R-regularity condition is due to Robinson and it was introduced in [105] in the context of the local solvability of generalized equations. There it is called strong regularity and is analogous to the nonsingularity condition imposed to the usual implicit-function theorem for nonlinear equations. The b-regularity condition was employed, e.g., in [61, 96, 20]. At a nondegenerate solution x^* of NCP(F) the b- and R-regularity coincide. The following example from [20] shows that b-regularity is a weaker assumption than R-regularity.

Example 3.19 Consider the NCP(F) with $F : \mathbb{R}^2 \to \mathbb{R}^2$ defined by

$$F(x) := \begin{pmatrix} -x_1 + x_2 \\ -x_2 \end{pmatrix}.$$

The unique solution $x^* = (0,0)^T$ is degenerate and b-regular. A simple calculation yields

$$\partial_B \Phi_P(x^*) = \left\{ \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}.$$

Hence, x^* is a BD-regular solution of the system $\Phi_P(x) = 0$. On the other hand, x^* is not R-regular, since $\alpha = \emptyset$ and $F'(x^*)_{\beta,\beta} = \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix}$ is not a P-matrix. Considering $x^k := \left(\frac{1}{k}, \frac{2}{k}\right) \to x^*$, where the operator Φ_{FB} is smooth, we see that

$$\Phi'_{FB}(x^k) \to \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} - 1 \\ 0 & \sqrt{2} \end{pmatrix} \in \partial_B \Phi_{FB}(x^*).$$

This shows that x^* is not a BD-regular solution of the system $\Phi_{FB}(x) = 0$.

As a matter of fact, BD-regularity respective to Φ_P at a solution of NCP can be established under a weaker assumption than BD-regularity respective to Φ_{FB}. Let $H \in \partial_B \Phi_P(x^*)$ be arbitrary, and let α, β, γ be the index sets defined above. Then there is an index set $\delta \subseteq \beta$ such that

$$H = \begin{pmatrix} F'(x^*)_{\alpha\cup\delta,\alpha\cup\delta} & F'(x^*)_{\alpha\cup\delta,\gamma\cup\bar{\delta}} \\ 0_{\gamma\cup\bar{\delta},\alpha\cup\delta} & I_{\gamma\cup\bar{\delta},\gamma\cup\bar{\delta}} \end{pmatrix},$$

where $\bar{\delta} := \beta \setminus \delta$, see [20]. The definition of b-regularity now directly gives the following proposition.

Proposition 3.20 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable and $x^* \in \mathbb{R}^n$ a b-regular solution of NCP(F). Then x^* is a BD-regular solution of the system $\Phi_P(x) = 0$.*

On the other hand, R-regularity of a solution implies the BD/CD-regularity with respect to Φ_{FB} and Φ_{CCK}.

Proposition 3.21 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable and $x^* \in \mathbb{R}^n$ a R-regular solution of NCP(F). Then*

(a) x^* is a CD-regular solution of the system $\Phi_{FB}(x) = 0$;

(b) x^* is a CD-regular solution of the system $\Phi_{CCK}(x) = 0$.

Proof. Statement (a) will play a central role in the subsequent chapters and we include the proof here, although it is identical to Lemma 5.3 in [19]. Let $H \in \partial_C \Phi_{FB}(x^*)$ be arbitrary but fixed. In view of the chain rule from Theorem 2.5 and the structure of the generalized gradient of ϕ_{FB} at a point $(x_i, F_i(x))$, there are diagonal matrices $D_a := D_a(x^*) \in \mathbb{R}^{n\times n}$ and $D_b := D_b(x^*) \in \mathbb{R}^{n\times n}$ such that $H = D_a + D_b M$, where $M := F'(x^*)$ and $D_a := \operatorname{diag}(a_1(x^*), \ldots, a_n(x^*))$, $D_b := \operatorname{diag}(b_1(x^*), \ldots, b_n(x^*)) \in \mathbb{R}^{n\times n}$ are diagonal matrices whose i-th diagonal element is given by

$$a_i(x^*) = \frac{x_i^*}{\|(x_i^*, F_i(x^*))\|} - 1, \quad b_i(x^*) = \frac{F_i(x^*)}{\|(x_i^*, F_i(x^*))\|} - 1$$

if $(x_i^*, F_i(x^*)) \neq (0, 0)$, and by

$$a_i(x^*) = \xi_i - 1, \quad b_i(x^*) = \chi_i - 1 \quad \text{with } (\xi_i, \chi_i) \in \mathbb{R}^2 \text{ such that } \|(\xi_i, \chi_i)\| \leq 1$$

if $(x_i^*, F_i(x^*)) = (0, 0)$. Write

$$M = \begin{pmatrix} M_{\alpha\alpha} & M_{\alpha\beta} & M_{\alpha\gamma} \\ M_{\beta\alpha} & M_{\beta\beta} & M_{\beta\gamma} \\ M_{\gamma\alpha} & M_{\gamma\beta} & M_{\gamma\gamma} \end{pmatrix}$$

and, accordingly,

$$D_a = \begin{pmatrix} D_{a,\alpha} & 0 & 0 \\ 0 & D_{a,\beta} & 0 \\ 0 & 0 & D_{a,\gamma} \end{pmatrix} \quad \text{and} \quad D_b = \begin{pmatrix} D_{b,\alpha} & 0 & 0 \\ 0 & D_{b,\beta} & 0 \\ 0 & 0 & D_{b,\gamma} \end{pmatrix},$$

where $D_{a,\alpha} := (D_a)_{\alpha\alpha}$, $D_{a,\beta} := (D_a)_{\beta\beta}$, etc. Now let $p \in \mathbb{R}^n$ be an arbitrary vector with $Hp = 0$. Partitioning $p = (p_\alpha, p_\beta, p_\gamma)$ we can rewrite $Hp = 0$ as follows:

$$D_{a,\alpha} p_\alpha + D_{b,\alpha}(M_{\alpha\alpha} p_\alpha + M_{\alpha\beta} p_\beta + M_{\alpha\gamma} p_\gamma) = 0_\alpha, \tag{3.19}$$

$$D_{a,\beta} p_\beta + D_{b,\beta}(M_{\beta\alpha} p_\alpha + M_{\beta\beta} p_\beta + M_{\beta\gamma} p_\gamma) = 0_\beta, \tag{3.20}$$

$$D_{a,\gamma}p_\gamma + D_{b,\gamma}(M_{\gamma\alpha}p_\alpha + M_{\gamma\beta}p_\beta + M_{\gamma\gamma}p_\gamma) = 0_\gamma. \tag{3.21}$$

Since we have $D_{a,\alpha} = 0_\alpha, D_{a,\gamma} = -I_\gamma, D_{b,\alpha} = -I_\alpha,$ and $D_{b,\gamma} = 0_\gamma$, (3.21) immediately gives

$$p_\gamma = 0_\gamma, \tag{3.22}$$

so that (3.19) reduces to

$$M_{\alpha\alpha}p_\alpha + M_{\alpha\beta}p_\beta = 0_\alpha.$$

The submatrix $M_{\alpha\alpha}$ is nonsingular (x^* is a R-regular solution of NCP(F)) and we obtain from the previous equation

$$p_\alpha = -M_{\alpha\alpha}^{-1}M_{\alpha\beta}p_\beta. \tag{3.23}$$

Inserting this into (3.20), using (3.22), and rearranging terms we obtain

$$[D_{a,\beta} + D_{b,\beta}(M_{\beta\beta} - M_{\beta\alpha}M_{\alpha\alpha}^{-1}M_{\alpha\beta})]p_\beta = 0_\beta,$$

Since the Schur complement is a P-matrix and both diagonal matrices $D_{a,\beta}, D_{b,\beta}$ are negative semidefinite such that their sum is negative definite it follows that $D_{a,\beta} + D_{b,\beta}(M_{\beta\beta} - M_{\beta\alpha}M_{\alpha\alpha}^{-1}M_{\alpha\beta})]$ is nonsingular (see Lemma 2.29), thus $p_\beta = 0_\beta$. We therefore have $p = 0$, which proves that $H \in \partial_C\Phi_{FB}(x^*)$ is regular. Since H was chosen arbitrarily, we obtain the regularity of all elements in $\partial_C\Phi_{FB}(x^*)$. This implies the desired result, since $\partial\Phi_{FB}(x^*) \subset \partial_C\Phi_{FB}(x^*)$.

Statement (b) can be proved similarly (see Theorem 2.6 in [11]). □

If $F : \mathbb{R}^n \to \mathbb{R}^n$ is a P_0-function, then every Jacobian $F'(x)$ is a P_0-matrix for all $x \in \mathbb{R}^n$, see Theorem 2.28. In this case, there is no difference between b- and R-regularity, as the following proposition suggests. Note that if $F'(x^*)$ is a P_0-matrix then the Schur-complement (3.18) is also a P_0-matrix.

Proposition 3.22 *[20, Thm. 2.5] Let $x^* \in \mathbb{R}^n$ be a solution of NCP(F). Then the following statements are equivalent:*

(a) x^* is a R-regular solution of NCP(F).

(b) x^* is a b-regular solution and the Schur-complement (3.18) *is a P_0-matrix.*

To roughly summarize the discussion, if one of the equivalent conditions of Proposition 3.22 is satisfied then Propositions 3.20 and 3.21 imply that the (penalized) Fischer-Burmeister as well as the minimum reformulation give rise to locally convergent Newton methods for solving complementarity problems. We conclude this section by noting that the R-regularity condition is strictly related to the similar condition used in [35] involving the normal map reformulation.

3.4 Global Methods

We have seen that the Newton- and Levenberg-Marquardt-type methods discussed above display local (fast) convergence under appropriate conditions. Obtaining iterations that achieve global convergence towards the desired solution is usually a much more subtle issue. Such a property, however, is indispensable for developing reliable solvers of mixed and nonlinear complementarity problems. In this section, we briefly discuss globalization strategies and other globally convergent methods.

3.4.1 Merit Functions

To facilitate the development of global methods it is important to provide a measure for monitoring the convergence of the iterates in our method of choice toward a desired solution. Merit functions provide such a measure and are formally defined as follows.

Definition 3.23 *A function $\Psi : \mathbb{R}^n \to \mathbb{R}$ is called a merit function for the nonlinear complementarity problem/mixed complementarity problem NCP(F)/MCP(F, l, u) if it has the following two properties:*

(a) $\Psi(x) \geq 0$ *for all* $x \in \mathbb{R}^n$*;*

(b) $\Psi(x) = 0$ *if and only if* x *solves NCP(F)/MCP(F, l, u).*

The above definition admits a large class of functions; to be useful in practice a merit function should satisfy further properties, such as being continuously differentiable. In such a case it is easy to enforce the global convergence of algorithms by using the gradient of the merit function.

Example 3.24 The following functions are merit functions for the nonlinear complementarity problem NCP(F).

(a) Given an equation reformulation $\Phi(x) = 0$ of the complementarity problem NCP(F), the so called *natural merit function* is simply obtained by setting

$$\Psi(x) := \frac{1}{2}\Phi(x)^T\Phi(x) = \frac{1}{2}\|\Phi(x)\|^2. \tag{3.24}$$

The natural merit functions associated with $\Phi \in \{\Phi_P, \Phi_{FB}, \Phi_{CCK}\}$ will be denoted by $\Psi_P, \Psi_{FB}, \Psi_{CCK}$, respectively.

(b) Another classical merit function is based on the normal map

$$\Psi_+(x) := \|F_+(x) + x - x_+\|.$$

(c) The *Luo-Tseng merit function* is defined as

$$\Psi_{LT}(x) := \frac{1}{2}\max^2\{0, x^T F(x)\} + \frac{1}{2}\sum_{i=1}^{n}\max^2\{0, \phi_{FB}(x_i, F_i(x))\};$$

(d) The *Kanzow-Yamashita-Fukushima merit function* is defined as

$$\Psi_{KYF}(x) := \frac{1}{2}\sum_{i=1}^{n}(\max^2\{0, x_iF_i(x)\} + \max^2\{0, \phi_{FB}(x_i, F_i(x))\}).$$

(e) The *Mangasarian-Solodov merit function* is defined as

$$\Psi_{MS}(x) := \sum_{i=1}^{n}\{x_iF_i(x)+\frac{1}{2\alpha}(\max^2\{0, x_i-\alpha F_i(x)\}-x_i^2+\max^2\{0, F_i(x)-\alpha x_i\}-F_i(x)^2)\},$$

where $\alpha > 1$ is a fixed parameter.

It is not difficult to see that the merit functions Ψ_{LT}, Ψ_{KYF} and Ψ_{MS} are continuously differentiable, whereas Ψ_P and Ψ_+ are, in general, not differentiable. On the other hand, the next theorem shows that also Ψ_{FB} and Ψ_{CCK} are continously differentiable (despite the fact that the underlying equation operators Φ_{FB} and Φ_{CCK} are nonsmooth). Hence, even if on the first view the reformulation of NCP via the operator Φ_P has an obvious advantage over the reformulations via the operators Φ_{FB} and Φ_{CCK} (cf. Section 3.3), the globalization of the local method is a much simpler issue for $\Phi \in \{\Phi_{FB}, \Phi_{CCK}\}$.

Theorem 3.25 *[19, Thm. 2.3],[11, Thm. 3.2] Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable. The following statement hold:*

(a) The merit function Ψ_{FB} is continuously differentiable with $\nabla\Psi_{FB}(x) = H^T\Phi_{FB}(x)$ for every $H \in \partial_C\Phi_{FB}(x)$.

(b) The merit function Ψ_{CCK} is continuously differentiable with $\nabla\Psi_{CCK}(x) = H^T\Phi_{CCK}(x)$ for every $H \in \partial_C\Phi_{CCK}(x)$.

Proof. (a) We only give the proof for the first statement since the second one can be verified in very much the same way. Let $x \in \mathbb{R}^n$ be arbitrary and define the index set $I = \{1, \ldots, n\}$. Let $\beta = \{i \in I \mid x_i = 0 = F_i(x)\}$ and let $\bar{\beta} := I \setminus \beta$ denote the complementarity subset of β in I. Then for every $i \in \bar{\beta}$ it holds that the i-th component function $\Phi_{FB,i}$ is continuously differentiable with

$$\partial\Phi_{FB,i}(x) = \partial\phi_{FB}(x_i, F_i(x)) = \{\nabla\Phi_{FB,i}(x)\}, \quad i \in \bar{\beta}. \tag{3.25}$$

We next show that the set $\{H^T\Phi_{FB}(x) \mid H \in \partial_C\Phi_{FB}(x)\}$ consists of one element only:

$$\begin{aligned}
S :=& \{H^T\Phi_{FB}(x) \mid H \in \partial_C\Phi_{FB}(x)\} \\
=& \{\sum_{i=1}^{m}\Phi_{FB,i}(x)H_i \mid H_i \in \partial\Phi_{FB,i}(x), i \in I\} \\
=& \{\sum_{i\in\bar{\beta}}\Phi_{FB,i}(x)H_i + \sum_{i\in\beta}\underbrace{\Phi_{FB,i}(x)}_{=0}H_i \mid H_i \in \partial\Phi_{FB,i}(x), i \in \bar{\beta}\cup\beta\} \\
\overset{(3.25)}{=}& \{\sum_{i\in\bar{\beta}}\Phi_{FB,i}(x)\nabla\Phi_{FB,i}(x)\}.
\end{aligned}$$

Now, using the relaxed chain rule, see Corollary 2.7, we obtain

$$\partial\Psi_{FB}(x) \subseteq \text{conv}(S),$$

and therefore $\partial\Psi_{FB}(x)$ is a singleton too. The assertion therefore follows from the fact that a locally Lipschitz continuous function is continuously differentiable if and only if its generalized gradient is a singleton at every point, see Example 2.2 (a). □

Since the most commonly used merit functions are once but not twice continuously differentiable, solving the complementarity problem using an off-the-shelf minimization method is not suggested. Nevertheless, the interplay between a gradient method and a Newton-type method applied to the underlying equation reformulation makes this minimization approach successful. However, obtaining a decreasing sequence $\{\Psi(x^k)\}$ is not sufficient to ensure the convergence of a sequence x^k of iterates toward a solution. Therefore, the common goal will be convergence toward a local minimizer of Ψ.

The next propositions summarize appropriate conditions for a stationary point of Ψ (provided that the merit function is differentiable) to be a solution of the complementarity problem. Most of this results can be verified in a similar way to the proof of Theorem 4.8.

Proposition 3.26 *[31, 11, 71, 78, 80] Let x^* be a stationary point for a merit function Ψ to be specified below. Then the following statements hold:*

(a) If $\Psi \in \{\Psi_{FB}, \Psi_{CCK}, \Psi_{KYF}\}$ and $F'(x^*)$ is a P_0-matrix, then x^* is a solution of $NCP(F)$.

(b) If $\Psi = \Psi_{LT}$ and $F'(x^*)$ is positive semidefinite, then x^* is a solution of $NCP(F)$.

(c) If $\Psi = \Psi_{MS}$ and $F'(x^*)$ is a P-matrix, then x^* is a solution of $NCP(F)$.

3.4.2 Line Search

The methods discussed in Section 3.2 compute at each iteration a new direction $d^k \neq 0$ which is added to the old iterate in order to obtain the new iterate. If the old iterate is not sufficiently close to the solution then it may happen that the new iterate is not closer to the desired solution, which can lead to stagnation or even divergence of the method. To avoid this to happen, the line search strategy dampens the effect of the update by scaling the direction with a positive parameter $t_k \leq 1$. The choice of this parameter can be met using the merit functions defined above.

Let x^k be the current iterate which is not a stationary point. The line search strategy is now to choose the step length $t_k \in (0, 1]$ such that the new iterate

$$x^{k+1} := x^k + t_k d^k$$

produces a sufficient decrease in the merit function Ψ. Considering the vector $x^k + td^k, t \in (0, 1]$, we have

$$\Psi(x^k + td^k) = \Psi(x^k) + t\nabla\Psi(x^k)^T d^k + o(t),$$

under the assumption that Ψ is continuously differentiable. Now, if d^k is a *descent condition* for Ψ in the sense that

$$\nabla\Psi(x^k)^T d^k < 0, \tag{3.26}$$

then for any constant $\sigma \in (0,1]$, one can show that there exists a $\bar{t}_k \in (0,1]$ such that for all $t \in (0, \bar{t}_k]$,

$$\Psi(x^k + td^k) \leq \Psi(x^k) + \sigma t \nabla\Psi(x^k)^T d^k.$$

By choosing our step length t_k to be such a particular $t_k \in (0, \bar{t}_k)$ we obtain a decrease in the merit function as

$$\Psi(x^{k+1}) \leq \Psi(x^k) + \sigma t_k \nabla\Psi(x^k)^T d^k,$$

in view of the descent property of d^k. There are many line search strategies ([21]) that provides such a t_k. One of the most popular is the Armijo-Goldstein line search rule [1, 46], which for a given parameter $\beta \in (0,1)$ evaluates the merit functions at the sequence of points $\{x^k + \beta^l d^k \mid l = 0, 1, \dots\}$ until a steplength $t_k = \max\{\beta^l \mid l = 0, 1, 2, \dots\}$ is found such that

$$\Psi(x^k + t_k d^k) \leq \Psi(x^k) + \sigma t_k \nabla\Psi(x^k)^T d^k. \tag{3.27}$$

In view of the above discussions this line search rule is well defined provided that d^k is a descent direction and Ψ is continuously differentiable. A generalization of the Armijo rule to the case of a B-differentiable merit function Ψ can be established provided that $\Psi'(x^k; d^k) < 0$, since B-differentiable merit functions have a similar first order expansion around x^k, see Definition 2.11. In analogy to the classical Armijo rule the steplength is given by $t_k = \beta^{l_k}$, where l_k is the first nonnegative integer l for which

$$\Psi(x^k + \beta^l d^k) \leq \Psi(x^k) + \sigma\beta^l \Psi'(x^k; d^k). \tag{3.28}$$

Remark 3.27 *(a) We note that it can be helpful to employ nonmonotone line search strategies, which admit a controlled increase of the merit function. This is mainly confirmed by computational experiments, see [48]. Roughly speaking, admitting such an increase can help the algorithm to avoid local minima that are not global ones. An implementation of a nonmonotone line search strategy is discussed in Section 4.5.1.*
(b) A large class of descent directions satisfying (3.26) is given by

$$d^k := -M_k \nabla\Psi(x^k),$$

where $M_k \in \mathbb{R}^{n\times n}$ is any symmetric positive definite matrix. Letting M_k be the identity matrix we obtain the steepest descent direction *$d^k = -\nabla\Psi(x^k)$. Considering $\Psi \in \{\Psi_{FB}, \Psi_{CCK}\}$, the Levenberg-Marquardt direction (see Section 3.2.3) reduces to*

$$d^k = -(H_k^T H_k + \nu_k I)^{-1} \nabla\Psi(x^k),$$

in view of Theorem 3.25. Accordingly, the Levenberg-Marquardt direction is a descent direction respective to these particular merit functions.

3.4.3 Path Search

A theoretical and practically relevant difficulty with the line search approach is that for some reasonable choices of merit functions the direction d^k is not guaranteed to be a descent direction. A strategy which avoids this effect for the normal map reformulation of NCPs and MCPs was proposed by Ralph [103]. Given an NCP(F), we consider the normal map, see Section 3.1, for the case $\mathcal{B} = [0, \infty)^n$:

$$F_+(x) := F(x_+) + x - x_+.$$

If $F_+(x) = 0$ then x_+ is a solution of NCP(F). Since $x \mapsto x_+$ is a piecewise linear operator, it is not sensible to approximate F_+ with a linear function. Instead, a first-order approximation with a piecewise linear normal map is used, for example

$$A_k(x) := F(x_+^k) + F'(x_+^k)(x_+ - x_+^k) + x - x_+,$$

where x^k is the current iterate. The zero of this approximation determines the Newton point x_N^k (which may not be unique). This is known to be equivalent to solving the LCP

$$y \geq 0, \quad F(y^k) + F'(y^k)(y - y^k) \geq 0, \quad y^T(F(y^k) + F'(y^k)(y - y^k)) = 0 \tag{3.29}$$

by setting $y^k = x_+^k$. Using the solution of this LCP results in a local method called the Josephy-Newton algorithm for NCPs or *sequential LCP* (SLCP) method in [82, 83]. Josephy [54] proved, in the context of generalized equations, local quadratic convergence for this method, under a strong regularity condition [105] at a solution. Global convergence results for the Josephy-Newton method were not established.

In contrast, the path search strategy generates a piecewise linear path $p^k(t)$ from x^k to the Newton point (if it exists) by applying a complementary pivot algorithm similar to Lemke's method; each pivot step results in a new linear segment of the path. This path is a so called *Newton path* [103], i.e., it is a continuous function $p^k : [0, T_k] \to \mathbb{R}^n$, which has the properties

$$\begin{aligned} p^k(0) &= x^k, \\ A_k(p^k(t)) &= (1-t)F_+(x^k), \quad \forall t \in [0, T_k], \end{aligned}$$

where $T_k \in [0, 1]$. This shows that, in first order, points on the path decrease the norm of the normal map. For larger t there might be no such decrease. In this case, the path is backtracked using an Armijo-type rule as follows. Given $\beta \in (0, 1)$, the points $\{p(\beta^0), p(\beta^1), p(\beta^2), \dots\}$ are tried until a value l is found for which

$$\|F_+(p^k(\beta^l))\| \leq (1 - \sigma\beta^l)\|F_+(x^k)\|, \tag{3.30}$$

where $\sigma > 0$ is a fixed parameter. The next iteration is then chosen to be $x^{k+1} = p^k(\beta^l)$.

For global convergence results concerning path search strategies, see [23, 103]. Similar to line search, there exist nonmonotone path search strategies that have the benefits mentioned in Remark 3.27 (a), see [103] for more details.

3.4.4 Trust Region

In this section, we consider a different strategy for designing global methods for CPs by considering as before a merit function $\Psi(x)$ associated with the CP under consideration. Solving the CP can be formulated as solving the unconstrained minimization problem

$$\min \Psi(x), \quad x \in \mathbb{R}^n.$$

In the following, we restrict ourselves to natural merit functions, which take the form $\Psi(x) = \frac{1}{2}\|\Phi(x)\|^2$, where $\Phi(x) = 0$ is the reformulation of the CP, and make the following assumption:

$$\nabla\Psi(x) = H^T\Phi(x) \quad \text{for an arbitrary} \quad H \in \partial_B\Phi(x).$$

This assumption certainly holds if Φ itself is continuously differentiable, but we have seen that it also holds in some situations where Φ is a nonsmooth mapping. We recall that in each step of the semismooth Newton method, one has to find the solution d^k of the linear system

$$H_k d + \Phi(x^k) = 0, \tag{3.31}$$

where $H_k \in \partial_B\Phi(x^k)$. In a small neighborhood of a BD-regular solution this is equivalent to solving the optimization problem

$$\min \frac{1}{2}\|H_k d + \Phi(x^k)\|^2 \quad \text{for all} \quad d \in \mathbb{R}^n.$$

Another point of view is to consider the quadratic form

$$q_k(d) := \frac{1}{2}\|H_k d + \Phi(x^k)\|^2$$

as a first-order approximation of $\Psi(x^k + \cdot)$. The idea of trust region methods is to *trust* this approximation only in a certain region, say for all $\|d\| \le \Delta_k$ with the *trust region radius* Δ_k. The update of Δ_k is done with respect to the decrease of the merit function. The subproblem to be solved at each iteration becomes a constrained optimization problem:

$$\min q_k(d), \quad \text{s.t.} \quad \|d\| \le \Delta_k. \tag{3.32}$$

The decision whether $x^k + d^k$, with d^k from (3.32) can be accepted as a new iterate depends on the ratio

$$r_k = \text{ared}_k(d^k)/\text{pred}_k(d^k), \tag{3.33}$$

where

$$\text{ared}_k(d) = \Psi(x^k) - \Psi(x^k + d), \qquad \text{pred}_k(d) = \Psi(x^k) - q_k(d)$$

denote the actual and predicted reduction of the merit function, respectively. Combining these findings leads to the following trust region algorithm. The only difference to a standard trust region method is the updating rule for the trust region radius after a successful iteration.

Algorithm 3.28 (Trust Region Method)

(S.0) Choose $x^0 \in \mathbb{R}^n$, $\Delta_0 > 0, 0 < \rho_1 < \rho_2 < 1$, $0 < \sigma_1 < 1 < \sigma_2$, $\Delta_{\min} > 0$ and set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_B \Phi(x^k)$, and compute d^k from (3.32).

(S.3) If $r_k \geq \rho_1$, with r_k as in (3.33), we call the iteration k successful and set $x^{k+1} := x^k + d^k$; otherwise we set $x^{k+1} := x^k$.

(S.4) Update the trust region radius as follows:

$$\Delta_{k+1} := \begin{cases} \sigma_1 \Delta_k, & \text{if } r_k < \rho_1, \\ \max\{\Delta_{\min}, \Delta_k\}, & \text{if } r_k \in [\rho_1, \rho_2), \\ \max\{\Delta_{\min}, \sigma_2 \Delta_k\}, & \text{if } r_k \geq \rho_2. \end{cases}$$

(S.5) Set $k \leftarrow k + 1$, and go to (S.1).

Several remarks concerning Algorithm 3.28 are in order. The choice of the norm when defining the trust region

$$\mathcal{B}_k := \{x \in \mathbb{R}^n | \|x - x^k\|_p \leq \Delta_k\}$$

determines the geometrical shape of the trust region. Although, this shape determines the position of the model minimizer, the choice of the norm that defines the trust region is in general irrelevant to the convergence of the method, but may have a serious impact on the computations. The $\|\cdot\|_1, \|\cdot\|_2, \|\cdot\|_\infty$ norms, or scaled variants of these, are preferred.

The algorithm uses a minimal radius $\Delta_{\min} > 0$ as a lower bound for the new radius, in order to ensure global and local superlinear/quadratic convergence. Under standard assumptions it can be shown that for k sufficiently large the generalized Newton direction from (3.31) (the solution of the unconstrained optimization problem) exists and is unique and coincides with the constrained optimization problem. Moreover, the iterations are successful. Thus, for sufficiently large k the trust region method reduces to the generalized Newton method, [57, 73].

Further we note that solving the subproblems is not a simple task. Each iteration requires the solution of the constrained quadratic programming problem (3.32). This subproblem has an optimal solution as its feasible region is nonempty and compact.

There exist efficient and reliable numerical methods to address (3.32), see, e.g., [17, 89, 50, 113].

On the first, line search strategies seem to be preferable as they only require the solution of a linear (least squares) problem in each iteration. To select the appropriate update of the iterate only a small number of merit function evaluations has to be performed. However, the higher cost of the trust-region method is typically more than compensated by its superior convergence properties [17]. There is also a nonmonotone variant of Algorithm 3.28, see, e.g., [118].

3.5 Other Methods

The need for nonsmooth Newton-type methods was motivated by the fact that reliable NCP reformulations of CPs yield nonsmooth equations. A possibility to maintain the reliability of these nonsmooth reformulations without having to use nonsmooth algorithms is presented in the following. In our discussion we restrict ourselves to the Fischer-Burmeister function, since it will naturally lead to another class of methods, the so called interior point methods.

The idea of *smoothing methods* is to approximate the NCP-function by a parameterized function, which is not NCP but leads to a smooth system of nonlinear equations. For example, the Fischer-Burmeister function is replaced by

$$\phi_\mu(a,b) := \sqrt{a^2+b^2+2\mu} - a - b, \tag{3.34}$$

so that $\phi_\mu(a,b) \to \phi_{FB}(a,b)$ as μ tends to zero [58]. Analogous to NCP reformulations, we obtain the following nonlinear equations:

$$\Phi_\mu(x) := \begin{pmatrix} \phi_\mu(x_1, F_1(x)) \\ \vdots \\ \phi_\mu(x_n, F_n(x)) \end{pmatrix}.$$

Now we can apply a standard Newton method to solve $\Phi_\mu(x) = 0$. Since the ultimate goal is to find a solution of $\Phi_{FB}(x) = \Phi_0(x) = 0$, we let the parameter μ converge to zero during the Newton iteration. Introducing μ_k, the value of μ at the k-th iteration, we thus compute the direction d^k as the solution of the linear system

$$\Phi'_{\mu_k}(x^k)d = -\Phi_{\mu_k}(x^k) \tag{3.35}$$

at each iteration. As in the standard Newton method, the next iterate is obtained by setting $x^{k+1} = x^k + d^k$. Choosing μ_k in an appropriate manner is a delicate task. There are several possibilities, which can be shown to yield superlinear or even quadratic local convergence under the R-regularity condition, see, e.g., [8, 30, 58]. To improve the global convergence properties, the smoothing algorithm described above should be combined with line search or other globalization strategies. For monotone NCPs, global convergence can be established [10]. Indeed, smoothing methods usually require F to be at least a P_0-function in order to guarantee that the linear systems (3.35) are solvable. However, the implementation of the smoothing technique by Chen and Mangasarian [12] seems to work quite well even applied to nonmonotone problems. We mention that there exists many other variants of smoothing methods. Among these Jacobian smoothing methods are often viewed as a mixture between the nonsmooth methods and smoothing methods, since these method try to solve at each iteration the mixed Newton equation

$$\Phi'_{\mu_k}(x^k)d = -\Phi(x^k),$$

using the smooth matrix from (3.35), but an unperturbed right-hand side, see, e.g., [70, 13, 101].

Kanzow [58] has shown a theoretical equivalence between the smoothed Fischer-Burmeister method and the *interior-point method*. Basically, the relationship between these two methods can be seen as follows. Considering ϕ_μ from (3.34), we see that

$$\phi_\mu(a,b) = 0 \quad \Leftrightarrow \quad a > 0, b > 0, ab = \mu.$$

It directly follows that solving $\Phi_\mu(x) = 0$ is equivalent to

$$x_i > 0, \quad F_i(x) > 0, \quad x_i F_i(x) = \mu, \quad \forall i = 1, \ldots, n. \tag{3.36}$$

It turns out that (3.36) constitute the central path conditions typically used in interior-point methods [124]. However, the subproblems associated with the two methods are solved in a different manner. In analogy to interior-point methods for linear programs [74], interior-point methods for linear complementarity problems have polynomial complexity, which means that the worst-case execution time of this algorithms is a polynomial function of the problem size. In practice, the run time grows slowly for large-scale linear problems. They are therefore preferable compared to pivotal methods such as Lemke's method. Returning to the nonlinear case, local fast convergence can be established for interior point methods, even in the absence of strong regularity conditions.

3.6 Software

In the following, we provide a brief overview of available software for addressing nonlinear and mixed complementarity problems. This survey is partly based on [5].

The SEMISMOOTH algorithm [19, 90] is based upon reformulating the MCP as a system of nonsmooth equations involving both the Fischer-Burmeister NCP-function ϕ_{FB} and the penalized Fischer-Burmeister function ϕ_{CCK}. SEMISMOOTH extends the approach used in [4, 19] reformulating the MCP using the reformulation $\Phi : \mathbb{R}^n \to \mathbb{R}^n$ given by

$$\Phi(x) := \begin{cases} \phi_{FB}(x_i - l_i, F_i(x)) & \text{if } i \in I_l, \\ -\phi_{FB}(u_i - x_i, -F_i(x)) & \text{if } i \in I_u, \\ \phi(x_i - l_i, \phi_{FB}(u_i - x_i, -F_i(x))) & \text{if } i \in I_{lu}, \\ -F_i(x) & \text{if } i \in I_f, \end{cases}$$

where $\phi \in \{\phi_{FB}, \phi_{CCK}\}$. Furthermore, I_l, I_u, I_{lu} and I_f denote the set of indices $i \in \{1, \ldots, n\}$ with finite lower bounds only, finite upper bounds only, finite lower and upper bounds and no finite bounds, respectively, on the variable x_i, see (4.35). This results in a semismooth system of equations $\Phi(x) = 0$ on which a nonsmooth generalized Newton method (see Section 3.2.1) is applied to obtain a Newton direction d^k. The natural merit function

$$\Psi(x) := \frac{1}{2}\|\Phi(x)\|^2 \tag{3.37}$$

is continuously differentiable, thus the local method can be globalized using standard line search techniques, provided d^k satisfies sufficient decrease. Otherwise, the negative gradient

of the merit function is taken. However, when the Newton system is (close to) singular solving the linear least squares problem via iterative solvers is preferred to the resort of taking the gradient step. To improve performance, iterative solvers are also used to compute the Newton direction when dealing with large-scale problems.

The SEMICOMP algorithm [4] is an extension to the SEMISMOOTH algorithm, which adds a proximal perturbation strategy that allows the iterates to escape local minima of the merit function from (3.37). If SEMISMOOTH stopped making satisfactory progress towards a solution of Φ at an iterate x^p, then a sequence of perturbed problems will be solved, which generates a sequence of solutions $\{y^k\}$ that lead to a better starting point $y^p =: x^{p+1}$. The perturbed problems replace F with a perturbed function

$$F^{\lambda,\bar{y}} := F(y) + \lambda(y - \bar{y}), \tag{3.38}$$

where the centering point is usually chosen to be the current iterate y^k and $\lambda > 0$ is chosen to be large enough to assure that $F^{\lambda,\bar{x}}$ is strongly monotone. Thus the sequence of subproblems MCP(F^{λ,y^k}, B) can be solved by SEMISMOOTH providing the next iterate y^{k+1}. In general, the perturbed problems MCP(F^{λ,y^k}, B) are not solved exactly. Whenever an iterate is found where the merit function Ψ of the unperturbed problem has been sufficiently reduced with respect to any other point computed so far, then the algorithm returns to the unperturbed problem, SEMISMOOTH starts from the last iterate and the perturbation strategy is stopped.

The BDIFF algorithm [52, 95] is based upon reformulating the NCP as a system of nonsmooth equations using the minimum function ϕ_P. The algorithms attempts to find a zero of the semismooth equation

$$\Phi_P(x) = \min\{x, F(x)\}$$

involving directional derivatives of Φ_P. Solving the subproblems

$$\Phi'_P(x^k; d) = -\Phi_P(x^k) \tag{3.39}$$

a direction d^k is obtained which is a descent direction, in the sense that $\Psi'_P(x^k; d^k) < 0$. Thus the Armijo-type rule from (3.28) is well defined, providing the globalization strategy for BDIFF. Recall that the natural merit function $\Psi_P(x^k)$ is in general not differentiable. However, (3.39) is a system of nonlinear equations. It is a nontrivial task to solve it. Pang [95] suggested to solve it inexactly.

The NE/SQP algorithm (for Nonsmooth Equations/Successive Quadratic Programming) [96] is based upon the same reformulation of the NCP via the B-differentiable operator Φ_P, but resulting into a nonnegatively constrained system of equations. In [4], this idea is extended to the MCP framework using the reformulation

$$\bar{\Phi}_{P,i}(x) := \min(x_i - l_i, \max(u_i - x_i, -F_i(x))), \quad x \in [l_i, u_i],$$

which leads to the B-differentiable merit function

$$\bar{\Psi}_P(x) = \frac{1}{2}\|\bar{\Phi}_P(x)\|^2.$$

The resulting nonlinear system of equations is solved by a damped Gauss-Newton method, which leads at each iteration to a convex quadratic program with box-constraints

$$\min q_k(x^k, d) \quad \text{s.t. } d \in \mathcal{B} - x^k,$$

where q_k is formed by squaring a linear approximation of $\bar{\Phi}_P$ at x^k, see [4]. The advantage of this approach is that the subproblems are always solvable. However, the performance of the method depends on the choice of a reliable QP solver. Once the direction is calculated, a slightly modified Armijo rule is used to determine the step length. The robustness of the NE/SQP algorithm is disappointing when applied to large scale problems, see [5].

The NE/SQP algorithm improved by a proximal perturbation strategy gives the QPCOMP algorithm [4].

The PROXI algorithm [4] uses the the minimum map reformulation of the mixed complementarity problem

$$\bar{\Phi}_P(x) = 0$$

and applies, opposed to NE/SQP, a nonsmooth version of Newton's method on this reformulation. At each iteration a linear approximation of $\bar{\Phi}_P$ is solved, choosing a particular element of its subdifferential at a point where the operator is nondifferentiable. PROXI is closely related to QPCOMP since it also relies on a proximal perturbation strategy to help iterates escape local minima of the merit function. This strategy is also extended to deal with singularities.

MILES [107] can be viewed as an extension of the classical Josephy-Newton method [54] for MCP. The latter attempts to solve the generalized equation (see (2.6))

$$0 \in F(x) + N_{\mathcal{B}}(x)$$

by solving at the k-th iteration the linearized subproblem

$$0 \in F(x^k) + F'(x^k)(x - x^k) + N_{\mathcal{B}}(x).$$

It can be directly seen from Definition 2.34 of the normal cone that the linearized subproblem is equivalent to the linear mixed complementarity problem

$$\mathrm{MCP}(F(x^k) + F'(x^k)(x - x^k), \mathcal{B}).$$

Similarly to the method developed in [82, 83], MILES computes the solution of each subproblem using an extension of Lemke's almost-complementary pivot algorithm in which upper and lower bounds are represented implicitly. This Newton point is used to define the Newton direction, which is then used in a damped line search. Note that this is theoretically unjustified since the Newton direction is not necessarily a descent direction for the merit function used. Furthermore, when Lemke's algorithm does not terminate successfully MILES has to resort to a restart procedure.

The PATH solver [23] is a path search damped Newton-type method applied to the nonsmooth reformulation of the MCP via the normal map

$$0 = F(P_{\mathcal{B}}(x)) + x - P_{\mathcal{B}}(x),$$

see Section 3.4.3. The algorithm consists of a sequence of major iterations, each consisting of an approximation or linearization step similar to that of MILES (sometimes called successive LCP) cast as a linear MCP of the form LMCP$(q^k, M_k, \mathcal{B})$, where

$$M_k := F'(P_{\mathcal{B}}(x^k)) \quad \text{and} \quad q_k := F(P_{\mathcal{B}}(x^k)) - M_k P_{\mathcal{B}}(x^k).$$

Then a path to the Newton point (the solution to the approximation, or equivalently, to the solution of LMCP$(q^k, M_k, \mathcal{B})$) is constructed using a pivotal technique, and a possible search of this path is performed. When the Newton point does not exist or the path cannot be entirely constructed, a step along the partially computed path is taken before the problem is relinearized. A nonmonotone watchdog strategy is employed when applying the path search; this helps avoid convergence to local minima of the norm function for the underlying nonsmooth equation and keeps the number of function evaluations required as small as possible. To solve the linearized subproblems PATH uses a pivotal based code similar to Lemke's method in which upper and lower bounds are represented implicitly. A limitation of the PATH solver is that the residual of the normal map, the merit function used by the former versions of PATH, is not differentiable. Newer versions consider alternative merit functions [33] for globalization purposes. When the subproblem solver fails, a projected gradient direction of a differentiable merit function is used. A further enhancement is a projected Newton preprocessor used in order to find an initial point that corresponds better to the optimal active set.

The SMOOTH algorithm [12] is based upon reformulating the NCP as a system of nonsmooth equations (see Proposition 2.35)

$$0 = x - P_{\mathbb{R}^n_+}(x - F(x)).$$

Similarly to smoothing techniques for NCP-reformulations, the method solves a sequence of smooth approximations, which lead to a zero of the nonsmooth system. The smooth approximation $\hat{p}(x, \beta)$ (see [12] for a definition) to $P_{\mathbb{R}^n_+}(x)$ are commonly used in machine learning and lead to the smooth equation

$$0 = x - \hat{p}(x - F(x), \beta).$$

The search direction is generated by applying only one Newton step to the smooth system. This direction is searched using a Armijo-type rule respective to the merit function

$$\|x - \hat{p}(x - F(x), \beta)\|.$$

Since the accuracy of the approximation is given by the residual of the current point $\|x_k - P_{\mathbb{R}^n_+}(x_k - F(x_k)\|$, assuming that the new point have a smaller residual, the next approximation will be tighter. An extension to the MCP framework is possible and the numerical test involving MCPLIB indicates good performance. In contrast to PATH which uses the preprocessor only to identify the active set (that is, determination of which variables are at their upper and lower bounds), SMOOTH uses the same preprocessor to solve the problem. If the preprocessor does not find a solution SMOOTH is then used to find it.

Chapter 4

A Least-Square Semismooth Method

We have seen that a number of important methods for the solution of the complementarity problem (1.3) are based on reformulating the complementarity problem via the Fischer-Burmeister function. The Fischer-Burmeister function $\phi_{FB}(a, b)$ is very effective in obtaining feasibility, since it becomes relatively large if a or b are significantly negative. However, it has some difficulties in reducing the complementarity gap, since $\phi_{FB}(a, b)$ is quite flat on the positive orthant, see Figure 4.1. For example, if a is a large number and b is, say, equal to one, then the product ab is a large number while $|\phi_{FB}(a, b)|$ is small. In this section, we propose an approach which overcomes these difficulties but retains the advantages of the Fischer-Burmeister function. To this end, we modify the nonlinear systems reformulation described in Section 3.1 by appending additional equations that incorporate product terms, see Section 4.1. This leads to a least-squares reformulation of the nonlinear complementarity problem, whose properties are discussed in Section 4.2. To solve the arising overdetermined system of equations we propose a semismooth Levenberg-Marquardt method equipped with line search, see Section 4.3. The global and local fast convergence results (under mild assumptions) are similar to some existing equation-based methods. In Section 4.4, this newly developed algorithm is extended to the more general case of mixed complementarity problems. The numerical results presented in Section 4.5 illustrate that our new approach is significantly more robust than the one based on the nonlinear systems reformulation.

4.1 A Least-Square Semismooth Reformulation

To introduce a least squares formulation of nonlinear complementarity problems, let us define the function

$$\phi_+(a, b) := a_+ b_+ \ ,$$

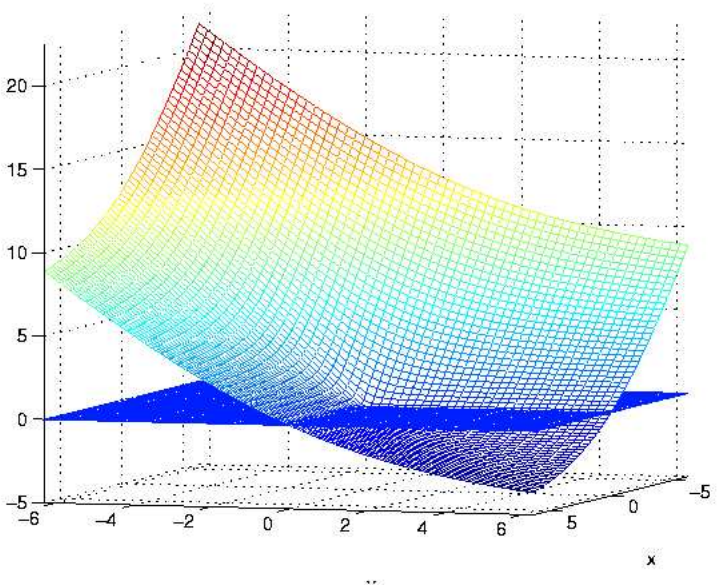

Figure 4.1: Graph of the Fischer-Burmeister function.

where $z_+ := \max\{0, z\}$ for $z \in \mathbb{R}$. We then define the mapping $\Phi : \mathbb{R}^n \to \mathbb{R}^{2n}$ by

$$\Phi(x) := \begin{pmatrix} \vdots \\ \lambda_1 \phi_{FB}(x_i, F_i(x)), \quad i = 1, \ldots, n \\ \vdots \\ \lambda_2 \phi_+(x_i, F_i(x)), \quad i = 1, \ldots, n \\ \vdots \end{pmatrix}, \tag{4.1}$$

where $\lambda_1, \lambda_2 \in \mathbb{R} \setminus \{0\}$ are fixed but arbitrary parameters used as weight parameters between the first type of terms and the second one. Hence we obtain Φ by adding some components to the definition of Φ_{FB}. These additional components are used in order to avoid the disadvantage of the Fischer-Burmeister function mentioned before.

A similar idea has been used before in [11] where the penalized Fischer-Burmeister function was introduced which, however, is based on a direct modification of ϕ_{FB} (see also Section 4.5.3). Moreover, the corresponding Newton-type method in [11] (essentially taken from [19]) might have to take a number of gradient steps for difficult problems, whereas this is completely avoided in our approach.

To describe this approach, first note that $\Phi(x) = 0$ is an overdetermined system of equations having the property that

$$x^* \text{ solves } \Phi(x) = 0 \Longleftrightarrow x^* \text{ solves NCP}(F).$$

Hence we have a nonlinear least squares formulation of the complementarity problem with the additional property that the residual at the solution is zero. We therefore suggest a

nonsmooth Gauss-Newton- or Levenberg-Marquardt-type method for the solution of this least squares problem. This method has the following advantages over existing methods based on Φ_{FB}:

- Faster reduction of the complementarity gap $x^T F(x)$.
- A Newton-type search direction can be taken at each iteration; in particular, no gradient steps are necessary in order to get global convergence.
- The numerical results indicate that the method is significantly more robust than those methods which are based on Φ_{FB}.

Moreover, in the following section it will be shown that the corresponding merit function

$$\Psi(x) := \frac{1}{2}\|\Phi(x)\|^2 \tag{4.2}$$

shares all the beneficial properties of Ψ_{CCK}.

Similarly the idea can also be used in order to modify other equation-based methods, see, for example, [114] for a summary of many of these equation reformulations. More precisely, assume we have a reformulation of the complementarity problem as a square system of equations $\Phi_A(x) = 0$ with $\Phi_A : \mathbb{R}^n \to \mathbb{R}^n$. Suppose further that $\Phi_B : \mathbb{R}^n \to \mathbb{R}^m$ is any mapping with the property that $\Phi_B(x) = 0$ whenever x is a solution of the NCP. Then it is easy to see that x^* is a solution of the complementarity problem if and only if x^* is a solution of the overdetermined system of equations $\tilde{\Phi}(x) = 0$, where $\tilde{\Phi} : \mathbb{R}^n \to \mathbb{R}^{n+m}$ is now defined by

$$\tilde{\Phi}(x) := \begin{pmatrix} \Phi_A(x) \\ \Phi_B(x) \end{pmatrix}.$$

Assuming that $\tilde{\Phi}$ and the corresponding merit function $\tilde{\Psi}(x) := \frac{1}{2}\|\tilde{\Phi}(x)\|^2$ have similar properties as those to be stated in the next Section 4.2 for the functions from (4.1) and (4.2), we could apply our the Levenberg-Marquardt method method also to the least squares problem

$$\min \tilde{\Psi}(x)$$

in order to solve the nonlinear complementarity problem. Of course, the crucial part is the definition of the mapping Φ_B which depends on the properties of the mapping Φ_A.

4.2 Properties of Φ and Ψ

In this section, we study several important properties of the mappings Φ and Ψ from (4.1) and (4.2), respectively. To this end, we begin with the equation operator Φ and note that it is (strongly) semismooth.

Theorem 4.1 *The mapping Φ from (4.1) is semismooth. If F is an LC^1 function, then Φ is strongly semismooth.*

Proof. The function Φ is (strongly) semismooth if every of its component functions is (strongly) semismooth. For each $i \in \{1, \ldots, n\}$, Φ_i is the composite of the strongly semismooth Fischer-Burmeister function ϕ_{FB} (see Example 2.20) and of the differentiable function $x \mapsto (x_i, F_i(x))^T : \mathbb{R}^n \to \mathbb{R}^2$. If F is an LC^1 function, then $x \mapsto (x_i, F_i(x))^T$ is strongly semismooth. Since the composite of (strongly) semismooth functions is again (strongly) semismooth, Φ_i is (strongly) semismooth for all $i \in \{1, \ldots, n\}$. On the other hand, Φ_{n+i} is for all $i \in \{1, \ldots, n\}$ the composite of the plus function ϕ_+ (which is strongly semismooth, since it is the product of two strongly semismooth functions), and the function $x \mapsto (x_i, F_i(x))^T : \mathbb{R}^n \to \mathbb{R}^2$. In turn, every component function of Φ is strongly semismooth. □

We next investigate the structure of the C-subdifferential of Φ at a given point $x \in \mathbb{R}^n$. To this end, we first state a standard result regarding the generalized gradients of ϕ_{FB} and ϕ_+, cf. [11].

Lemma 4.2 *The generalized gradient of the function $\phi_{FB} : \mathbb{R}^2 \to \mathbb{R}$ at a point $(a, b) \in \mathbb{R}^2$ is equal to the set of all $(g_a, g_b)^T \in \mathbb{R}^2$ with*

$$(g_a, g_b) = \begin{cases} \left(\frac{a}{\|(a,b)\|} - 1, \frac{b}{\|(a,b)\|} - 1\right), & \text{if } (a, b) \neq (0, 0), \\ (\xi - 1, \zeta - 1), & \text{if } (a, b) = (0, 0), \end{cases}$$

and where (ξ, ζ) is any vector satisfying $\|(\xi, \zeta)\| \leq 1$. The generalized gradient of the function $\phi_+ : \mathbb{R}^2 \to \mathbb{R}$ at a point $(a, b)^T \in \mathbb{R}^2$ is equal to $\partial\phi_+(a, b) = (b_+\partial a_+, a_+\partial b_+)^T$, where

$$\partial z_+ = \begin{cases} 1 & \text{if } z > 0, \\ [0, 1] & \text{if } z = 0, \\ 0 & \text{if } z < 0. \end{cases}$$

Proof. The Fischer-Burmeister function is the difference of the Euclidean norm function and the differentiable function $(a, b)^T \mapsto a + b$. Since

$$\partial\|(a, b)\| = \begin{cases} \left(\frac{a}{\|(a,b)\|}, \frac{b}{\|(a,b)\|}\right)^T, & \text{if } (a, b) \neq (0, 0), \\ (\xi, \zeta)^T, & \text{if } (a, b) = (0, 0), \end{cases}$$

where (ξ, ζ) is any vector satisfying $\|(\xi, \zeta)\| \leq 1$, and $\partial(a + b) = (1, 1)^T$, Corollary 2.8 part (a) provides the desired result for the Fischer-Burmeister function. To calculate the generalized gradient of the plus function ϕ_+ we first define $g_1, g_2 : \mathbb{R}^2 \to \mathbb{R}$ by $g_1(a, b) := a_+$ and $g_2(a, b) := b_+$. Note that both g_1 and g_2 are convex and nonnegative functions. Using well known calculus rules (see Corollary 2.8 part (b)) we obtain

$$\begin{aligned} \partial\phi_+(a, b) =& \partial(g_1 g_2)(a, b) = g_2(a, b)\partial g_1(a, b) + g_1(a, b)\partial g_2(a, b) \\ =& b_+ \begin{pmatrix} \partial a_+ \\ 0 \end{pmatrix} + a_+ \begin{pmatrix} 0 \\ \partial b_+ \end{pmatrix} = \begin{pmatrix} b_+\partial a_+ \\ a_+\partial b_+ \end{pmatrix}. \end{aligned}$$

This completes the proof. □

As a consequence of Lemma 4.2, we obtain the following result.

Theorem 4.3 *Let $x \in \mathbb{R}^n$ be given. Then any matrix $H \in \partial_C \Phi(x)$ has the representation*

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix},$$

where

$$H_1 \in \{D_a(x) + D_b(x)F'(x)\} \quad \text{and} \quad H_2 \in \{\tilde{D}_a(x) + \tilde{D}_b(x)F'(x)\}$$

with

$$D_a(x) = \operatorname{diag}\{a_i(x)\}, \;\; D_b(x) = \operatorname{diag}\{b_i(x)\}, \;\; \tilde{D}_a(x) = \operatorname{diag}\{\tilde{a}_i(x)\}, \;\; \tilde{D}_b(x) = \operatorname{diag}\{\tilde{b}_i(x)\}$$

being diagonal matrices with entries $(a_i(x), b_i(x)) \in \partial\phi_{FB}(x_i, F_i(x))$ and $(\tilde{a}_i(x), \tilde{b}_i(x)) \in \partial\phi_+(x_i, F_i(x))$, where $\partial\phi_{FB}(x_i, F_i(x))$ and $\partial\phi_+(x_i, F_i(x))$ denote the sets from Lemma 4.2, with (a, b) being replaced by $(x_i, F_i(x))$.

Proof. By our definition of the C-subdifferential, we have

$$\partial_C \Phi(x)^T = \partial\Phi_1(x) \times \cdots \times \partial\Phi_{2n}(x),$$

where $\partial\Phi_i(x)$ denotes the generalized gradient of the i-th component function of Φ. Using Lemma 4.2, it follows that

$$\partial\Phi_i(x) \subseteq \{\lambda_1\big(a_i(x)e_i^T + b_i(x)\nabla F_i(x)^T\big)\} \quad \forall i \in \{1, \ldots, n\} \tag{4.3}$$

and

$$\partial\Phi_{n+i}(x) \subseteq \{\lambda_2\big(\tilde{a}_i(x)e_i^T + \tilde{b}_i(x)\nabla F_i(x)^T\big)\} \quad \forall i \in \{1, \ldots, n\}, \tag{4.4}$$

with $(a_i(x), b_i(x))$ and $(\tilde{a}_i(x), \tilde{b}_i(x))$ being the elements specified in the statement of our theorem. □

In order to prove fast local convergence, we need to show that every element $H \in \partial_C \Phi(x^*)$ has full rank n under a suitable assumption. This assumption will be the R-regularity condition. We recall Definition 3.18, stating that a solution x^* of the complementarity problem is R-regular if the submatrix $F'(x^*)_{\alpha\alpha}$ is nonsingular and the Schur complement

$$F'(x^*)_{\beta\beta} - F'(x^*)_{\beta\alpha}F'(x^*)_{\alpha\alpha}^{-1}F'(x^*)_{\alpha\beta}$$

is a P-matrix, where the partition $I = \alpha \cup \beta \cup \gamma$ is given by the index sets

$$\alpha = \{i \mid x_i^* > 0, F_i(x^*) = 0\}, \tag{4.5}$$
$$\beta = \{i \mid x_i^* = 0, F_i(x^*) = 0\}, \tag{4.6}$$
$$\gamma = \{i \mid x_i^* = 0, F_i(x^*) > 0\}. \tag{4.7}$$

Then we have the following result.

Theorem 4.4 *Let $x^* \in \mathbb{R}^n$ be an R-regular solution of the complementarity problem. Then all elements from the C-subdifferential $\partial_C \Phi(x^*)$ have full rank.*

Proof. Let $H \in \partial_C \Phi(x^*)$. In view of Theorem 4.3, we then have

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix},$$

where H_1 is an element from $\partial_C \Phi_{FB}(x^*)$. It now follows from the proof Proposition 3.21 (a) that each element $H_1 \in \partial_C \phi_{FB}(x^*)$ is nonsingular under the assumed R-regularity condition. Therefore we have $\operatorname{rank}(H) = n$, i.e., H has full rank. □

We stress that the proof of Theorem 4.4 is based on known properties of the first block H_1. An interesting question is whether the second component H_2 contributes something so that the entire matrix $H \in \partial_C \Phi(x^*)$ could have full rank even if the first block H_1 is singular. However, the answer is negative. Let us consider a solution $x^* \in \mathbb{R}^n$ of the NCP together with the associated index sets α, β, γ from (4.5) and an arbitrary matrix $H \in \partial_C \Phi(x^*)$. We calculate the i-th row of H using Theorem 4.3 and obtain:
For $i \in \alpha$ there is a $t_i \in [0, 1]$ such that

$$H_i = -\nabla F_i(x^*)^T \quad \text{and} \quad H_{n+i} = t_i x_i^* \nabla F_i(x^*)^T;$$

for $i \in \beta$ there is a $(\xi_i, \zeta_i) \in \mathbb{R}^2$ satisfying $\|(\xi_i, \zeta_i)\| \leq 1$ such that

$$H_i = (\xi_i - 1)e_i^T + (\zeta_i - 1)\nabla F_i(x^*)^T \quad \text{and} \quad H_{n+i} = (0, \ldots, 0)^T;$$

for $i \in \gamma$ there is a $\tau_i \in [0, 1]$ such that

$$H_i = -e_i^T \quad \text{and} \quad H_{n+i} = \tau_i F_i(x^*) e_i^T.$$

This shows that the rows of H_2 are either completely zero or are multiples of the corresponding rows from the H_1-matrix. Nevertheless, it is interesting to note that, if we are far away from a solution x^*, then the H_2-block is sometimes quite helpful to guarantee the full rank of the entire matrix H.

We next state a consequence of Theorem 4.4 that will play an important role in our convergence analysis.

Lemma 4.5 *Let $x^* \in \mathbb{R}^n$ be an R-regular solution of the complementarity problem. Then there exist constants $\varepsilon > 0$ and $c > 0$ such that*

$$\|(H^T H)^{-1}\| \leq c$$

for all $H \in \partial_C \Phi(x)$ and all $x \in \mathbb{R}^n$ with $\|x - x^*\| \leq \varepsilon$.

Proof. The proof is similar to the one of Lemma 3.15, in view of Theorem 4.4, so we omit it. □

We next investigate the properties of the merit function Ψ from (4.2). To this end, it will be useful to rewrite this function as

$$\Psi(x) = \frac{1}{2}\|\Phi(x)\|^2 = \sum_{i=1}^{n} \psi(x_i, F_i(x))$$

with $\psi : \mathbb{R}^2 \to \mathbb{R}$ being defined by

$$\psi(a,b) := \frac{1}{2}\lambda_1^2 \phi_{FB}^2(a,b) + \frac{1}{2}\lambda_2^2 a_+^2 b_+^2. \tag{4.8}$$

The following properties of ψ are crucial in order to state several interesting results for the corresponding merit function Ψ. Basically, the next result says that ψ shares all the beneficial properties of the merit function corresponding to the Fischer-Burmeister function ϕ_{FB}.

Lemma 4.6 *The mapping $\psi : \mathbb{R}^2 \to \mathbb{R}$ defined in* (4.8) *has the following properties:*

(a) ψ is continuously differentiable on $\mathbb{R}^2$;

(b) $\psi(a,b) \geq 0$ for all $a, b \in \mathbb{R}^2$;

(c) $\psi(a,b) = 0 \iff a \geq 0, b \geq 0$ and $ab = 0$;

(d) $\frac{\partial \psi}{\partial a}(a,b)\frac{\partial \psi}{\partial b}(a,b) \geq 0$ for all $a, b \in \mathbb{R}^2$;

(e) $\psi(a,b) = 0 \iff \nabla\psi(a,b) = 0 \iff \frac{\partial \psi}{\partial a}(a,b) = 0 \iff \frac{\partial \psi}{\partial b}(a,b) = 0$.

Proof. Statements (a) and (b) follow directly from the definition of ψ together with the fact that ϕ_{FB}^2 is known to be continuously differentiable on $\mathbb{R}^2$, see [43, 31]. Property (c) follows from the fact that ϕ_{FB} is an NCP-function. Hence it remains to show statements (d) and (e). Since both statements obviously hold for $(a,b) = (0,0)$, we can assume without loss of generality that $(a,b) \neq (0,0)$ for the rest of this proof.

In order to verify part (d), first note that we have

$$\begin{aligned} &\frac{\partial \psi}{\partial a}(a,b)\frac{\partial \psi}{\partial b}(a,b) \\ &= \lambda_1^4 \phi_{FB}^2(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big)\Big(\frac{b}{\sqrt{a^2+b^2}} - 1\Big) + \lambda_2^4 a_+^3 b_+^3 + \lambda_1^2\lambda_2^2 t(a,b) \end{aligned}$$

with $t : \mathbb{R}^2 \to \mathbb{R}$ being defined by

$$t(a,b) := \phi_{FB}(a,b) a_+ b_+ \Big[\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big)a_+ + \Big(\frac{b}{\sqrt{a^2+b^2}} - 1\Big)b_+\Big].$$

It is easy to see that it suffices to prove that $t(a,b) \geq 0$. Now, we obviously have $t(a,b) \geq 0$ if $a \geq 0$ and $b \geq 0$. On the other hand, in all other cases, we have $t(a,b) = 0$, so that statement (d) follows.

To prove part (e), we first recall that we have $(a,b) \neq (0,0)$. Furthermore, taking into account the fact that an unconstrained minimum of a continuously differentiable function is always a stationary point of this function and using the symmetry of the function ψ with respect to its arguments a and b, we only have to verify the implication

$$\frac{\partial \psi}{\partial a}(a,b) = 0 \Longrightarrow \psi(a,b) = 0.$$

To this end, we first note that

$$\frac{\partial \psi}{\partial a}(a,b) = \lambda_1^2 \phi_{FB}(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big) + \lambda_2^2 a_+ b_+^2.$$

Using $\frac{\partial \psi}{\partial a}(a,b) = 0$, let us consider two cases: If $a \leq 0$ or $b \leq 0$, we have $a_+ b_+^2 = 0$ and therefore

$$0 = \frac{\partial \psi}{\partial a}(a,b) = \lambda_1^2 \phi_{FB}(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big).$$

This implies

$$\phi_{FB}(a,b) = 0 \quad \text{or} \quad \frac{a}{\sqrt{a^2+b^2}} - 1 = 0$$

which, in turn, is equivalent to

$$\phi_{FB}(a,b) = 0 \quad \text{or} \quad \big(a > 0 \text{ and } b = 0\big).$$

Hence we immediately have $\psi(a,b) = 0$.

Now consider the second case where $a > 0$ and $b > 0$. Then we get $\phi_{FB}(a,b) \leq 0$ and therefore

$$\phi_{FB}(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big) \geq 0.$$

Consequently, we obtain from

$$0 = \frac{\partial \psi}{\partial a}(a,b) = \lambda_1^2 \phi_{FB}(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big) + \lambda_2^2 a_+ b_+^2$$

that both sums must be equal to zero. In particular, we therefore have

$$0 = \lambda_1^2 \phi_{FB}(a,b)\Big(\frac{a}{\sqrt{a^2+b^2}} - 1\Big).$$

Hence we can argue as in the first case and see that $\psi(a,b) = 0$. □

Already from Lemma 4.6 part (a), we obtain the differentiability of the merit function Ψ. The next proposition is important from a computational point of view and shows how $\nabla\Psi$ can be computed making use of an arbitrary element $H \in \partial_C \Phi(x)$.

Theorem 4.7 *Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable. Then Ψ is continuously differentiable with $\nabla\Psi(x) = H^T\Phi(x)$, where $H \in \partial_C\Phi(x)$ can be chosen arbitrarily.*

Proof. Let $x \in \mathbb{R}^n$ be arbitrary, consider the index sets $I = \{1, \ldots, n\}$, $J = \{1, \ldots, 2n\}$ and define the following index sets associated with x:

$$\begin{array}{ll} \alpha = \{i \in I \mid x_i > 0 = F_i(x)\}, & \\ \gamma = \{i \in I \mid x_i = 0 < F_i(x)\}, & \overline{\alpha \cup \gamma} := I \setminus (\alpha \cup \gamma), \\ \beta = \{i \in I \mid x_i = 0 = F_i(x)\}, & \bar{\beta} := I \setminus \beta. \end{array}$$

Then for all $i \in \bar{\beta}$ the i-th component function Φ_i is continuously differentiable and

$$\partial\Phi_i(x) = \lambda_1 \partial\phi_{FB}(x_i, F_i(x)) = \{\nabla\Phi_i(x)\}, \quad i \in \bar{\beta} \tag{4.9}$$

holds. On the other hand,

$$\Phi_i(x) = \lambda_1 \phi_{FB}(x_i, F_i(x)) = 0, \quad \text{for all } i \in \beta. \tag{4.10}$$

For all $i \in \overline{\alpha \cup \gamma}$ the $(n+i)$-th component function Φ_{n+i} is continuously differentiable and

$$\partial\Phi_{n+i}(x) = \lambda_2 \partial\phi_+(x_i, F_i(x)) = \nabla\Phi_{n+i}(x), \quad i \in \overline{\alpha \cup \gamma} \tag{4.11}$$

holds. On the other hand,

$$\Phi_{n+i}(x) = \lambda_2 \phi_+(x_i, F_i(x)) = 0, \quad \text{for all } i \in \alpha \cup \gamma. \tag{4.12}$$

Taking into account (4.9)–(4.12) we can show that the set $\{H^T\Phi(x) \mid H \in \partial_C\Phi(x)\}$ consists only of one element:

$$\begin{aligned} S &:= \{H^T\Phi(x) \mid H \in \partial_C\Phi(x)\} \\ &= \{\lambda_1 \sum_{i=1}^{n} \phi_{FB}(x_i, F_i(x)) H_i + \lambda_2 \sum_{i=1}^{n} \phi_+(x_i, F_i(x)) H_{n+i} \mid H_i \in \partial\Phi_i(x), i \in J\} \\ &\overset{(4.10),(4.12)}{=} \{\lambda_1 \sum_{i \in \bar{\beta}} \phi_{FB}(x_i, F_i(x)) H_i + \lambda_2 \sum_{i \in \overline{\alpha\cup\gamma}} \phi_+(x_i, F_i(x)) H_{n+i} \mid H_i \in \partial\Phi_i(x), i \in J\} \\ &\overset{(4.9),(4.11)}{=} \{\lambda_1 \sum_{i \in \bar{\beta}} \phi_{FB}(x_i, F_i(x)) \nabla\Phi_i(x) + \lambda_2 \sum_{i \in \overline{\alpha\cup\gamma}} \phi_+(x_i, F_i(x)) \nabla\Phi_{n+i}(x)\} \end{aligned}$$

Now, using the relaxed chain rule, see Corollary 2.7, we obtain:

$$\partial\Psi(x) \subseteq \operatorname{conv}(S),$$

and therefore $\partial\Psi(x)$ is a singleton too. The assertion therefore follows from the fact that a locally Lipschitz continuous function is continuously differentiable if and only if its generalized gradient is a singleton at every point. □

We now prove our stationary point result. See also Proposition 3.26.

Theorem 4.8 *Suppose that $x^* \in \mathbb{R}$ is a stationary point of Ψ such that the Jacobian $F'(x^*)$ is a P_0-matrix. Then x^* is a solution of the nonlinear complementarity problem NCP(F).*

Proof. We first recall that we can write

$$\Psi(x^*) = \sum_{i=1}^{n} \psi(x_i^*, F_i(x^*))$$

with $\psi : \mathbb{R}^2 \to \mathbb{R}$ being defined in (4.8). Based on Lemma 4.6, the proof is essentially the same as the one given in [31, 65]. Since $x^* \in \mathbb{R}^n$ is a stationary point of Ψ, we have

$$0 = \nabla\Psi(x^*) = \frac{\partial\psi}{\partial a}(x^*, F(x^*)) + F'(x^*)^T \frac{\partial\psi}{\partial b}(x^*, F(x^*)) \tag{4.13}$$

where

$$\frac{\partial\psi}{\partial a}(x^*, F(x^*)) := \left(\ldots, \frac{\partial\psi}{\partial a}(x_i^*, F_i(x^*)), \ldots \right)^T \in \mathbb{R}^n$$

and, similarly,

$$\frac{\partial\psi}{\partial b}(x^*, F(x^*)) := \left(\ldots, \frac{\partial\psi}{\partial b}(x_i^*, F_i(x^*)), \ldots \right)^T \in \mathbb{R}^n.$$

Componentwise, equation (4.13) becomes

$$\frac{\partial\psi}{\partial a}(x_i^*, F_i(x^*)) + [F'(x^*)^T \frac{\partial\psi}{\partial b}(x^*, F(x^*))]_i = 0, \quad \forall i = 1, \ldots, n.$$

Premultiplying the i-th equation by $\frac{\partial\psi}{\partial b}(x_i^*, F_i(x^*))$ we obtain

$$\frac{\partial\psi}{\partial b}(x_i^*, F_i(x^*)) \frac{\partial\psi}{\partial a}(x_i^*, F_i(x^*)) + \frac{\partial\psi}{\partial b}(x_i^*, F_i(x^*))[F'(x^*)^T \frac{\partial\psi}{\partial b}(x^*, F(x^*))]_i = 0 \tag{4.14}$$

for all $i = 1, \ldots, n$. Now we assume that $\frac{\partial\psi}{\partial b}(x^*, F(x^*)) \neq 0$. By assumption, $F'(x^*)$ and therefore also $F'(x^*)^T$ is a P_0-matrix. Hence there is an index $i_0 \in \{1, \ldots, n\}$ such that $\frac{\partial\psi}{\partial b}(x_{i_0}^*, F_{i_0}(x^*)) \neq 0$ and

$$\frac{\partial\psi}{\partial b}(x_{i_0}^*, F_{i_0}(x^*))[F'(x^*)^T \frac{\partial\psi}{\partial b}(x^*, F(x^*))]_{i_0} \geq 0. \tag{4.15}$$

On the other hand, we also have

$$\frac{\partial\psi}{\partial a}(x_{i_0}^*, F_{i_0}(x^*)) \frac{\partial\psi}{\partial b}(x_{i_0}^*, F_{i_0}(x^*)) \geq 0. \tag{4.16}$$

by Lemma 4.6 (d). In view of (4.14)–(4.16), we obtain

$$\frac{\partial\psi}{\partial a}(x_{i_0}^*, F_{i_0}(x^*)) \frac{\partial\psi}{\partial b}(x_{i_0}^*, F_{i_0}(x^*)) = 0.$$

Lemma 4.6 (e) therefore implies

$$\psi(x^*_{i_0}, F_{i_0}(x^*)) = 0.$$

This, in turn, implies $\frac{\partial\psi}{\partial b}(x^*_{i_0}, F_{i_0}(x^*)) = 0$ by Lemma 4.6 (e), a contradiction to the choice of the index $i_0 \in \{1, \ldots, n\}$. Hence $\frac{\partial\psi}{\partial b}(x^*, F(x^*)) = 0$, which again by Lemma 4.6 (e), implies $\Psi(x^*) = 0$ so that x^* solves NCP(F). □

The proof of the next theorem uses a technique which was introduced by Geiger and Kanzow [43] in order to prove a similar theorem for the case of strongly monotone functions. Before, we require the following technical result.

Lemma 4.9 *If ϕ_P and ϕ_{FB} denote the minimum and Fischer-Burmeister NCP functions, respectively, then there exist positive constants c_1, c_2 such that*

$$c_1\phi_P^2(a, b) \le \phi_{FB}^2(a, b) \le c_2\phi_P^2(a, b).$$

Proof. The assertion follows directly from Lemma 3.1 in [117]. □

Theorem 4.10 *Let $c \in \mathbb{R}$ be an arbitrary constant, and let Ψ be the merit function defined in* (4.2)*. Then the level set*

$$\mathcal{L}_\Psi(c) := \{x \in \mathbb{R}^n \mid \Psi(x) \le c\}$$

is compact for all $c \in \mathbb{R}$, if F is a uniform P-function.

Proof. Since Ψ is continuous, the set $\mathcal{L}_\Psi(c)$ is obviously closed. Hence it suffices to show the boundedness of the level set $\mathcal{L}_\Psi(c)$. Assume this set is unbounded for some $c \in \mathbb{R}$. Then there is a sequence $\{x^k\} \subseteq \mathcal{L}_\Psi(c)$ such that $\lim_{k\to\infty} \|x^k\| = \infty$. Hence the index set

$$J := \{i \in \{1, \ldots, n\} \mid \{x_i^k\} \text{ is unbounded}\}$$

is nonempty. We now define a second sequence $\{z^k\} \subseteq \mathbb{R}^n$ by

$$z_i^k := \begin{cases} 0, & \text{if } i \in J, \\ x_i^k, & \text{if } i \notin J. \end{cases}$$

From the definition of $\{z^k\}$ and the fact that F is a uniform P-function, there is a scalar $\mu > 0$ such that

$$\begin{aligned} \mu \sum_{j\in J} (x_i^k)^2 =& \mu \|x^k - z^k\|^2 \\ &\le \max_{i\in\{1,\ldots,n\}} [x_i^k - z_i^k][F_i(x^k) - F_i(z^k)] \\ &= \max_{i\in J} \; x_i^k[F_i(x^k) - F_i(z^k)] \\ &\le \sqrt{\sum_{i\in J} (x_i^k)^2} \sum_{i\in J} |F_i(x^k) - F_i(z^k)|. \end{aligned} \tag{4.17}$$

Dividing by $\sqrt{\sum_{i\in J}(x_i^k)^2} \neq 0$, equation (4.17) then gives

$$\mu\sqrt{\sum_{i\in J}(x_i^k)^2} \leq \sum_{i\in J}|F_i(x^k) - F_i(z^k)|. \tag{4.18}$$

Since F is continuous and the sequence $\{z^k\}$ is bounded, the sequence $\{F_i(z^k)\}$ is also bounded for all $i \in \{1,\ldots,n\}$. Hence (4.18) implies the existence of an index $i_0 \in J$ such that

$$|F_{i_0}(x^k)| \to \infty.$$

On the other hand, since $i_0 \in J$, we also have

$$|x_{i_0}^k| \to \infty,$$

at least on a subsequence and together $\min^2\{x_{i_0}^k, F_{i_0}(x^k)\} \to \infty$ on a subsequence. Hence

$$\Psi(x^k) \geq \frac{\lambda_1^2}{2}\sum_{j\in J}\phi_{FB}^2(x_i^k, F_i(x^k)) \geq \frac{\lambda_1^2}{2}\phi_{FB}^2(x_{i_0}^k, F_{i_0}(x^k)) \overset{Lem.4.9}{\geq} \frac{c_1\lambda_1^2}{2}\min^2\{x_{i_0}^k, F_{i_0}(x^k)\} \to \infty$$

on a subsequence, contradicting the fact that the whole sequence $\{x^k\}$ lies in the level set $\mathcal{L}_\Psi(c)$. □

We next provide another condition for bounded level sets and note that it is not satisfied for the natural merit function related to the pure Fischer-Burmeister reformulation.

Theorem 4.11 *Let Ψ be the merit function defined in* (4.2)*. Assume that F is monotone and the complementarity problem $NCP(F)$ is strictly feasible, i.e., there exists a vector $\hat{x} \in \mathbb{R}^n$ such that $\hat{x} > 0$ and $F(\hat{x}) > 0$. Then the level sets $\mathcal{L}_\Psi(c)$ are compact for all $c \in \mathbb{R}$.*

Proof. We first rewrite

$$\Psi(x) = \frac{\lambda_1^2}{2}\sum_{i=1}^n \phi_{FB}^2(x_i, F_i(x)) + \frac{\lambda_2^2}{2}\sum_{i=1}^n \max^2\{0, x_i\}\max^2\{0, F_i(x)\}$$

and assume that there exists an unbounded sequence $\{x^k\} \subseteq \mathcal{L}_\Psi(c)$ for some $c \in \mathbb{R}$. We note that there is no index $i \in \{1,\ldots,n\}$ such that $x_i^k \to -\infty$ or $F_i(x^k) \to -\infty$ on a subsequence, because otherwise we would have $\phi_{FB}(x_i^k, F_i(x^k)) \to \infty$, which in turn would imply $\Psi(x^k) \to \infty$ on a subsequence. Hence all components of the two sequence $\{x^k\}$ and $\{F(x^k)\}$ are bounded from below, i.e., there is a constant $c > 0$ such that

$$x_i^k > -c \quad \text{and} \quad F_i(x^k) > -c \quad \text{for all } k \in \mathbb{N} \text{ and } i \in \{1,\ldots,n\}. \tag{4.19}$$

On the other hand, the sequence $\{x^k\}$ is unbounded by assumption. Hence there exists an index $i_0 \in \{1,\ldots,n\}$ such that $x_{i_0}^k \to \infty$ on a subsequence. Now let $\hat{x}$ satisfy the strict feasibility condition for the complementarity problem. Since F is monotone, we have

$$(x^k)^T F(\hat{x}) + \hat{x}^T F(x^k) \leq (x^k)^T F(x^k) + \hat{x}^T F(\hat{x}). \tag{4.20}$$

Hence the left-handside of (4.20) tends to infinity, since $\hat{x} > 0$ and $F(\hat{x}) > 0$, which implies that also $(x^k)^T F(x^k) \to \infty$ on a subsequence. Thus, there is a subset $K \subset \mathbb{N}$, a $k_0 \in K$ and an index j such that

$$x_j^k F_j(x^k) > c^2 > 0 \quad \text{for all} \quad k \geq k_0, k \in K. \tag{4.21}$$

Hence, there is an index $k_1 \in \mathbb{N}$ such that

$$x_j^k > 0 \quad \text{and} \quad F_j(x^k) > 0 \quad \text{for all} \quad k \geq k_1, k \in K, \tag{4.22}$$

since otherwise there would exist a subset $\bar{K} \subseteq K$ such that $x_j^k < 0$ or $F_j(x^k) < 0$ for all $k \in \bar{K}$. But this together with (4.19) would imply that

$$x_j^k F_j(x^k) < c^2 \quad \text{for all} \quad k \in \bar{K},$$

which contradicts (4.21). Taking (4.22) into account, we obtain

$$\Psi(x^k) \geq \frac{\lambda_2^2}{2}(\max\{0, x_j^k\}\max\{0, F_j(x^k)\})^2 \overset{(4.22)}{=} \frac{\lambda_2^2}{2}(x_j^k F_j(x^k))^2,$$

for all $k \geq k_1, k \in K$. Now (4.21) obviously implies $\{\Psi(x^k)\}_K \to \infty$, a contradiction to our assumption that $\{x^k\} \subseteq \mathcal{L}_\Psi(c)$. □

As a corollary of the previous results, we give the next existence result, consistently with Section 2.4.2.

Corollary 4.12 *Assume that F is either a uniform P-function or F is monotone and the complementarity problem* (1.3) *is strictly feasible. Then the NCP has a nonempty and bounded solution set.*

Proof. Let $c \in \mathbb{R}_+$ be large enough such that the level set $\mathcal{L}_\Psi(c)$ is nonempty. By Theorem 4.10 or respectively 4.11 the level set $\mathcal{L}_\Psi(c)$ is compact. Since Ψ is continuous it has a global minimum x^* in $\mathcal{L}_\Psi(c)$. In particular x^* is a stationary point of Ψ, since Ψ is continuously differentiable by Theorem 4.7. Since both assumptions on F imply that $F'(x^*)$ is a P_0-matrix (see Theorem 2.28 or respectively Proposition 2.24) we obtain in view of Theorem 4.8 that x^* is also a solution of the NCP. Hence $x^* \in \mathcal{L}_\Psi(0)$. The boundedness of the solution set $\mathcal{L}_\Psi(0)$ follows from the fact that $\mathcal{L}_\Psi(c)$ is bounded and $\mathcal{L}_\Psi(0) \subset \mathcal{L}_\Psi(c)$ obviously holds.

□

We close this section by noting that there are some other merit functions which share the properties of the merit function Ψ see Section 3.4.1 and [71, 11]. However, we are not aware of any merit function having stronger properties, while there are a couple of merit functions (including the Fischer-Burmeister merit function) which satisfy only some weaker conditions, see [80, 78, 43].

4.3 Algorithm and Convergence

We first state our algorithm for the solution of the complementarity problem (1.3). It is a Levenberg-Marquardt-type method (see Algorithm 3.12) equipped with line search (see Section 3.4.2) applied to the nonlinear least squares problem

$$\min \Psi(x) = \frac{1}{2}\|\Phi(x)\|^2,$$

where Φ and Ψ denote the mappings from (4.1) and (4.2), respectively.

Algorithm 4.13 (Semismooth Levenberg-Marquardt Method)

(S.0) Let $\beta \in (0,1)$, $\sigma \in (0, \frac{1}{2})$ and $\varepsilon \geq 0$. Choose any $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If $\|\nabla\Psi(x^k)\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C\Phi(x^k), \nu_k > 0$ and find a solution $d^k \in \mathbb{R}^n$ of

$$\big(H_k^T H_k + \nu_k I\big)d = -\nabla\Psi(x^k). \tag{4.23}$$

(S.3) Compute $t_k = \max\{\beta^l \mid l = 0, 1, 2, \dots\}$ such that

$$\Psi(x^k + t_k d^k) \leq \Psi(x^k) + \sigma t_k \nabla\Psi(x^k)^T d^k. \tag{4.24}$$

Set $x^{k+1} = x^k + t_k d^k$, $k \leftarrow k+1$, and go to (S.1).

We now investigate the convergence properties of our algorithm. To this end, we assume that the termination parameter ε is equal to zero and that Algorithm 4.13 generates an infinite sequence. We further note that Algorithm 4.13 is well defined since $\nu_k > 0$ and since one can easily see that the search direction d^k is always a descent direction for the merit function Ψ.

We first state a global convergence result. For the sake of simplicity, we assume that ν_k is given by

$$\nu_k := \|\nabla\Psi(x^k)\|, \tag{4.25}$$

although several other choices of ν_k yield the same result, including the more realistic choices

$$\nu_k := \min\{c_1, c_2\|\nabla\Psi(x^k)\|\} \quad \text{or} \quad \nu_k := \min\{c_1, c_2\|\Phi(x^k)\|\}$$

for certain constants $c_1, c_2 > 0$. Note that these choices are consistent with the requirements for local superlinear/quadratic convergence stated in Theorem 4.15 below.

Theorem 4.14 *Algorithm 4.13 is well defined for an arbitrary nonlinear complementarity problem. Furthermore, every accumulation point of a sequence $\{x^k\}$ generated by Algorithm 4.13 is a stationary point of Ψ.*

Proof. As noticed above the algorithm is well defined. Let x^* be any accumulation point of the sequence $\{x^k\}$ and $\{x^k\}_K$ a subsequence converging to x^*. Suppose that $\nabla\Psi(x^*) \neq 0$. Due to the monotone decrease of the sequence $\{\Psi(x^k)\}$ and the fact that $\{\Psi(x^k)\}_K$ converges to $\Psi(x^*)$, it follows that the entire sequence $\{\Psi(x^k)\}$ converges to $\Psi(x^*)$. In particular, we have

$$\Psi(x^{k+1}) - \Psi(x^k) \to 0.$$

On the other hand, we obtain

$$\Psi(x^{k+1}) - \Psi(x^k) \leq \sigma t_k \nabla\Psi(x^k)^T d^k \leq 0$$

by Step (S.3) in Algorithm 4.13 and the descent property of the search direction d^k. Hence we have

$$\{t_k \nabla\Psi(x^k)^T d^k\}_K \to 0. \tag{4.26}$$

Using the definition of the Levenberg-Marquardt direction gives

$$t_k \nabla\Psi(x^k)^T d^k = -t_k \nabla\Psi(x^k)^T (H_k^T H_k + \nu_k I)^{-1} \nabla\Psi(x^k). \tag{4.27}$$

Since $\{x^k\}_K \to x^*$, we get from the upper semicontinuity of the C-subdifferential that the sequence $\{H_k\}_K$ is bounded. Without loss of generality, we therefore have $\{H_k\}_K \to H_*$ for some matrix $H_* \in \partial_C \Phi(x^*)$. Since $\nabla\Psi$ is continuous, we also obtain $\{\nabla\Psi(x^k)\}_K \to \nabla\Psi(x^*)$ and therefore $\{\nu_k\}_K \to \nu_*$ with $\nu_* := \|\nabla\Psi(x^*)\| > 0$, cf. (4.25). Using these arguments, it follows that the matrices

$$H_k^T H_k + \nu_k I$$

converge to the symmetric positive definite matrix $H_*^T H_* + \nu_* I$ on the subset $K \subseteq \mathbb{N}$. From (4.26) and (4.27) we therefore obtain

$$\{t_k\}_K \to 0.$$

Now, for each $k \in \mathbb{N}$, let $l_k \in \mathbb{N}$ be the uniquely defined exponent such that $t_k = \beta^{l_k}$. It follows that the Armijo rule in Step (S.3) is not satisfied for $\beta^{l_k - 1}$ for sufficiently large $k \in K$. Hence, we have

$$\frac{\Psi(x^k + \beta^{l_k - 1} d^k) - \Psi(x^k)}{\beta^{l_k - 1}} > \sigma \nabla\Psi(x^k)^T d^k \tag{4.28}$$

for all these $k \in K$. From the Levenberg-Marquardt equation we obtain $\{d^k\}_K \to d^*$, with d^* being the solution of the linear system

$$\big(H_*^T H_* + \nu_* I\big) d = -\nabla\Psi(x^*).$$

Taking into account that $\{d^k\}_K \to d^*$, $\{x^k\}_K \to x^*$ and $\{t_k\}_K \to 0$, we obtain from (4.28) that

$$\nabla\Psi(x^*)^T d^* \geq \sigma \nabla\Psi(x^*)^T d^*.$$

Hence $\nabla\Psi(x^*)^T d^* \geq 0$, since $\sigma \in (0, \frac{1}{2})$.

On the other hand, we have

$$\nabla\Psi(x^*)^T d^* = -\nabla\Psi(x^*)^T (H_*^T H_* + \nu_* I)^{-1} \nabla\Psi(x^*) < 0.$$

This contradiction shows that x^* is a stationary point of Ψ. □

Recall that Theorem 4.8 gives a relatively mild condition for a stationary point of Ψ to be a solution of the complementarity problem (1.3). Furthermore, the existence of a stationary point follows, e.g., under the assumptions of Theorem 4.10 and 4.11.

We next investigate the rate of convergence of Algorithm 4.13. Obviously, this rate of convergence depends on the choice of the Levenberg-Marquardt parameter ν_k.

Theorem 4.15 *Let $\{x^k\}$ be a sequence generated by Algorithm 4.13. Assume that x^* is an accumulation point of $\{x^k\}$ such that x^* is an R-regular solution of the complementarity problem* (1.3)*. Then the following statements hold:*

(a) The entire sequence $\{x^k\}$ converges to x^* if $\{\nu_k\}$ is bounded.

(b) The full stepsize $t_k = 1$ is always accepted for k sufficiently large so that $x^{k+1} = x^k + d^k$ provided that $\nu_k \to 0$.

(c) The rate of convergence is Q-superlinear if $\nu_k \to 0$.

(d) The rate of convergence is Q-quadratic if $\nu_k = O(\|\nabla\Psi(x^k)\|)$ and, in addition, F is an LC^1-function.

Proof. (a) To establish that the entire sequence $\{x^k\}$ converges to x^*, we first note that an R-regular solution is an isolated solution of the complementarity problem, see Lemma 6.13 or [105]. Since Algorithm 4.13 generates a decreasing sequence $\{\Psi(x^k)\}$ and x^* is a solution of the complementarity problem, it follows that the entire sequence $\{\Psi(x^k)\}$ converges to zero. Hence every accumulation point of the sequence $\{x^k\}$ is a solution of (1.3). Consequently, x^* is an isolated accumulation point of the sequence $\{x^k\}$.

Now let $\{x^k\}_K$ denote any subsequence converging to x^*, and note that x^* is a stationary point of Ψ. For all $k \in \mathbb{N}$, we have

$$\|x^{k+1} - x^k\| = t_k \|d^k\| \leq \|d^k\| \leq \|(H_k^T H_k + \nu_k I)^{-1}\| \, \|\nabla\Psi(x)\|.$$

From $\{\nabla\Psi(x^k)\}_K \to 0$, Lemma 4.5 and the assumed boundedness of $\{\nu_k\}$, we immediately obtain $\{\|x^{k+1} - x^k\|\}_K \to 0$. Hence statement (a) follows from [89, Lemma 4.10].

(b), (c) First we prove that

$$\|x^k + d^k - x^*\| = o(\|x^k - x^*\|) \tag{4.29}$$

for all $k \in \mathbb{N}$ sufficiently large. In view of part (a), we know that the entire sequence $\{x^k\}$ converges to the R-regular solution x^*. Hence it follows from Lemma 4.5 that there is a constant $c > 0$ such that

$$\|(H_k^T H_k + \nu_k I)^{-1}\| \leq c \quad \forall k \in \mathbb{N}.$$

Furthermore, the sequence $\{H_k\}$ is bounded. We can therefore assume without loss of generality that we also have

$$\|H_k^T\| \leq c \quad \forall k \in \mathbb{N}.$$

Using Theorem 4.7 and $\Phi(x^*) = 0$, we then obtain for all $k \in \mathbb{N}$ sufficiently large that

$$\begin{aligned}
\|x^k + d^k - x^*\| &= \|x^k - (H_k^T H_k + \nu_k I)^{-1} \nabla \Psi(x^k) - x^*\| \\
&\leq \|(H_k^T H_k + \nu_k I)^{-1}\| \, \|\nabla \Psi(x^k) - (H_k^T H_k + \nu_k I)(x^k - x^*)\| \\
&\leq c \, \|H_k^T \Phi(x^k) - H_k^T H_k (x^k - x^*) - \nu_k (x^k - x^*)\| \\
&= c \, \|H_k^T \big(\Phi(x^k) - \Phi(x^*) - H_k (x^k - x^*)\big) - \nu_k (x^k - x^*)\| \\
&\leq c \, \big(\|H_k^T\| \, \|(\Phi(x^k) - \Phi(x^*) - H_k (x^k - x^*)\| + \nu_k \|x^k - x^*\|\big) \\
&\leq c\big(c\|\Phi(x^k) - \Phi(x^*) - H_k (x^k - x^*)\| + \nu_k \|x^k - x^*\|\big).
\end{aligned}$$

Since Φ is semismooth by Theorem 4.1, it follows that

$$\|\Phi(x^k) - \Phi(x^*) - H_k (x^k - x^*)\| = o(\|x^k - x^*\|),$$

see Proposition 2.13. Using the fact that $\nu_k \to 0$ by assumption, we therefore obtain (4.29).

In order to prove that the full step is eventually accepted, we next show that

$$\lim_{k \to \infty} \frac{\Psi(x^k + d^k)}{\Psi(x^k)} = 0 \tag{4.30}$$

and

$$1 + \sigma \frac{\nabla \Psi(x^k)^T d^k}{\Psi(x^k)} \geq 1 - 2\sigma > 0 \tag{4.31}$$

holds for all sufficiently large $k \in \mathbb{N}$. Since $\Psi(x^k) \neq 0$ for all $k \in \mathbb{N}$, we get from Theorem 4.7 that

$$\begin{aligned}
\frac{\nabla \Psi(x^k)^T d^k}{\Psi(x^k)} &= -\frac{(H_k^T \Phi(x^k))^T (H_k^T H_k + \nu_k I)^{-1} H_k^T \Phi(x_k)}{\frac{1}{2}\|\Phi(x^k)\|^2} \\
&\geq -\frac{\Phi(x^k)^T H_k (H_k^T H_k)^{-1} H_k^T \Phi(x_k)}{\frac{1}{2}\|\Phi(x^k)\|^2} \\
&\geq -\frac{\Phi(x^k)^T \Phi(x_k)}{\frac{1}{2}\|\Phi(x^k)\|^2} \\
&= -2,
\end{aligned} \tag{4.32}$$

for all sufficiently large $k \in \mathbb{N}$. Here, the second inequality in (4.32) follows from the fact that

$$d^T A d \leq \lambda_{\max}(A)\|d\|^2 \quad \forall d \in \mathbb{R}^n$$

holds for all symmetric matrices $A \in \mathbb{R}^{n\times n}$, by noting that the maximal eigenvalue of the symmetric matrix $A := H_k(H_k^T H_k)^{-1}H_k^T$ is equal to one.

Indeed, H_k has full rank for sufficiently large $k \in \mathbb{N}$ and a singular value decomposition $H_k = U_k\hat{\Sigma}_k V_k^T$, where $U_k \in \mathbb{R}^{2n\times 2n}$ and $V_k \in \mathbb{R}^{n\times n}$ are orthogonal matrices, $\hat{\Sigma}_k \in \mathbb{R}^{2n\times n}$ is of the form $\hat{\Sigma}_k = \begin{pmatrix}\Sigma_k \\ 0\end{pmatrix}$, with $\Sigma_k = \operatorname{diag}(\sigma_1, \ldots, \sigma_n) \in \mathbb{R}^n$ a diagonal matrix with positive diagonal elements in decreasing order. Then it holds

$$\begin{aligned} H_k(H_k^T H_k)^{-1}H_k^T =& U_k\hat{\Sigma}_k V_k^T (V_k\hat{\Sigma}_k^T U_k^T U_k\hat{\Sigma}_k V_k^T)^{-1} V_k\hat{\Sigma}_k^T U_k^T \\ =& U_k\hat{\Sigma}_k V_k^T V_k \big(\Sigma_k\Sigma_k\big)^{-1} V_k^T V_k\hat{\Sigma}_k^T U_k^T \\ =& U_k\hat{\Sigma}_k \big(\Sigma_k\big)^{-1}\big(\Sigma_k\big)^{-1}\hat{\Sigma}_k^T U_k^T \\ =& U_k \begin{pmatrix} I & 0 \\ 0 & 0\end{pmatrix} U_k^T. \end{aligned}$$

The inequality (4.31) now follows from (4.32). To verify (4.30), we only have to show that

$$\lim_{k\to\infty} \frac{\|\Phi(x^k + d^k)\|}{\|\Phi(x^k)\|} = 0 \tag{4.33}$$

holds. To this end, we first note that there exists a constant $\alpha > 0$ such that

$$\|\Phi(x^k)\| \geq \alpha\|x^k - x^*\| \tag{4.34}$$

for all $k \in \mathbb{N}$ sufficiently large. This follows from the simple observation that $\|\Phi(x)\| \geq \lambda\|\Phi_{FB}(x)\|$ together with the fact that all elements $V \in \partial\Phi_{FB}(x^*)$ are nonsingular under the R-regularity condition. Using (4.34) and (4.29), we obtain

$$\begin{aligned} \frac{\|\Phi(x^k + d^k)\|}{\|\Phi(x^k)\|} &\leq \frac{\|\Phi(x^k + d^k)\|}{\alpha\|x^k - x^*\|} \\ &= \frac{\|\Phi(x^k + d^k) - \Phi(x^*)\|}{\alpha\|x^k - x^*\|} \\ &\leq \frac{L\|x^k + d^k - x^*\|}{\alpha\|x^k - x^*\|} \\ &\to 0, \end{aligned}$$

where $L > 0$ denotes the local Lipschitz constant of Φ. Hence (4.33) holds.

Using (4.30) and (4.31), we see that the condition

$$\Psi(x^k + d^k) \leq \Psi(x^k) + \sigma\nabla\Psi(x^k)^T d^k$$

or, equivalently,

$$\frac{\Psi(x^k + d^k)}{\Psi(x^k)} \leq 1 + \sigma \frac{\nabla\Psi(x^k)^T d^k}{\Psi(x^k)}$$

is satisfied for all $k \in \mathbb{N}$ sufficiently large. Hence the stepsize $t_k = 1$ is eventually accepted in the line search criterion, and we have $x^{k+1} = x^k + d^k$ for all $k \in \mathbb{N}$ large enough. Hence Q-superlinear convergence of $\{x^k\}$ to x^* follows from (4.29).

(d) The proof is essentially the same as for the local superlinear convergence. We only note that F being an LC^1 function implies that Φ is strongly semismooth by Theorem 4.1, and that the relation

$$\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| = O(\|x^k - x^*\|^2)$$

holds for strongly semismooth functions. □

Note that the previous proof is similar to one given in [56]. We stress, however, that [56] considers a Levenberg-Marquardt-type method for a square system of equations, whereas we are dealing with a nonsquare (overdetermined) system.

4.4 Extension to Mixed Complementarity Problems

In this section, we would like to point out that the approach presented for the standard nonlinear complementarity problem (1.3) can actually be extended to the more general mixed complementarity problem.

In order to present a reformulation of this mixed complementarity problem, let us introduce the following partition of the index set $I := \{1, \ldots, n\}$:

$$\begin{aligned} I_l &:= \{i \in I \mid -\infty < l_i < u_i = \infty\}, \\ I_u &:= \{i \in I \mid -\infty = l_i < u_i < \infty\}, \\ I_{lu} &:= \{i \in I \mid -\infty < l_i < u_i < \infty\}, \\ I_f &:= \{i \in I \mid -\infty = l_i < u_i = \infty\}. \end{aligned} \tag{4.35}$$

We now define the operator $\bar{\Phi} : \mathbb{R}^n \to \mathbb{R}^{2n}$ componentwise as follows ($i = 1, \ldots, n$):

$$\bar{\Phi}_i(x) := \begin{cases} \lambda_1 \phi_{FB}(x_i - l_i, F_i(x)) & \text{if } i \in I_l, \\ -\lambda_1 \phi_{FB}(u_i - x_i, -F_i(x)) & \text{if } i \in I_u, \\ \lambda_1 \phi_{FB}(x_i - l_i, \phi_{FB}(u_i - x_i, -F_i(x))) & \text{if } i \in I_{lu}, \\ -\lambda_1 F_i(x) & \text{if } i \in I_f, \end{cases} \tag{4.36}$$

$$\bar{\Phi}_{n+i}(x) := \begin{cases} \lambda_2 \phi_+(x_i - l_i, F_i(x)) & \text{if } i \in I_l, \\ \lambda_2 \phi_+(u_i - x_i, -F_i(x)) & \text{if } i \in I_u, \\ \lambda_2(\phi_+(x_i - l_i, F_i(x)) + \phi_+(u_i - x_i, -F_i(x))) & \text{if } i \in I_{lu}, \\ -\lambda_2 F_i(x) & \text{if } i \in I_f. \end{cases}$$

Note that the first n components of $\bar{\Phi}$ correspond to the Fischer-Burmeister-type reformulation of the mixed complementarity problem first introduced by Billups [4] and further investigated in [33]. The last n components are again used in order to reduce the complementarity gap at the current point x. Further in this section we will often make use of the following notation:

$$\begin{aligned} \bar{\Phi}_{FB,i}(x^*) &:= \frac{1}{\lambda_1}\bar{\Phi}_i(x^*) \quad \forall i \in \{1, \ldots, n\}, \\ \bar{\Phi}_{+,i}(x^*) &:= \frac{1}{\lambda_2}\bar{\Phi}_{n+i}(x^*) \quad \forall i \in \{1, \ldots, n\}. \end{aligned} \tag{4.37}$$

It follows in a relatively simple way that the mixed complementarity problem is equivalent to the overdetermined system of equations $\bar{\Phi}(x) = 0$. The proof is a simple extension of that given in [4, Prop. 3.2.7].

Proposition 4.16 *x^* is a solution of the mixed complementarity problem if and only if x^* solves the nonlinear overdetermined system of equations $\bar{\Phi}(x) = 0$.*

Proof. If x^* solves MCP(F, l, u), then for any $i \in I$, one of the following cases holds:

$$\begin{array}{lllll} \textit{Case 1:} & x_i^* = l_i & \text{and} & F_i(x^*) > 0, \\ \textit{Case 2:} & x_i^* = u_i & \text{and} & F_i(x^*) < 0, \\ \textit{Case 3:} & x_i^* \in [l_i, u_i] & \text{and} & F_i(x^*) = 0. \end{array}$$

If the first case holds for some i, then $i \in I_l$ or $i \in I_{lu}$. For $i \in I_l$ we obtain $\bar{\Phi}_i(x^*) = 0$ and $\bar{\Phi}_{n+i}(x^*) = 0$, since $\phi_{FB}(x_i^* - l_i, F_i(x^*)) = 0$ and $\phi_+(x_i^* - l_i, F_i(x^*)) = 0$. Further we have $u_i - x_i^* > 0$ and $-F_i(x^*) < 0$, which implies $\phi_{FB}(u_i - x_i^*, -F_i(x^*)) > 0$. Thus,

$$\phi_{FB}(x_i^* - l_i, \phi_{FB}(u_i - x_i^*, -F_i(x^*))) = 0,$$

since $x_i^* - l_i = 0$, and so $\bar{\Phi}_i(x^*) = 0$ for $i \in I_{lu}$. For $i \in I_{lu}$ it also follows that $\bar{\Phi}_{n+i}(x^*) = 0$, since $\phi_+(x_i^* - l_i, F_i(x^*)) = 0$ and $\phi_+(u_i - x_i^*, -F_i(x^*)) = 0$ for Case 1.

If the second case holds for some i, then $i \in I_u$ or $i \in I_{lu}$. For $i \in I_{lu}$ we obtain $\bar{\Phi}_i(x^*) = 0$, since $\phi_{FB}(u_i - x_i^*, -F_i(x^*)) = 0$ and $x_i^* - l_i > 0$. Furthermore, we have $\bar{\Phi}_{n+i}(x^*) = 0$, since $(x_i^* - l_i)_+(F_i(x^*))_+ = 0$ and $(u_i - x_i^*)_+(-F_i(x^*))_+ = 0$. For $i \in I_u$ we have $\bar{\Phi}_i(x^*) = 0$ and $\bar{\Phi}_{n+i}(x^*) = 0$, since $\phi_{FB}(u_i - x_i^*, -F_i(x^*)) = 0$ and $(x_i^* - l_i)_+(F_i(x^*))_+ = 0$.

Assume that the third case holds for some i. If $i \in I_f$, we obtain $\bar{\Phi}_i(x^*) = 0$ and $\bar{\Phi}_{n+i}(x^*) = 0$, since $F_i(x^*) = 0$. Further $u_i - x_i^* \geq 0$ and $-F_i(x^*) = 0$ holds, thus $\phi_{FB}(u_i - x_i^*, -F_i(x^*)) = 0$ and therefore also

$$\phi_{FB}(x^* - l_i, \phi_{FB}(u_i - x_i^*, -F_i(x^*))) = 0,$$

since $x^* - l_i \geq 0$. Thus, for $i \in I_u$ or $i \in I_{lu}$ we have $\bar{\Phi}_i(x^*) = 0$ and since $F_i(x^*) = 0$ holds in Case 3, also $\bar{\Phi}_{n+i}(x^*) = 0$ holds. For $i \in I_l$ we obtain $\bar{\Phi}_i(x^*) = 0$ and $\bar{\Phi}_{n+i}(x^*) = 0$, since $x_i^* - l_i \geq 0$ and $F_i(x^*) = 0$.

To prove the opposite direction, let us first consider an index $i \in I_l$. Since $\bar{\Phi}_i(x^*) = 0$, we have $x_i^* - l_i \geq 0, F_i(x^*) \geq 0$ and $(x_i^* - l_i)F_i(x^*) = 0$. Thus, either Case 1 or Case 3 occurs. From $\bar{\Phi}_i(x^*) = 0$ for $i \in I_u$, it follows that $u_i - x_i^* \geq 0, -F_i(x^*) \geq 0$ and $(u_i - x_i^*)F_i(x^*) = 0$. Thus, either Case 2 or Case 3 holds. If $i \in I_f$ and $\bar{\Phi}_i(x^*) = 0$, we directly obtain Case 3. If $i \in I_{lu}$ and $\bar{\Phi}_i(x^*) = 0$, then we have either

$$\text{(a):} \quad x_i^* - l_i > 0 \text{ and } \phi_{FB}(u_i - x_i^*, -F_i(x^*)) = 0$$

or

$$\text{(b):} \quad x_i^* - l_i = 0 \text{ and } \phi_{FB}(u_i - x_i^*, -F_i(x^*)) \geq 0.$$

If (a) holds, the complementarity conditions $u_i - x_i^* \geq 0, F_i(x^*) \leq 0, (u_i - x_i^*)F_i(x^*) = 0$, are satisfied, which in turn, imply either Case 2 or Case 3.

If (b) holds, $u_i - x_i^* = u_i - l_i > 0$. Thus, since ϕ_{FB} is negative only on the positive orthant (see Figure 4.1), we see that $-F(x^*) \leq 0$. Thus, the complementarity condition $x_i^* - l_i \geq 0, F_i(x^*) \geq 0, (x_i^* - l_i)F_i(x^*) = 0$ holds. Hence either Case 1 or Case 3 holds. □

We next analyze the structure of the C-subdifferential of the operator $\bar{\Phi}$.

Proposition 4.17 *Let $x \in \mathbb{R}^n$. Then any matrix $H \in \partial_C \bar{\Phi}(x)$ has the representation*

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix},$$

where

$$H_1 \in \{D_a(x) + D_b(x)F'(x)\} \quad \textit{and} \quad H_2 \in \{\tilde{D}_a(x) + \tilde{D}_b(x)F'(x)\},$$

and $D_a(x) \in \mathbb{R}^{n \times n}$ and $D_b(x) \in \mathbb{R}^{n \times n}$ are diagonal matrices whose diagonal elements are defined as follows:
(a) If $i \in I_l$, then if $(x_i - l_i, F_i(x)) \neq (0, 0)$,

$$D_a(x)_{ii} = \frac{x_i - l_i}{\|(x_i - l_i, F_i(x))\|} - 1,$$
$$D_b(x)_{ii} = \frac{F_i(x)}{\|(x_i - l_i, F_i(x))\|} - 1,$$

but if $(x_i - l_i, F_i(x)) = (0, 0)$,

$$(D_a(x)_{ii}, D_b(x)_{ii}) \in \{(\xi - 1, \zeta - 1) \in \mathbb{R}^2 \mid \|(\xi, \zeta)\| \leq 1\}.$$

Further, if $x_i > l_i$ and $F_i(x) > 0$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= F_i(x), \\ \tilde{D}_b(x)_{ii} &= x_i - l_i, \end{aligned}$$

if $x_i > l_i$ *and* $F_i(x) = 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(0, \zeta(x_i - l_i)) \in \mathbb{R}^2 \mid \zeta \in [0,1]\},$$

if $x_i = l_i$ *and* $F_i(x) > 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(\xi F_i(z), 0) \in \mathbb{R}^2 \mid \xi \in [0,1]\},$$

but if $x_i < l_i$ *or* $F_i(x) < 0$, *or if* $(x_i - l_i, F_i(x)) = (0,0)$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= 0, \\ \tilde{D}_b(x)_{ii} &= 0. \end{aligned}$$

(b) If $i \in I_u$, *then if* $(u_i - x_i, F_i(x)) \neq (0,0)$,

$$\begin{aligned} D_a(x)_{ii} &= \frac{u_i - x_i}{\|(u_i - x_i, F_i(x))\|} - 1, \\ D_b(x)_{ii} &= \frac{-F_i(x)}{\|(u_i - x_i, F_i(x))\|} - 1, \end{aligned}$$

but if $(u_i - x_i, F_i(x)) = (0,0)$,

$$(D_a(x)_{ii}, D_b(x)_{ii}) \in \{(\xi - 1, \zeta - 1) \in \mathbb{R}^2 \mid \|(\xi, \zeta)\| \leq 1\}.$$

Further, if $x_i < u_i$ *and* $F_i(x) < 0$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= F_i(x), \\ \tilde{D}_b(x)_{ii} &= x_i - u_i, \end{aligned}$$

if $x_i < u_i$ *and* $F_i(x) = 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(0, \zeta(x_i - u_i)) \in \mathbb{R}^2 \mid \zeta \in [0,1]\},$$

if $x_i = u_i$ *and* $F_i(x) < 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(\xi F_i(z), 0) \in \mathbb{R}^2 \mid \xi \in [0,1]\},$$

but if $u_i < x_i$ *or* $F_i(x) > 0$, *or if* $(u_i - x_i, F_i(x)) = (0,0)$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= 0, \\ \tilde{D}_b(x)_{ii} &= 0. \end{aligned}$$

(c) If $i \in I_{lu}$, *then, for certain* $a_i(x), b_i(x), c_i(x), d_i(x) \in \mathbb{R}$ *defined below, it holds*

$$\begin{aligned} D_a(x)_{ii} &= a_i(x) + b_i(x)c_i(x), \\ D_b(x)_{ii} &= b_i(x)d_i(x). \end{aligned}$$

If $(x_i - l_i, F_i(x)) \neq (0,0)$,

$$a_i(x) = \frac{x_i - l_i}{\|(x_i - l_i, \phi_{FB}(u_i - x_i, -F_i(x)))\|} - 1,$$
$$b_i(x) = \frac{\phi_{FB}(u_i - x_i, -F_i(x)}{\|(x_i - l_i, \phi_{FB}(u_i - x_i, -F_i(x)))\|} - 1,$$

but if $(x_i - l_i, F(x)) = (0,0)$,

$$(a_i(x), b_i(x)) \in \{(\xi - 1, \zeta - 1) \in \mathbb{R}^2 \mid \|(\xi, \zeta)\| \leq 1\}.$$

Further, if $(u_i - x_i, F(x)) \neq (0,0)$,

$$c_i(x) = \frac{x_i - u_i}{\|(u_i - x_i, F_i(x))\|} + 1, \quad d_i(x) = \frac{F_i(x)}{\|(u_i - x_i, F_i(x))\|} + 1,$$

but if $(u_i - x_i, F(x)) = (0,0)$,

$$(c_i(x), d_i(x)) \in \{(\xi + 1, \zeta + 1) \in \mathbb{R}^2 | \|(\xi, \zeta)\| \leq 1\}.$$

Further, if $x_i < u_i$ *and* $F_i(x) < 0$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= F_i(x), \\ \tilde{D}_b(x)_{ii} &= x_i - u_i, \end{aligned}$$

if $x_i > l_i$ *and* $F_i(x) > 0$

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= F_i(x), \\ \tilde{D}_b(x)_{ii} &= x_i - l_i, \end{aligned}$$

if $x_i = l_i$ *and* $F_i(x) > 0$ *or* $x_i = u_i$ *and* $F_i(x) < 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(\xi F_i(x), 0) \in \mathbb{R}^2 \mid \xi \in [0,1]\}.$$

Further, if $x_i > u_i$ *and* $F_i(x) < 0$, *or, if* $x_i < l_i$ *and* $F_i(x) > 0$,

$$\begin{aligned} \tilde{D}_a(x)_{ii} &= 0, \\ \tilde{D}_b(x)_{ii} &= 0. \end{aligned}$$

If $x_i \leq l_i$ *and* $F_i(x) = 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(0, \zeta(x_i - u_i)) \in \mathbb{R}^2 \mid \zeta \in [0,1]\},$$

if $l_i < x_i < u_i$ *and* $F_i(x) = 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(0, \xi(x_i - l_i) + \zeta(x_i - u_i)) \in \mathbb{R}^2 \mid \xi, \zeta \in [0,1]\},$$

if $x_i \geq u_i$ *and* $F_i(x) = 0$,

$$(\tilde{D}_a(x)_{ii}, \tilde{D}_b(x)_{ii}) \in \{(0, \zeta(x_i - l_i)) \in \mathbb{R}^2 \mid \zeta \in [0,1]\}.$$

(d) If $i \in I_f$, *then* $D_a(x)_{ii} = 0 = \tilde{D}_a(x)_{ii}$ *and* $D_b(x)_{ii} = -1 = \tilde{D}_b(x)_{ii}$.

Proof. Taking into account the definition of $\bar{\Phi}$ using the different index sets I_l, I_u, I_{lu}, I_f and Lemma 4.2 the computation of the elements of $D_a(x), D_b(x), \tilde{D}_a(x)$ and $\tilde{D}_b(x)$ is rather tedious, but straightforward (see also [4, Lem. 3.2.10]). Note that the C-subdifferential exists, since all component functions of $\bar{\Phi}$ are locally Lipschitz continuous. □

We now investigate the properties of the merit function

$$\bar{\Psi}(x) := \frac{1}{2}\|\bar{\Phi}(x)\|^2, \tag{4.38}$$

and the properties of the associated operator $\bar{\Phi}$.

Theorem 4.18 *If $F : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable, then the following statements hold:*

(a) The mapping $\bar{\Phi}$ from (4.36) is semismooth. If, in addition, F is an LC^1 function, then $\bar{\Phi}$ is strongly semismooth.

(b) The merit function $\bar{\Psi}$ from (4.38) is continuously differentiable with $\nabla\bar{\Psi}(x) = H^T\bar{\Phi}(x)$, where $H \in \partial_C\bar{\Phi}(x)$ can be chosen arbitrarily.

Proof. (a) Since $\bar{\Phi}$ is (strongly) semismooth if and only if all component functions are (strongly) semismooth and since the composite of (strongly) semismooth functions is (strongly) semismooth (see Proposition 2.21), we obtain the above result as an immediate consequence of the fact that ϕ_{FB} and ϕ_+ are strongly semismooth.

(b) The merit function $\bar{\Psi}$ is locally Lipschitz continuous, since it is the composite of the locally Lipschitz continuous mapping $\bar{\Phi}$ and the Lipschitz continuous square Euclidean norm function. Hence its generalized gradient exists, and using the relaxed chain rule from Corollary 2.7 we obtain:

$$\partial\bar{\Psi}(x) \subseteq \{H^T\bar{\Phi}(x) \mid H \in \partial_C\bar{\Phi}(x)\} =: \partial_C\bar{\Phi}(x)^T\bar{\Phi}(x).$$

Now we show that the set $\partial_C\bar{\Phi}(x)^T\bar{\Phi}(x)$ consists only of one element because the zero components of $\bar{\Phi}(x)$ cancel out the possibly multivalued columns of $\partial_C\bar{\Phi}(x)^T$. Let $x \in \mathbb{R}^n$ be arbitrary, define $\mathcal{K} := \{(a,b) \in \mathbb{R}^2 \mid ab = 0, a \geq 0, b \geq 0\} \setminus (0,0)$ and the following index sets associated with x:

$$\begin{array}{ll}
J_l^0 := \{i \in I_l \mid (x_i - l_i, F_i(x)) = (0,0)\}, & \bar{J}_l^0 := I_l \setminus J_l^0, \\
J_u^0 := \{i \in I_u \mid (u_i - x_i, -F_i(x)) = (0,0)\}, & \bar{J}_u^0 := I_u \setminus J_u^0, \\
J_{lu}^0 := \{i \in I_{lu} \mid (x_i - l_i, F_i(x)) = (0,0) \text{ or } (u_i - x_i, -F_i(x)) = (0,0)\}, & \bar{J}_{lu}^0 := I_{lu} \setminus J_{lu}^0, \\
J_l^+ := \{i \in I_l \mid (x_i - l_i, F_i(x)) \in \mathcal{K}\}, & \bar{J}_l^+ := I_l \setminus J_l^+, \\
J_u^+ := \{i \in I_u \mid (u_i - x_i, -F_i(x)) \in \mathcal{K}\}, & \bar{J}_u^+ := I_u \setminus J_u^+, \\
J_{lu}^+ := \{i \in I_{lu} \mid (x_i - l_i, F_i(x)) \in \mathcal{K} \text{ or } (u_i - x_i, -F_i(x)) \in \mathcal{K}\}, & \bar{J}_{lu}^+ := I_{lu} \setminus J_{lu}^+.
\end{array}$$

Then for all $i \in \bar{J}_l^0 \cup \bar{J}_u^0 \cup \bar{J}_{lu}^0 \cup I_f =: D_{FB}$ the i-th component function $\bar{\Phi}_i$ is continuously differentiable and

$$\partial\bar{\Phi}_i(x) = \{\nabla\bar{\Phi}_i(x)\}$$

holds, for all these i. On the other hand,

$$\bar{\Phi}_i(x) = 0, \quad \text{for all } i \in J_l^0 \cup J_u^0 \cup J_{lu}^0 =: \Theta_{FB}.$$

For all $i \in \bar{J}_l^+ \cup \bar{J}_u^+ \cup \bar{J}_{lu}^+ \cup I_f =: D_+$ the $(n+i)$-th component function of $\bar{\Phi}$ is continuously differentiable and

$$\partial\bar{\Phi}_{n+i}(x) = \{\nabla\bar{\Phi}_{n+i}(x)\}$$

holds, for all these i, in view of Proposition 4.17. On the other hand, it is not difficult to see that for all $i \in J_l^+ \cup J_u^+ \cup J_{lu}^+ =: \Theta_+$

$$\bar{\Phi}_i(x) = 0$$

holds. Taking these observations into account we can see that the set

$$\begin{aligned}
&\partial_C\bar{\Phi}(x)^T\bar{\Phi}(x)\\
&= \Big\{ \sum_{i=1}^{n} \bar{\Phi}_i(x)H_i + \sum_{i=1}^{n} \bar{\Phi}_{n+i}(x)H_{n+i} \mid H_i \in \partial\bar{\Phi}_i(x), i \in \{1,2,\ldots,2n\} \Big\}\\
&= \Big\{ \sum_{i\in\Theta_{FB}} \underbrace{\bar{\Phi}_i(x)}_{=0}\partial\bar{\Phi}_i(x) + \sum_{i\in D_{FB}} \bar{\Phi}_i(x)\nabla\bar{\Phi}_i(x) + \sum_{i\in\Theta_+} \underbrace{\bar{\Phi}_{n+i}(x)}_{0}\partial\bar{\Phi}_{n+i}(x) + \sum_{i\in D_+} \bar{\Phi}_{n+i}(x)\nabla\bar{\Phi}_{n+i}(x) \Big\}\\
&= \Big\{ \sum_{i\in D_{FB}} \bar{\Phi}_i(x)\nabla\bar{\Phi}_i(x) + \sum_{i\in D_+} \bar{\Phi}_{n+i}(x)\nabla\bar{\Phi}_{n+i}(x) \Big\}
\end{aligned}$$

consists only of one element.

The assertion therefore follows from the fact that a locally Lipschitz continuous function is continuously differentiable if and only if its generalized gradient is a singleton at every point. □

In order to prove fast local convergence towards a solution x^* of the mixed complementarity problem we need to show that every element $H \in \partial_C\bar{\Phi}(x^*)$ has full rank n under a suitable regularity condition. This assumption will be the strong regularity condition in the sense of Robinson [105], restated in the context of mixed complementarity problems, using yet another partition of $I = \{1,\ldots,n\}$:

$$\begin{aligned}
\alpha &:= \{i \in I \mid l_i < x_i^* < u_i, F_i(x^*) = 0\},\\
\beta &:= \{i \in I \mid x_i^* \in \{l_i, u_i\}, F_i(x^*) = 0\},\\
\gamma &:= \{i \in I \mid x_i^* \in \{l_i, u_i\}, F_i(x^*) \neq 0\}.
\end{aligned}$$

This condition will also be called R-regularity to be consistent with the analogous concept for standard complementarity problems.

Definition 4.19 *A solution of the mixed complementarity problem is called R-regular if the submatrix $F'(x^*)_{\alpha\alpha}$ is nonsingular and the Schur complement*

$$F'(x^*)_{\beta\beta} - F'(x^*)_{\beta\alpha}F'(x^*)_{\alpha\alpha}^{-1}F'(x^*)_{\alpha\beta}$$

is a P-matrix.

Note that, in the case of a nonlinear complementarity problem (i.e., $l_i = 0$ and $u_i = \infty$ for all $i \in I$), the two R-regularity conditions coincide. We stress that the original definition of strong regularity from [105] is different, but it was shown in [27] that the two definitions are equivalent.

Theorem 4.20 *If x^* is a strongly regular solution of the mixed complementarity problem, then all elements $H \in \partial_C \bar{\Phi}(x^*)$ are nonsingular.*

Proof. Let $H \in \partial_C \bar{\Phi}(x^*)$. In view of Proposition 4.17, we have

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix},$$

where H_1 is an element from $\partial_C \bar{\Phi}_{FB}(x^*)$ (here we used the notation from (4.37)). It now follows from [33, Thm. 2.7] that each element $H_1 \in \partial_C \bar{\Phi}_{FB}(x^*)$ is nonsingular under the assumed strong regularity condition. Therefore we have $\operatorname{rank}(H) = n$, i.e., H has full rank. □

Lemma 4.21 *Let $x \in \mathbb{R}^n$ be arbitrary and $H \in \partial_C \bar{\Phi}(x)$, where $H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix}$, $H_1 = D_a(x) + D_b(x)F'(x)$ and $H_2 = \tilde{D}_a(x) + \tilde{D}_b(x)F'(x)$, with diagonal matrices $D_a(x)$, $D_b(x)$, $\tilde{D}_a(x)$, $\tilde{D}_b(x) \in \mathbb{R}^{n \times n}$ as defined in Proposition 4.17. Further define*

$$u_i(x) := \lambda_1^2 D_a(x)_{ii} \bar{\Phi}_i(x) + \lambda_2^2 \tilde{D}_a(x)_{ii} \bar{\Phi}_{n+i}(x)$$

and

$$v_i(x) := \lambda_1^2 D_b(x)_{ii} \bar{\Phi}_i(x) + \lambda_2^2 \tilde{D}_b(x)_{ii} \bar{\Phi}_{n+i}(x)$$

for all $i \in I$. Further we denote $I_{\bar{f}} := I \setminus I_f$. Then the following statements hold:

(a) For all $i \in I_{\bar{f}}$,

$$\big(D_a(x)_{ii} \bar{\Phi}_i(x)\big)\big(D_b(x)_{ii} \bar{\Phi}_i(x)\big) \geq 0, \tag{4.39}$$

$$\big(D_a(x)_{ii} \bar{\Phi}_i(x)\big)\big(\tilde{D}_a(x)_{ii} \bar{\Phi}_{n+i}(x)\big) \geq 0, \tag{4.40}$$

$$\big(D_b(x)_{ii} \bar{\Phi}_i(x)\big)\big(\tilde{D}_b(x)_{ii} \bar{\Phi}_{n+i}(x)\big) \geq 0. \tag{4.41}$$

(b) For all $i \in I_{\bar{f}}$, $u_i(x) = 0 \iff \bar{\Phi}_i(x) \iff v_i = 0$.

(c) For all $i \in I_{\bar{f}}$, $u_i(x) v_i(x) \geq 0$.

Proof. (a) Considering the three cases $i \in I_l, i \in I_u, i \in I_{lu}$ separately, it is easy to see that $D_a(x)_{ii} \leq 0$ and $D_b(x)_{ii} \leq 0$. Hence (4.39) holds, since

$$\big(D_a(x)_{ii} \bar{\Phi}_i(x)\big)\big(D_b(x)_{ii} \bar{\Phi}_i(x)\big) = D_a(x)_{ii} D_b(x)_{ii} \bar{\Phi}_i^2(x) \geq 0.$$

To establish (4.40) and (4.41), we consider these three cases separately.

Case 1: $i \in I_{lu}$.
If $i \in J_l := \{i : x_i > l_i \text{ and } F_i(x) > 0\}$, we have $\bar{\Phi}_{n+i}(x) > 0$ and by Proposition 4.17

$$\tilde{D}_a(x)_{ii} = F_i(x) > 0,$$
$$\tilde{D}_b(x)_{ii} = x_i - l_i > 0.$$

Thus

$$\tilde{D}_a(x)_{ii}\bar{\Phi}_{n+i}(x) \geq 0 \quad \text{and} \quad \tilde{D}_b(x)_{ii}\bar{\Phi}_{n+i}(x) \geq 0. \tag{4.42}$$

On the other hand,

$$\bar{\Phi}_i(x) = \lambda_1 \phi_{FB}(x_i - l_i, \underbrace{\phi_{FB}(u_i - x_i, -F_i(x))}_{>0}) < 0,$$

since the Fischer-Burmeister function is negative on $\{(a,b) \in \mathbb{R}^2 : a > 0, b > 0\}$ and positive on $\mathbb{R}^2 \setminus \{(a,b) \in \mathbb{R}^2 : a \geq 0, b \geq 0\}$. Since $D_a(x)_{ii} \leq 0$ and $D_b(x)_{ii} \leq 0$, we have

$$D_a(x)_{ii}\bar{\Phi}_i(x) \geq 0 \quad \text{and} \quad D_b(x)_{ii}\bar{\Phi}_i(x) \geq 0. \tag{4.43}$$

From (4.42) and (4.43) we obtain both (4.40) and (4.41).
If $i \in J_u := \{i : x_i < u_i \text{ and } F_i(x) < 0\}$, we have $\bar{\Phi}_{n+i}(x) > 0$ and by Proposition 4.17

$$\tilde{D}_a(x)_{ii} = F_i(x) < 0,$$
$$\tilde{D}_b(x)_{ii} = x_i - u_i < 0.$$

Thus

$$\tilde{D}_a(x)_{ii}\bar{\Phi}_{n+i}(x) \leq 0 \quad \text{and} \quad \tilde{D}_b(x)_{ii}\bar{\Phi}_{n+i}(x) \leq 0. \tag{4.44}$$

On the other hand,

$$\bar{\Phi}_i(x) = \lambda_1 \phi_{FB}(x_i - l_i, \underbrace{\phi_{FB}(u_i - x_i, -F_i(x))}_{<0}) > 0.$$

This implies

$$D_a(x)_{ii}\bar{\Phi}_i(x) \leq 0 \quad \text{and} \quad D_b(x)_{ii}\bar{\Phi}_i(x) \leq 0, \tag{4.45}$$

since $D_a(x)_{ii} \leq 0$ and $D_b(x)_{ii} \leq 0$. The inequalities (4.44) and (4.45) now imply (4.40) and (4.41).
If $i \notin J_l \cup J_u$ then $\bar{\Phi}_{n+i}(x) = 0$, thus (4.40) and (4.41) hold trivially.
Case 2: $i \in I_l$.
The subcase $i \in J_l = \{i : x_i > l_i \text{ and } F_i(x) > 0\}$, can be shown very similar to the one shown above. For $i \notin J_l$, $\bar{\Phi}_{n+i}(x) = 0$. This immediately implies (4.40) and (4.41).
Case 3: $i \in I_u$.
For $i \in J_u = \{i : x_i > u_i \text{ and } F_i(x) < 0\}$ we can argue similarly as in Case 1. For $i \notin J_u$, $\bar{\Phi}_{n+i}(x) = 0$, thus (4.40) and (4.41) hold.

(b) If $\bar{\Phi}_i(x) = 0$ for $i \in I_{\bar{f}}$, we also have $\bar{\Phi}_{n+i}(x) = 0$ (see Proposition 4.16). Thus $u_i(x) = 0$ and $v_i(x) = 0$ follow immediately.
Conversely, assume that $u_i(x) = 0$ for some index $i \in I_{\bar{f}}$ (the proof is analogous if $v_i(x) = 0$ and we omit the details). Since the two summands of $u_i(x)$ have the same sign by (4.40), we must have $D_a(x)_{ii}\bar{\Phi}_i(x) = 0$ and therefore $D_a(x)_{ii} = 0$ or $\bar{\Phi}_i(x) = 0$. Suppose that $D_a(x)_{ii} = 0$ (in the later case, there is nothing to show). We distinguish three cases:
Case 1: $i \in I_l$.
If $(x_i - l_i, F_i(x)) = (0, 0)$, then $\bar{\Phi}_i(x) = 0$ follows immediately. Otherwise, due to the definition of $D_a(x)_{ii}$ in Proposition 4.17, we have

$$0 = \frac{x_i - l_i}{\|(x_i - l_i, F_i(x))\|} - 1,$$

which implies $x_i > l_i$ and $F_i(x) = 0$, so that $\bar{\Phi}_i(x) = 0$.
Case 2: $i \in I_u$.
This case is analogous to the above Case 1.
Case 3: $i \in I_{lu}$.
If $(x_i - l_i, F_i(x)) = (0, 0)$, then $(x_i - l_i, \phi_{FB}(u_i - x_i, -F_i(x))) = (0, 0)$ and $\bar{\Phi}_i(x) = 0$ follows from the definition of the operator $\bar{\Phi}$. Otherwise, we have

$$0 = D_a(x)_{ii} = a_i(x) + b_i(x)c_i(x),$$

with certain numbers $a_i(x) \le 0$, $b_i(x) \le 0$, $c_i(x) \ge 0$ specified in Proposition 4.17 (c). Since the sum of two nonpositive expressions can be zero only if both expressions are zero, we have in particular $a_i(x) = 0$. In view of the definition of $a_i(x)$, this implies that $x_i - l_i > 0$ and $\phi_{FB}(u_i - x_i, -F_i(x)) = 0$. Thus $\bar{\Phi}_i(x) = 0$.

(c) The inequalities (4.39)–(4.40) imply that the two summands in $u_i(x)$ and $v_i(x)$ have the same sign for all $i \in I_{\bar{f}}$. Thus statement (c) hold. □

In the following result we will use the shortcut $\nabla F(x^*)_{ff}$ to denote the submatrix $\nabla F(x^*)_{I_f I_f}$. A similar notation is used for submatrices and subvectors defined by other index sets.

Theorem 4.22 *Let $x^* \in \mathbb{R}^n$ be a stationary point of $\bar{\Psi}$. Assume that*

(a) the principal submatrix $\nabla F(x^*)_{ff}$ is nonsingular, and

(b) the Schur complement $\nabla F(x^*)/\nabla F(x^*)_{ff}$ is a P_0-matrix.

Then x^* is a solution of the mixed complementarity problem.

Proof. Let x^* be a stationary point of $\bar{\Psi}$. Then by Proposition 4.18 (b) we have

$$\nabla\bar{\Psi}(x^*) = H^T\bar{\Phi}(x^*) = 0, \tag{4.46}$$

for an arbitrary $H \in \partial_C \bar{\Phi}(x^*)$. By Proposition 4.17, there exist diagonal matrices $D_a(x^*)$, $D_b(x^*)$, $\tilde{D}_a(x^*)$ and $\tilde{D}_b(x^*)$, such that the matrix $H \in \partial_C \bar{\Phi}(x^*)$ has the representation

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix},$$

with

$$H_1 = D_a(x^*) + D_b(x^*)F'(x^*) \quad \text{and} \quad H_2 = \tilde{D}_a(x^*) + \tilde{D}_b(x^*)F'(x^*).$$

Using the notation (4.37) we have

$$\bar{\Phi}(x^*) = \begin{pmatrix} \lambda_1 \bar{\Phi}_{FB}(x^*) \\ \lambda_2 \bar{\Phi}_{+}(x^*) \end{pmatrix},$$

and (4.46) therefore becomes

$$\lambda_1^2(D_a(x^*) + \nabla F(x^*)D_b(x^*))\bar{\Phi}_{FB}(x^*) + \lambda_2^2(\tilde{D}_a(x^*) + \nabla F(x^*)\tilde{D}_b(x^*))\bar{\Phi}_{+}(x^*) = 0. \quad (4.47)$$

Writing

$$D_a(x^*) = \begin{pmatrix} D_a(x^*)_{ff} & D_a(x^*)_{f\bar{f}} \\ D_a(x^*)_{\bar{f}f} & D_a(x^*)_{\bar{f}\bar{f}} \end{pmatrix}, \quad \tilde{D}_a(x^*) = \begin{pmatrix} \tilde{D}_a(x^*)_{ff} & \tilde{D}_a(x^*)_{f\bar{f}} \\ \tilde{D}_a(x^*)_{\bar{f}f} & \tilde{D}_a(x^*)_{\bar{f}\bar{f}} \end{pmatrix},$$

$$D_b(x^*) = \begin{pmatrix} D_b(x^*)_{ff} & D_b(x^*)_{f\bar{f}} \\ D_b(x^*)_{\bar{f}f} & D_b(x^*)_{\bar{f}\bar{f}} \end{pmatrix}, \quad \tilde{D}_b(x^*) = \begin{pmatrix} \tilde{D}_b(x^*)_{ff} & \tilde{D}_b(x^*)_{f\bar{f}} \\ \tilde{D}_b(x^*)_{\bar{f}f} & \tilde{D}_b(x^*)_{\bar{f}\bar{f}} \end{pmatrix}$$

and

$$\nabla F(x^*) = \begin{pmatrix} \nabla F(x^*)_{ff} & \nabla F(x^*)_{f\bar{f}} \\ \nabla F(x^*)_{\bar{f}f} & \nabla F(x^*)_{\bar{f}\bar{f}} \end{pmatrix},$$

where $I_{\bar{f}} = I \setminus I_f$, and taking into account that

$$\begin{aligned} D_a(x^*)_{ii} &= 0 = \tilde{D}_a(x^*)_{ii}, \quad i \in I_f, \\ D_b(x^*)_{ii} &= -1 = \tilde{D}_b(x^*)_{ii}, \quad i \in I_f, \end{aligned}$$

by Proposition 4.17 (d), we can rewrite (4.47) as

$$\begin{aligned} 0 =& \lambda_1^2\big(- \nabla F(x^*)_{ff}\bar{\Phi}_{FB}(x^*)_f + \nabla F(x^*)_{f\bar{f}} D_b(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{FB}(x^*)_{\bar{f}}\big) \\ &+ \lambda_2^2\big(- \nabla F(x^*)_{ff}\bar{\Phi}_{+}(x^*)_f + \nabla F(x^*)_{f\bar{f}}\tilde{D}_b(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{+}(x^*)_{\bar{f}}\big), \end{aligned} \quad (4.48)$$

$$\begin{aligned} 0 =& \lambda_1^2\big(D_a(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{FB}(x^*)_{\bar{f}} - \nabla F(x^*)_{\bar{f}f}\bar{\Phi}_{FB}(x^*)_f + \nabla F(x^*)_{\bar{f}\bar{f}} D_b(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{FB}(x^*)_{\bar{f}}\big) \\ &+ \lambda_2^2\big(\tilde{D}_a(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{+}(x^*)_{\bar{f}} - \nabla F(x^*)_{\bar{f}f}\bar{\Phi}_{+}(x^*)_f + \nabla F(x^*)_{\bar{f}\bar{f}}\tilde{D}_b(x^*)_{\bar{f}\bar{f}}\bar{\Phi}_{+}(x^*)_{\bar{f}}\big). \end{aligned} \quad (4.49)$$

In order to simplify the notation we define

$$u_i(x^*) := \lambda_1^2 D_a(x^*)_{ii}\bar{\Phi}_{FB,i}(x^*) + \lambda_2^2 \tilde{D}_a(x^*)_{ii}\bar{\Phi}_{+,i}(x^*)$$

and

$$v_i(x^*) := \lambda_1^2 D_b(x^*)_{ii}\bar{\Phi}_{FB,i}(x^*) + \lambda_2^2 \tilde{D}_b(x^*)_{ii}\bar{\Phi}_{+,i}(x^*)$$

for all $i \in I$, as in Lemma 4.21. Since $\nabla F(x^*)_{ff}$ is assumed to be nonsingular, we obtain from (4.48):

$$\lambda_1^2\bar{\Phi}_{FB}(x^*)_f + \lambda_2^2\bar{\Phi}_+(x^*)_f = \nabla F(x^*)_{ff}^{-1}\nabla F(x^*)_{f\bar{f}}\; v(x^*)_{\bar{f}}. \tag{4.50}$$

Substituting expression (4.50) into (4.49) and rearranging terms gives

$$u(x^*)_{\bar{f}} + (\nabla F(x^*)/\nabla F(x^*)_{ff})v(x^*)_{\bar{f}} = 0_{\bar{f}}. \tag{4.51}$$

Our next aim is to prove that

$$\bar{\Phi}_{FB}(x^*)_{\bar{f}} = 0. \tag{4.52}$$

Suppose the contrary. Then $\bar{\Phi}_{FB}(x^*)_{\bar{f}} \neq 0$ and both $u(x^*)_{\bar{f}} \neq 0, v(x^*)_{\bar{f}} \neq 0$ are different from 0 and have their nonzero elements in the same positions, according to Lemma 4.21 (b). Moreover, these nonzero elements have the same sign by Lemma (4.21) (c). Then for all $j \in I_{\bar{f}}$ with $\bar{\Phi}_{FB,j}(x^*) \neq 0 (\iff v_j(x^*) \neq 0)$ we obtain from (4.51)

$$v_j(x^*)[(\nabla F(x^*)/\nabla F(x^*)_{ff})v(x^*)]_j = -u_j(x^*)v_j(x^*) < 0. \tag{4.53}$$

But (4.53) contradicts the fact that $\nabla F(x^*)/\nabla F(x^*)_{ff}$ is a P_0-matrix. Hence (4.52) holds. This immediately implies $v(x^*)_{\bar{f}} = 0$ in view of Lemma 4.21 (b). Thus (4.50) gives

$$\big(\lambda_1^2 + \lambda_2^2\big)\bar{\Phi}_{FB}(x^*)_f = 0, \tag{4.54}$$

since $\bar{\Phi}_{FB}(x^*)_f = \bar{\Phi}_+(x^*)_f$. Now (4.52) and (4.54) gives $\bar{\Phi}_{FB}(x^*) = 0$, and therefore $\bar{\Phi}(x^*) = 0$. Hence x^* is a solution of the mixed complementarity problem. □

The generalization of Algorithm 4.13 to the MCP framework is stated below, where $\bar{\Phi}$ and $\bar{\Psi}$ denote the mappings defined in (4.36) and (4.38), respectively.

Algorithm 4.23 (Semismooth Levenberg-Marquardt Method for MCPs)

(S.0) Let $\beta \in (0,1)$, $\sigma \in (0, \frac{1}{2})$ and $\varepsilon \geq 0$. Choose any $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If $\|\nabla\bar{\Psi}(x^k)\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C\bar{\Phi}(x^k), \nu_k > 0$ and find a solution $d^k \in \mathbb{R}^n$ of

$$\big(H_k^T H_k + \nu_k I\big)d = -\nabla\bar{\Psi}(x^k). \tag{4.55}$$

(S.3) Compute $t_k = \max\{\beta^l \,|\, l = 0, 1, 2, \dots\}$ such that

$$\bar{\Psi}(x^k + t_k d^k) \leq \bar{\Psi}(x^k) + \sigma t_k \nabla\bar{\Psi}(x^k)^T d^k. \tag{4.56}$$

Set $x^{k+1} = x^k + t_k d^k$, $k \leftarrow k+1$, and go to (S.1).

Note that Algorithm 4.23 is well defined for an arbitrary mixed complementarity problem. The main convergence result for this algorithm is given by the following theorem, whose proof is identical to the proof of the analogous statements for Algorithm 4.13.

Theorem 4.24 *The following statements hold.*

1. *Every accumulation point of a sequence $\{x^k\}$ generated by Algorithm 4.23 is a stationary point of $\bar{\Psi}$.*

2. *Let $\{x^k\}$ be a sequence generated by Algorithm 4.23. Assume that x^* is an accumulation point of $\{x^k\}$ such that x^* is a R-regular solution of the mixed complementarity problem. Then the following statements hold:*

   (a) *The entire sequence $\{x^k\}$ converges to x^* if $\{\nu_k\}$ is bounded.*

   (b) *The full stepsize $t_k = 1$ is always accepted for k sufficiently large so that $x^{k+1} = x^k + d^k$ provided that $\nu_k \to 0$.*

   (c) *The rate of convergence is Q-superlinear if $\nu_k \to 0$.*

   (d) *The rate of convergence is Q-quadratic if $\nu_k = O(\|\nabla\bar{\Psi}(x^k)\|)$ and, in addition, F is an LC^1-function.*

Recall that Theorem 4.22 gives a relatively mild condition for a stationary point of $\bar{\Psi}$ to be a solution of the mixed complementarity problem.

4.5 Numerical Experiments

4.5.1 Implementation Details

We implemented Algorithm 4.23 in MATLAB and tested the algorithm on the MCPLIB test problem collection, see [22] (note that we used a newer version of this test problem collection, as currently available from `http://www.gams.com/mpec/mcplib.htm`). The implementation is along the lines of Algorithm 4.23 except that we use a nonmonotone line search as introduced by Grippo, Lampariello and Lucidi [48], together with a watchdog stabilization technique (see [49]).

The *nonmonotone line search* can be stated as follows. Let $m \geq 0$ be a prespecified constant and let $m_k \geq 1$ be an integer which is adjusted at each iteration k. We calculate a steplength $t_k = \max\{\beta^l : l = 0, 1, 2, \dots\} > 0$ satisfying the nonmonotone Armijo-rule by

$$\bar{\Psi}(x^k + t_k d^k) \leq \mathcal{W}_k + \sigma t_k \nabla\bar{\Psi}(x^k)^T d^k,$$

where $\mathcal{W}_k := \max\{\bar{\Psi}(x^j) \mid j = k+1-m_k, \dots, k\}$ denotes the maximal function value of $\bar{\Psi}$ over the last m_k iterations. Note that $m_k = 1$ corresponds to the monotone Armijo-rule. In the implementation, we used the following adjustment of m_k:

1. Set $m_k = 1$ for $k = \{0, \ldots, 5\}$. In other words, start the algorithm using the monotone Armijo-rule for the first five steps.

2. $m_{k+1} = \min\{m_k + 1, m\}$ at all remaining iterations (with $m = 10$ in our implementation).

As already mentioned, the method from Algorithm 4.23 is enhanced with a so-called *watchdog* feature. If after 20 steps the best function value of $\bar{\Psi}$ found so far has not been reduced sufficiently, we return to that point using a monotone line search. The starting point x^0 is the standard one provided by the MCPLIB collection. We terminate the iteration if one of the following conditions are satisfied

$$\|\bar{\Phi}(x^k)\| \leq 10^{-11} \quad \text{or} \quad \|\nabla\bar{\Psi}(x^k)\| \leq 10^{-6} \quad \text{or} \quad k > 300.$$

The Levenberg-Marquardt parameter ν_k is chosen as follows: For smaller problems with $n < 100$, we first estimate the condition number of the matrix $H_k^T H_k$, see [53, Ch. 15]. If this estimated condition number is larger than 10^{25}, we set $\nu_k := 0.1/(k+1)$. In all other cases, we take $\nu_k := 0$. This latter choice is motivated by some preliminary numerical experiments which showed that small values of ν_k give much better results than larger once so that, in the end, we decided to take the limiting value $\nu_k = 0$. The other parameters used in our implementation are $\lambda_1 = 0.1, \lambda_2 = 0.9, \beta = 0.55, \sigma = 10^{-4}$. The procedure for calculating an element $H_k \in \partial_C\Phi(x^k)$ is similar to one given in [4] for the Fischer-Burmeister equation operator $\bar{\Phi}_{FB}$.

4.5.2 Numerical Results

The obtained numerical results are summarized in Table 4.1 for small dimensional problems and in Table 4.2 for large dimensional ones. In these tables, the first column gives the name of the problem; Dim is the number of the variables in the problem; $\bar{\Psi}(x^0)$ gives the value of the merit function at the starting point; Nit denotes the number of iterations; Nwd gives the number of times the watchdog was activated; $\bar{\Psi}(x^f)$ and $\|\nabla\bar{\Psi}(x^f)\|$ denote the values of $\bar{\Psi}(x)$ and $\|\nabla\bar{\Psi}(x)\|$ at the final iterate $x = x^f$. Note that Nit is equal to the number of linear subproblems solved.

Table 4.1: Numerical results for (small) MCPLIB test problems

Problem	Dim	$\Psi(x^0)$	Nit	Nwd	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|$
`badfree`	5	4.600000e-01	7	0	9.268389e-12	7.457793e-07
`bertsekas`	15	3.936098e-03	38	0	2.753981e-16	1.468192e-07
`billups`	1	3.451182e-05	30	1	2.204422e-12	7.627348e-06
`choi`	13	7.709002e-03	5	0	2.649619e-16	1.278982e-09
`colvdual`	20	5.488000e+01	19	0	8.785821e-12	1.096167e-05
`colvnlp`	15	6.207596e+01	6	0	4.033072e-15	2.298059e-07

Table 4.1: Numerical results for (small) MCPLIB test problems (continued)

Problem	Dim	$\Psi(x^0)$	Nit	Nwd	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|$
cycle	1	5.173835e+01	5	0	3.703547e-21	7.746281e-10
degen	2	1.000000e-01	5	0	6.295417e-17	1.122182e-09
duopoly	63	2.132546e+02	—	—	—	—
ehl-k40	41	1.042178e+04	32	0	2.335817e-14	6.724182e-06
ehl-k60	61	3.797546e+04	43	1	4.583750e-14	1.039919e-05
ehl-k80	81	9.363011e+04	50	1	1.115490e-12	3.133144e-03
ehl-kost	101	1.878951e+05	113	4	1.021911e-12	5.417297e-03
electric	158	2.609736e+08	33	0	8.195661e-13	2.421314e-06
explcp	16	3.200000e-01	19	0	5.723100e-16	3.383225e-09
forcebsm	184	3.944244e+03	239	8	3.095727e-12	2.489442e-07
forcedsa	186	3.948661e+03	25	0	2.971468e-16	2.437821e-09
freebert	15	1.509811e+04	10	0	6.212865e-14	2.194618e-06
gafni	5	1.300358e+03	10	0	6.470323e-13	3.651867e-05
games	16	6.006634e+01	6	0	7.154607e-12	8.895455e-05
hanskoop	14	1.185959e+02	8	0	1.052035e-16	3.867725e-09
hydroc06	29	1.766604e+05	5	0	6.762849e-15	6.397969e-04
hydroc20	99	4.104414e+05	9	0	6.304574e-16	1.026980e-04
jel	6	9.561221e+02	7	0	5.187227e-18	2.058262e-08
josephy	4	2.281054e-02	3	0	1.059211e-22	1.355775e-10
kojshin	4	2.281054e-02	3	0	1.079806e-22	1.368936e-10
mathinum	3	6.215376e+02	4	0	3.024771e-12	6.673325e-07
mathisum	4	5.216473e+00	8	0	2.199525e-16	1.559273e-08
methan08	31	6.463832e+06	4	0	2.488877e-14	4.527827e-03
nash	10	5.426293e+02	4	0	2.354633e-19	7.457201e-09
ne-hard	3	1.155892e+04	—	—	1.448421e-10	2.179638e-04
pgvon106	106	1.536653e+02	21	0	6.110093e-12	8.964999e-07
pies	42	5.267785e+08	27	0	7.026880e-13	8.659392e-03
powell	16	6.807131e-04	5	0	8.057887e-17	1.061372e-08
powell-mcp	8	9.316746e+01	2	0	2.728284e-13	6.048681e-06
qp	4	3.300000e+00	5	0	6.295416e-17	1.122089e-09
scarfanum	13	6.994871e-05	3	0	3.605079e-12	2.824943e-06
scarfasum	14	6.994871e-05	3	0	3.604873e-12	2.809442e-06
scarfbsum	40	1.123239e+02	27	0	6.331156e-17	2.098521e-06
shubik	45	1.638873e-01	290	0	8.777558e-17	1.805669e-08
simple-ex	17	9.561639e+00	53	1	7.317284e-13	9.444120e-07
simple-red	13	2.250785e+02	11	0	1.037776e-19	3.444468e-10
sppe	27	1.216934e+02	6	0	5.936441e-19	5.100155e-09

Table 4.1: Numerical results for (small) MCPLIB test problems (continued)

Problem	Dim	$\Psi(x^0)$	Nit	Nwd	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|$
`tinloi`	146	4.001771e-01	9	0	1.416760e-12	1.286753e-03
`tobin`	42	3.236481e+00	2	0	1.474633e-14	1.354525e-05

Table 4.1 shows that the algorithm was able to solve almost all problems from the MCPLIB collection including a number of examples which are known to be very hard. We have failures only on problems `duopoly` and `ne-hard`. By changing our parameters, we are also able to solve these problems with high precision. In very few cases, like the `billups` problem from [4], we view it as a mere coincidence that we are able to solve them. In general, however, the method seems to be extremely robust.

Table 4.2: Numerical results for (large) MCPLIB test problems

Problem	Dim	$\Psi(x^0)$	Nit	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|$
bert-oc	5000	5.129446e+01	10	6.254441e–12	3.734828e–07
bratu	5625	7.886962e+00	10	1.800397e–14	2.026905e–08
bishop	1645	2.157671e+11	—	—	—
lincont	419	3.956019e+03	21	5.335966e–18	9.678748e–07
obstacle	2500	3.371445e–04	7	3.232956e–12	1.645663e–06
opt-cont	288	8.693982e+02	8	3.973421e–14	3.040037e–08
opt-cont31	1024	2.435888e+02	9	1.175346e–12	1.578468e–07
opt-cont127	4096	7.867371e+01	12	3.232490e–12	2.584229e–07
opt-cont255	8192	5.184548e+01	41	4.567335e–12	3.173779e–07
opt-cont511	16384	3.848816e+01	17	4.924145e–13	1.000753e–07
trafelas	2904	5.124999e+03	143	6.567286e–17	1.585157e–09

In Table 4.2 we see that we are also able to solve all larger problems with the only exception of problem `bishop`. In particular, we can solve the relatively difficult examples `lincont` and `trafelas`.

4.5.3 Comparison with Fischer-Burmeister Function

We consider the following one-dimensional NCP:

$$x \geq 0, \quad F(x) := \frac{1}{x} \geq 0, \quad xF(x) = 0. \tag{4.57}$$

Obviously, this problem has no solution, since the complementarity gap is always 1. To indicate the difference between the merit functions, Figure 4.2 plots them for this simple

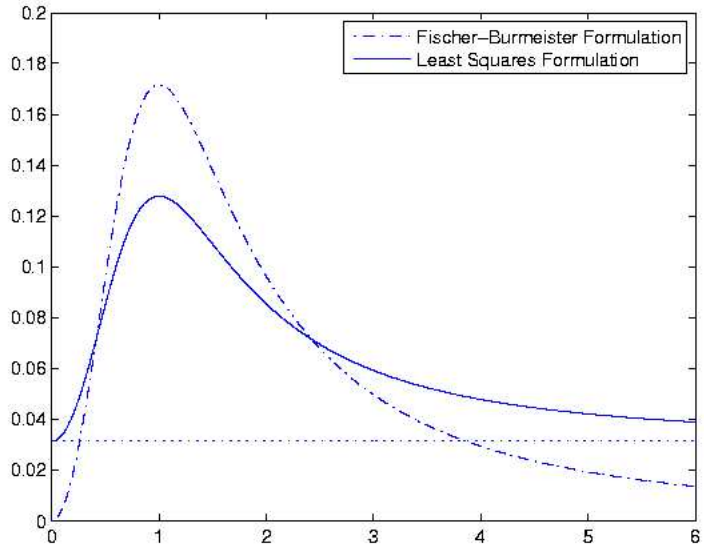

Figure 4.2: Merit functions for Fischer-Burmeister and least squares reformulation of the one-dimensional NCP (4.57).

example. Here Ψ is plotted for $\lambda_1 = 0.75, \lambda_2 = 0.25$. Further we observe that Ψ_{FB} tends to 0 as $x \to 0$. From this measure we might think $x = 0$ is a solution. However, F is not defined at $x = 0$. Indeed, applying our algorithm with $\lambda_1 = 1, \lambda_2 = 0$ to this simple example choosing various starting points < 1 the (Fischer-Burmeister) merit function value (less then 10^{-16}) indicate that we have solved the problem in a few iterations (less than 16). Using the new merit function this phenomenon is avoided by obvious reasons and our algorithm will fail (pleasantly in this case).

A more reasonable comparison with the pure Fischer-Burmeister approach can be obtained considering the MCPLIB test suite. To this end, we make the following remarks:

- During all the iterations, no domain violations occurred, i.e., the function F was always defined at the iterates x^k. This is very much in contrast to the pure Fischer-Burmeister approach where domain violations occur quite frequently and special (heuristic) rules have to be used so that the method can go on. We admit, however, that we have no theoretical justification for this observation since no special care is taken in order to avoid domain violations when using our least squares approach.

- If we apply our algorithm with $\lambda_1 = 1, \lambda_2 = 0$ in the definition of Φ or $\bar{\Phi}$, then our method reduces to the standard Fischer-Burmeister approach since the last n components in the definition of Φ or $\bar{\Phi}$ get canceled. Doing so, we get failures on eleven (compared to two) test problems among the small-dimensional examples, namely `duopoly`, `ehl-k40`, `ehl-k60`, `ehl-k80`, `electric`, `forcebsm`, `forcedsa`, `ne-hard`,

pgvon106, shubik, simple-ex. Furthermore, we sometimes have to take a significantly higher number of iterations for some other examples, e.g., the solution of ehl-kost now takes more than 200 iterations. The new approach scores well also applied to the large-scale problems. The Fischer-Burmeister approach fails on bishop and opt-cont511, and takes more than 150 iterations on opt-cont127.

- A further comparison with the pure Fischer-Burmeister approach can be obtained by having a look at the numerical results presented in [118] where four different Fischer-Burmeister-type algorithms are compared with each other (two of them use constrained reformulations of the complementarity problem and therefore have to solve more complicated subproblems). Even the best method in [118] produces more failures than our algorithm. This is interesting to note especially because many of the more difficult test problems from the MCPLIB collection (like electric, forcebsm, forcedsa) have been completely excluded from the numerical results in [118].

Altogether this indicates that our new approach is certainly more robust and sometimes also more efficient than the underlying Fischer-Burmeister method.

4.5.4 Comparison with Penalized Fischer-Burmeister Function

The penalized Fischer-Burmeister function from [11] (see Figure 4.3) is given by

$$\tilde{\phi}(a,b) := \lambda\phi_{FB}(a,b) - (1-\lambda)\phi_{+}(a,b).$$

It can be used in order to reformulate the complementarity problem as a square system of equations $\tilde{\Phi}(x) = 0$ with

$$\tilde{\Phi}_i(x) := \tilde{\phi}(x_i, F_i(x)) \quad \forall i = 1, \ldots, n.$$

The corresponding merit function $\tilde{\Psi} : \mathbb{R}^n \to \mathbb{R}$ is then given by

$$\tilde{\Psi}(x) := \frac{1}{2}\tilde{\Phi}(x)^T\tilde{\Phi}(x)$$

and can be rewritten as

$$\tilde{\Psi}(x) = \sum_{i=1}^{n} \tilde{\psi}(x_i, F_i(x))$$

with

$$\tilde{\psi}(x_i, F_i(x)) := \frac{1}{2}\tilde{\phi}(x_i, F_i(x))^2 = u_i + v_i + w_i,$$

where the terms u_i, v_i, and w_i are given by

$$\begin{aligned} u_i &:= \frac{1}{2}\lambda^2\phi_{FB}(x_i, F_i(x))^2, \\ v_i &:= \frac{1}{2}(1-\lambda)^2\phi_{+}(x_i, F_i(x))^2, \end{aligned}$$

$$w_i \;:=\; \lambda(\lambda-1)\phi_{FB}(x_i,F_i(x))\phi_+(x_i,F_i(x)).$$

Note that u_i is used in order to get an equivalent reformulation of the complementarity problem as a system of equations or an unconstrained minimization. Furthermore, v_i is responsible for making the complementarity gap as small as possible, whereas the contribution of the mixed term w_i is not quite clear and, in fact, not necessary. This is reflected by our merit function which, in the above notation, can be written as

$$\Psi(x)=\sum_{i=1}^{n}\psi(x_i,F_i(x)) \quad \text{with} \quad \psi(x_i,F_i(x)) := u_i+v_i,$$

where $\lambda_1=\lambda$ and $\lambda_2=1-\lambda$. Of course, this is not the only difference since we also compute a totally different search direction for example.

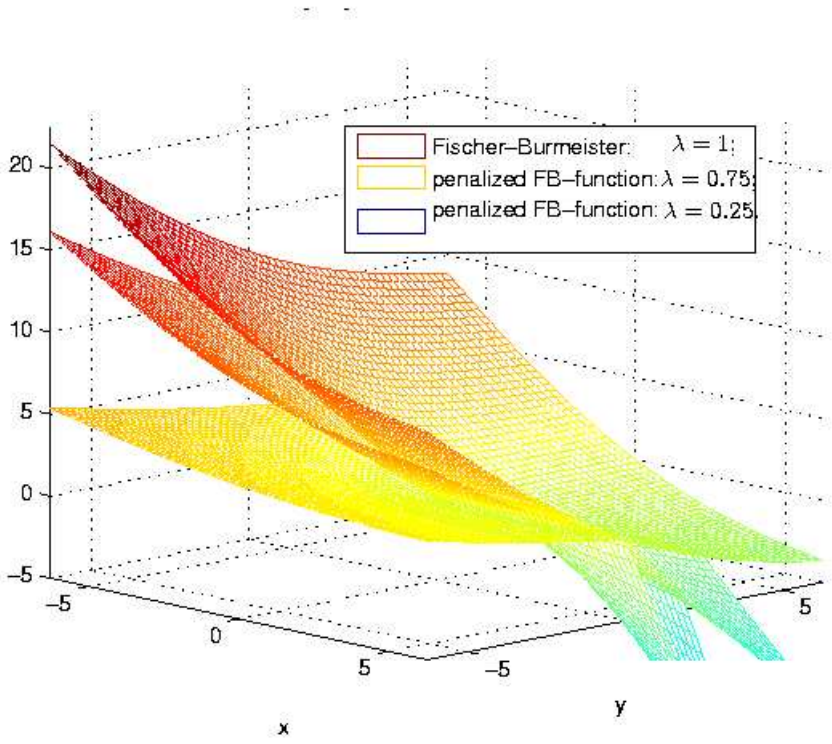

Figure 4.3: Graph of the penalized Fischer-Burmeister function for three values of λ.

Numerically, the experiments indicate our new method is also more robust. In order to see this, we made another test run with our current implementation of the nonsmooth Newton method from [11] applied to the nonlinear equation $\tilde{\Phi}(x)=0$. Instead of giving the details of this test run here, we only summarize the results: The nonsmooth Newton method from [11] is also quite robust and able to solve some of the difficult test problems like `billups`, `forcebsm`, and `forcedsa`. Nevertheless, it produces a significantly higher

number of errors: Within the small dimensional examples, it produces failures on problems `colvdual`, `duopoly`, `electric`, `ne-hard`, `pgvon106`, and `shubik`, and within the set of large dimensional problems, it is not able to solve the three examples `bishop`, `lincont`, and `trafelas`. Hence, altogether, there are nine failures compared to only three for our least squares formulation.

Chapter 5

An Inexact Semismooth Method

Similar to standard Newton- and Levenberg-Marquardt methods, Algorithm 4.23 is of limited practical value for large scale complementarity problems, simply due to the fact that the linear system (4.55) can in general not be solved exactly by direct methods for larger n. Instead, iterative methods have to be used, leading to inexact solutions of (4.55). The main purpose of this chapter is to discuss the influence of this inexactness on the convergence of Algorithm 4.23. Since the newly inexact variant allows us to address a much larger range of applications, we also discuss the application of the new variant to optimal control and obstacle problems, additionally to the examples from the MCPLIB.

5.1 Description of Algorithm

The method to be considered exploits a reformulation of the (mixed) complementarity problem as an overdetermined nonlinear system of equations $\Phi(x) = 0$ with $\Phi : \mathbb{R}^n \to \mathbb{R}^{2n}$ being defined in (4.36), as presented in the previous chapter.

Algorithm 5.1 (Inexact Semismooth Levenberg-Marquardt Method)

(S.0) Let $\beta \in (0,1)$, $\sigma \in (0, \frac{1}{2})$, $\rho > 0$, $p > 2$ and $\varepsilon \geq 0$. Choose any $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If $\|\nabla\Psi(x^k)\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C\Phi(x^k), \nu_k > 0$ and find an *approximate* solution $d^k \in \mathbb{R}^n$ of

$$\big(H_k^T H_k + \nu_k I\big)d = -\nabla\Psi(x^k), \tag{5.1}$$

where ν_k is the Levenberg-Marquardt parameter. If the condition

$$\nabla\Psi(x^k)^T d^k \leq -\rho\|d^k\|^p \tag{5.2}$$

is not satisfied, set $d^k = -\nabla\Psi(x^k)$.

(S.3) Compute $t_k = \max\{\beta^\ell \mid \ell = 0, 1, 2, \dots\}$ such that

$$\Psi(x^k + t_k d^k) \leq \Psi(x^k) + \sigma t_k \nabla\Psi(x^k)^T d^k. \tag{5.3}$$

(S.4) Set $x^{k+1} = x^k + t_k d^k$, $k \leftarrow k + 1$, and go to (S.1).

Algorithm 5.1 is very similar to the one presented in [28] (see also [56]), which, however, is based on a different reformulation of the complementarity problem as a square system of equations. Nevertheless, this observation will simplify the convergence analysis of Algorithm 5.1 significantly, and we will come back to this point in the next section.

Before investigating the convergence properties of Algorithm 5.1, however, we need to say what we mean by solving the subproblem (5.1) inexactly in Step (S.2). To specify this point, we will assume that the inexact solution d^k of (5.1) satisfies a relation of the form

$$(H_k^T H_k + \nu_k I)d^k = -\nabla\Psi(x^k) + r^k \tag{5.4}$$

for some residual vector r^k such that

$$\|r^k\| \leq \alpha_k \|\nabla\Psi(x^k)\| \tag{5.5}$$

for some a priori chosen number $\alpha_k \geq 0$. Note that the choice $\alpha_k = 0$ corresponds to an exact solution of the regularized linear least squares subproblem from (4.23).

5.2 Convergence Properties

In this section, we investigate the convergence properties of our algorithm. To this end, we assume that the termination parameter ε is equal to zero and that Algorithm 5.1 generates an infinite sequence. We further assume throughout this section that the subproblems (5.1) are solved inexactly in such a way that conditions (5.4) and (5.5) hold for some sequence $\{\alpha_k\}$. We first state a global convergence result for Algorithm 5.1. Its proof is essentially the same as the one from [28, Theorem 12], and we include it here for the sake of completeness.

Theorem 5.2 *Assume that the sequence $\{\nu_k\}$ is bounded and that the sequence of residual vectors $\{r^k\}$ satisfies condition (5.5) for some sequence of positive numbers $\{\alpha_k\}$ such that $\alpha_k \leq \bar{\alpha}$ for some $\bar{\alpha} \in [0, 1)$. Then every accumulation point of a sequence $\{x^k\}$ generated by Algorithm 5.1 is a stationary point of Ψ.*

Proof. We show that the sequence $\{d^k\}$ is uniformly gradient related to $\{x^k\}$, according to [2]), i.e., for every convergent subsequence $\{x^k\}_K$ for which

$$\lim_{k\to\infty, k\in K} \nabla\Psi(x^k) \neq 0, \tag{5.6}$$

there holds

$$\limsup_{k\to\infty, k\in K} \|d^k\| < \infty, \tag{5.7}$$

$$\liminf_{k\to\infty,k\in K} |\nabla\Psi(x^k)^T d^k| > 0. \tag{5.8}$$

Let $\{x^k\}_K$ be any convergent subsequence for which (5.6) holds. To show that $\{d^k\}_K$ satisfies condition (5.7) and (5.8) we can assume without loss of generality that d^k is always given by (5.1), since any subsequence of $\{\nabla\Psi(x)\}_K$ is uniformly gradient related to the corresponding subsequence of $\{x^k\}_K$.

We now show first that $\{d^k\}_K$ is bounded. From (5.4) we get

$$\|d^k\| \geq \frac{\|\nabla\Psi(x^k) - r^k\|}{\|H_k^T H_k + \nu_k I\|}, \tag{5.9}$$

and since ν_k is bounded by assumption and the generalized Jacobian is upper semicontinuous (recall that the sequence $\{x^k\}_K$ converges), there exists a constant $\kappa > 0$ such that

$$\|H_k^T H_k + \nu_k I\| \leq \kappa \text{ for all } k \in K.$$

We now obtain

$$\begin{aligned} \|d^k\| &\geq \frac{\|\nabla\Psi(x^k) - r^k\|}{\kappa} \geq \frac{\|\nabla\Psi(x^k)\| - \|r^k\|}{\kappa} \\ &\overset{(5.5)}{\geq} \frac{1-\alpha_k}{\kappa}\|\nabla\Psi(x^k)\| \geq \frac{1-\bar{\alpha}}{\kappa}\|\nabla\Psi(x^k)\| =: \kappa_1\|\nabla\Psi(x^k)\|, \end{aligned} \tag{5.10}$$

for all $k \in K$ sufficiently large. Since the direction d^k satisfies (5.2) we have

$$\|d^k\|^p \leq -\frac{1}{\rho}\nabla\Psi(x^k)^T d^k \leq \frac{1}{\rho}\|\nabla\Psi(x^k)\|\|d^k\| \overset{(5.10)}{\leq} \frac{1}{\rho\kappa_1}\|d^k\|^2$$

and the boundedness of the sequence $\{d^k\}$ now readily follows from the above inequality dividing by $\|d^k\|^2$ together with $p > 2$. Note that $\|d^k\| \neq 0$, since otherwise we would have $\nabla\Psi(x^k) - r^k = 0$ by (5.9) which, in turn, since $\|r^k\| \leq \alpha_k\|\nabla\Psi(x^k)\|$ with $\alpha_k < 1$, would be possible only if $\|\nabla\Psi(x^k)\| = 0$, so that x^k would be a stationary point and the algorithm would have stopped.

For proving (5.8), we assume that there exists a subsequence $\{x^k\}_{K'}$ of $\{x^k\}_K$ for which $\lim_{k\to\infty,k\in K'} |\nabla\Psi(x^k)^T d^k| = 0$. By (5.2), this implies, that $\lim_{k\to\infty,k\in K'} \|d^k\| = 0$. This in turn implies $\lim_{k\to\infty,k\in K'} \|\nabla\Psi(x^k)\| = 0$, in view of (5.10), but contradicting (5.6). Thus $\{d^k\}$ is uniformly gradient related to $\{x^k\}$ and the assertion of the theorem now follows from Proposition 1.8 in [2].

□

In order to show local fast convergence, we need a regularity assumption. This will be the R-regularity assumption. For our subsequent analysis, we note that the R-regularity assumption implies that, if the sequence $\{x^k\}$ converges to an R-regular solution x^*, then the matrices $H_k^T H_k$ are uniformly positive definite, i.e., there is a constant $\gamma > 0$ such that

$$\|H_k d^k\|^2 = (d^k)^T H_k^T H_k d^k \geq \gamma\|d^k\|^2 \tag{5.11}$$

for all k sufficiently large, see Lemma 4.5. We are now in the position to state a local convergence result.

Theorem 5.3 *Let $\{x^k\}$ be a sequence generated by Algorithm 5.1, let the sequence $\{\nu_k\}$ be bounded and assume that $\{\alpha_k\} \to 0$ with $\{\alpha_k\}$ being the sequence from (5.5). Assume that x^* is an accumulation point of $\{x^k\}$ such that x^* is an R-regular solution of the complementarity problem (1.3). Then the following statements hold:*

(a) The entire sequence $\{x^k\}$ converges to x^*.

(b) Eventually d^k is always given by the inexact solution of system (5.1).

(c) The full stepsize $t_k = 1$ is always accepted for k sufficiently large so that $x^{k+1} = x^k + d^k$ provided that $\nu_k \to 0$.

(d) The rate of convergence is Q-superlinear if $\nu_k \to 0$.

(e) The rate of convergence is Q-quadratic if $\nu_k = O(\|\Phi(x^k)\|)$, $\alpha_k = O(\|\Phi(x^k)\|)$ and, in addition, F' is locally Lipschitzian.

Proof. (a) Using the R-regularity assumption, we can argue exactly as in Theorem 4.15 (a) for proving that x^* is an isolated accumulation point of the sequence $\{x^k\}$. Let $\{x^k\}_K$ denote any subsequence converging to x^*, and note that x^* is a stationary point of Ψ by Theorem 5.2. For all $k \in \mathbb{N}$ such that d^k is an inexact solution of (4.23), we have

$$\begin{aligned}
\|x^{k+1} - x^k\| &= t_k\|d^k\| \\
&\leq \|d^k\| \\
&\overset{(5.4)}{\leq} \|(H_k^T H_k + \nu_k I)^{-1}\| \, \| - \nabla\Psi(x^k) + r^k\| \\
&\leq \|(H_k^T H_k + \nu_k I)^{-1}\| \big(\|\nabla\Psi(x^k)\| + \|r^k\|\big) \\
&\overset{(5.5)}{\leq} (1 + \alpha_k)\|(H_k^T H_k + \nu_k I)^{-1}\| \, \|\nabla\Psi(x^k)\|.
\end{aligned}$$

On the other hand, for all $k \in \mathbb{N}$ with $d^k = -\nabla\Psi(x^k)$, we have

$$\|x^{k+1} - x^k\| = t_k\|d^k\| \leq \|d^k\| = \|\nabla\Psi(x^k)\|.$$

Together, it follows from $\{\nabla\Psi(x^k)\}_K \to 0$, the assumed boundedness of $\{\nu_k\}$ and Lemma 4.5 that $\{\|x^{k+1} - x^k\|\}_K \to 0$. Hence statement (a) follows from [89, Lemma 4.10].

(b) First we prove that there is a constant $\kappa > 0$ such that

$$\nabla\Psi(x^k)^T d^k \leq -\kappa\|d^k\|^2 \tag{5.12}$$

for all $k \in \mathbb{N}$ sufficiently large, where d^k denotes an inexact solution of (4.23) in the sense that (5.4) and (5.5) are satisfied.

Since $\{\nu_k\}$ is bounded by assumption, $x^k \to x^*$ by (a) and the generalized Jacobian is upper semicontinuous, the sequence $\{H_k^T H_k + \nu_k I\}$ is bounded. Furthermore, it follows from $x^k \to x^*$, the assumed R-regularity and Lemma 4.5 that the corresponding inverse matrices are also uniformly bounded. Hence there is a constant $c > 0$ such that

$$\|H_k^T H_k + \nu_k I\| \le c \quad \text{and} \quad \|(H_k^T H_k + \nu_k I)^{-1}\| \le c \quad \forall k \in \mathbb{N}. \tag{5.13}$$

Since

$$\|H_k^T H_k + \nu_k I\| = \lambda_{\max}(H_k^T H_k + \nu_k I) =: \lambda_{\max}^k$$

and

$$\|(H_k^T H_k + \nu_k I)^{-1}\| = \frac{1}{\lambda_{\min}(H_k^T H_k + \nu_k I)} =: \frac{1}{\lambda_{\min}^k},$$

we obtain from (5.13)

$$\frac{1}{c}\|d^k\|^2 \le \lambda_{\min}^k \|d^k\|^2 \le (d^k)^T (H_k^T H_k + \nu_k I) d^k \le \lambda_{\max}^k \|d^k\|^2 \le c\|d^k\|^2. \tag{5.14}$$

Furthermore, we have

$$\|\nabla\Psi(x^k) - r^k\| \overset{(5.4)}{=} \|(H_k^T H_k + \nu_k I) d^k\| \le \|H_k^T H_k + \nu_k I\| \, \|d^k\|$$

and therefore

$$\begin{aligned} \|d^k\| \ge \frac{\|\nabla\Psi(x^k) - r^k\|}{\|H_k^T H_k + \nu_k I\|} &\overset{(5.13)}{\ge} \frac{1}{c}\|\nabla\Psi(x^k) - r^k\| \\ &\ge \frac{1}{c}\big(\|\nabla\Psi(x^k)\| - \|r^k\|\big) \\ &\overset{(5.5)}{\ge} \frac{1}{c}\big(\|\nabla\Psi(x^k)\| - \alpha_k\|\nabla\Psi(x^k)\|\big) \\ &= \frac{1}{c}(1-\alpha_k)\|\nabla\Psi(x^k)\|. \end{aligned} \tag{5.15}$$

The Cauchy-Schwarz inequality therefore implies

$$\begin{aligned} \nabla\Psi(x^k)^T d^k &\overset{(5.4)}{=} -(d^k)^T (H_k^T H_k + \nu_k I) d^k + (r^k)^T d^k \\ &\le -(d^k)^T (H_k^T H_k + \nu_k I) d^k + \|r^k\| \, \|d^k\| \\ &\overset{(5.5)}{\le} -(d^k)^T (H_k^T H_k + \nu_k I) d^k + \alpha_k \|\nabla\Psi(x^k)\| \|d^k\| \\ &\overset{(5.14)}{\le} -\frac{1}{c}\|d^k\|^2 + \alpha_k \|\nabla\Psi(x^k)\| \|d^k\| \\ &\overset{(5.15)}{\le} -\frac{1}{c}\|d^k\|^2 + c\frac{\alpha_k}{1-\alpha_k}\|d^k\|^2. \end{aligned}$$

Hence inequality (5.12) follows immediately from the fact that $\alpha_k \to 0$.

Using (5.12), the Cauchy-Schwarz inequality implies

$$\kappa\|d^k\|^2 \leq \|\nabla\Psi(x^k)\|\,\|d^k\|$$

and therefore $\{\|d^k\|\} \to 0$. This together with $p > 2$ gives statement (b).
(c), (d) We first show that

$$\|x^k + d^k - x^*\| = o(\|x^k - x^*\|) \tag{5.16}$$

holds for all $k \in \mathbb{N}$ sufficiently large. To this end, we recall that, for any $k \in \mathbb{N}$, the matrix $H_k^T H_k + \nu_k I$ is nonsingular with $\|(H_k^T H_k + \nu_k I)^{-1}\| \leq c$ by (5.13). Furthermore, the sequence $\{H_k\}$ is bounded (since $\{x^k\}$ is convergent) and we can assume without loss of generality that we also have $\|H_k^T\| \leq c$. Since $\nabla\Psi(x^k) = H_k^T\Phi(x^k)$ in view of Theorem 4.7, we obtain for all x^k sufficiently close to x^* that

$$\begin{aligned}
&\|x^k + d^k - x^*\| \\
&\overset{(5.4)}{=} \|x^k + (H_k^T H_k + \nu_k I)^{-1}(-\nabla\Psi(x^k) + r^k) - x^*\| \\
&\leq \|(H_k^T H_k + \nu_k I)^{-1}\|\,\|\nabla\Psi(x^k) - r^k - (H_k^T H_k + \nu_k I)(x^k - x^*)\| \\
&\leq c\|H_k^T\Phi(x^k) - H_k^T H_k(x^k - x^*) - \nu_k(x^k - x^*) - r^k\| \\
&\leq c\big(\|H_k^T(\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*))\| + \nu_k\|x^k - x^*\| + \|r^k\|\big) \\
&\overset{(5.5)}{\leq} c\big(\|H_k^T\|\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| + \nu_k\|x^k - x^*\| + \alpha_k\|H_k^T\Phi(x^k)\|\big) \\
&\leq c\big(c\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| + \nu_k\|x^k - x^*\| + \alpha_k c\|\Phi(x^k) - \Phi(x^*)\|\big) \\
&= o(\|x^k - x^*\|) + o(\|x^k - x^*\|) + o(\|x^k - x^*\|) \\
&= o(\|x^k - x^*\|)
\end{aligned}$$

since $\nu_k \to 0, \alpha_k \to 0$, and Φ is locally Lipschitz and semismooth. Hence (5.16) holds.

In order to verify statement (c), we have to show that the full step $t_k = 1$ is eventually accepted by the line search rule in Algorithm 5.1. This fact may be derived from a general result in [25] using some additional properties of the merit function Ψ. However, we prefer to give a direct proof here which does not exploit any further properties of this merit function.

First note that (5.16) implies

$$\|x^k - x^*\| \leq \|x^k + d^k - x^*\| + \|d^k\| = o(\|x^k - x^*\|) + \|d^k\|.$$

Hence we have

$$\|x^k - x^*\| = O(\|d^k\|). \tag{5.17}$$

Together with (5.16), the local Lipschitz property of Φ and the fact that $\Phi(x^*) = 0$, we therefore obtain

$$\begin{aligned}\Psi(x^k + d^k) &= \frac{1}{2}\|\Phi(x^k + d^k)\|^2 \\ &= \frac{1}{2}\|\Phi(x^k + d^k) - \Phi(x^*)\|^2 \\ &= O(\|x^k + d^k - x^*\|^2) \\ &= o(\|x^k - x^*\|^2) \\ &= o(\|d^k\|^2).\end{aligned} \tag{5.18}$$

In a similar way, we also get from (5.5) and $\nabla\Psi(x^k) = H_k^T\Phi(x^k)$ that

$$\|r^k\| = o(\|\nabla\Psi(x^k)\|) = o(\|\Phi(x^k) - \Phi(x^*)\|) = o(\|x^k - x^*\|) = o(\|d^k\|). \tag{5.19}$$

Exploiting the semismoothness of Φ once again, we have

$$\big|\|\Phi(x^k) - \Phi(x^*)\| - \|H_k(x^k - x^*)\|\big| \le \|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| = o(\|x^k - x^*\|). \tag{5.20}$$

This means that there is a positive sequence $\tau_k \to 0$ such that

$$\big|\|\Phi(x^k) - \Phi(x^*)\| - \|H_k(x^k - x^*)\|\big| \le \tau_k\|x^k - x^*\|$$

for all k sufficiently large. Consequently, we have

$$\tau_k\|x^k - x^*\| + \|H_k(x^k - x^*)\| - \|\Phi(x^k) - \Phi(x^*)\| \ge 0$$

and

$$\tau_k\|x^k - x^*\| - \|H_k(x^k - x^*)\| + \|\Phi(x^k) - \Phi(x^*)\| \ge 0 \tag{5.21}$$

for all k large enough. Multiplying the last two inequalities, we obtain

$$\tau_k^2\|x^k - x^*\|^2 - \|H_k(x^k - x^*)\|^2 + 2\|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| \ge \|\Phi(x^k) - \Phi(x^*)\|^2.$$

We therefore have

$$\frac{1}{2}\|\Phi(x^k) - \Phi(x^*)\|^2 \le -\frac{1}{2}\|H_k(x^k - x^*)\|^2 + \|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| + o(\|x^k - x^*\|^2).$$

On the other hand, multiplying (5.21) with $\|\Phi(x^k) - \Phi(x^*)\|$ and rearranging terms, we get

$$\begin{aligned}&-\|\Phi(x^k) - \Phi(x^*)\|^2 \\ &\le \tau_k\|x^k - x^*\|\,\|\Phi(x^k) - \Phi(x^*)\| - \|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| \\ &\le -\|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| + o(\|x^k - x^*\|^2)\end{aligned}$$

since Φ is locally Lipschitz. Adding the last two inequalities and using (5.17) gives

$$-\frac{1}{2}\|\Phi(x^k)-\Phi(x^*)\|^2 \leq -\frac{1}{2}\|H_k(x^k-x^*)\|^2 + o(\|d^k\|^2). \tag{5.22}$$

Since

$$\big|\|H_k(x^k+d^k-x^*)\| - \|H_k d^k\|\big| \leq \|H_k(x^k+d^k-x^*) - H_k d^k\| = \|H_k(x^k-x^*)\|$$

holds and the left-hand term is nonnegative, squaring both sides gives

$$\|H_k(x^k+d^k-x^*)\|^2 - 2\|H_k(x^k+d^k-x^*)\|\,\|H_k d^k\| + \|H_k d^k\|^2 \leq \|H_k(x^k-x^*)\|^2.$$

Multiplying this inequality by $-\frac{1}{2}$ and using (5.16), (5.17) as well as the boundedness of the sequence $\{H_k\}$, we obtain

$$\begin{aligned}
&-\frac{1}{2}\|H_k(x^k-x^*)\|^2 \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 - \frac{1}{2}\|H_k(x^k+d^k-x^*)\|^2 + \|H_k(x^k+d^k-x^*)\|\,\|H_k d^k\| \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 - \frac{1}{2}\|H_k(x^k+d^k-x^*)\|^2 + o(\|d^k\|^2) \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 + o(\|d^k\|^2).
\end{aligned} \tag{5.23}$$

Summarizing our previous discussion, we now obtain for all x^k sufficiently close to x^* that

$$\begin{aligned}
&\Psi(x^k+d^k) - \Psi(x^k) - \sigma\nabla\Psi(x^k)^T d^k \\
&\overset{(5.4),(5.18)}{=} o(\|d^k\|^2) - \frac{1}{2}\|\Phi(x^k)\|^2 + \sigma(d^k)^T(H_k^T H_k + \nu_k I)d^k - \sigma(r^k)^T d^k \\
&\leq -\frac{1}{2}\|\Phi(x^k)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + \sigma\nu_k\|d^k\|^2 + o(\|d^k\|^2) + \sigma|(r^k)^T d^k| \\
&\overset{\nu_k\to 0}{\leq} -\frac{1}{2}\|\Phi(x^k)-\Phi(x^*)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + o(\|d^k\|^2) + \sigma\|r^k\|\|d^k\| \\
&\overset{(5.22),(5.19)}{\leq} -\frac{1}{2}\|H_k(x^k-x^*)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + o(\|d^k\|^2) \\
&\overset{(5.23)}{\leq} -\frac{1}{2}\|H_k d^k\|^2 + \sigma\|H_k d^k\|^2 + o(\|d^k\|^2) \\
&= (\sigma-\frac{1}{2})\|H_k d^k\|^2 + o(\|d^k\|^2) \\
&\overset{(5.11)}{\leq} (\sigma-\frac{1}{2})\gamma\|d^k\|^2 + o(\|d^k\|^2) \\
&< 0,
\end{aligned}$$

where the last two inequalities follow from the fact that $\sigma \in (0, 1/2)$. This implies that the full step is eventually accepted, i.e., we have $x^{k+1} = x^k + d^k$ for all k sufficiently large.

Consequently, (5.16) shows that $\{x^k\}$ converges Q-superlinearly to x^*.

(e) The proof is essentially the same as for the local superlinear convergence. To this end, we only note that F' being locally Lipschitz implies that Φ is strongly semismooth, and that the relation

$$\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| = O(\|x^k - x^*\|^2).$$

holds for strongly semismooth functions, see 2.16 (b). □

Note that statement (e) of Theorem 5.3 remains true if the two sequences $\{\nu_k\}$ and $\{\alpha_k\}$ satisfy $\nu_k = O(\|\nabla\Psi(x^k)\|)$ and $\alpha_k = O(\|\nabla\Psi(x^k)\|)$.

5.3 Numerical Experiments

Since the previous sections showed that the good theoretical properties of the exact semismooth Newton method in Chapter 4 also hold for the inexact version from Algorithm 5.1, we now look at the practical behavior of the algorithm. Here we are mainly interested in large-scale problems where the exact method may not necessarily be applied to because the solution of the linearized least squares problem at each iteration is either too time-consuming or simply not possible due to storage problems.

We first give some general comments regarding the implementation of Algorithm 5.1 in Subsection 5.3.1. We then give some more details and present our numerical results in Subsections 5.3.2 (for the large-scale problems from MCPLIB), 5.3.3 (for some problems from optimal control), and 5.3.4 (for a discretized obstacle problem).

5.3.1 General Considerations

We first note that Algorithm 5.1 can be extended in a relatively simple way to the more general class of mixed complementarity problems. The details are given in Chapter 4. Our implementation is therefore able to deal with mixed complementarity problems. Note, however, that we still write $\Phi(x) = 0$ for the corresponding reformulation as an overdetermined nonlinear system of equations, and we still write $\Psi(x) := \frac{1}{2}\|\Phi(x)\|^2$ for the associated merit function, i.e., we do not change our notation from the previous sections although Φ and Ψ are defined in a slightly different way.

We have implemented Algorithm 5.1 in MATLAB. The implementation is along the lines of Algorithm 5.1, except that we use a nonmonotone line search. To be more precise, we use the standard (monotone) Armijo rule during the first five iterations and then switch to the nonmonotone line search where the maximum of the function values $\Psi(x^k)$ is taken over the last ten iterations.

Some preliminary numerical experiments indicated that small values of the Levenberg-Marquardt parameter ν_k give much better results than larger ones so that we decided to

take the limiting value $\nu_k = 0$ for all k, i.e., the Levenberg-Marquardt step from (5.1) reduces to a Gauss-Newton step

$$\min_d \|H_k d + \Phi(x^k)\|. \tag{5.24}$$

The search direction d^k is always given by the inexact solution of system (5.24).

We terminate the iteration in step (S.1) of Algorithm 5.1 if one of the following conditions are satisfied:

$$\Psi(x^k) \leq 10^{-8} \quad \text{or} \quad \|\nabla\Psi(x^k)\|_\infty \leq 10^{-6} \quad \text{or} \quad k > 100.$$

The other parameters used in our implementation are $\lambda_1 = 0.9, \lambda_2 = 0.1, \beta = 0.9$ and $\sigma = 10^{-4}$.

For the inexact solution of the linearized least squares subproblems, we use the LSQR method from [94]. An implementation of LSQR is provided by MATLAB. LSQR is an iterative method for the solution of linear least squares problems and does not need any matrix factorizations. This allows us to apply LSQR to large-scale problems. The forcing sequence $\{\alpha_k\}$ from Algorithm 5.1, which determines the accuracy with which we actually solve the subproblems, is defined as

$$\alpha_k = \min\Big\{\frac{10^{-2}}{k+1}, \Psi(x^k), \|\nabla\Psi(x^k)\|_\infty\Big\}.$$

LSQR employs several termination criteria (see [94]). The two main criteria used in our implementation are

$$\frac{\|r_{LS}^k\|}{\|\Phi(x^k)\|} \leq \alpha_k \tag{5.25}$$

and

$$\|H_k^T r_{LS}^k\| \leq \max\Big\{10^{-8}, \min\Big\{\alpha_k, \theta\|H_k^T\Phi(x^k)\|\Big\}\Big\} \quad \text{with } \theta = 0.01, \tag{5.26}$$

where $r_{LS}^k := H_k d + \Phi(x^k)$ denotes the residual vector of (5.24) (note that this vector is different from the vector r^k occurring in (5.4)). Basically, the first criterion (5.25) checks whether the relative residuum is sufficiently small. In general, this condition will be satisfied only if the linearized least squares problem has a zero or small residuum in the solution d^k, and this will usually happen only if we are getting close to a solution x^* of our mixed complementarity problem.

The other condition (5.26) is applicable in more general situations and checks whether the error in the normal equation is small enough. Note that we use an absolute lower bound of 10^{-8} so that we do not force this error to become too small. The other two terms in (5.26) are easy to understand: We require the relative error in the normal equation to be at least as small as α_k, and, in addition, it has to satisfy the bound

$$\|H_k^T r_{LS}^k\| \leq \theta\|H_k^T\Phi(x^k)\|$$

for some constant $\theta \in (0,1)$. This latter condition is important because otherwise it happens quite often that the zero vector (used as a starting point for the inner LSQR iteration) is accepted by this criterion, meaning that $x^{k+1} = x^k$ in the corresponding outer iteration, and this useless situation has to be avoided.

We also note that estimates of the quantities $\|r_{LS}^k\|$ and $\|H_k^T r_{LS}^k\|$ used within the inner termination criterion can be obtained at minimal cost from the LSQR method itself, see [94] for more details.

Finally, we turn to the question of a suitable preconditioner. Like all iterative methods for the solution of linear systems of equations, the practical performance of LSQR for the iterative solution of the linear least squares subproblem (5.24) may often be accelerated by the choice of a suitable preconditioner. Note, however, that we only have the possibility to choose a right preconditioner M since

$$\min_d \|Hd + \Phi(x)\| = \min_z \|HM^{-1}z + \Phi(x)\|, \quad \text{where } z = Md,$$

whereas a left preconditioner would change the subproblem. In order to find an appropriate preconditioner M, recall that any matrix $H \in \partial_C \Phi(x)$ has the representation

$$H = \begin{pmatrix} \lambda_1 H_1 \\ \lambda_2 H_2 \end{pmatrix}, \tag{5.27}$$

where

$$H_1 \subseteq D_a(x) + D_b(x)F'(x) \quad \text{and} \quad H_2 \subseteq \tilde{D}_a(x) + \tilde{D}_b(x)F'(x) \tag{5.28}$$

with certain diagonal matrices $D_a(x), D_b(x), \tilde{D}_a(x), \tilde{D}_b(x)$, see Theorem 4.3 and Proposition 4.17.

Taking into account this structure, a natural choice for M seems to be the first block matrix H_1 provided this matrix is nonsingular and the size and structure of H_1 allows the solution of linear systems of equations with this matrix. Note also that H_1 is the leading block since $\lambda_1 = 0.9, \lambda_2 = 0.1$ in our implementation, i.e., we put much more emphasis on this block than on the second part.

However, for some large-scale problems, it may not be possible to use H_1 or a suitable modification of this matrix as a preconditioner, and then we have to take a closer look at the particular structure of this matrix in order to find a suitable preconditioner. We will illustrate this point in more detail in some of the following subsections.

5.3.2 MCPLIB Test Problems

Our first test problems are the larger ones taken from the MCPLIB. We note again that the test problem library used here is an updated version of the MCPLIB originally introduced in [22], see also Section 4.5.1. The starting point x^0 is the standard one provided by the MCPLIB collection.

Since the examples from the MCPLIB are difficult, but still of reasonable size, we basically take the suggestion from the previous subsection and use the slightly regularized

H_1-block $M := H_1 + 10^{-4}I$ as a preconditioner. We note, however, that nonsingularity of this matrix M is not guaranteed, but the addition of the scaled identity seems to be quite helpful in order to avoid singularity problems at the solution of some test examples.

Our numerical results are summarized in Table 5.1. In this table, the first column gives the name of the problem; Dim is the number of the variables in the problem; o.it. denotes the number of outer iterations; column avg.i.it. presents the average number of inner LSQR iterations needed to solve the corresponding linear least squares problem (5.24) inexactly; $\Psi(x^0)$ gives the value of the merit function at the starting point; and $\Psi(x^f)$ and $\|\nabla\Psi(x^f)\|_\infty$ denote the values of $\Psi(x)$ and $\|\nabla\Psi(x)\|_\infty$ at the final iterate $x = x^f$.

Table 5.1: Numerical results for (large) MCPLIB test problems

Problem	Dim	o.it.	avg.i.it.	$\Psi(x^0)$	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|_\infty$
`bert_oc`	5000	5	1.8	5.13e+01	2.99e-12	1.07e-06
`bratu`	5625	8	1.6	1.41e+01	4.22e-10	4.21e-05
`bishop`	1645	—	—	1.00e+11	—	—
`lincont`	419	34	45.2	7.11e+03	1.19e-11	7.37e-06
`obstacle`	2500	7	1.0	2.36e-02	6.79e-10	4.88e-05
`opt_cont`	288	8	1.9	6.09e+01	5.86e-09	8.92e-05
`opt_cont31`	1024	10	1.5	6.76e+01	7.57e-10	3.36e-05
`opt_cont127`	4096	11	2.0	3.89e+01	1.12e-09	4.77e-05
`opt_cont255`	8192	10	2.9	2.64e+01	4.78e-09	1.37e-05
`opt_cont511`	16384	13	3.6	1.84e+01	2.54e-14	3.26e-07
`trafelas`	2904	39	4.2	5.28e+03	1.10e-11	3.86e-06

With the only exception of example `bishop`, we see from Table 5.1 that we can solve all other test examples. These other examples include some problems like `lincont` or `trafelas` which are usually regarded as being quite difficult. We also stress that the average number of inner iterations is extremely small for all problems except `lincont`. This indicates the effectiveness of our preconditioner.

5.3.3 Optimal Control Problems

In this section we look at the practical behavior of the algorithm by considering a variety of large-scale complementarity problems resulting from suitable discretizations of optimal control problems. We consider both control problems with control constraints and control problems with control and state constraints.

Control Problems with Control Constraints

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with boundary $\Gamma = \partial\Omega$, and let $y_d, u_d, \psi \in L^2(\Omega)$ be given functions such that y_d represents a desired state, u_d a desired control, and ψ describes

the upper bounds on the control variable. Furthermore, let $\alpha \geq 0$ denote a regularization parameter. Our aim is then to find a control u and a corresponding state y minimizing the functional

$$J(y,u) = \frac{1}{2}\int_\Omega \big(y(x) - y_d(x)\big)^2 dx + \frac{\alpha}{2}\int_\Omega \big(u(x) - u_d(x)\big)^2 dx,$$

subject to the elliptic state equation

$$-\Delta y(x) = u(x), \quad \text{for } x \in \Omega,$$

the Dirichlet boundary conditions

$$y(x) = 0, \quad \text{for } x \in \Gamma,$$

and the control constraints

$$u(x) \leq \psi(x) \quad \text{a.e. in } \Omega.$$

To be more specific, consider the two-dimensional case $\Omega = (0,1) \times (0,1) \subseteq \mathbb{R}^2$, and let A denote the standard five-point finite difference approximation to the negative Laplacian with uniform stepsize $h := 1/(N+1)$ for some $N \in \mathbb{N}$, so that we have $n := N^2$ interior nodes. Then the discretized optimal control problem becomes

$$\min_{u,y} \frac{1}{2}\|y - y_d\|_2^2 + \frac{\alpha}{2}\|u - u_d\|_2^2 \quad \text{s.t.} \quad Ay = u, \;\; \psi - u \geq 0,$$

where, for simplicity of notation, the discretized functions u, y etc. are denoted by the same letters as their continuous counterparts.

Because the state variable is not constrained, we can remove the control variable using $u = Ay$ and obtain the equivalent problem

$$\min_{y} \frac{1}{2}\|y - y_d\|_2^2 + \frac{\alpha}{2}\|Ay - u_d\|_2^2 \quad \text{s.t.} \quad \psi - Ay \geq 0.$$

Setting $v := \psi - Ay$, we obtain

$$\min_{v} \frac{1}{2}\|A^{-1}(\psi - v) - y_d\|_2^2 + \frac{\alpha}{2}\|\psi - v - u_d\|_2^2 \quad \text{s.t.} \quad v \geq 0.$$

Defining $v_d := y_d - A^{-1}\psi$ and $\psi_d := u_d - \psi$, we finally obtain the convex problem

$$\min_{v} f(v) := \frac{1}{2}\|A^{-1}v + v_d\|_2^2 + \frac{\alpha}{2}\|v + \psi_d\|_2^2 \quad \text{s.t.} \quad v \geq 0.$$

Using the KKT theory, it follows that this convex quadratic optimization problem is equivalent to the linear complementarity problem

$$v \geq 0, \quad F(v) \geq 0, \quad v^T F(v) = 0$$

with

$$F(v) := \nabla f(v) = (A^{-1}A^{-1} + \alpha I)v + A^{-1}v_d + \alpha\psi_d.$$

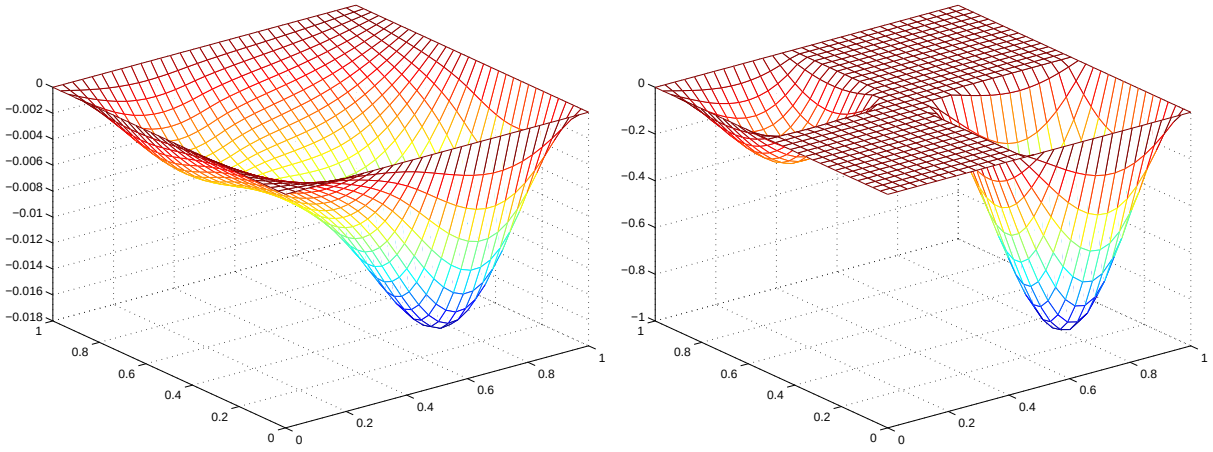

Figure 5.1: Optimal state (left) and optimal control (right) for Example 5.4

Table 5.2: Numerical results for Example 5.4

N	50	100	150	200	250	300
o. it.	10	10	9	13	16	15
avg. i. it.	6.3	20.7	38.0	25.1	31.0	37.5

At this stage we can apply Algorithm 5.1 using the same parameter setting as in the previous subsection. In order to solve the corresponding linear least squares problem (5.24) inexactly, we apply the LSQR method with the same termination criteria as described above.

The matrix H_k arising in the subproblem (5.24) has the structure from (5.27), (5.28) with $F'(v) = A^{-1}A^{-1} + \alpha I$. Since we only need to compute matrix-vector products of the form $H_k v$ and $H_k^T u$ for certain vectors v and u, respectively, and since the matrix A corresponds to the standard five-point finite difference approximation of the negative Laplacian, these matrix-vector products can be computed quite efficiently by, e.g., a fast sine transform in only $O(N^2 \log_2 N)$ arithmetic operations which is not much more than $O(n)$ flops.

We apply our method to two examples taken from [3] (also used as test problems in, e.g., [119, 62]).

Example 5.4 (**Control Constraints**) The data are $\alpha = 0.01, \psi \equiv 0, u_d \equiv 0$ and $y_d(x_1, x_2) = \sin(2\pi x_1)\sin(2\pi x_2)\exp(2x_1)/6$. The optimal state and control are depicted in Figure 5.1.

We present our numerical results (number of outer iterations and average number of inner LSQR iterations) for this example in Table 5.2 using different discretizations $N \in \mathbb{N}$. Note that the dimension of the corresponding complementarity problem is $n = N^2$.

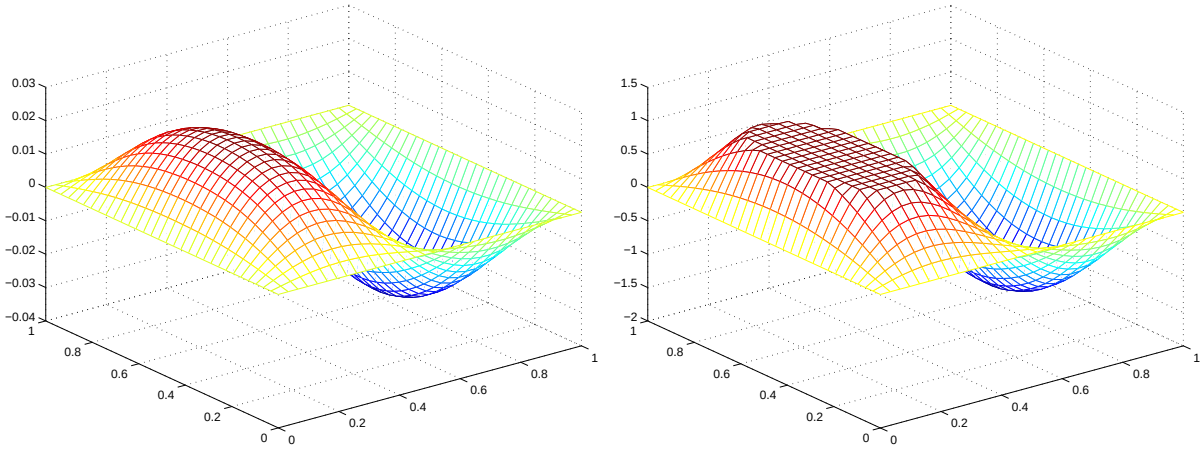

Figure 5.2: Optimal state (left) and optimal control (right) for Example 5.5

Table 5.3: Numerical results for Example 5.5

N	50	100	150	200	250	300
o. it.	12	16	10	10	11	11
avg.i. it.	6.2	12.6	21.2	37.5	45.6	45.2

Note also that the average number of inner iterations is relatively small for this example, so there was no need to use a fancy preconditioner for the LSQR method.

Example 5.5 (**Control Constraints**) The data are $\alpha = 0.01, \psi \equiv 1, u_d \equiv 0$ and

$$y_d(x_1, x_2) = \begin{cases} 200x_1x_2(x_1 - 0.5)^2(1 - x_2), & \text{if } 0 < x_1 \leq 0.5, \\ 200x_2(x_1 - 1)(x_1 - 0.5)^2(1 - x_2), & \text{if } 0.5 < x_1 \leq 1. \end{cases}$$

The optimal state and control are depicted in Figure 5.2.

Table 5.3 contains the number of inner and outer iterations needed by our method to solve Example 5.5. Again, we observe a relatively small number of average inner iterations, so there is no need to use a suitable preconditioner for this example.

Both examples clearly indicate that our inexact semismooth method can be applied very successfully to optimal control problems with control constraints.

Control Problems with Control and State Constraints

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with boundary $\Gamma = \partial\Omega$. Given $y_d \in L^2(\Omega), u_d, u_1, u_2, \psi \in L^2(\Gamma), \alpha \geq 0$, and suitable functions $d : \Omega \times \mathbb{R} \to \mathbb{R}, b : \Gamma \times \mathbb{R} \to \mathbb{R}$, our aim is to find a control function $u \in L^2(\Gamma)$ and a corresponding state y minimizing the functional

$$J(y, u) = \frac{1}{2} \int_\Omega \big(y(x) - y_d(x)\big)^2 dx + \frac{\alpha}{2} \int_\Gamma \big(u(x) - u_d(x)\big)^2 dx, \tag{5.29}$$

subject to the state equation

$$-\Delta y(x) + d(x, y(x)) = 0, \quad \text{for } x \in \Omega, \tag{5.30}$$

the Dirichlet boundary conditions

$$y(x) = b(x, u(x)), \quad \text{for } x \in \Gamma, \tag{5.31}$$

and the control and state constraints

$$y(x) \leq \psi(x) \text{ a.e. in } \Omega, \quad u_1(x) \leq u(x) \leq u_2(x) \text{ a.e. in } \Gamma. \tag{5.32}$$

We discretize this problem in a similar way as described in the previous subsection, where Ω is again the unit square $(0,1) \times (0,1) \subset \mathbb{R}^2$. After discretization we obtain a nonlinear programming problem of the form

$$\min f(z) \quad \text{s.t.} \quad g(z) \leq 0, \quad h(z) = 0. \tag{5.33}$$

The corresponding KKT conditions of (5.33) form a mixed complementarity problem which may be reformulated as an overdetermined nonlinear system of equations $\Phi(w) = 0$, with $\Phi : \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^m \to \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^{2m}$ being defined by

$$\Phi(w) := \Phi(z, \zeta, \xi) := \begin{pmatrix} \nabla f(z) + g'(z)^T \xi + h'(z)^T \zeta \\ h(z) \\ \lambda_1 \ \varphi_{FB}(\xi, g(z)) \\ \lambda_2 \varphi_+(\xi, g(z)) \end{pmatrix}, \tag{5.34}$$

for some $\lambda_1, \lambda_2 \in \mathbb{R} \setminus \{0\}$ (again, we use $\lambda_1 = 0.9, \lambda_2 = 0.1$ in our implementation),

$$\varphi_{FB}(\xi, g(z)) := (\phi_{FB}(\xi_1, g_1(z)), \ldots, \phi_{FB}(\xi_m, g_m(z))^T \in \mathbb{R}^m$$

and

$$\varphi_+(\xi, g(z)) := (\phi_+(\xi_1, g_1(z)), \ldots, \phi_+(\xi_m, g_m(z))^T \in \mathbb{R}^m.$$

We note that the last m components are again used in order to reduce the complementarity gap at the current point z.

We now follow [84] and try to achieve the form (5.33) by choosing a number $N \in \mathbb{N}$, a stepsize $h = 1/(N+1)$, considering the mesh points

$$x_{ij}, \quad 0 \leq i, j \leq N+1,$$

and defining the following sets of indices (i, j), residing either in the domain Ω or on the boundary Γ:

$$\begin{aligned} I(\Omega) &:= \{(i,j) \mid 1 \leq i, j \leq N+1\}, \\ I(\Gamma) &:= \{(i,j) \mid i = 1, \ldots, N, \ j = 0 \text{ or } j = N+1, \\ &\qquad\qquad j = 1, \ldots, N, \ i = 0 \text{ or } i = N+1 \ \}. \end{aligned}$$

Obviously, these index sets have the cardinality $|I(\Omega)| = N^2$ and $|I(\Gamma)| = 4N$, respectively.

The optimization variable z in (5.33) is taken as the vector

$$z := ((y_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma)}, (u_{ij})_{(i,j)\in I(\Gamma)}) \in \mathbb{R}^{N^2+8N}.$$

Since we have Dirichlet boundary conditions, the dimension of the optimization variable z can be reduced to a vector in the smaller space $\mathbb{R}^{N^2+4N}$ by determining the state variables $(y_{ij})_{(i,j)\in I(\Gamma)}$ out of the Dirichlet conditions (5.31).

The discretized form of the cost function (5.29) then becomes

$$f(z) := \frac{h^2}{2} \sum_{(i,j)\in I(\Omega)} (y_{ij} - y_{d,ij})^2 + \frac{\alpha h}{2} \sum_{(i,j)\in I(\Gamma)} (u_{ij} - u_{d,ij})^2.$$

The application of the five-point finite difference approximation of $-\Delta$ to the elliptic equation (5.30) yields the following equality constraints for all $(i,j) \in I(\Omega)$:

$$h_{ij}(z) := 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2 d(x_{ij}, y_{ij}) = 0.$$

Note that the Dirichlet conditions (5.31) are used in the above equation to substitute the variables $(y_{ij})_{(i,j)\in I(\Gamma)}$, so we have $h : \mathbb{R}^{N^2+4N} \to \mathbb{R}^{N^2}$.

The control and state inequality constraints (5.32) yield the inequality constraints $g : \mathbb{R}^{N^2+4N} \to \mathbb{R}^{N^2+8N}$ defined by

$$\begin{array}{lll} g_{ij}(z) & := y_{ij} - \psi_{ij} \le 0 & \forall (i,j) \in I(\Omega), \\ g_{ij}(z) & := -u_{ij} + u_{1,ij} \le 0 & \forall (i,j) \in I(\Gamma), \\ g_{n+i,n+j}(z) & := u_{ij} - u_{2,ij} \le 0 & \forall (i,j) \in I(\Gamma). \end{array}$$

In summary, we obtain a problem of the form (5.33) and therefore get the corresponding equation reformulation $\Phi(w) = 0$ using certain Lagrange multipliers $\zeta = (\zeta_{ij})_{(i,j)\in I(\Omega)}$ and $\xi = (\xi_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma)\cup I(\Gamma)}$.

Example 5.6 (**Control and State Constraints**) This example is taken from [84] and has the following data

$$\begin{array}{ll} \text{on } \Omega & : -\Delta y(x) = 20,\ y(x) \le 3.5, \quad y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1), \\ \text{on } \Gamma & : y(x) = u(x),\ 0 \le u(x) \le 10, \quad u_d(x) \equiv 0,\ \alpha = 0.01. \end{array}$$

The cost function evaluated at the optimal control and state by the authors in [84] is $f(\bar{y}, \bar{u}) = 0.196525$ for a discretization factor $N = 99$. The optimal state and adjoint variable ζ are depicted in Figure 5.3. The control variable is depicted in Figure 5.4.

Example 5.7 (**Control and State Constraints**) This example is again taken from [84] and has the same data as Example 5.6 except that $\alpha = 0$. A singular control is obtained. The cost function evaluated at the optimal control and state by the authors in [84] is $f(\bar{y}, \bar{u}) = 0.096695$ for a discretization factor $N = 99$. The optimal state and adjoint variable ζ are depicted in Figure 5.5. The control variable is shown in Figure 5.6.

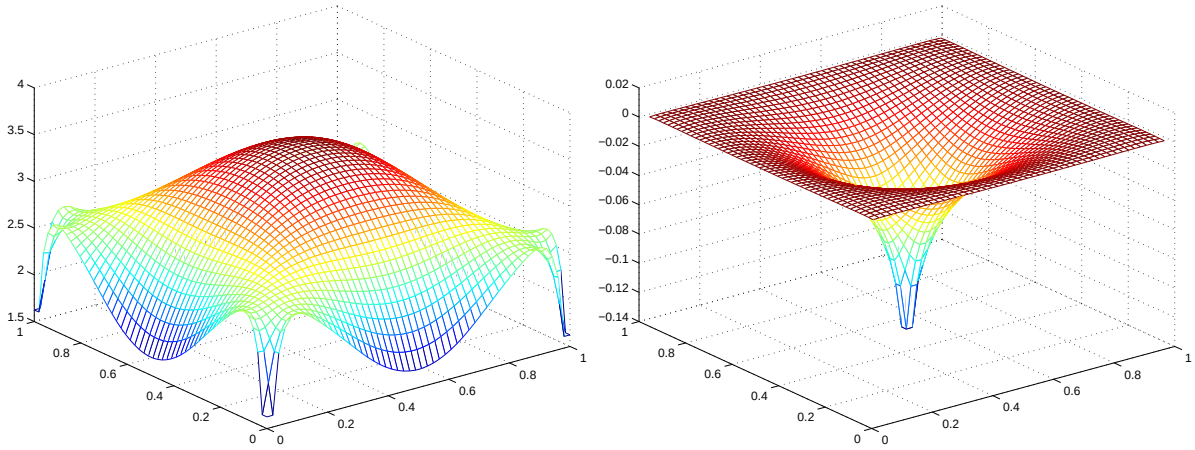

Figure 5.3: Optimal state (left) and adjoint variable (right) for Example 5.6

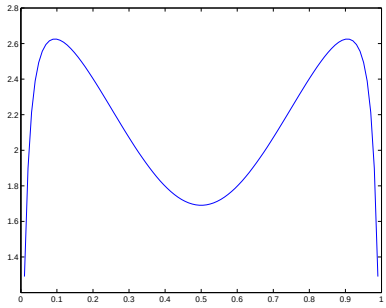

Figure 5.4: Optimal control for Example 5.6

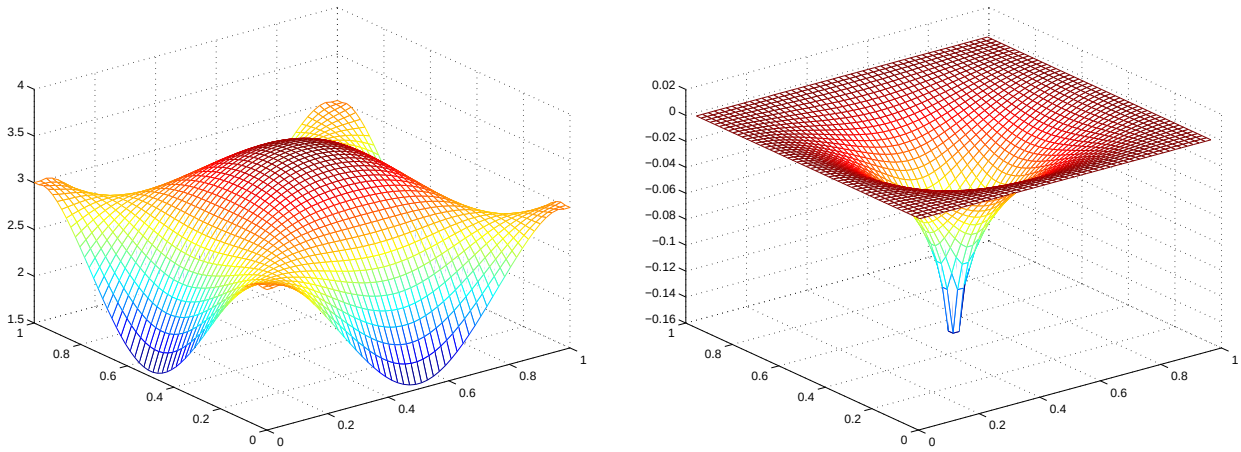

Figure 5.5: Optimal state (left) and adjoint variable (right) for Example 5.7

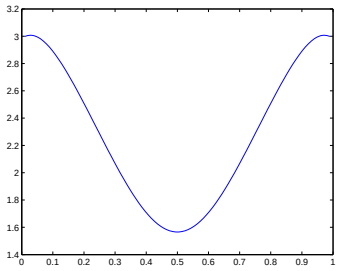

Figure 5.6: Optimal control for Example 5.7

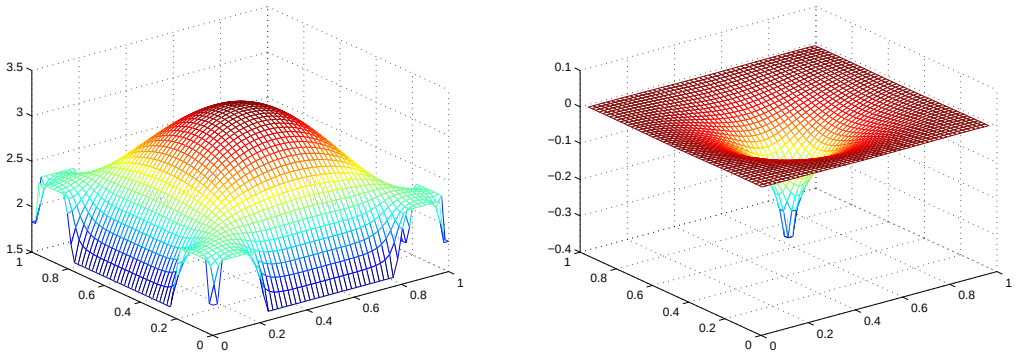

Figure 5.7: Optimal state (left) and adjoint variable (right) for Example 5.8

Example 5.8 (**Control and State Constraints**) This is the third example from [84] and has the same data as Example 5.6 except that the state and control constraints are more restrictive:

$$\begin{array}{lll} \text{on } \Omega & : -\Delta y(x) = 20,\ y(x) \le 3.2, & y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1), \\ \text{on } \Gamma & : y(x) = u(x),\ 1.6 \le u(x) \le 2.3 & u_d(x) \equiv 0,\ \alpha = 0.01. \end{array}$$

The optimal state and adjoint variable ζ are depicted in Figure 5.7. The control variable is shown in Figure 5.8. The cost function evaluated at the optimal control and state by the authors in [84] is $f(\bar{y}, \bar{u}) = 0.321010$ when using $N = 99$.

Example 5.9 (**Control and State Constraints**) This is the fourth example from [84] and has the same data as Example 5.8 except that $\alpha = 0$. We obtain a bang-bang optimal control. The optimal state and adjoint variable ζ are depicted in Figure 5.9. The control variable is shown in Figure 5.10. The cost function evaluated at the optimal control and state by the authors in [84] is $f(\bar{y}, \bar{u}) = 0.249178$ for $N = 99$.

Note that, after the discretization of these examples, we obtain a nonlinear programming problem (5.33) with convex objective function f and linear equality and linear in-

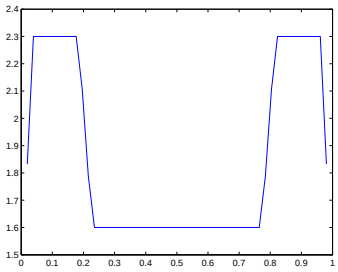

Figure 5.8: Optimal control for Example 5.8

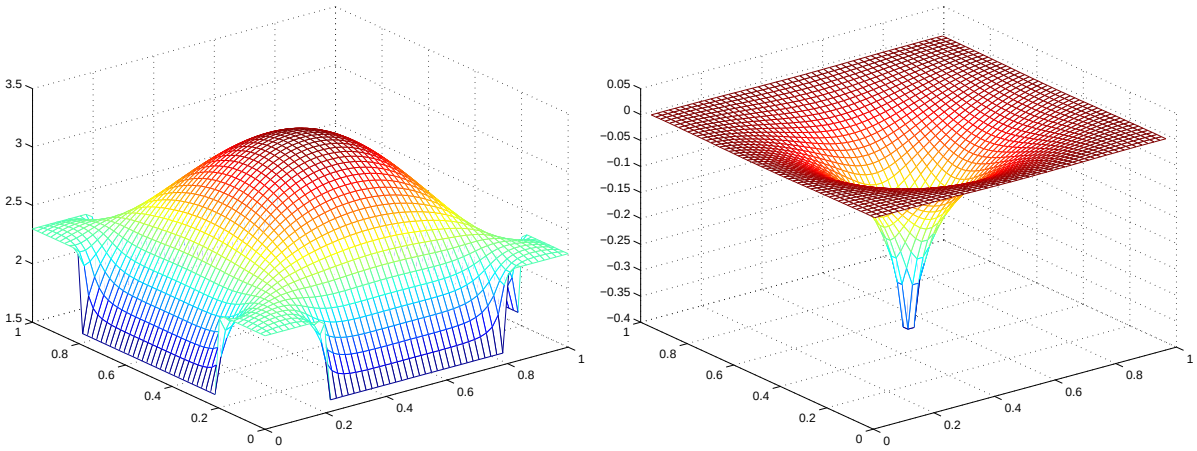

Figure 5.9: Optimal state (left) and adjoint variable (right) for Example 5.9

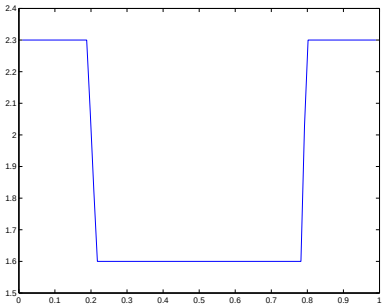

Figure 5.10: Optimal control for Example 5.9

equality constraints h and g. This implies the equivalence between (5.33) and the overdetermined system of equations $\Phi(x) = 0$ from (5.34).

We therefore applied Algorithm 5.1 using the same parameters as in the previous subsections. However, without a suitable preconditioner, LSQR was not able to solve the larger subproblems successfully. Therefore we had to find a suitable preconditioner M in order to improve the performance of the LSQR method. To this end, we note that the matrix H_k from the least squares subproblem (5.24) has the following structure for all test problems from Examples 5.6–5.9:

$$H_k = \left(\begin{array}{ccc|ccc} \frac{1}{(N+1)^2}I & 0 & A & I & 0 & 0 \\ 0 & \frac{\alpha}{N+1}I & B & 0 & -I & I \\ A & B^T & 0 & 0 & 0 & 0 \\ \hline \lambda_1 D_1 & 0 & 0 & & & \\ 0 & -\lambda_1 D_2 & 0 & & \lambda_1 D_4 & \\ 0 & \lambda_1 D_3 & 0 & & & \\ \hline -\lambda_2 \tilde{D}_1 & 0 & 0 & & & \\ 0 & \lambda_2 \tilde{D}_2 & 0 & & \lambda_2 \tilde{D}_4 & \\ 0 & -\lambda_2 \tilde{D}_3 & 0 & & & \end{array}\right),$$

where the matrix $A \in \mathbb{R}^{N^2 \times N^2}$ is the five-point difference approximation to the negative Laplace operator, $B \in \mathbb{R}^{4N \times N^2}$ a sparse matrix with entries 0 or -1, and $D_i, \tilde{D}_i, i = 1, 2, 3$ are diagonal matrices of suitable dimension.

Taking into account this structure, we decided to take the matrix

$$M = \left(\begin{array}{ccc|c} 0 & 0 & A & \\ 0 & \frac{1}{N+1}I & B & 0 \\ A & B^T & 0 & \\ \hline & 0 & & I \end{array}\right)$$

as a preconditioner for the LSQR matrix since this matrix is both nonsingular and may be viewed as a suitable approximation to the leading block of H_k. Moreover, we can solve linear systems involving M once again very efficiently by a fast sine transform. The numerical results obtained with Algorithm 5.1 using this preconditioner are summarized in Table 5.4 using different discretizations $N \in \mathbb{N}$. The columns in Table 5.4 have the same meaning as those for Table 5.1 except that we now have one additional column which shows the optimal value $f(\bar{y}, \bar{u})$ of the cost function obtained by our method. Note that, for $N = 100$, this value is always very close to the corresponding results presented in [84].

Table 5.4: Numerical results for optimal control problems with mixed constraints

Example	N	Dim	o.it.	avg.i.it.	$\Psi(w^f)$	$\|\nabla\Psi(w^f)\|_\infty$	$f(\bar{y}, \bar{u})$
5.6	50	8100	14	42.4	7.99e-09	6.19e-05	1.882782e-01
	100	31200	13	55.1	3.79e-10	8.48e-06	1.965488e-01
	150	69300	23	96.5	3.53e-09	3.62e-05	1.993628e-01

Table 5.4: Numerical results for optimal control problems with mixed constraints (continued)

Example	N	Dim	o.it.	avg.i.it.	$\Psi(w^f)$	$\|\nabla\Psi(w^f)\|_\infty$	$f(\bar{y},\bar{u})$
5.7	50	8100	12	53.1	5.30e-10	2.63e-06	8.939136e-02
	100	31200	14	56.9	9.17e-07	9.79e-07	9.659419e-02
	150	69300	21	116.3	3.37e-07	7.93e-07	1.000500e-01
5.8	50	8100	77	1004.5	3.37e-09	5.09e-05	3.069800e-01
	100	31200	55	516.1	2.48e-06	6.35e-07	3.195118e-01
	150	69300	67	596.4	2.64e-06	7.88e-07	3.230811e-01
5.8	50	8100	84	1172.1	3.67e-09	5.02e-05	2.358106e-01
	100	31200	57	484.4	2.48e-06	4.45e-07	2.474559e-01
	150	69300	75	702.1	2.27e-06	5.43e-07	2.506512e-01

Table 5.4 shows that we are able to solve all optimal control problems with mixed constraints from Examples 5.6–5.9. The number of outer iterations is quite reasonable for all test runs. Also the number of inner iterations is at least acceptable taking into account the overall dimension of the problems.

5.3.4 Obstacle Problems

Let $\Omega \subset \mathbb{R}^2$ be a given domain with boundary $\Gamma = \partial\Omega$. The obstacle problem consists in finding the equilibrium position of an elastic membrane subject to an external force f and an obstacle ψ. Hence the infinite-dimensional problem is to minimize the total energy

$$E(u) := \frac{1}{2}\int_\Omega \|\nabla u\|^2 dx - \int_\Omega f u dx,$$

subject to the constraint

$$u \geq \psi \text{ a.e. in } \Omega.$$

The optimality conditions for this infinite-dimensional problem lead to a variational inequality which, under a weak regularity condition, is equivalent to the following complementarity problem

$$\begin{aligned} -\Delta u &\geq f \quad \text{on } \Omega, \\ u &\geq \psi \quad \text{on } \Omega, \\ (-\Delta u - f)(u-\psi) &= 0 \quad \text{on } \Omega, \\ u &\equiv 0 \quad \text{on } \Gamma. \end{aligned} \tag{5.35}$$

In order to discretize this problem, we take once again the standard rectangle $\Omega = (0,1) \times (0,1)$ and denote by A the five-point finite difference approximation to the negative Laplace operator on a uniform grid with stepsize $h := 1/(N+1)$ for some $N \in \mathbb{N}$. Then, setting

$v := u - \psi$, the discretized problem can be reformulated as a nonlinear complementarity problem

$$v \geq 0, F(v) \geq 0, v^T F(v) = 0 \tag{5.36}$$

with $F(v) := A(v + \psi) - f$. Using $f = f(v) := \lambda e^{-\psi - v}$ for some parameter $\lambda \geq 0$, we obtain the obstacle Bratu problem from [87].

We apply Algorithm 5.1 to this problem using the particular data $\psi \equiv -4, \lambda := 1$ and the same parameters as in the previous subsections. We use the matrix A as a preconditioner for the inner LSQR method. Note again that a linear system with this matrix can be solved very efficiently. The numerical results are summarized for different discretizations in Table 5.5.

Table 5.5: Numerical results for the obstacle Bratu problem

N	o.it	avg.i.it	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|_\infty$
100	7	9.9	2.67e-15	4.13e-05
200	7	11.6	3.28e-11	5.58e-02
300	8	13.9	3.55e-12	1.78e-04
400	8	14.1	6.59e-12	4.86e-04
500	8	14.2	1.05e-11	1.15e-03

Note that both the number of outer iterations and the average number of inner iterations is extremely small for this example. This is consistent with the observation made in [62] for a somewhat different method.

Chapter 6

A Projected Trust Region Filter Method

In this chapter, we aim at improving the exact method from Chapter 4 further. To this end, we incorporate two additional features: First, we incorporate the bound constraints explicitly into the reformulation of the mixed complementarity problem as a least squares system, so that all iterates stay feasible with respect to these constraints. This should improve the robustness of the method since it avoids spurious stationary points outside the box $\mathcal{B} = [l, u]$, for example. Second, we add a filter in our trust region method in order to improve the efficiency of the method. In fact, preliminary numerical experiments showed that the local method presented in Section 3.2.4 behaves very good, so we try to accept the full (Levenberg-Marquardt-type) step as often as possible.

The organization of this chapter is as follows. We begin by presenting a projected Levenberg-Marquardt-type method for the solution of mixed complementarity problems in Section 6.1. The global and local convergence properties of this method are investigated in Sections 6.2 and 6.3, respectively. We then incorporate a filter technique into the globalized method in Section 6.4 and show that all global and local convergence results still hold for this filter trust region method. Finally, numerical results are presented in Section 6.5.

6.1 Projected Levenberg-Marquardt Method

We reconsider the reformulation of the mixed complementarity as an overdetermined system of equation $\Phi(x) = 0$, with the operator $\Phi : \mathbb{R}^n \to \mathbb{R}^{2n}$ being the operator $\bar{\Phi} : \mathbb{R}^n \to \mathbb{R}^{2n}$ defined in (4.36). Then it was noted in Proposition 4.16 that the overdetermined system of equations $\Phi(x) = 0$ is equivalent to the mixed complementarity problem. Obviously, the same holds for the box constrained reformulation $\Phi(x) = 0, x \in [l, u]$, which we prefer here because this avoids some problems like mappings F which are not defined outside the feasible region $\mathcal{B} = [l, u]$ or possible stationary points outside this set. Hence we arrive at a problem of the form (3.13). Now the mixed complementarity problem is

equivalent to the box constrained overdetermined system

$$\Phi(x) = 0, \quad x \in \mathcal{B}, \tag{6.1}$$

and therefore fits into the framework (3.13) discussed in Section 3.2.4. For the readers convenience we restate the local projected Levenberg-Marquardt Algorithm 3.14.

Algorithm 6.1 (Projected Levenberg-Marquardt Method for MCPs)

(S.0) Choose $x^0 \in \mathcal{B}$, and set $k := 0$.

(S.1) If x^k satisfies a suitable termination criterion: STOP.

(S.2) Choose $H_k \in \partial_C \Phi(x^k), \nu_k > 0$, and compute p^k_{LM} as the solution of the linear system

$$\big(H_k^T H_k + \nu_k I\big) p_{LM} = -H_k^T \Phi(x^k), \qquad H_k \in \partial_C \Phi(x^k). \tag{6.2}$$

(S.3) Compute the projected Levenberg-Marquardt direction

$$p^k_{PLM} := P_{\mathcal{B}}(x^k + p^k_{LM}) - x^k = P_{\mathcal{B}-x^k}(p^k_{LM}). \tag{6.3}$$

(S.4) Set $x^{k+1} = x^k + p^k_{PLM}, k \leftarrow k+1$, and go to (S.1).

We now want to develop a globalized version of Algorithm 6.1 for the solution of the mixed complementarity problem. For this purpose we note the equivalence between the box constrained reformulation (6.1) of the MCP and the bound constraint least squares problem

$$\min \Psi(x) := \frac{1}{2}\|\Phi(x)\|^2 \quad \text{s.t.} \quad x \in \mathcal{B}. \tag{6.4}$$

Then it was noted in Theorem 4.18 (b) that the merit function Ψ is continuously differentiable. In view of this observation the Levenberg-Marquardt direction p^k_{LM} may equivalently be computed by solving the linear system

$$\big(H_k^T H_k + \nu_k I\big) p_{LM} = -\nabla \Psi(x^k),$$

see (6.2).

Our globalized method is a trust-region algorithm that contains elements from affine-scaling methods. In fact, we exploit an observation by Coleman and Li [16] who noted that the first-order optimality conditions of the least squares problem (6.4) are equivalent to the nonlinear system of equations

$$G(x) = 0 \quad \text{with} \quad G(x) := D(x)^r \nabla \Psi(x),$$

where $r > 0$ and

$$D(x) := \operatorname{diag}\big(d_1(x), \ldots, d_n(x)\big)$$

is a suitable *scaling matrix* satisfying the following conditions:

$$d_i(x) \begin{cases} = 0, & \text{if } x_i = l_i \text{ and } [\nabla\Psi(x)]_i > 0, \\ = 0, & \text{if } x_i = u_i \text{ and } [\nabla\Psi(x)]_i < 0, \\ \geq 0, & \text{if } x_i \in \{l_i, u_i\} \text{ and } [\nabla\Psi(x)]_i = 0, \\ > 0, & \text{else.} \end{cases} \qquad i = 1, \ldots, n. \tag{6.5}$$

Several different scaling matrices may be found in the literature, see, e.g., [16, 66, 122]. For the sake of simplicity, we will always use the following scaling matrix in this paper:

$$d_i(x) := \begin{cases} \min\{1, x_i - l_i\}, & \text{if } [\nabla\Psi(x)]_i > 0, \\ \min\{1, u_i - x_i\}, & \text{if } [\nabla\Psi(x)]_i < 0, \\ \min\{1, x_i - l_i, u_i - x_i\}, & \text{if } [\nabla\Psi(x)]_i = 0. \end{cases} \quad i = 1, \ldots, n. \tag{6.6}$$

This scaling matrix was suggested by Ulbrich [118] and satisfies some additional properties that will be used in our convergence analysis, see Lemmas 6.5 and 6.10. We note, however, that other choices are possible, like the one from [66].

For notational convenience, we write

$$D_k := D(x^k) \quad \text{and} \quad g^k := \nabla\Psi(x^k).$$

Let

$$q_k(p) := p^T g^k + \frac{1}{2} p^T \big(H_k^T H_k + \nu_k I\big) p$$

be a quadratic approximation of $\Psi(x^k + p) - \Psi(x^k)$, where x^k denotes the current iterate. We then compute a search direction p^k as an approximate solution of the trust region subproblem

$$\min\ q_k(p) \quad \text{s.t.} \quad x^k + p \in \mathcal{B}, \ \ \|p\|_\infty \leq \Delta_k \tag{6.7}$$

for some trust region radius $\Delta_k > 0$. Note that this is a box constrained quadratic program with feasible set

$$X_k := [l - x^k, u - x^k] \cap [-\Delta_k, +\Delta_k]^n.$$

Whether $x^k + p^k$ can be accepted as the new iterate x^{k+1} then depends on the ratio

$$r_k := \frac{\text{ared}_k(p^k)}{\text{pred}_k(p^k)} \tag{6.8}$$

of the actual and predicted reductions

$$\text{ared}_k(p) := \Psi(x^k) - \Psi(x^k + p) \quad \text{and} \quad \text{pred}_k(p) := -q_k(p),$$

respectively. In order to guarantee nice global convergence results, the approximate solution p^k of the trust region subproblem (6.7) has to satisfy at least the *feasibility condition*

$$p^k \in X_k \iff x^k + p^k \in \mathcal{B},\ \|p^k\|_\infty \leq \Delta_k, \tag{6.9}$$

and the *fraction of Cauchy decrease* condition

$$q_k(p^k) \leq \alpha q_k(p_C^k), \tag{6.10}$$

where $\alpha \in (0, 1]$ is a given constant, and $p_C^k = p(t_k)$ denotes the scaled *Cauchy step*, where t_k is defined as the solution of the one-dimensional subproblem

$$\begin{array}{ll} \min_t q_k\big(p(t)\big) \quad \text{s.t.} & p(t) = -tD_k^2 g^k, \;\; t \geq 0, \\ & \|p(t)\|_\infty \leq \Delta_k, \;\; x^k + p(t) \in \mathcal{B}. \end{array} \tag{6.11}$$

Note that, since $q_k(p_C^k) \leq q_k(0) = 0$, we may take the Cauchy step $p^k = p_C^k$ itself in order to get a suitable approximate solution of the trust region subproblem (6.7) satisfying (6.10). The overall method is as follows.

Algorithm 6.2 (Scaled Trust Region Method)

(S.0) Choose $x^0 \in \mathcal{B}$, $\Delta_0 > 0, 0 < \rho_1 < \rho_2 < 1$, $0 < \sigma_1 < 1 < \sigma_2$, $\varepsilon \geq 0$, $\eta \in (0, 1)$, $\Delta_{\min} > 0$, $\alpha \in (0, 1]$, and set $k := 0$.

(S.1) If $\|D_k g^k\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C \Phi(x^k), \nu_k > 0$, and compute p_{LM}^k using (6.2).

(S.3) Compute p_{PLM}^k from (6.3). If $\|\Phi(x^k + p_{PLM}^k)\| \leq \eta \|\Phi(x^k)\|$ holds, set $x^{k+1} := x^k + p_{PLM}^k$, $\Delta_{k+1} := \max\{\Delta_{\min}, \sigma_2 \Delta_k\}$, and go to step (S.6); otherwise go to step (S.4).

(S.4) Compute an approximate solution p^k of the trust region subproblem (6.7) satisfying (6.9) and (6.10), and define r_k by (6.8). If $r_k \geq \rho_1$, we call the iteration k successful and set $x^{k+1} := x^k + p^k$; otherwise we set $x^{k+1} := x^k$.

(S.5) Update the trust region radius as follows:

$$\Delta_{k+1} := \begin{cases} \sigma_1 \Delta_k, & \text{if } r_k < \rho_1, \\ \max\{\Delta_{\min}, \Delta_k\}, & \text{if } r_k \in [\rho_1, \rho_2), \\ \max\{\Delta_{\min}, \sigma_2 \Delta_k\}, & \text{if } r_k \geq \rho_2. \end{cases}$$

(S.6) Set $k \leftarrow k + 1$, and go to (S.1).

Throughout the rest of this paper, we denote by

$$\hat{g}^k := D_k g^k$$

the scaled gradient. Using this notation, we can state the following result which is standard for trust region methods and provides a lower bound for the predicted reduction pred_k, cf. [16, Lemma 3.1].

Lemma 6.3 *Let p^k be an approximate solution of the subproblem* (6.7) *satisfying the fraction of Cauchy decrease condition* (6.10)*. Then*

$$\mathrm{pred}_k(p^k) \geq \frac{1}{2}\alpha\|\hat{g}^k\| \min\Big\{\frac{\|\hat{g}^k\|}{\|H_k^T H_k + \nu_k I\|}, \Delta_k, 1\Big\}.$$

Proof. Consider a fixed iterate $x^k \in \mathcal{B}$, and recall that the Cauchy step $p_C^k = p(t_k)$ is given by the solution t_k of the one-dimensional problem (6.11) in the variable $t = t_k$. By definition, the stepsize $t \geq 0$ has to satisfy the two requirements

$$\|tD_k\hat{g}^k\|_\infty \leq \Delta_k \quad \text{and} \quad l - x^k \leq -tD_k\hat{g}^k \leq u - x^k.$$

Let t_Δ and $t_\mathcal{B}$ denote the maximum stepsize such that these two conditions hold. Then an elementary calculation shows that

$$\begin{aligned} t_\Delta &= \frac{\Delta_k}{\|D_k\hat{g}^k\|_\infty} \qquad \text{and} \\ t_\mathcal{B} &= \min\Big\{\min_{i:[D_k\hat{g}^k]_i<0} \frac{u_i - x_i^k}{-[D_k\hat{g}^k]_i}, \min_{i:[D_k\hat{g}^k]_i>0} \frac{x_i^k - l_i}{[D_k\hat{g}^k]_i}\Big\} \end{aligned}$$

(note that $D_k\hat{g}^k = D_k^2 g^k \neq 0$, since otherwise Algorithm 6.2 would have stopped at iteration k in step (S.1), hence the two maximum stepsizes are finite numbers).

Now, the definition (6.6) of the scaling matrix D_k implies that, for all i such that $[D_k\hat{g}^k]_i < 0$, we have $d_i(x^k) = \min\{1, u_i - x_i^k\}$, and therefore

$$\frac{u_i - x_i^k}{-[D_k\hat{g}^k]_i} = \frac{u_i - x_i^k}{-d_i(x^k)\hat{g}_i^k} \geq \frac{d_i(x^k)}{d_i(x^k)|\hat{g}_i^k|} = \frac{1}{|\hat{g}_i^k|} \geq \frac{1}{\|\hat{g}^k\|_\infty}.$$

In a similar way, we obtain for all i such that $[D_k\hat{g}^k]_i > 0$ the lower bound

$$\frac{x_i^k - l_i}{[D_k\hat{g}^k]_i} = \frac{x_i^k - l_i}{d_i(x^k)\hat{g}_i^k} \geq \frac{d_i(x^k)}{d_i(x^k)|\hat{g}_i^k|} = \frac{1}{|\hat{g}_i^k|} \geq \frac{1}{\|\hat{g}^k\|_\infty}.$$

Consequently, we have $t_\mathcal{B} \geq \frac{1}{\|\hat{g}^k\|_\infty}$. Using the definition (6.6) of the scaling matrix D_k once again, we get $\|D_k\hat{g}^k\|_\infty \leq \|D_k\|_\infty\|\hat{g}^k\|_\infty \leq \|\hat{g}^k\|_\infty$. Therefore, we obtain the following lower bound for the maximum stepsize $\bar{t}$ of the one-dimensional subproblem (6.11):

$$\bar{t} = \min\{t_\Delta, t_\mathcal{B}\} \geq \frac{1}{\|\hat{g}^k\|_\infty} \min\{1, \Delta_k\}. \tag{6.12}$$

We now derive an upper bound for $q_k(p^k)$. Using the fraction of Cauchy decrease condition (6.10) and the choice of the optimal stepsize t_k, we have

$$q_k(p^k) \leq \alpha q_k(p_C^k) = \alpha q_k(p(t_k)). \tag{6.13}$$

Further, recall that the one-dimensional objective function is given by

$$q_k\big(p(t)\big) = -t(g^k)^T D_k \hat{g}^k + \frac{1}{2}t^2(\hat{g}^k)^T D_k(H_k^T H_k + \nu_k I)D_k\hat{g}^k = -t\|\hat{g}^k\|^2 + \frac{1}{2}t^2\mu_k,$$

where

$$\mu_k := (\hat{g}^k)^T D_k(H_k^T H_k + \nu_k I)D_k\hat{g}^k > 0.$$

The strict inequality follows from the fact that $D_k\hat{g}^k = D_k^2 g^k \neq 0$ (otherwise we would have stopped in step (S.1) of Algorithm 6.2) together with the positive definiteness of the matrix $H_k^T H_k + \nu_k I$. Obviously, this quadratic function attains its global unconstrained minimum at $t_{\min} = \|\hat{g}^k\|^2/\mu_k$. Then we either have $t_k < t_{\min}$ (if $t_{\min} > \bar{t}$), or $t_k = t_{\min}$ (if $t_{\min} \leq \bar{t}$).

We consider these two cases separately. If $t_k < t_{\min}$, we have $t_k = \bar{t} < \frac{\|\hat{g}^k\|^2}{\mu_k}$, and therefore, using (6.12),

$$q_k\big(p(t_k)\big) = -\bar{t}\|\hat{g}^k\|^2 + \frac{1}{2}\bar{t}^2\mu_k < -\frac{1}{2}\bar{t}\|\hat{g}^k\|^2 \leq -\frac{1}{2}\frac{\|\hat{g}^k\|^2}{\|\hat{g}^k\|_\infty}\min\{\Delta_k, 1\}.$$

On the other hand, if $t_k = t_{\min}$, we have $t_k = \|\hat{g}^k\|^2/\mu_k$, and therefore

$$q_k\big(p(t_k)\big) = -t_{\min}\|\hat{g}^k\|^2 + \frac{1}{2}t_{\min}^2\mu_k = -\frac{1}{2}t_{\min}\|\hat{g}^k\|^2 = -\frac{1}{2}\frac{\|\hat{g}^k\|^4}{\mu_k} \leq -\frac{1}{2}\frac{\|\hat{g}^k\|^2}{\|H_k^T H_k + \nu_k I\|}.$$

Here, we used the fact that $\mu_k \leq \|\hat{g}^k\|^2\|D_k\|^2\|H_k^T H_k + \nu_k I\| \leq \|\hat{g}^k\|^2\|H_k^T H_k + \nu_k I\|$, since $\|D_k\| \leq 1$ in view of (6.6).

Since $\|\hat{g}^k\|_\infty \leq \|\hat{g}^k\|$, we obtain from the last two inequalities that

$$q_k\big(p(t_k)\big) \leq -\frac{1}{2}\|\hat{g}^k\| \min\Big\{\Delta_k, 1, \frac{\|\hat{g}^k\|}{\|H_k^T H_k + \nu_k I\|}\Big\}.$$

The statement now follows from (6.13). □

As a direct consequence of Lemma 6.3, we have that Algorithm 6.2 is well-defined, since the denominator $\mathrm{pred}_k(p^k) = -q_k(p^k)$ in the definition of r_k is nonzero for all $k \in \mathbb{N}$, otherwise the algorithm would have stopped at step (S.1). More precisely, Lemma 6.3 shows that the denominator $\mathrm{pred}_k(p^k)$ is always positive. This, in turn, implies that $\Psi(x^{k+1}) \leq \Psi(x^k)$ for all iterations $k \in \mathbb{N}$ for which the test in step (S.3) does not hold. On the other hand, if this test is satisfied, we also have $\Psi(x^{k+1}) \leq \Psi(x^k)$. Consequently, the entire sequence $\{\Psi(x^k)\}$ is monotonically decreasing. We will use this fact several times in our subsequent convergence analysis.

Moreover, the proof of Lemma 6.3 clearly shows how the scaled Cauchy step p_C^k can be computed in practice.

6.2 Global Convergence

The aim of this section is to prove some global convergence results for Algorithm 6.2. To this end, we assume that Algorithm 6.2 does not terminate after a finite number of iterations. Furthermore, we recall that Algorithm 6.2 uses two different search directions, namely the projected Levenberg-Marquardt step p^k_{PLM} and the Cauchy-like step p^k. The former will be used in order to prove fast local convergence, whereas the latter is the main tool for proving global convergence results. Our first result basically shows that the global convergence properties are not destroyed by using the projected Levenberg-Marquardt direction.

Theorem 6.4 *If the direction p^k_{PLM} is accepted an infinite number of times in step (S.3) of Algorithm 6.2, we have*

$$\lim_{k\to\infty} \|\Phi(x^k)\| = 0.$$

Proof. We already observed that the entire sequence $\{\Psi(x^k)\}$ is monotonically decreasing. Obviously, this implies that the whole sequence $\{\|\Phi(x^k)\|\}$ is also monotonically decreasing. Since the test $\|\Phi(x^k + p^k_{PLM})\| \leq \eta\|\Phi(x^k)\|$ is accepted an infinite number of times in view of our assumptions, we therefore get $\|\Phi(x^k)\| \to 0$ for $k \to \infty$ since $\eta \in (0, 1)$. □

For a complete convergence analysis of Algorithm 6.2, it remains to consider the case where the direction p^k_{PLM} from step (S.3) is accepted only a finite number of times. In the following global convergence analysis, we therefore assume without loss of generality that the direction p^k_{PLM} is never accepted in step (S.3). Hence, in all iterations $k \in \mathbb{N}$, we take the approximate solution p^k from step (S.4).

The technique of proof is similar to the one in [57, 73] for a square system of equations. In addition, we present another convergence result which is based on a stronger smoothness property of the mapping $x \mapsto D(x)\nabla\Psi(x)$. We first note that $\nabla\Psi$ is continuous on $\mathcal{O}$ since Ψ is continuously differentiable on this set. However, the scaling $x \mapsto D(x)$ is discontinuous at certain points x. Nevertheless, our first result states that the mapping $x \mapsto D(x)\nabla\Psi(x)$ is continuous, see also [118, Lemma 6.1].

Lemma 6.5 *The mapping $x \mapsto D(x)\nabla\Psi(x)$ is continuous on $\mathcal{O}$.*

Proof. Let $x \in \mathcal{O}$ be given, and let $i \in \{1, \ldots, n\}$ be an arbitrary component. If either $[\nabla\Psi(x)]_i > 0$ or $[\nabla\Psi(x)]_i < 0$, then it follows immediately from the definition (6.6) of the scaling matrix $D(x)$ that the mapping $x \mapsto [D(x)\nabla\Psi(x)]_i = d_i(x)[\nabla\Psi(x)]_i$ is continuous in x. Hence it remains to consider the case where $[\nabla\Psi(x)]_i = 0$. Let $\{x^k\}$ denote an arbitrary sequence converging to x. Since $\nabla\Psi$ is continuous and the scaling matrix $D(x)$ is bounded, we obtain $[D(x^k)\nabla\Psi(x^k)]_i \to 0 = [D(x)\nabla\Psi(x)]_i$, and this completes the proof. □

From now on, we always assume that the following condition is satisfied.

(A) The sequence $\{\nu_k\}$ is bounded.

The following result will be used in order to show that every accumulation point of a sequence generated by Algorithm 6.2, is a KKT-point of (6.4).

Lemma 6.6 *Let $\{x^k\}$ be a sequence generated by Algorithm 6.2, and let $\{x^k\}_K$ be a subsequence converging to a point $x^* \in \mathcal{B}$. If x^* is not a KKT-point of* (6.4)*, then* $\liminf_{k\to\infty, k\in K} \Delta_k > 0$.

Proof. Let $\bar{K} := \{k-1 \mid k \in K\}$. Then $\{x^{k+1}\}_{k\in\bar{K}} \to x^*$, and we have to show that $\liminf_{k\to\infty, k\in\bar{K}} \Delta_{k+1} > 0$. Assume this is not true. Subsequencing if necessary, we may suppose that

$$\lim_{k\to\infty, k\in\bar{K}} \Delta_{k+1} = 0. \tag{6.14}$$

In view of the updating rules for Δ_{k+1} in step (S.5), this implies that none of the iterations $k \in \bar{K}$, with k sufficiently large, is successful. Hence we have

$$r_k < \rho_1 \tag{6.15}$$

and $x^k = x^{k+1}$ for all $k \in \bar{K}$ large enough. Consequently, we also have $\{x^k\}_{k\in\bar{K}} \to x^*$. Moreover, since $\Delta_{k+1} = \sigma_1 \Delta_k$ for all $k \in \bar{K}$ sufficiently large, it follows from (6.14) that

$$\lim_{k\to\infty, k\in\bar{K}} \Delta_k = 0. \tag{6.16}$$

Since x^* is not a KKT-point of (6.4) by assumption, it follows from Lemma 6.5 that there exists a constant $\beta_1 > 0$ such that

$$\|\hat{g}^k\| \geq \beta_1 \tag{6.17}$$

for all $k \in \bar{K}$. From the upper semicontinuity of the generalized Jacobian and Assumption (A), we get the existence of a constant $\beta_2 > 0$ such that

$$\|H_k^T H_k + \nu_k I\| \leq \beta_2 \tag{6.18}$$

for all $k \in \bar{K}$. Using Lemma 6.3, (6.16), (6.17), and (6.18), we obtain

$$\begin{aligned}
\mathrm{pred}_k(p^k) &\geq \frac{\alpha}{2}\|\hat{g}^k\| \min\left\{\frac{\|\hat{g}^k\|}{\|H_k^T H_k + \nu_k I\|}, \Delta_k, 1\right\} \\
&\geq \frac{\alpha}{2}\beta_1 \min\left\{\frac{\beta_1}{\beta_2}, \Delta_k, 1\right\} \\
&\overset{(6.16)}{=} \frac{\alpha}{2}\beta_1 \Delta_k \\
&\overset{(6.9)}{\geq} \frac{\alpha}{2}\beta_1 \|p^k\|_\infty \\
&\geq \frac{\alpha\beta_1}{2\sqrt{n}}\|p^k\|
\end{aligned} \tag{6.19}$$

for all $k \in \bar{K}$ sufficiently large. Since Ψ is continuously differentiable, there exists, for each $k \in \mathbb{N}$, a vector $\xi^k \in [x^k, x^k + p^k]$ such that $\Psi(x^k + p^k) = \Psi(x^k) + \nabla\Psi(\xi^k)^T p^k$. This implies

$$\begin{aligned}
|r_k - 1| &= \left| \frac{\mathrm{ared}_k(p^k)}{\mathrm{pred}_k(p^k)} - 1 \right| \\
&= \frac{\left|\Psi(x^k) - \Psi(x^k + p^k) + q_k(p^k)\right|}{-q_k(p^k)} \\
&= \frac{\left|\Psi(x^k) - \Psi(x^k + p^k) + \nabla\Psi(x^k)^T p^k + \frac{1}{2}(p^k)^T (H_k^T H_k + \nu_k I) p^k\right|}{-q_k(p^k)} \\
&= \frac{\left|(\nabla\Psi(x^k) - \nabla\Psi(\xi^k))^T p^k + \frac{1}{2}(p^k)^T (H_k^T H_k + \nu_k I) p^k\right|}{-q_k(p^k)} \\
&\overset{(6.19)}{\leq} \frac{2\sqrt{n}}{\alpha\beta_1} \frac{\left|(\nabla\Psi(x^k) - \nabla\Psi(\xi^k))^T p^k + \frac{1}{2}(p^k)^T (H_k^T H_k + \nu_k I) p^k\right|}{\|p^k\|} \\
&\overset{(6.18)}{\leq} \frac{2\sqrt{n}}{\alpha\beta_1} \left(\|\nabla\Psi(x^k) - \nabla\Psi(\xi^k)\| + \frac{1}{2}\beta_2 \|p^k\| \right) \\
&\leq \frac{2\sqrt{n}}{\alpha\beta_1} \left(\|\nabla\Psi(x^k) - \nabla\Psi(\xi^k)\| + \frac{1}{2}\beta_2 \sqrt{n}\Delta_k \right) \\
&\overset{\bar{K}}{\to} 0,
\end{aligned}$$

where $\{\|\nabla\Psi(x^k) - \nabla\Psi(\xi^k)\|\}_{\bar{K}} \to 0$ follows from $\{x^k\}_{\bar{K}} \to x^*, \{\xi^k\}_{\bar{K}} \to x^*$ (since $\|p^k\|_\infty \leq \Delta_k \to 0$ for $k \in \bar{K}$ in view of (6.16)) and the continuity of $\nabla\Psi$. Hence $\{r_k\}_{k\in\bar{K}} \to 1$, which contradict (6.15). □

As a direct consequence of Lemma 6.6, we now show that there are infinitely many successful iterations (provided that Algorithm 6.2 does not terminate at a stationary point of (6.4) after a finite number of iterations).

Lemma 6.7 *Let $\{x^k\}$ be a sequence generated by Algorithm 6.2. Then there are infinitely many successful iterations.*

Proof. Assume that the number of successful iterations in (S.4) is finite. Then there exists an index $k_0 \in \mathbb{N}$ such that $r_k < \rho_1$ and $x^k = x^{k_0}$ for all $k \geq k_0$. Hence $\{\Delta_k\} \to 0$ and $\{x^k\} \to x^{k_0}$. This contradicts Lemma 6.6, since $\hat{g}^{k_0} = D(x^{k_0})\nabla\Psi(x^{k_0}) \neq 0$. □

We are now in the position to state our first global convergence result.

Theorem 6.8 *Let $\{x^k\}$ be any sequence generated by Algorithm 6.2. Then every accumulation point of $\{x^k\}$ is a KKT-point of* (6.4).

Proof. We first recall that, as a consequence of Theorem 6.4, we may assume without loss of generality that the search direction is always computed by step (S.4) of Algorithm 6.2.

Let x^* be an accumulation point of $\{x^k\}$, and let $\{x^k\}_K$ be a subsequence converging to x^*. In view of Lemma 6.7, we can assume, without loss of generality, that all $k \in K$ are successful iterations, since $x^{k+1} = x^k$ for all nonsuccessful iterations k. Suppose that x^* is not a KKT-point of (6.4). Then it follows from Lemma 6.5, the upper semicontinuity of the generalized Jacobian, and Assumption (A) that there exist suitable constants $\beta_1 > 0$ and $\beta_2 > 0$ such that

$$\|\hat{g}^k\| \geq \beta_1 \quad \text{and} \quad \|H_k^T H_k + \nu_k I\| \leq \beta_2 \tag{6.20}$$

for all $k \in K$. Since the iterations $k \in K$ are successful, we have $r_k \geq \rho_1$ for all $k \in K$. By Lemma 6.3 and the fact that the entire sequence $\{\Psi(x^k)\}$ is decreasing and bounded from below, we have

$$\begin{aligned}
\Psi(x^0) &\geq \sum_{k=0}^{\infty} \big(\Psi(x^k) - \Psi(x^{k+1})\big) \\
&\geq \sum_{k=0}^{\infty} \rho_1 \operatorname{pred}_k(p^k) \\
&\geq \rho_1 \sum_{k \in K} \operatorname{pred}_k(p^k) \\
&\geq \frac{\alpha\rho_1}{2} \sum_{k \in K} \|\hat{g}^k\| \min\Big\{ \frac{\|\hat{g}^k\|}{\|H_k^T H_k + \nu_k I\|}, \Delta_k, 1 \Big\} \\
&\geq \frac{\alpha\rho_1\beta_1}{2} \sum_{k \in K} \min\Big\{ \frac{\beta_1}{\beta_2}, \Delta_k, 1 \Big\}.
\end{aligned}$$

This implies $\{\Delta_k\}_K \to 0$, a contradiction to Lemma 6.6. □

We want to give two additional global convergence results which are more traditional in the context of trust region methods, see, e.g., [17]. To this end, we first introduce the following assumption.

(B) The sequence $\{H_k\}$ is bounded.

Then we can state the following result which is weaker than Theorem 6.8 in the sense that it does not guarantee that every accumulation point is a KKT-point. However, it will be used in the subsequent result in order to state a stronger convergence theorem.

Theorem 6.9 *Suppose that Assumptions (A) and (B) hold, and let $\{x^k\}$ be any sequence generated by Algorithm 6.2. Then*

$$\liminf_{k \to \infty} \|\hat{g}^k\| = 0. \tag{6.21}$$

Proof. The proof is by contradiction. Suppose there exists a constant $\beta_1 > 0$ such that $\|\hat{g}^k\| \geq \beta_1$ for all $k \in \mathbb{N}$. Assumptions (A) and (B) imply the existence of a constant $\beta_2 > 0$

such that $\|H_k^T H_k + \nu_k I\| \leq \beta_2$ for all $k \in \mathbb{N}$. We denote the set of all successful iterates by S and note that it has infinite cardinality by Lemma 6.7. Since the entire sequence $\{\Psi(x^k)\}$ is monotonically decreasing, we get from Lemma 6.3 that

$$\begin{aligned}
\Psi(x^0) &\geq \sum_{k=0}^{\infty} \big(\Psi(x^k) - \Psi(x^{k+1})\big) \\
&\geq \sum_{k\in S} \big(\Psi(x^k) - \Psi(x^{k+1})\big) \\
&\geq \sum_{k\in S} \rho_1 \operatorname{pred}_k(p^k) \\
&\geq \frac{\alpha\rho_1}{2} \sum_{k\in S} \|\hat{g}^k\| \min\Big\{\frac{\|\hat{g}^k\|}{\|H_k^T H_k + \nu_k I\|}, \Delta_k, 1\Big\} \\
&\geq \frac{\alpha\rho_1\beta_1}{2} \sum_{k\in S} \min\Big\{\frac{\beta_1}{\beta_2}, \Delta_k, 1\Big\}.
\end{aligned}$$

This implies $\sum_{k\in S} \Delta_k < \infty$. Taking into account that $\|x^{k+1} - x^k\|_\infty = \|p^k\|_\infty \leq \Delta_k$ for all $k \in S$, we get $\sum_{k\in S} \|x^{k+1} - x^k\|_\infty < \infty$. Since $\|x^{k+1} - x^k\|_\infty = 0$ for all $k \notin S$, we obtain

$$\sum_{k=0}^{\infty} \|x^{k+1} - x^k\|_\infty < \infty.$$

Hence $\{x^k\}$ is a Cauchy sequence and therefore convergent to a point x^*. Theorem 6.8 then implies that x^* is a KKT-point of (6.4). Consequently, we have $\hat{g}^* := D(x^*)\nabla\Psi(x^*) = 0$. However, Lemma 6.5 implies that $\hat{g}^k \to \hat{g}^* = 0$, a contradiction to our assumption. Hence (6.21) holds. □

In order to state our final convergence result, we need to introduce another assumption.

(C) The function $\nabla\Psi$ is uniformly continuous and bounded on the box $\mathcal{B}$.

Note that Assumption (C) automatically holds if the box $\mathcal{B}$ is a compact set. As a consequence of Assumption (C), we get the following preliminary result, see also [118].

Lemma 6.10 *Under Assumption (C), the mapping $x \mapsto D(x)\nabla\Psi(x)$ is uniformly continuous on $\mathcal{B}$.*

Proof. Let $\varepsilon > 0$ and $i \in \{1, \ldots, n\}$ be arbitrary. Since, by assumption, $\nabla\Psi$ is bounded on $\mathcal{B}$, there is a constant $b > 0$ such that $\|\nabla\Psi(x)\|_\infty \leq b$ for all $x \in \mathcal{B}$. Since $\nabla\Psi$ is uniformly continuous, we have the existence of a constant $\bar{\delta} > 0$ such that

$$-\frac{\varepsilon}{4} \leq [\nabla\Psi(y)]_i - [\nabla\Psi(x)]_i \leq \frac{\varepsilon}{4} \tag{6.22}$$

holds for all $x, y \in \mathcal{B}$ with $|y_i - x_i| \leq \bar{\delta}$. Now define $\delta := \min\{\bar{\delta}, \frac{3\varepsilon}{4b}\}$, let $x, y \in \mathcal{B}$ with $\|y - x\|_\infty \leq \delta$ be arbitrary, and set $T(x, y) := D(y)\nabla\Psi(y) - D(x)\nabla\Psi(x)$. Then

$$\begin{aligned} \big|[T(x,y)]_i\big| &= \big|d_i(y)[\nabla\Psi(y)]_i - d_i(x)[\nabla\Psi(x)]_i\big| \\ &\leq d_i(y)\big|[\nabla\Psi(y)]_i - [\nabla\Psi(x)]_i\big| + \big|d_i(y) - d_i(x)\big|\,\big|[\nabla\Psi(x)]_i\big| \\ &\overset{(6.6)}{\leq} \big|[\nabla\Psi(y)]_i - [\nabla\Psi(x)]_i\big| + \big|d_i(y) - d_i(x)\big|\,\big|[\nabla\Psi(x)]_i\big|. \end{aligned} \tag{6.23}$$

We now distinguish several cases.
Case 1. If $[\nabla\Psi(x)]_i = 0$, we immediately obtain $\big|[T(x,y)]_i\big| \leq \varepsilon$ from (6.23) and (6.22).
Case 2. If $[\nabla\Psi(x)]_i > 0$, we consider two subcases:
Case 2.1. If $[\nabla\Psi(x)]_i \leq \frac{3\varepsilon}{8}$ we obtain $\big|[T(x,y)]_i\big| \leq \frac{\varepsilon}{4} + 2\frac{3\varepsilon}{8} = \varepsilon$ from (6.23).
Case 2.2. If $[\nabla\Psi(x)]_i > \frac{3\varepsilon}{8}$, we obtain

$$[\nabla\Psi(y)]_i = \big([\nabla\Psi(y)]_i - [\nabla\Psi(x)]_i\big) + [\nabla\Psi(x)]_i \geq -\frac{\varepsilon}{4} + \frac{3\varepsilon}{8} = \frac{\varepsilon}{8} > 0$$

from the first inequality in (6.22). Hence both $[\nabla\Psi(x)]_i$ and $[\nabla\Psi(y)]_i$ are positive, and (6.23) together with the definition of the scaling matrix $D(x)$ becomes

$$\begin{aligned} \big|[T(x,y)]_i\big| &\leq \big|[\nabla\Psi(y)]_i - \nabla\Psi(x)]_i\big| + \big|\min\{1, y_i - l_i\} - \min\{1, x_i - l_i\}\big|[\nabla\Psi(x)]_i \\ &\leq \big|[\nabla\Psi(y)]_i - \nabla\Psi(x)]_i\big| + \big|y_i - x_i\big|\,[\nabla\Psi(x)]_i \leq \frac{\varepsilon}{4} + \frac{3\varepsilon}{4b}b = \varepsilon. \end{aligned}$$

Case 3. Analogously, for $[\nabla\Psi(x)]_i < 0$, we consider the following two subcases:
Case 3.1. If $[\nabla\Psi(x)]_i \geq -\frac{3\varepsilon}{8}$, we obtain $\big|[T(x,y)]_i\big| \leq \frac{\varepsilon}{4} + 2\frac{3\varepsilon}{8} = \varepsilon$ from (6.23).
Case 3.2. If $[\nabla\Psi(x)]_i < -\frac{3\varepsilon}{8}$, the second inequality in (6.22) implies

$$[\nabla\Psi(y)]_i = \big([\nabla\Psi(y)]_i - [\nabla\Psi(x)]_i\big) + [\nabla\Psi(x)]_i \leq \frac{\varepsilon}{4} - \frac{3\varepsilon}{8} = -\frac{\varepsilon}{8} < 0.$$

Hence $[\nabla\Psi(x)]_i$ and $[\nabla\Psi(y)]_i$ are both negative, and we obtain

$$\begin{aligned} \big|[T(x,y)]_i\big| &\leq \big|[\nabla\Psi(y)]_i - \nabla\Psi(x)]_i\big| + \big|\min\{1, u_i - y_i\} - \min\{1, u_i - x_i\}\big|\,\big|[\nabla\Psi(x)]_i\big| \\ &\leq \big|[\nabla\Psi(y)]_i - \nabla\Psi(x)]_i\big| + \big|y_i - x_i\big|\,\big|[\nabla\Psi(x)]_i\big| \leq \frac{\varepsilon}{4} + \frac{3\varepsilon}{4b}b = \varepsilon \end{aligned}$$

from (6.23).

Summarizing all three cases, we obtain $\|T(x,y)\|_\infty \leq \varepsilon$ for all $\|y - x\|_\infty \leq \delta$. The assertion of the lemma therefore holds. □

We are now in the position to state our final global convergence result.

Theorem 6.11 *Suppose that Assumptions (A), (B) and (C) hold, and let $\{x^k\}$ be any sequence generated by Algorithm 6.2. Then*

$$\lim_{k\to\infty} \|\hat{g}^k\| = 0. \tag{6.24}$$

Proof. Suppose that (6.24) does not hold. Then there is a constant $\varepsilon > 0$ and a subsequence $\{x^k\}_K, K \subseteq \mathbb{N}$, such that

$$\|\hat{g}^k\| \geq 2\varepsilon \quad \forall k \in K. \tag{6.25}$$

In view of Theorem 6.9, we can find, for each $k \in K$, an index $\ell(k) > k$ such that

$$\|\hat{g}^\ell\| \geq \varepsilon \ \forall k \leq \ell < \ell(k) \quad \text{and} \quad \|\hat{g}^{\ell(k)}\| < \varepsilon. \tag{6.26}$$

Let $\beta_2 > 0$ be a constant such that $\|H_k^T H_k + \nu_k I\| \leq \beta_2$ for all $k \in \mathbb{N}$, cf. Assumptions (A) and (B). Given $k \in K$, take an arbitrary index ℓ with $k \leq \ell < \ell(k)$ and suppose, for the moment, that iteration ℓ is successful. Then Lemma 6.3 implies

$$\begin{aligned}
\Psi(x^\ell) - \Psi(x^{\ell+1}) &\geq \rho_1 \operatorname{pred}_\ell(p^\ell) \\
&\geq \frac{1}{2}\alpha\rho_1\|\hat{g}^\ell\| \min\Big\{\frac{\|\hat{g}^\ell\|}{\|H_\ell^T H_\ell + \nu_\ell I\|}, \Delta_\ell, 1\Big\} \\
&\geq \frac{1}{2}\alpha\rho_1\varepsilon \min\Big\{\frac{\varepsilon}{\beta_2}, \Delta_\ell, 1\Big\} \\
&\geq \frac{1}{2}\alpha\rho_1\varepsilon \min\Big\{\frac{\varepsilon}{\beta_2}, \|x^{\ell+1} - x^\ell\|_\infty, 1\Big\}.
\end{aligned}$$

Since $\{\Psi(x^k)\}$ converges, we therefore get

$$\Psi(x^\ell) - \Psi(x^{\ell+1}) \geq \frac{1}{2}\alpha\rho_1\varepsilon\|x^{\ell+1} - x^\ell\|_\infty$$

for all these ℓ sufficiently large. Trivially, this inequality also holds for all nonsuccessful iterations. Consequently, we get

$$\begin{aligned}
\frac{1}{2}\alpha\rho_1\varepsilon\|x^{\ell(k)} - x^k\|_\infty &\leq \frac{1}{2}\alpha\rho_1\varepsilon \sum_{\ell=k}^{\ell(k)-1} \|x^{\ell+1} - x^\ell\|_\infty \\
&\leq \sum_{\ell=k}^{\ell(k)-1} \big(\Psi(x^\ell) - \Psi(x^{\ell+1})\big) \\
&= \Psi(x^k) - \Psi(x^{\ell(k)})
\end{aligned}$$

for all $k \in K$. The convergence of the entire sequence $\{\Psi(x^k)\}$ therefore implies $\{\|x^{\ell(k)} - x^k\|\}_K \to 0$. In view of Lemma 6.10, we then get $\{\|\hat{g}^{\ell(k)} - \hat{g}^k\|\}_K \to 0$. On the other hand, it follows from (6.25) and (6.26) that

$$\|\hat{g}^{\ell(k)} - \hat{g}^k\| \geq \|\hat{g}^k\| - \|\hat{g}^{\ell(k)}\| \geq 2\varepsilon - \varepsilon = \varepsilon.$$

This contradiction completes the proof. □

6.3 Local Convergence

In this section, we consider the local behavior of Algorithm 6.2. Taking into account Theorem 3.16, it follows that we only have to show that the projected Levenberg-Marquardt direction p^k_{PLM} from step (S.3) is automatically accepted in a neighborhood of a solution of (6.1). In order to do this we begin with the following preliminary result.

Lemma 6.12 *Let $x^* \in \mathbb{R}^n$ be a solution of (6.1) such that all elements from $\partial_C \Phi(x^*)$ have full rank, and let $\bar{\nu} > 0$. Then there exist constants $\varepsilon > 0$ and $\kappa > 0$ such that*

$$p^T(H^T H + \nu I)p \geq \kappa \|p\|^2$$

for all $H \in \partial_C \Phi(x)$ and all $x \in \mathbb{R}^n$ with $\|x - x^*\| \leq \varepsilon$ and all $\nu \in [0, \bar{\nu}]$, i.e., the matrices $H^T H + \nu I$ are uniformly positive definite.

Proof. It follows from Lemma 3.15 that there exist constants $\varepsilon > 0$ and $c > 0$ such that

$$\|(H^T H + \nu I)^{-1}\| \leq c \quad \forall x \in B_\varepsilon(x^*),\ \forall H \in \partial_C \Phi(x),\ \forall \nu \in [0, \bar{\nu}]. \tag{6.27}$$

Since

$$\|(H^T H + \nu I)^{-1}\| = \frac{1}{\lambda_{\min}(H^T H + \nu I)} =: \frac{1}{\lambda^x_{\min}}$$

for all $x \in B_\varepsilon(x^*)$, all $H \in \partial_C \Phi(x)$ and all $\nu \in [0, \bar{\nu}]$, we obtain from (6.27)

$$(p)^T(H^T H + \nu I)p \geq \lambda^x_{\min}\|p\|^2 \geq \frac{1}{c}\|p\|^2 \quad \forall x \in B_\varepsilon(x^*),\ \forall H \in \partial_C \Phi(x),\ \forall \nu \in [0, \bar{\nu}].$$

Hence the assertion holds with $\kappa := \frac{1}{c}$. □

As noticed in Theorem 4.20 the full rank assumption for all elements in the C-subdifferential $\partial_C \Phi(x^*)$ at a solution x^* of the MCP is satisfied under the R-regularity condition according to the Definition in 4.19.

In order to establish our main local convergence theorem we also need the following result.

Lemma 6.13 *Let $x^* \in \mathbb{R}^n$ be an R-regular solution of the mixed complementarity problem. Then there exist constants $\varepsilon > 0$ and $\gamma > 0$ such that*

$$\|\Phi(x)\| \geq \gamma \|x - x^*\| \quad \textit{for all } x \in B_\varepsilon(x^*).$$

Proof. Lemma 6.12 implies that there are constants $\varepsilon_1 > 0$ and $\kappa > 0$ such that

$$\|H(x - x^*)\|^2 = (x - x^*)^T H^T H(x - x^*) \geq \kappa \|x - x^*\|^2 \tag{6.28}$$

holds for all $x \in B_{\varepsilon_1}(x^*)$ and all $H \in \partial_C \Phi(x)$. Furthermore, the semismoothness of Φ implies that there is a constant $\varepsilon_2 > 0$ such that

$$\|\Phi(x) - \Phi(x^*) - H(x - x^*)\| \leq \frac{\sqrt{\kappa}}{2}\|x - x^*\| \tag{6.29}$$

holds for all $x \in B_{\varepsilon_2}(x^*)$ and all $H \in \partial_C \Phi(x)$, cf. Proposition 2.18. Setting $\varepsilon := \min\{\varepsilon_1, \varepsilon_2\}$, we obtain from (6.28) and (6.29) that, for all $x \in B_\varepsilon(x^*)$ and all $H \in \partial_C \Phi(x)$, we have

$$\begin{aligned}\|\Phi(x)\| &= \big\|H(x-x^*) + \big(\Phi(x) - \Phi(x^*) - H(x-x^*)\big)\big\| \\ &\geq \|H(x-x^*)\| - \|\Phi(x) - \Phi(x^*) - H(x-x^*)\| \\ &\geq \sqrt{\kappa}\|x-x^*\| - \frac{\sqrt{\kappa}}{2}\|x-x^*\| \\ &= \frac{\sqrt{\kappa}}{2}\|x-x^*\|.\end{aligned}$$

The statement therefore holds with $\gamma := \frac{\sqrt{\kappa}}{2}$. □

We are now in the position to state the main convergence result of this section.

Theorem 6.14 *Suppose that Assumption (A) hold, and let $\{x^k\}$ be a sequence generated by Algorithm 6.2. Assume that $x^* \in \mathcal{B}$ is an accumulation point of $\{x^k\}$ such that x^* is a R-regular solution of problem* (6.1)*. Then the following statements hold:*

(a) The entire sequence $\{x^k\}$ converges to x^*.

(b) The direction p^k_{PLM} in (S.3) is always accepted for k sufficiently large so that the next iterate is given by $x^{k+1} = x^k + p^k_{PLM}$, provided that $\nu_k \to 0$.

(c) The rate of convergence is Q-superlinear if $\nu_k \to 0$.

(d) The rate of convergence is Q-quadratic if $\nu_k = O(\|\Phi(x^k)\|)$ and, in addition, F is an LC^1 function.

Proof. (a) To establish that the entire sequence $\{x^k\}$ converges to x^*, we first note that x^* is an isolated solution of (6.1). This follows immediately from Lemma 6.13. Since Algorithm 6.2 generates a decreasing sequence $\{\Psi(x^k)\}$ and x^* is a zero of Φ (and Ψ), it follows that the entire sequence $\{\Psi(x^k)\}$ converges to zero. Hence every accumulation point of the sequence $\{x^k\}$ is a solution of (3.13). Consequently, x^* is an isolated accumulation point of the sequence $\{x^k\}$.

Now let $\{x^k\}_K$ denote any subsequence converging to x^*, and note that $\Phi(x^*) = 0$ and, therefore, $\nabla\Psi(x^*) = 0$.

For all $k \in \mathbb{N}$ with the search direction p^k_{PLM} coming from (S.3), we have

$$\begin{aligned}\|x^{k+1} - x^k\| = \|p^k_{PLM}\| &= \|P_{\mathcal{B}}(x^k + p^k_{LM}) - x^k\| \\ &= \|P_{\mathcal{B}}(x^k + p^k_{LM}) - P_{\mathcal{B}}(x^k)\| \\ &\leq \|x^k + p^k_{LM} - x^k\| \\ &= \| - (H_k^T H_k + \nu_k I)^{-1}\nabla\Psi(x^k)\| \\ &\leq \|(H_k^T H_k + \nu_k I)^{-1}\|\,\|\nabla\Psi(x^k)\|.\end{aligned} \tag{6.30}$$

We now consider the iterates $k \in \mathbb{N}$ where the search direction is the Cauchy-like step p^k coming from (S.4). Using Lemma 6.12, it follows that there is a constant $\kappa > 0$ such that

$$\kappa \|p^k\|^2 \leq (p^k)^T (H_k^T H_k + \nu_k I) p^k \tag{6.31}$$

for all $k \in K$ sufficiently large. On the other hand, since $q_k(p^k) \leq 0$, we get

$$\frac{1}{2}(p^k)^T (H_k^T H_k + \nu_k I) p^k \leq -\nabla \Psi(x^k)^T p^k. \tag{6.32}$$

From (6.31), (6.32), and the Cauchy-Schwarz inequality, we obtain

$$\kappa \|p^k\|^2 \leq 2 \|\nabla \Psi(x^k)\| \, \|p^k\|.$$

This implies

$$\|x^{k+1} - x^k\| \leq \|p^k\| \leq \frac{2}{\kappa} \|\nabla \Psi(x^k)\|. \tag{6.33}$$

Since $\{\nabla \Psi(x^k)\}_K \to \nabla \Psi(x^*) = 0$, we obtain from (6.30), (6.33), and the boundedness of the sequence $\{\|(H_k^T H_k + \nu_k I)^{-1}\|\}$ (see Lemma 4.5) that $\{\|x^{k+1} - x^k\|\}_K \to 0$. Hence statement (a) follows from [89, Lemma 4.10].

(b), (c), (d) We only have to prove statement (b), since (c) and (d) then follow directly from Theorem 3.16.

To this end, we first recall from the proof of Theorem 3.16 that

$$\|x^k + p_{LM}^k - x^*\| = o(\|x^k - x^*\|), \tag{6.34}$$

provided that $\nu_k \to 0$. Furthermore, Lemma 6.13 implies that there is a constant $\gamma > 0$ such that

$$\|\Phi(x^k)\| \geq \gamma \|x^k - x^*\| \tag{6.35}$$

for all $k \in \mathbb{N}$ sufficiently large. Using (6.35) and (6.34), we obtain

$$\begin{aligned} \frac{\|\Phi(x^k + p_{LM}^k)\|}{\|\Phi(x^k)\|} &\leq \frac{\|\Phi(x^k + p_{LM}^k)\|}{\gamma \|x^k - x^*\|} \\ &= \frac{\|\Phi(x^k + p_{LM}^k) - \Phi(x^*)\|}{\gamma \|x^k - x^*\|} \\ &\leq \frac{L \|x^k + p_{LM}^k - x^*\|}{\gamma \|x^k - x^*\|} \\ &\to 0, \end{aligned}$$

where $L > 0$ denotes the local Lipschitz constant of Φ (note that Φ is semismooth and therefore, in particular, locally Lipschitzian). Hence we have

$$\|\Phi(x^k + p_{LM}^k)\| = o(\|\Phi(x^k)\|). \tag{6.36}$$

Using the definition of p^k_{PLM} and exploiting the definition of the projection $P_{\mathcal{B}}$, we obtain

$$\begin{aligned}\|p^k_{PLM} - p^k_{LM}\| &= \|P_{\mathcal{B}}(x^k + p^k_{LM}) - (x^k + p^k_{LM})\| \\ &\overset{x^* \in \mathcal{B}}{\leq} \|x^* - (x^k + p^k_{LM})\| \\ &\overset{(6.34)}{=} o(\|x^k - x^*\|) \\ &\overset{(6.35)}{=} o(\|\Phi(x^k)\|).\end{aligned} \tag{6.37}$$

From (6.37) and (6.36), we now get

$$\begin{aligned}\|\Phi(x^k + p^k_{PLM})\| &\leq \|\Phi(x^k + p^k_{PLM}) - \Phi(x^k + p^k_{LM})\| + \|\Phi(x^k + p^k_{LM})\| \\ &\leq L\|p^k_{PLM} - p^k_{LM}\| + \|\Phi(x^k + p^k_{LM})\| \\ &= o(\|\Phi(x^k)\|),\end{aligned}$$

and this shows that the test in (S.3) is passed by the direction p^k_{PLM} for all $k \in \mathbb{N}$ sufficiently large. □

6.4 A Projected Filter Trust Region Method

In this section, we present a variant of Algorithm 6.2 by adding a filter technique into our projected Levenberg-Marquardt trust region method. We will show that this method has essentially the same global and local convergence properties as Algorithm 6.2 itself. However, the filter allows a nonmonotone behavior of the sequence $\{\Psi(x^k)\}$ by accepting the full projected Levenberg-Marquardt step even in some situations where we get no decrease of the merit function Ψ.

Originally, filter methods were proposed in the year 2002 by Fletcher and Leyffer [40] for the solution of constrained optimization problems, see also [39, 47, 121, 123] for some further developments in this direction. Extensions of the filter idea to the solution of nonlinear systems of equations can be found in Fletcher and Leyffer [41] as well as in Gould et al. [47]. Here we adapt the multidimensional filter approach from [47] and incorporate that idea into our method for the solution of problem (3.13).

More precisely, we simplify the approach from [47] to some extent and present a special case of that filter approach only. This version is tailored to the case where we apply our method to mixed complementarity problems. To describe the filter idea, let $r \in \{1, \ldots, m-1\}$ be any given number, and partition the mapping $\Phi : \mathbb{R}^n \to \mathbb{R}^m$ into

$$\Phi(x) := \begin{pmatrix} \Phi_A(x) \\ \Phi_B(x) \end{pmatrix} \quad \text{with} \quad \Phi_A : \mathbb{R}^n \to \mathbb{R}^r, \;\; \Phi_B : \mathbb{R}^n \to \mathbb{R}^{m-r}.$$

Then define a mapping $\theta : \mathbb{R}^n \to \mathbb{R}^2$ by

$$\theta(x) := \big(\theta_1(x), \theta_2(x)\big)^T := \big(\|\Phi_A(x)\|, \|\Phi_B(x)\|\big)^T.$$

We say that a vector $x \in \mathbb{R}^n$ *dominates* another vector $y \in \mathbb{R}^n$ if $\theta_i(x) \leq \theta_i(y)$ for both $i = 1$ and $i = 2$. Now suppose that we are at the kth iteration of a suitable method and that we have generated certain iterates $x^0, x^1, \ldots, x^k$. Then a *filter* $\mathcal{F}_k$ at the kth iteration is a subset

$$\mathcal{F}_k \subseteq \{\theta(x^0), \theta(x^1), \ldots, \theta(x^k)\}$$

such that none of the elements $\theta(x^l) \in \mathcal{F}_k$ dominates another element from the set $\mathcal{F}_k$.

Assume that a filter $\mathcal{F}_k$ is given, and that we have computed a new vector y (which we hope to become x^{k+1}). The question is when $\theta(y)$ becomes an element of the new filter $\mathcal{F}_{k+1}$. A straightforward idea would be to add $\theta(y)$ to the old filter $\mathcal{F}_k$ if $\theta(y)$ is not dominated by any element from $\mathcal{F}_k$. However, this notion is not strong enough in order to prove suitable convergence results.

Following [47], we therefore call y *acceptable* for the filter $\mathcal{F}_k$ if there is a constant $\gamma_\theta > 0$ such that, for each element $\theta(x^l) \in \mathcal{F}_k$, there is an index $j \in \{1, 2\}$ with

$$\theta_j(y) \leq \theta_j(x^l) - \gamma_\theta \|\theta(y)\|.$$

Loosely speaking, this means that $\theta(y)$ is acceptable if, for each element $\theta(x^l) \in \mathcal{F}_k$, the new candidate $\theta(y)$ is sufficiently smaller than $\theta(x^l)$ in at least one of the two components. In this case we define the new filter by

$$\mathcal{F}_{k+1} := \mathcal{F}_k \cup \{\theta(y)\}$$

and remove all elements from $\mathcal{F}_k$ that are dominated by $\theta(y)$. Moreover, we accept $x^{k+1} := y$ as our new iterate. On the other hand, if y is not acceptable for the filter $\mathcal{F}_k$, we simply set $\mathcal{F}_{k+1} := \mathcal{F}_k$.

Finally, we note that, in a very natural way, the definition of Φ from (4.36) leads to the partition $\Phi = (\Phi_A, \Phi_B)$, where Φ_A denotes the first n components and Φ_B the last n components of Φ. Hence we can apply our filter technique described above with $r := n$ to this reformulation of mixed complementarity problems.

Incorporating this filter idea into Algorithm 6.2, we obtain the following method.

Algorithm 6.15 (Scaled Filter Trust Region Method)

(S.0) Choose $x^0 \in \mathcal{B}$, $\Delta_0 > 0, 0 < \rho_1 < \rho_2 < 1$, $0 < \sigma_1 < 1 < \sigma_2$, $\varepsilon \geq 0$, $\eta \in (0, 1)$, $\Delta_{\min} > 0$, $\alpha \in (0, 1], M > 0$, and set $\mathcal{F}_0 := \{\theta(x^0)\}, k := 0$.

(S.1) If $\|D_k g^k\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C \Phi(x^k), \nu_k > 0$, and compute p^k_{LM} using (6.2).

(S.3) Compute p^k_{PLM} from (6.3). If $x^k + p^k_{PLM}$ is acceptable for the filter $\mathcal{F}_k$ and $\|\Phi(x^k + p^k_{PLM})\| \leq M$, set $x^{k+1} := x^k + p^k_{PLM}$, $\Delta_{k+1} := \max\{\Delta_{\min}, \sigma_2 \Delta_k\}, \mathcal{F}_{k+1} := \mathcal{F}_k \cup \{\theta(x^{k+1})\}$ (and remove all entries from $\mathcal{F}_k$ that are dominated by $\theta(x^{k+1})$), and go to step (S.7); otherwise set $\mathcal{F}_{k+1} := \mathcal{F}_k$, and go to (S.4).

(S.4) If $\|\Phi(x^k+p^k_{PLM})\| \leq \eta\|\Phi(x^k)\|$ holds, set $x^{k+1} := x^k+p^k_{PLM}$, $\Delta_{k+1} := \max\{\Delta_{\min}, \sigma_2\Delta_k\}$, and go to (S.7); otherwise, go to step (S.5).

(S.5) Compute an approximate solution p^k of the trust region subproblem (6.7) satisfying (6.9) and (6.10), and define r_k by (6.8). If $r_k \geq \rho_1$, we call the iteration k successful and set $x^{k+1} := x^k + p^k$; otherwise we set $x^{k+1} := x^k$.

(S.6) Update the trust region radius as follows:

$$\Delta_{k+1} := \begin{cases} \sigma_1\Delta_k, & \text{if } r_k < \rho_1, \\ \max\{\Delta_{\min}, \Delta_k\}, & \text{if } r_k \in [\rho_1, \rho_2), \\ \max\{\Delta_{\min}, \sigma_2\Delta_k\}, & \text{if } r_k \geq \rho_2. \end{cases}$$

(S.7) Set $k \leftarrow k+1$, and go to (S.1).

Note that Algorithm 6.15 differs from Algorithm 6.2 only in (S.3) where we added the filter strategy. Furthermore, note that we have a constant M which we assume to be sufficiently large in practice such that the test $\|\Phi(x^k + p^k_{PLM})\| \leq M$ is always satisfied. From a theoretical point of view, however, this constant M is needed and plays the role of a safeguard in order to prevent the sequence $\{\|\Phi(x^k)\|\}$ to become too large. In fact, we have the following simple note.

Remark 6.16 The sequence $\{x^k\}$ generated by Algorithm 6.15 has the property that $\|\Phi(x^k)\| \leq \max\{\|\Phi(x^0)\|, M\}$ for all $k \in \mathbb{N}$. This can be seen by induction. For $k = 0$, this inequality holds trivially. Hence suppose that it holds for some $k \geq 0$, and consider the iterate x^{k+1}. If this iterate is computed in step (S.3), we have $\|\Phi(x^{k+1})\| \leq M$. Otherwise, we have $\|\Phi(x^{k+1})\| \leq \|\Phi(x^k)\|$, and the statement then follows from the induction hypothesis.

The following result shows what happens if the new vector $x^k+p^k_{PLM}$ is accepted an infinite number of times by our filter step in (S.3).

Theorem 6.17 *Assume there are infinitely many iterations k such that $x^{k+1} = x^k+p^k_{PLM}$ is accepted in the filter step (S.3) of Algorithm 6.15. Then*

$$\lim_{k\to\infty} \|\Phi(x^k)\| = 0.$$

Proof. Let $K \subseteq \mathbb{N}$ denote the infinite subset such that $x^{k+1} = x^k + p^k_{PLM}$ is accepted for all $k \in K$ in step (S.3) of Algorithm 6.15. In the first part of the proof, we show that

$$\lim_{k\in K} \|\theta(x^{k+1})\| = 0. \tag{6.38}$$

Suppose this is not true. Then we may assume that there is a infinite subset $\bar{K} \subseteq K$ and a constant $\varepsilon > 0$ such that

$$\|\theta(x^{k+1})\| \geq \varepsilon \quad \forall k \in \bar{K}. \tag{6.39}$$

In view of step (S.3) of Algorithm 6.15, the sequence $\{\theta(x^{k+1})\}_{k\in\bar{K}}$ is bounded. Hence there is another subset $\hat{K} \subseteq \bar{K}$ with

$$\lim_{k\in\hat{K}} \theta(x^{k+1}) = \theta^* \tag{6.40}$$

for some number $\theta^* \in \mathbb{R}^2$ satisfying $\|\theta^*\| \geq \varepsilon$.

For the moment, consider a fixed index $k \in \hat{K}$. Furthermore, let $l_k \in \hat{K}$ denote the index in $\hat{K}$ previous to k. Since x^{k+1} was acceptable for the filter $\mathcal{F}_k$, we have

$$\theta_j(x^{k+1}) \leq \theta_j(x^{l_k+1}) - \gamma_\theta\|\theta(x^{k+1})\| \tag{6.41}$$

for at least one index $j \in \{1, 2\}$. This statement does not depend on $\theta(x^{l_k+1})$ still being in the filter $\mathcal{F}_k$. Indeed, if $\theta(x^{l_k+1}) \notin \mathcal{F}_k$, it must be dominated by an entry $\theta(x^l)$ in the filter $\mathcal{F}_k$. Since $x^{k+1}, k \in \hat{K}$, is acceptable for $\theta(x^l) \in \mathcal{F}_k$, there is an index $j \in \{1, 2\}$ such that

$$\theta_j(x^{k+1}) \leq \theta_j(x^l) - \gamma_\theta\|\theta(x^{k+1})\| \leq \theta_j(x^{l_k+1}) - \gamma_\theta\|\theta(x^{k+1})\|,$$

where the last inequality holds since $\theta(x^l)$ dominates $\theta(x^{l_k+1})$. Hence (6.41) holds. Together with (6.39), we obtain

$$\theta_j(x^{k+1}) - \theta_j(x^{l_k+1}) \leq -\gamma_\theta\varepsilon$$

for at least one index $j \in \{1, 2\}$. However, the left-hand side converges to zero for at least one index $j \in \{1, 2\}$ because of (6.40). This contradiction shows that (6.38) holds.

As an immediate consequence of (6.38), we also obtain $\lim_{k\in K} \|\Phi(x^{k+1})\| = 0$. However, for all $k \notin K$, we have $\|\Phi(x^{k+1})\| \leq \|\Phi(x^k)\|$. Hence we obtain $\lim_{k\to\infty} \|\Phi(x^k)\| = 0$, and this completes the proof. □

Theorem 6.17 shows that every accumulation point of a sequence generated by Algorithm 6.15 is actually a solution of (6.1) and not just a stationary point of (6.4), provided the filter is accepted an infinite number of times. Hence we get a very strong global convergence result in this case. Moreover, it is easy to see that all statements of the local convergence result from Theorem 6.14 remain true in this case.

On the other hand, if the filter is accepted only a finite number of times, then Algorithm 6.15 eventually reduces to Algorithm 6.2, and in this case Algorithm 6.15 has precisely the same convergence properties of Algorithm 6.2 as described in the previous sections.

6.5 Numerical Experiments

We implemented Algorithm 6.15 in MATLAB and tested the algorithm on a number of mixed complementarity problems from the MCPLIB collection (see [22]) using the reformulation from the previous section.

Preliminary numerical experiments showed that the local method behaves extremely good. We therefore decided to use the local method as a preprocessor before starting the

main algorithm. More precisely, we first allow at most 20 iterations of the local method, and then switch to the globalized trust-region filter method from Algorithm 6.15. Moreover, we follow an idea by Ulbrich [118] and compute the direction p^k_{PLM} using a projection onto the intersection of the box $\mathcal{B}$ and the trust-region bound rather than a projection onto $\mathcal{B}$ alone. Note that, locally, this does not change anything since $p^k_{PLM} \to 0$ whereas the trust-region radius $\Delta_k \geq \Delta_{\min}$ is bounded away from zero. In particular, neither the global nor the local convergence theory is affected by this modification.

We next describe the initialization of our method: The starting point x^0 is the one from the MCPLIB collection. It always belongs to the box $\mathcal{B}$, so there is no need to project it onto the feasible set. The Levenberg-Marquardt parameter ν_k is chosen as follows: For smaller problems with $n < 100$, we first estimate the condition number of the matrix $H_k^T H_k$. If this estimated condition number is larger than 10^{25}, we set $\nu_k := 10^{-6}/(k+1)$, otherwise we set $\nu_k := 10^{-16}$. In all other cases, we take $\nu_k := 0$. (Note the condition estimator becomes expensive for larger problems, so we do not use it for problems with $n \geq 100$.) We terminate our iteration if one of the following conditions hold:

$$\Psi(x^k) \leq 10^{-10} \quad \text{or} \quad \|\hat{g}(x^k)\| \leq 10^{-6} \quad \text{or} \quad k > 500 \quad \text{or} \quad \Delta_k \leq 10^{-12}.$$

The remaining parameters used by our method are $\lambda_1 = 0.1, \lambda_2 = 0.9, \alpha = 10^{-4}, \rho_1 = 10^{-4}, \rho_2 = 0.75, \sigma_1 = 0.5, \sigma_2 = 2, \Delta_0 = 10$, and $\Delta_{\min} = 10^{-6}$.

If the preprocessor is not able to solve a problem or if $\|p^k_{PLM}\| \leq 10^{-12}$, we switch to Algorithm 6.15 starting with the best point computed so far. We then test whether our slightly modified projected step p^k_{PLM} is acceptable for the current filter or satisfies the descent condition in (S.4). If this is not the case and p^k_{PLM} also fails to satisfy the fraction of Cauchy decrease condition, we compute p^k in (S.5) by solving the trust-region subproblem (6.7) exactly. Here, the QP-solver MINQ from Neumaier [92] is used. This is a MATLAB routine for bound constrained quadratic programs, and we allow at most n inner iterations for each call of this QP-solver. Unfortunately, sometimes we do not succeed in solving the trust-region subproblem even with a higher number of inner QP-iterations. The number of errors produced by MINQ grows with the dimension n of the mixed complementarity problem. For this reason, we exclude from our test all problems of the MCPLIB with size $n > 160$. Alternatively, we could compute an approximate solution of the trust-region subproblem like a Cauchy step or a simple dogleg step, however, according to our numerical tests, it is better to solve (or try to solve) the QP-subproblem exactly.

Our numerical results are summarized in Table 6.1. In this table the first column gives the name of the problem; i_{tot} gives the total number of outer iterations (adding the iteration numbers from the preprocessor and the main algorithm). The entry '–' is used to indicate that the algorithm terminated unsuccessfully; $\Psi(x^f)$ and $\|\hat{g}(x^f)\|$ denote the values of $\Psi(x)$ and $\|\hat{g}(x)\|$ at the final iterate $x = x^f$; i_{fil} gives the number of filter steps taken and i_{des} the number of descent steps satisfying the criterion in (S.4) of Algorithm 6.15. The remaining two columns contain nonzero numbers only if we solve our QP-subproblem using MINQ. The entries of column i_{TR} report the number of successful (left) and the number of unsuccessful trust-region steps (right); moreover, column i_{QP} gives the number of QP-problems that were solved successfully (left) and unsuccessfully (right). In the latter case,

we do not stop our iteration if the final approximate solution provided by MINQ satisfies the fraction of Cauchy decrease condition.

Table 6.1: Numerical results for MCPLIB test problems

Problem	i_{tot}	$\Psi(x^f)$	$\|\hat{g}(x^f)\|$	i_{fil}	i_{des}	i_{TR}		i_{QP}	
						succ	unsucc	solv	unsolv
badfree	4	1.589642e-14	3.088351e-08	0	0	0	0	0	0
bertsekas	11	1.276482e-11	3.156252e-05	0	0	0	0	0	0
billups	–	2.000000e-06	0.000000e+00	0	0	0	0	0	0
choi	5	2.649619e-16	4.405966e-10	0	0	0	0	0	0
colvdual	14	9.073964e-11	9.450997e-05	0	0	0	0	0	0
colvnlp	6	4.885855e-16	4.901420e-08	0	0	0	0	0	0
cycle	4	8.921959e-12	4.224224e-07	0	0	0	0	0	0
degen	4	3.151895e-17	1.122835e-09	0	0	0	0	0	0
duopoly	–	5.163723e+00	4.977950e-07	14	0	22	5	14	13
ehl_k40	12	1.511446e-13	1.842138e-04	0	0	0	0	0	0
ehl_k60	15	3.103870e-11	6.406644e-04	0	0	0	0	0	0
ehl_k80	14	9.474365e-13	3.872440e-03	0	0	0	0	0	0
ehl_kost	17	5.651902e-12	1.512516e-02	0	0	0	0	0	0
electric	52	1.745588e-11	1.238040e-02	23	0	4	5	4	0
explcp	4	7.407629e-14	3.849074e-08	0	0	0	0	0	0
freebert	11	4.545773e-11	5.974924e-05	0	0	0	0	0	0
gafni	10	6.420657e-13	9.795657e-06	0	0	0	0	0	0
games	13	4.384397e-13	1.618921e-05	0	0	0	0	0	0
hanskoop	14	1.231700e-11	3.573738e-06	0	0	0	0	0	0
hydroc06	7	5.792347e-19	1.566474e-09	0	0	0	0	0	0
hydroc20	10	2.322843e-16	5.090809e-05	0	0	0	0	0	0
jel	8	3.651083e-18	1.601171e-08	0	0	0	0	0	0
josephy	2	2.989144e-11	6.436729e-05	0	0	0	0	0	0
kojshin	2	3.004186e-11	6.452607e-05	0	0	0	0	0	0
mathinum	4	3.024771e-12	6.673325e-07	0	0	0	0	0	0
mathisum	8	2.199503e-16	1.559264e-08	0	0	0	0	0	0
methan08	4	6.252855e-13	2.274457e-02	0	0	0	0	0	0
nash	4	2.354633e-19	7.457045e-09	0	0	0	0	0	0
ne-hard	20	5.337625e-11	1.323158e-04	0	0	0	0	0	0
pgvon106	69	1.387117e-12	1.325755e-01	4	0	11	34	42	3
pies	29	1.739675e-13	1.328305e-03	8	0	0	1	0	0
powell	4	5.659114e-11	7.740843e-06	0	0	0	0	0	0
powell_mcp	2	2.728284e-13	6.048681e-06	0	0	0	0	0	0

Table 6.1: Numerical results for MCPLIB test problems (continued)

Problem	i_{tot}	$\Psi(x^f)$	$\|\hat{g}(x^f)\|$	i_{fil}	i_{des}	i_{TR}		i_{QP}	
						succ	unsucc	solv	unsolv
qp	2	1.603357e-31	1.025472e-15	0	0	0	0	0	0
scarfanum	3	3.605079e-12	1.796300e-06	0	0	0	0	0	0
scarfasum	3	3.604872e-12	2.255827e-06	0	0	0	0	0	0
scarfbsum	120	1.507297e-11	9.669907e-04	7	1	57	35	89	2
shubik	–	1.407769e-07	4.303409e-03	74	8	161	237	290	91
simple-ex	25	1.079537e-13	4.142756e-07	5	0	0	0	0	0
simple-red	10	2.173645e-11	5.866415e-06	0	0	0	0	0	0
sppe	3	4.251553e-11	1.849914e-04	0	0	0	0	0	0
tinloi	6	7.639515e-12	7.292264e-04	0	0	0	0	0	0
tobin	2	1.474605e-14	1.352957e-05	0	0	0	0	0	0

Table 6.1 shows that our method was able to solve the majority of all test examples. Most of them were solved in less than 20 iterations and, therefore, by our preprocessor which turns out to be very effective. We have failures only on three problems, namely `billups`, `duopoly`, and `shubik`. For `billups` and `duopoly`, we terminate with a stationary point, whereas the function value in the final iteration of `shubik` is very small, but does not satisfy our termination criterion. We also stress that we have a relatively high number of unsolved QP-subproblems for the two examples `duopoly` and `shubik` which might be the reason for the failure of the overall algorithm. However, we also tried some other QP-solvers, but, in general, MINQ seems to be a good choice for bound constrained quadratic programs. Finally, we mention that we changed example `pgvon106` slightly by adding a small number to the lower bounds. This prevents difficulties in computing the function value $F(x)$ when x is close to the lower bounds.

Conclusions

The contributions of this thesis are concerned with solving nonlinear and mixed complementarity problems.

- In Section 3.2.4, we developed a local projected Levenberg-Marquardt method for box constrained least squares problems, which in turn can be used to address mixed complementarity problems. The convergence was shown to be locally fast.

- In Chapter 4, a new reformulation of nonlinear and mixed complementarity problems was given, whose properties were shown to be similar to the Fischer-Burmeister reformulation. However, the new reformulation avoids certain drawbacks of the latter approach. Proposing a Levenberg-Marquardt-type method with line search, global and fast local convergence were established. This new method turns out to be very reliable for the examples from the MCPLIB.

- In Chapter 5, we developed an inexact variant of the method from Chapter 4 which was shown to be able to solve large-scale mixed complementarity problems, such as those arising from optimal control and obstacle problems. It was proven that the global and fast local convergence properties are preserved.

- In Chapter 6, we proposed yet another approach for solving mixed complementarity problems by combining the ideas developed in Section 3.2.4 and Chapter 4 with a trust region globalization strategy. Additionally, a filter technique is incorporated to improve the efficiency of the overall method. Again, superior global and fast local convergence properties are established. Surprisingly, the numerical experiments revealed the robustness of the method even without any globalization strategy. On the other hand, it turned out that, when applying globalization, the attained robustness was inferior compared to the method from Chapter 4.

As a result of our theoretical and algorithmic investigations, MATLAB functions for solving mixed complementarity problems were developed. This implementation combines the local method from Chapter 6 with the global method from Chapter 4. These functions are online available from `http://www.mathematik.uni-wuerzburg.de/~petra/`.

The work presented in this thesis admits several extensions.

- The regularity conditions for local convergence presented in the preceding chapters can possibly be weakened. One direction to obtain improvements could be the construction of other least squares formulations of the complementarity problem.

- The method of Chapter 6 is of limited value for large scale problems. To address such problems, it is necessary to use solvers for large scale QP-problems with box constraints.

- Although LMMCP has been demonstrated to be a robust solver, the current implementation admits further possibilities for improvements, which will be incorporated in future versions of this program.

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