

**AN INTERIOR-POINT AFFINE-SCALING
TRUST-REGION METHOD FOR SEMISMOOTH
EQUATIONS WITH BOX CONSTRAINTS**

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Abstract. An algorithm for the solution of a semismooth system of equations with box constraints is described. The method is an affine-scaling trust-region method. All iterates generated by this method are strictly feasible. In this way, possible domain violations outside or on the boundary of the box are avoided. The method is shown to have strong global and local convergence properties under suitable assumptions, in particular, when the method is used with a special scaling matrix. Numerical results are presented for a number of problems arising from different areas.

Key Words. Affine scaling, trust-region method, nonlinear equations, box constraints, semismooth functions, Newton's method.

1 Introduction

We consider the nonlinear system of equations with bound constraints

$$F(x) = 0, \quad x \in \Omega := \{x \in \mathbb{R}^n \mid l_i \leq x_i \leq u_i \quad \forall i = 1, \dots, n\}, \quad (1)$$

where $F : \mathcal{O} \rightarrow \mathbb{R}^n$ is at least semismooth on the open set \mathcal{O} containing the box Ω and where the lower and upper bounds satisfy the relation $-\infty \leq l_i < u_i \leq +\infty$ for all $i = 1, \dots, n$.

The corresponding unconstrained problem with $\Omega = \mathbb{R}^n$ and F continuously differentiable is discussed in several books including [1, 16, 18, 31, 32, 40]. Extensions of the classical Newton method for the solution of the unconstrained problem with F being semismooth may be found in [43, 42, 41, 22]. Despite the popularity of the unconstrained system of nonlinear equations, the number of references dealing with the box constrained problem (1) (and with F being either smooth or nonsmooth) is still very limited. Currently, we are only aware of the papers [2, 3, 4, 5, 28, 29, 33, 44, 47].

Most of these papers, however, appeared during the last few years, and we believe that the box constrained problem (1) is of increasing interest and quite important for several reasons. In fact, in a number of applications, the mapping F is not defined outside the box Ω . In some other situations, the unconstrained problem $F(x) = 0$ might have solutions outside the box Ω which have no physical meaning, e.g., negative concentrations in chemical equilibrium problems are completely useless. Furthermore, if one has a good idea that a solution should exist in a certain area, this kind of information can be used by putting suitable bounds on the variables.

The main motivation for the current work is a series of papers by Bellavia et al. [2, 3, 4]. These authors consider a class of affine-scaling interior-point methods for the solution of problem (1) which seem to have very good numerical properties. In particular, in our experience, the practical performance of these methods is better than the behaviour of the active-set type methods discussed in [28, 29, 44]. However, Bellavia et al. consider smooth equations only, and in order to show that a certain inner iteration is finite, they assume that the Jacobian $F'(x)$ is nonsingular. Our aim is therefore to generalize their method to the class of semismooth equations (which is important if we want to apply our method to complementarity problems, for example) and to get rid of the nonsingularity assumption. We also try to simplify their method and the corresponding convergence analysis by using a simple rule for the transition from global to local fast convergence.

The method suggested by Ulbrich [47] is also able to deal with semismooth equations and has similar global and local convergence properties. However, it is not an interior-point method. The iterates in Ulbrich's method belong to Ω , but not to the interior of this set. This causes some practical problems in those applications where the mapping F is not defined on certain parts of the boundary of Ω due to some logarithmic terms, for example. Difficulties of this kind occur quite frequently in some economic equilibrium problems, cf. [24]. Therefore, although we assume for our theoretical analysis that F is defined on the open neighbourhood \mathcal{O} of Ω , we feel that it is quite important from a practical point of view that all iterates stay in the interior of the box Ω .

While there are not so many papers dealing with problem (1), there is a huge literature with different methods for the solution of box constrained optimization problems, and we refer the reader to [6, 7, 10, 11, 12, 13, 17, 20, 21, 26, 27, 30, 34, 35, 36, 45, 48, 49, 50], for example. These references include active set-type methods, projected Newton methods, penalty methods, pattern search, and affine-scaling interior-point methods. The latter class of methods is of particular interest for our work and is the subject of the papers [10, 11, 17, 27, 48, 49]. They play an important role for the construction of our algorithm because we will use a certain bound constrained optimization problem in order to globalize our local method for the solution of the box constrained system of nonlinear equations (1).

We stress, however, that there is a significant difference in applying affine-scaling methods to either bound constrained optimization problems or to nonlinear equations with box constraints. In the former case, the affine-scaling approach is used in order to get good local convergence properties, while in the latter the local convergence is, more or less, guaranteed by a suitable modification of the standard Newton step for the unconstrained problem $F(x) = 0$, whereas the affine-scaling approach is used in order to get suitable global convergence properties. Therefore, we either use different assumptions on the affine-scaling matrices depending on the kind of problem we want to solve, or we use the same assumptions, but then they play a different role.

The paper is organized as follows: We derive our affine-scaling trust-region method for the solution of (1) in Section 2. The global and local convergence properties of this method are investigated in Sections 3 and 4, respectively. Implementation details and numerical results for different classes of problems are given in Section 5, and we close with some final remarks in Section 6.

A few words regarding our notation: The symbol $\|\cdot\|$ denotes the Euclidean vector norm or the induced (spectral) matrix norm, whereas $\|\cdot\|_\infty$ is the maximum norm in \mathbb{R}^n . The Euclidean projection of a vector $x \in \mathbb{R}^n$ onto the box Ω is denoted by $P_\Omega(x)$. The symbol $B_\varepsilon(x^*)$ stands for the Euclidean ball of radius $\varepsilon > 0$ around the point $x^* \in \mathbb{R}^n$. Given a positive semidefinite matrix $A \in \mathbb{R}^{n \times n}$, we write $A^{1/2}$ for its positive semidefinite square root. Furthermore, given a mapping $G : \mathbb{R}^n \rightarrow \mathbb{R}^m$, we write $G'(x)$ for the Jacobian of G at x (if G is differentiable), and $\partial G(x)$ for the generalized Jacobian of G at x (if G is locally Lipschitz), see Clarke [9]. Note, in particular, that $\partial G(x) = \{G'(x)\}$ if G is continuously differentiable in x . We often use the short-hand notation G_k for the mapping G evaluated at a point $x^k \in \mathbb{R}^n$. Finally, several properties of (strongly) semismooth functions will be exploited in our proofs. Although we give precise references in all cases, the reader not familiar with this class of functions may consult the original works [43, 42] or have a look at the corresponding section in the book [22] for further details.

2 Description of the Method

This section gives a detailed description of our trust-region-type method for the solution of problem (1). To this end, we first note that (1) is closely related to the box constrained

optimization problem

$$\text{minimize } f(x) := \frac{1}{2} \|F(x)\|^2 \quad \text{s.t. } x \in \Omega. \quad (2)$$

In fact, every solution x^* of (1) is a global minimum of (2). Conversely, if x^* is a minimum of (2) such that $f(x^*) = 0$, then x^* is also a solution of (1).

Regarding the mapping f defined in (2), we make the following assumption which we assume to hold throughout the remaining part of this paper.

(A) The mapping f from (2) is continuously differentiable.

Assumption (A) obviously holds if F itself is continuously differentiable. However, there are also some interesting situations where f is continuously differentiable although F is not differentiable (but semismooth), see, e.g., [23, 15, 8] for some examples in the context of complementarity problems.

We exploit the relation between the two problems (1) and (2) and follow an idea by Coleman and Li [10, 11] who observed that the first order optimality conditions of (2) are equivalent to the nonlinear system of equations

$$D(x)\nabla f(x) = 0, \quad x \in \Omega, \quad (3)$$

with a suitable *scaling matrix*

$$D(x) = \text{diag}(d_1(x), \dots, d_n(x)).$$

Originally, Coleman and Li [10, 11] consider only one particular choice of the scaling matrix $D(x)$. However, it was noted by Heinkenschloss et al. [27], for example, that the equivalence between (3) and the optimality conditions of (2) holds for a rather general class of scaling matrices satisfying the conditions

$$d_i(x) \begin{cases} = 0, & \text{if } x_i = l_i \text{ and } [\nabla f(x)]_i > 0, \\ = 0, & \text{if } x_i = u_i \text{ and } [\nabla f(x)]_i < 0, \\ \geq 0, & \text{if } x_i \in \{l_i, u_i\} \text{ and } [\nabla f(x)]_i = 0, \\ > 0, & \text{else} \end{cases} \quad (4)$$

for all $i = 1, \dots, n$ and all $x \in \Omega$. In fact, the reader may find some other scaling matrices (satisfying these conditions and sometimes having better convergence properties than the original Coleman-Li-scaling) in [27, 30, 49].

In this work, we allow the scaling matrix satisfying (4) to be from a rather general class, see Assumption (C) below. Several existing scaling matrices from the literature satisfy our assumptions, for example, we may take the Coleman-Li-scaling [10, 11], defined by

$$d_i^{CL}(x) := \begin{cases} x_i - l_i, & \text{if } [\nabla f(x)]_i > 0 \text{ and } l_i > -\infty, \\ u_i - x_i, & \text{if } [\nabla f(x)]_i < 0 \text{ and } u_i < \infty, \\ \min\{x_i - l_i, u_i - x_i\}, & \text{if } [\nabla f(x)]_i = 0 \text{ and } (l_i > -\infty \text{ or } u_i < \infty), \\ 1, & \text{else,} \end{cases} \quad (5)$$

for $x \in \Omega$ (more precisely, this is the modified Coleman-Li-scaling suggested by Heinken-schloss et al. [27]), or the minimum-scaling

$$d_i^{MIN}(x) := \begin{cases} 1, & \text{if } l_i = -\infty \text{ and } u_i = +\infty, \\ \min \{x_i - l_i + \gamma \max\{0, -[\nabla f(x)]_i\}, u_i - x_i + \gamma \max\{0, [\nabla f(x)]_i\}\}, & \text{else,} \end{cases} \quad (6)$$

where $\gamma > 0$ is a given constant, cf. [30]. Both scaling matrices may be used in order to prove suitable global and local convergence results. Nevertheless, we stress that the minimum-scaling has some additional properties (see Assumption (D) below) that allows us to prove stronger global convergence results than for the Coleman-Li-scaling (see Theorem 3.4 below).

In order to construct a suitable method for the solution of problem (1), we follow an interior-point trust-region approach for (2) similar to those in [11, 17, 49]. Given an iterate $x^k \in \text{int } \Omega$, we consider the quadratic model

$$m_k(p) := \frac{1}{2} \|F(x^k) + H_k p\|^2 \approx \frac{1}{2} \|F(x^k + p)\|^2$$

on the scaled trust-region

$$\{p \in \mathbb{R}^n \mid \|D(x^k)^{-1/2} p\| \leq \Delta_k\},$$

where $\Delta_k > 0$ denotes the trust-region radius, and where $H_k \in \partial F(x^k)$ is an element of the generalized Jacobian of F at x^k . In order to get the next iterate $x^{k+1} \in \text{int } \Omega$, we first compute an approximate solution $p^k \in \mathbb{R}^n$ of the subproblem

$$\text{minimize } m_k(p) \quad \text{s.t. } x^k + p \in \text{int } \Omega, \quad \|D(x^k)^{-1/2} p\| \leq \Delta_k. \quad (7)$$

Following the standard trust-region philosophy, we then define the predicted and actual reductions by

$$\begin{aligned} \text{ared}_k(p^k) &:= f(x^k) - f(x^k + p^k) \quad \text{and} \\ \text{pred}_k(p^k) &:= m_k(0) - m_k(p^k) = f(x^k) - m_k(p^k), \end{aligned}$$

respectively. If the quotient

$$r_k := \frac{\text{ared}_k(p^k)}{\text{pred}_k(p^k)} \quad (8)$$

is sufficiently large, we accept the quadratic model, compute $x^{k+1} := x^k + p^k$, and possibly increase the trust-region radius Δ_k . Otherwise we reject the step, set $x^{k+1} := x^k$ again and decrease the radius Δ_k .

Hence it remains to specify the computation of our approximate solution p^k . To this end, we first define the modified Cauchy-step

$$p_{CP}^k := -\tau_{CP} D_k \nabla f(x^k),$$

where $D_k := D(x^k)$ and $\tau_{CP} = \tau_{CP}^k \in \mathbb{R}$ is a solution of the one-dimensional problem

$$\begin{aligned} \text{minimize } m_k(p(\tau)) \quad \text{s.t. } \quad & p(\tau) = -\tau D_k \nabla f(x^k), \quad \|D_k^{-1/2} p(\tau)\| \leq \Delta_k \\ & \theta(l - x^k) \leq p(\tau) \leq \theta(u - x^k), \tau \geq 0, \end{aligned} \quad (9)$$

where $\theta \in (0, 1)$ is a given constant which guarantees that $x^k + p_{CP}^k \in \text{int } \Omega$, see also Dennis and Vicente [17]. We then compute a vector $p^k \in \mathbb{R}^n$ satisfying the fraction of Cauchy-decrease condition

$$m_k(p^k) \leq m_k(p_{CP}^k), \quad x^k + p^k \in \text{int } \Omega, \quad \|D_k^{-1/2} p^k\| \leq \Delta_k; \quad (10)$$

in particular, we may take $p^k = p_{CP}^k$. With such a choice of p^k , it is possible to prove a global convergence result. In order to get fast local convergence, we also use a projected interior-point Newton-type step. Since the (generalized) Newton direction

$$p_N^k := -H_k^{-1} F(x^k) \quad (\text{where } H_k \in \partial F(x^k)) \quad (11)$$

for the unconstrained problem $F(x) = 0$ does, in general, not satisfy the condition $x^k + p_N^k \in \text{int } \Omega$, we use the projected and truncated Newton direction

$$p_{PN}^k := \sigma_k (P_\Omega(x^k + p_N^k) - x^k), \quad (12)$$

with

$$\sigma_k := \max \{ \sigma, 1 - \|P_\Omega(x^k + p_N^k) - x^k\| \} \quad (13)$$

for some constant $\sigma \in (0, 1)$. We then have $x^{k+1} := x^k + p_{PN}^k \in \text{int } \Omega$, and we will see in our convergence analysis that this choice guarantees local fast convergence under suitable conditions.

In order to get a simple transition from the global method with a direction p^k satisfying (10) to the local method with the direction p_{PN}^k from (12), we also incorporate the test

$$\|F(x^k + p_{PN}^k)\| \leq \eta \|F(x^k)\| \quad (14)$$

in our method, where $\eta \in (0, 1)$ denotes another constant. We will see that (14) holds automatically in a neighbourhood of a solution of (1) under suitable assumptions.

We are now in a position to give a precise statement of the overall method.

Algorithm 2.1 (Interior-Point Trust-Region Method)

(S.0) Choose $x^0 \in \text{int } \Omega$, $\Delta_0 > 0$, $\varepsilon > 0$, $\eta, \sigma, \theta \in (0, 1)$, $0 < \rho_1 < \rho_2 < 1$, and $0 < \omega_1 < 1 < \omega_2$, set $k := 0$.

(S.1) If $\|D_k^{1/2} \nabla f(x^k)\| \leq \varepsilon$: STOP.

(S.2) Choose a matrix $H_k \in \partial F(x^k)$ and compute (if possible) p_{PN}^k using (12). If (14) holds, set $x^{k+1} := x^k + p_{PN}^k$, $\Delta_{k+1} := \omega_2 \Delta_k$, and go to (S.5); otherwise go to (S.3).

- (S.3) Compute $p^k \in \mathbb{R}^n$ satisfying (10), and define r_k by (8). If $r_k \geq \rho_1$, we call iteration k "successful" and set $x^{k+1} := x^k + p^k$; otherwise, we set $x^{k+1} := x^k$.
- (S.4) Update the trust-region radius according to the following rules:
 If $r_k < \rho_1$, set $\Delta_{k+1} := \omega_1 \Delta_k$.
 If $r_k \in [\rho_1, \rho_2)$, set $\Delta_{k+1} := \Delta_k$.
 If $r_k \geq \rho_2$, set $\Delta_{k+1} := \omega_2 \Delta_k$.
- (S.5) Set $k \leftarrow k + 1$, and go to (S.1).

We give a number of comments with some simple properties of Algorithm 2.1.

- Remark 2.2** (a) The termination criterion in step (S.1) checks whether the current iterate x^k is an approximate stationary point of the box constrained optimization problem (2).
- (b) All iterates x^k belong to the interior of the box Ω . Hence the inverse diagonal matrices $D_k^{-1/2}$ occurring, e.g., in (9), (10), always exist since the elements $d_i(x^k)$ are positive according to (4).
- (c) The computation of p_{PN}^k in step (S.2) requires the (generalized) Jacobian H_k from (11) to be nonsingular. If this matrix turns out to be singular, we immediately switch to step (S.3).
- (d) Taking into account the previous comments, Algorithm 2.1 is well-defined in the sense that all steps can actually be carried out without any additional assumptions on problem (1).
- (e) The entire sequence $\{f(x^k)\}$ is monotonically decreasing. Equivalently, this means that we have $\|F(x^{k+1})\| \leq \|F(x^k)\|$ for all $k \in \mathbb{N}$. In fact, this is obvious if the test (14) gets accepted in step (S.2) of Algorithm 2.1. Otherwise, we compute p^k satisfying (10) in step (S.3). If the iteration is not successful, we have $\|F(x^{k+1})\| = \|F(x^k)\|$, otherwise we have

$$r_k \geq \rho_1 \iff f(x^k) - f(x^k + p^k) \geq \rho_1 (f(x^k) - m_k(p^k)).$$

Here, the expression on the right-hand side is nonnegative because we have

$$m_k(p^k) \leq m_k(p_{CP}^k) \leq m_k(0) = f(x^k)$$

in view of (10) and the definition of the Cauchy step p_{CP}^k . Hence, the inequality $f(x^k) \geq f(x^k + p^k) = f(x^{k+1})$ also holds for all successful iterations in step (S.3).

In our subsequent convergence analysis, we assume throughout that $\varepsilon = 0$ and that Algorithm 2.1 generates an infinite sequence, i.e., it does not terminate after a finite number of iterations satisfying the first order optimality conditions of problem (2).

3 Global Convergence

The aim of this section is to prove a global convergence result for Algorithm 2.1. To this end, we need two more assumptions. The first is a boundedness assumption which is rather standard in trust-region methods (see, e.g., [14]), and the second one is a condition regarding the choice of the diagonal scaling matrix $D(x)$.

(B) The sequence $\{H_k\}$ generated by Algorithm 2.1 is bounded.

(C) The scaling matrix $D(x)$ satisfies (4) and is bounded on Ω . Furthermore, there exists a constant $\alpha > 0$ such that

$$\alpha d_i(x) \leq \begin{cases} x_i - l_i, & \text{if } [\nabla f(x)]_i > 0 \text{ and } l_i > -\infty, \\ u_i - x_i, & \text{if } [\nabla f(x)]_i < 0 \text{ and } u_i < +\infty \end{cases}$$

for all $i = 1, \dots, n$ and all $x \in \text{int } \Omega$.

Note that the last part of (C) is satisfied both by the modified Coleman-Li-scaling (5) and the minimum-scaling (6) with $\alpha = 1$. Furthermore, all remaining conditions hold automatically if Ω itself is bounded, i.e., if all lower and upper bounds l_i and u_i are finite (this follows, e.g., from the upper semicontinuity of the generalized Jacobian, see [9]). This assumption is quite realistic in many cases since otherwise one may replace infinite bounds by sufficiently large bounds.

There is a simple consequence of Assumption (B) that will play a crucial role in our subsequent analysis and that is therefore stated explicitly in the following remark.

Remark 3.1 Suppose that Assumptions (A) and (B) hold. Then the sequence $\{\nabla f(x^k)\}$ is bounded. To see this, note that Assumption (A) and [9, Proposition 2.2.4 and Theorem 2.6.6] together imply that we can write the gradient as $\nabla f(x^k) = H_k^T F(x^k)$ with H_k being the matrix from step (S.2) of Algorithm 2.1. Now $\{H_k\}$ is bounded in view of Assumption (B). Moreover, $\{\|F(x^k)\|\}$ is also bounded because of Remark 2.2 (e), so that $\{\nabla f(x^k)\}$ must indeed be bounded.

We now state a technical lemma that leads to a lower bound for the predicted reduction. Results of this kind are standard for trust-region methods, see, in particular, [49, Lemma 6.1] and [17, Lemma 4.1].

Lemma 3.2 *Suppose that Assumptions (A) and (C) hold, and let $p^k \in \mathbb{R}^n$ satisfy the fraction of Cauchy-decrease condition (10). Then*

$$\text{pred}_k(p^k) \geq \frac{1}{2} \|D_k^{1/2} g^k\| \min \left\{ \Delta_k, \frac{\|D_k^{1/2} g^k\|}{\|D_k^{1/2} H_k^T H_k D_k^{1/2}\|}, \theta \alpha \frac{\|D_k^{1/2} g^k\|}{\|g^k\|_\infty} \right\} \quad (15)$$

where $g^k := \nabla f(x^k)$ denotes the gradient of f at x^k . If, in addition, Assumption (B) holds, then there exists a constant $C > 0$ such that

$$\text{pred}_k(p^k) \geq C \|D_k^{1/2} g^k\|^2 \min\{\Delta_k, 1\}. \quad (16)$$

Proof. The proof is essentially the same as in [49, 17], except that we have a different quadratic model since we deal with box constrained nonlinear equations instead of bound constrained optimization problems. For the sake of completeness, however, we include the full proof here.

Consider a fixed iterate $x^k \in \text{int } \Omega$, and recall that the stepsize $\tau \geq 0$ in (9) has to satisfy the two feasibility requirements

$$\|D_k^{-1/2}p(\tau)\| \leq \Delta_k \quad (17)$$

and

$$\theta(l - x^k) \leq p(\tau) \leq \theta(u - x^k). \quad (18)$$

Let τ_Δ and τ_Ω denote the two maximum stepsizes such that (17) and (18) hold, respectively. Since $p(\tau) = -\tau D_k g^k$, an elementary calculation shows that

$$\begin{aligned} \tau_\Delta &= \frac{\Delta_k}{\|D_k^{1/2}g^k\|} \quad \text{and} \\ \tau_\Omega &= \theta \min \left\{ \min_{i:[D_k g^k]_i < 0} \left\{ \frac{u_i - x_i^k}{-[D_k g^k]_i} \right\}, \min_{i:[D_k g^k]_i > 0} \left\{ \frac{l_i - x_i^k}{-[D_k g^k]_i} \right\} \right\}. \end{aligned}$$

Hence the solution $\tau_{CP} = \tau_{CP}^k$ of the one-dimensional problem (9) has to belong to the interval $[0, \tau_+]$, where

$$\tau_+ := \min\{\tau_\Delta, \tau_\Omega\}.$$

(Note that τ_Δ, τ_Ω and, therefore, τ_+ are well-defined because $D_k g^k \neq 0$ since otherwise we would have stopped in step (S.1) of Algorithm 2.1.) From the Cauchy-decrease condition (10), we therefore obtain

$$m_k(p^k) \leq m_k(p_{CP}^k) = \min_{\tau \in [0, \tau_+]} \phi(\tau)$$

with

$$\phi(\tau) := m_k(-\tau D_k g^k).$$

Let $\tau^*(= \tau_{CP})$ be a solution of

$$\text{minimize } \phi(\tau) \quad \text{s.t. } \tau \in [0, \tau_+].$$

Using the notation

$$F_k := F(x^k), \quad \hat{g}^k := D_k^{1/2}g^k, \quad \text{and} \quad \hat{M}_k := D_k^{1/2}H_k^T H_k D_k^{1/2},$$

and recalling that $g^k = H_k^T F_k$ (see Remark 3.1), the function ϕ may be rewritten as

$$\phi(\tau) = \frac{1}{2}\|F_k\|^2 - \tau F_k^T H_k D_k g^k + \frac{1}{2}\tau^2 (g^k)^T D_k H_k^T H_k D_k g^k$$

$$= \frac{1}{2} \|F_k\|^2 - \tau \|\hat{g}^k\|^2 + \frac{1}{2} \tau^2 (\hat{g}^k)^T \hat{M}_k \hat{g}^k.$$

Note that \hat{M}_k is always positive semidefinite. We now distinguish four cases.

Case 1: Suppose that $\tau^* \in (0, \tau_+)$. Then τ^* is an unconstrained minimum of ϕ , and we therefore get

$$0 = \phi'(\tau^*) = -\|\hat{g}^k\|^2 + \tau^* (\hat{g}^k)^T \hat{M}_k \hat{g}^k. \quad (19)$$

This gives the explicit formula

$$\tau^* = \frac{\|\hat{g}^k\|^2}{(\hat{g}^k)^T \hat{M}_k \hat{g}^k}.$$

(Note that the denominator is nonzero, because otherwise (19) would lead to $D_k^{1/2} g^k = 0$ and we would have stopped in step (S.1) of Algorithm 2.1.) This implies

$$\phi(\tau^*) = \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \frac{\|\hat{g}^k\|^4}{(\hat{g}^k)^T \hat{M}_k \hat{g}^k} \leq \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \frac{\|\hat{g}^k\|^2}{\|\hat{M}_k\|}.$$

Case 2: Assume that $\tau^* = \tau_+$ and $\tau_+ = \tau_\Delta$. If, in addition, we have $(\hat{g}^k)^T \hat{M}_k \hat{g}^k > 0$, the necessary optimality condition $\phi'(\tau^*) \leq 0$ implies

$$\tau^* \leq \frac{\|\hat{g}^k\|^2}{(\hat{g}^k)^T \hat{M}_k \hat{g}^k}. \quad (20)$$

We therefore get

$$\begin{aligned} \phi(\tau^*) &\leq \frac{1}{2} \|F_k\|^2 - \tau_\Delta \|\hat{g}^k\|^2 + \frac{1}{2} \tau_\Delta \left(\frac{\|\hat{g}^k\|^2}{(\hat{g}^k)^T \hat{M}_k \hat{g}^k} \right) (\hat{g}^k)^T \hat{M}_k \hat{g}^k \\ &= \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \tau_\Delta \|\hat{g}^k\|^2 \\ &= \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \Delta_k \|\hat{g}^k\| \end{aligned}$$

from the definition of τ_Δ . On the other hand, if we have $(\hat{g}^k)^T \hat{M}_k \hat{g}^k = 0$, we also obtain

$$\phi(\tau^*) = \frac{1}{2} \|F_k\|^2 - \tau_\Delta \|\hat{g}^k\|^2 = \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \Delta_k \|\hat{g}^k\|.$$

Case 3: Suppose that $\tau^* = \tau_+$ and $\tau_+ = \tau_\Omega$. Here we first take a closer look at τ_Ω . Using Assumption (C), we get the following lower bound for the maximum stepsize τ_Ω :

$$\begin{aligned} \tau_\Omega &= \theta \min \left\{ \min_{i: [D_k g^k]_i < 0} \left\{ \frac{u_i - x_i^k}{-[D_k g^k]_i} \right\}, \min_{i: [D_k g^k]_i > 0} \left\{ \frac{l_i - x_i^k}{-[D_k g^k]_i} \right\} \right\} \\ &= \theta \min \left\{ \min_{i: [D_k g^k]_i < 0} \left\{ \frac{u_i - x_i^k}{d_i(x^k) |g_i^k|} \right\}, \min_{i: [D_k g^k]_i > 0} \left\{ \frac{x_i^k - l_i}{d_i(x^k) |g_i^k|} \right\} \right\} \end{aligned}$$

$$\begin{aligned}
&\geq \theta \min \left\{ \min_{i: [D_k g^k]_i < 0} \left\{ \frac{u_i - x_i^k}{d_i(x^k) \|g^k\|_\infty} \right\}, \min_{i: [D_k g^k]_i > 0} \left\{ \frac{x_i^k - l_i}{d_i(x^k) \|g^k\|_\infty} \right\} \right\} \\
&\geq \frac{\theta \alpha}{\|g^k\|_\infty}.
\end{aligned}$$

Therefore, if we have $(\hat{g}^k)^T \hat{M}_k \hat{g}^k > 0$, then $\phi'(\tau^*) \leq 0$, hence (20) holds, and we get

$$\phi(\tau^*) \leq \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \tau_\Omega \|\hat{g}^k\|^2 \leq \frac{1}{2} \|F_k\|^2 - \frac{\theta \alpha}{2} \frac{\|\hat{g}^k\|^2}{\|g^k\|_\infty}.$$

On the other hand, if $(\hat{g}^k)^T \hat{M}_k \hat{g}^k = 0$, we also obtain

$$\phi(\tau^*) = \frac{1}{2} \|F_k\|^2 - \tau^* \|\hat{g}^k\|^2 = \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \tau_\Omega \|\hat{g}^k\|^2 \leq \frac{1}{2} \|F_k\|^2 - \frac{\theta \alpha}{2} \frac{\|\hat{g}^k\|^2}{\|g^k\|_\infty}.$$

Case 4: Suppose that $\tau^* = 0$. Then the necessary optimality condition $-\|\hat{g}^k\|^2 = \phi'(\tau^*) \geq 0$ implies $\hat{g}^k = 0$, a contradiction to $D_k^{1/2} g^k \neq 0$. Hence this case does not occur.

Taking all cases together, we get

$$m_k(p^k) \leq \phi(\tau^*) \leq \frac{1}{2} \|F_k\|^2 - \frac{1}{2} \min \left\{ \Delta_k \|\hat{g}^k\|, \frac{\|\hat{g}^k\|^2}{\|\hat{M}_k\|}, \theta \alpha \frac{\|\hat{g}^k\|^2}{\|g^k\|_\infty} \right\}.$$

Consequently, we obtain the lower bound

$$\text{pred}_k(p^k) = m_k(0) - m_k(p^k) \geq \frac{1}{2} \|\hat{g}^k\| \min \left\{ \Delta_k, \frac{\|\hat{g}^k\|}{\|\hat{M}_k\|}, \theta \alpha \frac{\|\hat{g}^k\|}{\|g^k\|_\infty} \right\} \quad (21)$$

for the predicted reduction, which is precisely the statement from (15).

Now suppose that Assumptions (A)–(C) hold. Then the sequences $\|H_k\|$, $\|g^k\|_\infty$ and $\|D_k^{1/2}\|$ are bounded, cf. Remark 3.1. Hence $\|\hat{M}_k\|$ and $\|\hat{g}^k\|$ are bounded as well. Therefore, (21) yields the existence of a constant $C > 0$ such that

$$\begin{aligned}
\text{pred}_k(p^k) &\geq \frac{1}{2} \|\hat{g}^k\| \min \left\{ \frac{\Delta_k \|\hat{g}^k\|}{\|\hat{g}^k\|}, \frac{\|\hat{g}^k\|}{\|\hat{M}_k\|}, \theta \alpha \frac{\|\hat{g}^k\|}{\|g^k\|_\infty} \right\} \\
&= \frac{1}{2} \|\hat{g}^k\|^2 \min \left\{ \frac{\Delta_k}{\|\hat{g}^k\|}, \frac{1}{\|\hat{M}_k\|}, \frac{\theta \alpha}{\|g^k\|_\infty} \right\} \\
&\geq C \|\hat{g}^k\|^2 \min\{\Delta_k, 1\}
\end{aligned}$$

for all $k \in \mathbb{N}$, and this proves the second statement. \square

Note that the proof of Lemma 3.2 shows, in particular, how the Cauchy step p_{CP}^k can be computed in practice.

We are now in the position to state the first main global convergence result for Algorithm 2.1. To this end, note that we are dealing with two different search directions p_{PN}^k

(the projected Newton-like step) and p^k (the Cauchy-like step). While the former will play a central role for the local rate of convergence, the Cauchy-like step is the main tool for showing global convergence. This is similar to some existing results stated in [11, 17, 49], for example. Note that the local direction p_{PN}^k does not destroy the global convergence of the overall method.

Theorem 3.3 *Suppose that Assumptions (A)–(C) hold. Then*

$$\liminf_{k \rightarrow \infty} \|D_k^{1/2} \nabla f(x^k)\| = 0. \quad (22)$$

Moreover, if the direction p_{PN}^k is accepted an infinite number of times in step (S.2) of Algorithm 2.1, we have

$$\lim_{k \rightarrow \infty} \|F(x^k)\| = 0. \quad (23)$$

Proof. First recall from Remark 2.2 (e) that the entire sequence $\{\|F(x^k)\|\}$ is monotonically decreasing. Hence, if the test (14) in step (S.2) of Algorithm 2.1 is satisfied an infinite number of times, we immediately obtain (23). In particular, this implies $\|\nabla f(x^k)\| \rightarrow 0$ and therefore (22) since the sequence $\{D_k\}$ stays bounded in view of Assumption (C).

It remains to consider the case where the direction p_{PN}^k is accepted only a finite number of times. Without loss of generality, we may assume that this never happens, so we always compute the direction p^k . Suppose that (22) does not hold. Then there is a constant $\delta > 0$ such that

$$\|\hat{g}^k\| \geq \delta \quad \forall k \in \mathbb{N}, \quad (24)$$

where, again, we write $\hat{g}^k := D_k^{1/2} \nabla f(x^k)$.

In the first part of this proof, we show that this implies

$$\sum_{k=0}^{\infty} \Delta_k < \infty. \quad (25)$$

In fact, if there is only a finite number of successful iterations, we have $\Delta_{k+1} = \omega_1 \Delta_k$ for all $k \in \mathbb{N}$ sufficiently large, and (25) follows from $\omega_1 \in (0, 1)$ and the convergence of the geometric series. Otherwise, there is an infinite number of successful iterations. Let k_i denote the indices of the successful iterations. Since $\{f(x^k)\}$ is monotonically decreasing and bounded from below, the entire sequence $\{f(x^k)\}$ converges. In particular, we have

$$\sum_{k=0}^{\infty} (f(x^k) - f(x^{k+1})) < \infty. \quad (26)$$

From (16) and (24), we obtain

$$f(x^{k_i}) - f(x^{k_i+1}) = \text{ared}_{k_i}(p^{k_i}) \geq \rho_1 \text{pred}_{k_i}(p^{k_i}) \geq \rho_1 C \delta^2 \min\{\Delta_{k_i}, 1\} > 0 \quad (27)$$

for all successful iterations. Since the expression on the left-hand side of (27) converges to zero, it follows that $\min\{\Delta_{k_i}, 1\} = \Delta_{k_i}$ for all sufficiently large k_i . Consequently, (27) implies

$$\Delta_{k_i} \leq \frac{1}{\rho_1 C \delta^2} (f(x^{k_i}) - f(x^{k_i+1})).$$

Since $\{f(x^k)\}$ is monotonically decreasing, it therefore follows from (26) that

$$\sum_{i=0}^{\infty} \Delta_{k_i} \leq \frac{1}{\rho_1 C \delta^2} \sum_{i=0}^{\infty} (f(x^{k_i}) - f(x^{k_i+1})) \leq \sum_{k=0}^{\infty} (f(x^k) - f(x^{k+1})) < \infty. \quad (28)$$

If there are unsuccessful iterations between two successful ones, say k_i and k_{i+1} , we have

$$\Delta_{k_{i+1}} \leq \omega_2 \Delta_{k_i} \quad \text{and} \quad \Delta_{l+1} = \omega_1 \Delta_l \quad \forall l \in \{k_i + 1, \dots, k_{i+1} - 1\}.$$

This implies

$$\sum_{l=k_{i+1}}^{k_{i+1}-1} \Delta_l \leq \Delta_{k_{i+1}} \sum_{j=0}^{\infty} \omega_1^j = \frac{1}{1 - \omega_1} \Delta_{k_{i+1}} \leq \frac{\omega_2}{1 - \omega_1} \Delta_{k_i}.$$

Together, we obtain from (28) that

$$\begin{aligned} \sum_{k=0}^{\infty} \Delta_k &= \sum_{k \in \{k_i\}} \Delta_k + \sum_{k \notin \{k_i\}} \Delta_k \\ &\leq \sum_{i=0}^{\infty} \Delta_{k_i} + \frac{\omega_2}{1 - \omega_1} \sum_{i=0}^{\infty} \Delta_{k_i} \\ &= \left(1 + \frac{\omega_2}{1 - \omega_1}\right) \sum_{i=0}^{\infty} \Delta_{k_i} < \infty, \end{aligned}$$

and the proof of (25) is complete.

As a consequence of (25), it follows that

$$\min\{\Delta_k, 1\} = \Delta_k \quad \text{for all } k \in \mathbb{N} \text{ sufficiently large,} \quad (29)$$

and

$$\|p^k\| \leq \|D_k^{1/2}\| \|D_k^{-1/2} p^k\| \leq \|D_k^{1/2}\| \Delta_k \leq C_1 \Delta_k \longrightarrow 0 \quad (30)$$

since there is a constant $C_1 > 0$ such that $\|D_k^{1/2}\| \leq C_1$ for all $k \in \mathbb{N}$ in view of Assumption (C). Moreover, we obtain from (30) that

$$\|x^{k+p} - x^k\| \leq \sum_{j=0}^{p-1} \|x^{k+j+1} - x^{k+j}\| \leq \sum_{j=0}^{p-1} \|p^{k+j}\| \leq C_1 \sum_{j=0}^{p-1} \Delta_{k+j}.$$

Consequently, (25) implies that $\{x^k\}$ is a Cauchy sequence and therefore convergent.

In the next part of the proof, we show that $\lim_{k \rightarrow \infty} r_k = 1$. To this end, first note that

$$\begin{aligned} |\text{pred}_k(p^k)| |r_k - 1| &= |\text{pred}_k(p^k)| \left| \frac{\text{ared}_k(p^k)}{\text{pred}_k(p^k)} - 1 \right| \\ &= |\text{ared}_k(p^k) - \text{pred}_k(p^k)| \\ &= |f(x^k + p^k) - f(x^k) + m_k(0) - m_k(p^k)|. \end{aligned}$$

From the mean-value theorem, we therefore get the existence of a vector ξ^k between x^k and $x^k + p^k$ such that

$$\begin{aligned} |\text{pred}_k(p^k)| |r_k - 1| &= |\nabla f(\xi^k)^T p^k - \nabla f(x^k)^T p^k - \frac{1}{2}(p^k)^T H_k^T H_k p^k| \\ &\leq \|\nabla f(\xi^k) - \nabla f(x^k)\| \|p^k\| + \frac{1}{2} \|H_k p^k\|^2 \\ &\leq \|\nabla f(\xi^k) - \nabla f(x^k)\| C_1 \Delta_k + \frac{1}{2} \|H_k\|^2 C_1^2 \Delta_k^2, \end{aligned}$$

where the last inequality follows from (30). Dividing this expression by $\Delta_k > 0$, using Assumption (B), noting that $\Delta_k \rightarrow 0$ and $\|\nabla f(\xi^k) - \nabla f(x^k)\| \rightarrow 0$ since ∇f is continuous and both sequences $\{x^k\}, \{\xi^k\}$ converge to the same point (see (30)), we obtain

$$\frac{|\text{pred}_k(p^k)|}{\Delta_k} |r_k - 1| \rightarrow 0. \quad (31)$$

However, using (16), (24), and (29), we have

$$\frac{\text{pred}_k(p^k)}{\Delta_k} \geq C \|D_k^{1/2} g^k\|^2 \geq C \delta^2$$

for all $k \in \mathbb{N}$ sufficiently large. This implies $|r_k - 1| \rightarrow 0$ because of (31). This, in turn, gives $\Delta_{k+1} \geq \Delta_k$ for all these k , a contradiction to (25). \square

Note that, if the entire sequence $\{x^k\}$ remains bounded, then (22) guarantees that at least one accumulation point of this sequence is a stationary point of the optimization problem (2), whereas (23) guarantees that every accumulation point is a solution of the box constrained system of equations (1).

In order to prove a stronger convergence result than Theorem 3.3 with the limes inferior in (22) being replaced by the limes, we need to introduce another assumption, see also [49, Assumption (A.6)].

(D) The scaled gradient $D(x)^{1/2} \nabla f(x)$ is uniformly continuous.

Note that Assumption (D) is satisfied automatically on compact sets if $D(x)$ denotes the minimum-scaling from (6). This follows from the fact that both ∇f and $D(x)^{1/2}$ are continuous and therefore uniformly continuous on compact sets. This is in contrast to the scaling from (5) which is not continuous.

Theorem 3.4 *Suppose that Assumptions (A)–(D) hold. Then*

$$\lim_{k \rightarrow \infty} \|D_k^{1/2} \nabla f(x^k)\| = 0.$$

Proof. Similar to the proof of Theorem 3.3, we may assume that the test (14) in step (S.2) of Algorithm 2.1 is never accepted, so we always compute the direction p^k in step (S.3).

Suppose our statement is not true. Then there exists a constant $\delta > 0$ and a subsequence $\{x^k\}_K$ such that

$$\|D_k^{1/2} \nabla f(x^k)\| \geq 2\delta \quad \forall k \in K. \quad (32)$$

In view of Theorem 3.3, we have $\liminf_{k \rightarrow \infty} \|D_k^{1/2} \nabla f(x^k)\| = 0$. Therefore, we can find for each $k \in K$ an iteration index $\ell(k) > k$ such that

$$\|D_\ell^{1/2} \nabla f(x^\ell)\| \geq \delta \quad \forall k \leq \ell < \ell(k) \quad (33)$$

and

$$\|D_{\ell(k)}^{1/2} \nabla f(x^{\ell(k)})\| < \delta, \quad k \in K.$$

Using Assumptions (B), (C), there exist constants $C_1 > 0$ and $C_2 > 0$ such that $\|D_k^{1/2}\| \leq C_1$ and $\|H_k\| \leq C_2$ for all $k \in \mathbb{N}$.

Now, let $k \in K$ be fixed for the moment, take an arbitrary ℓ with $k \leq \ell < \ell(k)$, and assume that the ℓ -th iteration is successful. Then we obtain from Lemma 3.2 that

$$f(x^\ell) - f(x^{\ell+1}) \geq \rho_1 (f(x^\ell) - m_\ell(p^\ell)) \geq \rho_1 C \|D_\ell^{1/2} \nabla f(x^\ell)\|^2 \min\{\Delta_\ell, 1\}.$$

Since the left-hand side converges to zero and since

$$\|x^{\ell+1} - x^\ell\| = \|p^\ell\| \leq \|D_\ell^{1/2}\| \|D_\ell^{-1/2} p^\ell\| \leq \|D_\ell^{1/2}\| \Delta_\ell \leq C_1 \Delta_\ell,$$

we obtain

$$f(x^\ell) - f(x^{\ell+1}) \geq \rho_1 C \|D_\ell^{1/2} \nabla f(x^\ell)\|^2 \Delta_\ell \geq \frac{\delta^2 \rho_1 C}{C_1} \|x^{\ell+1} - x^\ell\|.$$

Trivially, this inequality also holds if the ℓ -th iteration is not successful. Consequently, we get

$$\begin{aligned} \frac{\delta^2 \rho_1 C}{C_1} \|x^{\ell(k)} - x^k\| &\leq \frac{\delta^2 \rho_1 C}{C_1} \sum_{\ell=k}^{\ell(k)-1} \|x^{\ell+1} - x^\ell\| \\ &\leq \sum_{\ell=k}^{\ell(k)-1} (f(x^\ell) - f(x^{\ell+1})) \\ &= f(x^k) - f(x^{\ell(k)}) \end{aligned}$$

for all $k \in K$. Since $\{f(x^k)\}$ converges, this implies

$$\{\|x^{\ell(k)} - x^k\|\}_{k \in K} \rightarrow 0.$$

In view of Assumption (D), we therefore have

$$\{\|D_{\ell(k)}^{1/2} \nabla f(x^{\ell(k)}) - D_k^{1/2} \nabla f(x^k)\|\}_{k \in K} \rightarrow 0.$$

On the other hand, it follows from (32) and (33) that

$$\|D_{\ell(k)}^{1/2} \nabla f(x^{\ell(k)}) - D_k^{1/2} \nabla f(x^k)\| \geq \|D_k^{1/2} \nabla f(x^k)\| - \|D_{\ell(k)}^{1/2} \nabla f(x^{\ell(k)})\| \geq 2\delta - \delta = \delta.$$

This contradiction completes the proof. \square

4 Local Convergence

In this section, we consider the local convergence properties of Algorithm 2.1. More precisely, we show in the following result that, locally, the projected and truncated Newton direction is always accepted in step (S.2), and that this direction guarantees superlinear and even quadratic convergence under suitable assumptions.

Theorem 4.1 *Let $\{x^k\}$ be a sequence generated by Algorithm 2.1, and let x^* be an accumulation point of this sequence such that $F(x^*) = 0$ and all elements $H_* \in \partial F(x^*)$ are nonsingular. Then the following statements hold:*

- (a) *The entire sequence $\{x^k\}$ converges to x^* .*
- (b) *The rate of convergence is Q -superlinear.*
- (c) *If F is strongly semismooth, the rate of convergence is Q -quadratic.*

Proof. Since all elements $H_* \in \partial F(x^*)$ are nonsingular, it follows from [43, Proposition 3.1] that there exist constants $\varepsilon_1 > 0$ and $c > 0$ such that

$$\|H(x)^{-1}\| \leq c \quad \forall x \in B_{\varepsilon_1}(x^*), \quad \forall H(x) \in \partial F(x). \quad (34)$$

Moreover, being semismooth, F is locally Lipschitz continuous. Hence there exist constants $\varepsilon_2 > 0$ and $L_1 > 0$ with

$$\|F(x) - F(y)\| \leq L_1 \|x - y\| \quad \forall x, y \in B_{\varepsilon_2}(x^*). \quad (35)$$

Furthermore, the nonsingularity assumption and [9, Theorem 7.1.1] implies that the inverse function F^{-1} exists in a sufficiently small neighbourhood of $F(x^*)$, and this function is also

locally Lipschitz. Consequently, we get the existence of two constants $\varepsilon_3 > 0$ and $L_2 > 0$ such that

$$\|F^{-1}(F(x)) - F^{-1}(F(y))\| \leq L_2 \|F(x) - F(y)\| \quad \forall x, y \in B_{\varepsilon_3}(x^*). \quad (36)$$

Using [41, Proposition 1] and the semismoothness of F , we see that there is another constant $\varepsilon_4 > 0$ such that

$$\|F(x) - F(x^*) - H(x)(x - x^*)\| \leq \min \left\{ \frac{\eta}{2cL_1L_2}, \frac{1}{4c} \right\} \|x - x^*\| \quad (37)$$

for all $x \in B_{\varepsilon_4}(x^*)$ and all $H(x) \in \partial F(x)$, where η denotes the constant from (14). Moreover, by continuity, there is a constant $\varepsilon_5 > 0$ with

$$\|F(x)\| \leq \min \left\{ \frac{\eta}{2cL_1L_2}, \frac{1 - \sigma}{c} \right\} \quad \forall x \in B_{\varepsilon_5}(x^*), \quad (38)$$

where $\sigma \in (0, 1)$ denotes the constant from Algorithm 2.1. Finally, the nonsingularity assumption implies that there is another constant $\varepsilon_6 > 0$ such that σ_k from (13) satisfies

$$\sigma_k = 1 - \|P_{\Omega}(x^k + p_N^k) - x^k\| \geq \frac{3}{4} \quad \forall x^k \in B_{\varepsilon_6}(x^*). \quad (39)$$

Now define $\varepsilon := \min\{\varepsilon_i \mid i = 1, \dots, 6\}$. Since x^* is an accumulation point of the sequence $\{x^k\}$, we can choose an iterate x^k (the index k is fixed for the moment) such that $x^k \in B_{\varepsilon}(x^*) \cap \text{int } \Omega$. We will show that the next iterate also belongs to this neighbourhood and, in fact, is actually much closer to x^* than x^k is. The proof of statement (a) then follows by a simple induction argument.

To this end, we first note that H_k is nonsingular in view of (34), and we therefore obtain from (37) that

$$\begin{aligned} \|x^k + p_N^k - x^*\| &= \|x^k - H_k^{-1}F(x^k) - x^*\| \\ &= \|H_k^{-1}\| \|F(x^k) - F(x^*) - H_k(x^k - x^*)\| \\ &\leq \min \left\{ \frac{\eta}{2L_1L_2}, \frac{1}{4} \right\} \|x^k - x^*\|, \end{aligned} \quad (40)$$

in particular, $x^k + p_N^k$ also belongs to the neighbourhood $B_{\varepsilon}(x^*)$ of the solution x^* . Since we can write

$$x^k + p_N^k - x^* = \sigma_k (P_{\Omega}(x^k + p_N^k) - x^*) + (1 - \sigma_k)(x^k - x^*), \quad (41)$$

it is easy to see that this also implies that the vector $x^k + p_N^k$ is in the neighbourhood $B_{\varepsilon}(x^*)$ of x^* . Using $x^k \in \text{int } \Omega$, (34), (38), and the nonexpansiveness of the projection operator, we get

$$\|P_{\Omega}(x^k + p_N^k) - x^k\| = \|P_{\Omega}(x^k + p_N^k) - P_{\Omega}(x^k)\| \leq \|p_N^k\| \leq \|H_k^{-1}\| \|F(x^k)\| \leq 1 - \sigma.$$

In view of (13), (39), this yields

$$1 - \sigma_k = \|P_\Omega(x^k + p_N^k) - x^k\| \leq \|H_k^{-1}\| \|F(x^k)\| \leq c \|F(x^k)\|. \quad (42)$$

Using (35), (41), (40), (42), (38), (36), $\sigma_k \leq 1$, and the nonexpansiveness of the projection operator, we get

$$\begin{aligned} \|F(x^k + p_{PN}^k)\| &= \|F(x^k + p_{PN}^k) - F(x^*)\| \\ &\leq L_1 \|x^k + p_{PN}^k - x^*\| \\ &\leq L_1 \sigma_k \|x^k + p_N^k - x^*\| + L_1 (1 - \sigma_k) \|x^k - x^*\| \\ &\leq \frac{\eta}{2L_2} \|x^k - x^*\| + L_1 c \|F(x^k)\| \|x^k - x^*\| \\ &\leq \frac{\eta}{2L_2} \|x^k - x^*\| + \frac{\eta}{2L_2} \|x^k - x^*\| \\ &= \frac{\eta}{L_2} \|F^{-1}(F(x^k)) - F^{-1}(F(x^*))\| \\ &\leq \eta \|F(x^k) - F(x^*)\| \\ &= \eta \|F(x^k)\|. \end{aligned}$$

Hence the projected Newton direction is accepted in step (S.2), and the next iterate is given by $x^{k+1} = x^k + p_{PN}^k$. Together with (39), (40), and (41), this implies

$$\begin{aligned} \|x^{k+1} - x^*\| &= \|x^k + p_{PN}^k - x^*\| \\ &\leq \sigma_k \|x^k + p_N^k - x^*\| + (1 - \sigma_k) \|x^k - x^*\| \\ &\leq \|x^k + p_N^k - x^*\| + \frac{1}{4} \|x^k - x^*\| \\ &\leq \frac{1}{2} \|x^k - x^*\|. \end{aligned}$$

Therefore, we also have $x^{k+1} \in B_\varepsilon(x^*)$. Using an induction argument, it follows that the test $\|F(x^k + p_{PN}^k)\| \leq \eta \|F(x^k)\|$ is satisfied for all sufficiently large $k \in \mathbb{N}$, so that we have $x^{k+1} = x^k + p_{PN}^k$ and

$$\|x^{k+1} - x^*\| \leq \frac{1}{2} \|x^k - x^*\| \quad (43)$$

for all $k \in \mathbb{N}$ large enough. In particular, the sequence $\{x^k\}$ is well-defined and converges (at least) linearly to x^* .

To prove superlinear convergence, we consider the inequality

$$\|x^{k+1} - x^*\| \leq \sigma_k \|x^k + p_N^k - x^*\| + (1 - \sigma_k) \|x^k - x^*\| \quad (44)$$

again, cf. (41). For sufficiently large $k \in \mathbb{N}$, it follows from (42) and (35) that

$$1 - \sigma_k \leq c \|F(x^k)\| = c \|F(x^k) - F(x^*)\| = O(\|x^k - x^*\|).$$

Using [41, Proposition 1] and the semismoothness of F , we get

$$\|x^k + p_N^k - x^*\| \leq \|H_k^{-1}\| \|F(x^k) - F(x^*) - H_k(x^k - x^*)\| = o(\|x^k - x^*\|).$$

Since $\sigma_k \rightarrow 1$, we therefore obtain from (44) that $\|x^{k+1} - x^*\| = o(\|x^k - x^*\|)$. Hence the local rate of convergence is superlinear.

If F is strongly semismooth, it follows from [22, Theorem 7.4.3] that

$$\|x^k + p_N^k - x^*\| \leq \|H_k^{-1}\| \|F(x^k) - F(x^*) - H_k(x^k - x^*)\| = O(\|x^k - x^*\|^2).$$

Since $1 - \sigma_k = O(\|x^k - x^*\|)$, we therefore get $\|x^{k+1} - x^*\| = O(\|x^k - x^*\|^2)$ from (44). Hence the rate of convergence is locally quadratic in the strongly semismooth case. \square

The assumptions for local quadratic convergence in Theorem 4.1 are satisfied, e.g., if F is continuously differentiable with F' being locally Lipschitz continuous and $F'(x^*)$ being nonsingular. However, in some applications the assumptions of Theorem 4.1 also hold for nonsmooth F , especially in the context of complementarity problems and variational inequalities, see, for example, [15, 22].

5 Numerical Experiments

In this section, we apply Algorithm 2.1 to several test problems of different types. Some of these problems are originally not given in the form of a nonlinear system of equations with box constraints, but can be reformulated in this way. We implemented Algorithm 2.1 in MATLAB using the scaling matrix from (6) and the following constants:

$$\sigma = 0.995, \theta = 0.95, \eta = 0.9, \gamma = 1, \omega_1 = 0.25, \omega_2 = 2, \rho_1 = 0.1, \rho_2 = 0.75, \Delta_0 = 1.$$

We terminate the iteration

$$\|D_k^{1/2} \nabla f(x^k)\| \leq 10^{-6} \text{ or } \|F(x^k)\|_\infty \leq 10^{-6} \text{ or } k \geq k_{\max} := 500 \text{ or } \Delta_k \leq \Delta_{\min} := 10^{-8}.$$

The last two criteria are used as a safeguard. The search direction p^k satisfying (10) in step (S.3) is computed in the following way: We first check whether a truncated or a projected and truncated Newton direction satisfies (10). If this is not the case, we use a dogleg strategy from the Cauchy point to the Newton direction such that strict feasibility of the iterates is guaranteed.

We next give a summary of the test problems that are used in our numerical experiments:

1. **The Chandrasekhar H-equation.** A discretization of Chandrasekhar's H-equation leads to a nonlinear system of equations that depends on a parameter $c \in [0, 1]$, see [31, p. 87] for more details. Since this system has two solutions and only one has a

physical meaning, we use the bounds $l_i := 0$ and $u_i := \infty$ for all $i = 1, \dots, n$. We choose $x^0 \in \mathbb{R}^n$ with $x_i^0 := 1$ for all i and consider the cases $c = 0.99$, $c = 0.9999$, and $c = 1$ with $n = 1000$.

2. **The seven-diagonal problem.** This is a nonlinear system of equations of variable dimension that can be found in [37]. The Jacobians have the structure of band matrices, which allows us to consider high dimensional cases. The system has several solutions, so we use the bounds $l_i := 0$ and $u_i := \infty$, $i = 1, \dots, n$, to avoid negative ones. We choose $n = 100000$ and $x_i^0 := 1$ for all $i = 1, \dots, n$.
3. **A countercurrent reactor problem.** This problem can be found in [37] as well. Again the problem has variable dimension, several solutions, and the Jacobians are band matrices. We consider $n = 10000$, $n = 100000$ and set $l_i := -1$, $u_i := \infty$ and $x_i^0 := 1$ for $i = 1, \dots, n$.
4. **A chemical equilibrium problem.** In [38, system 1], a nonlinear system of 11 equations and variables is described. A solution of this system is only physically meaningful if all components of the solution are real and positive. Following [4] we augment the system given in [38] to the size of $n = 11000$ and use $l_i := 0$, $u_i := \infty$ and $x_i^0 := 1$ for $i = 1, \dots, n$.
5. **Boundary value problems.** Discretizing a boundary value problem leads to a nonlinear system of equations. If this problem has several solutions, the use of bound constraints is quite helpful to avoid, for example, negative solutions. We use three different boundary value problems for our numerical test runs, called BVP1, BVP2, and BVP3 in the following. BVP1 is a two-point boundary value problem from [32, Example 2.7.4] which has at least two solutions. We use the discretization given in [32] ($n = 800$) to approximate the function and the first derivative. In order to get positive function values, we set $l_i := 0$ for all odd i , $l_i := -\infty$ for all even i and $u_i = \infty$ for $i = 1, \dots, n$. BVP2 is taken from [39]. The discretization given in [39] leads to a nonlinear system that has a unique solution in the box defined by $l_i = -0.5$ and $u_i = 0$ for $i = 1, \dots, n$. We set $n = 500$, use the given bounds and start with $x_i^0 := -0.25$ for all $i = 1, \dots, n$. Finally, BVP3 is taken from [46, p. 504]. The problem has two solutions, but only one is positive. We use the same discretization as for BVP2 and approximate the positive solution by setting $l_i := 0$, $u_i := \infty$. The dimension of this problem is $n = 500$, and we take $x_i^0 := 1$ for all $i = 1, \dots, n$.
6. **The Floudas et al. collection.** In [25, Section 14.1], Floudas et al. present a collection of box constrained nonlinear systems of equations. This collection contains nine examples. The dimension of these examples is small, nevertheless, some of these problems are challenging. All examples have finite lower and upper bounds. We choose $x^0 := l + 0.25(u - l)$ as initial iterate for all test problems.

7. **Complementarity problems.** Here one tries to find a solution of the system

$$x \geq 0, G(x) \geq 0, x^T G(x) = 0,$$

where $G : \mathbb{R}_+^n \rightarrow \mathbb{R}^n$ is a given function that is sometimes not defined outside the nonnegative orthant. This complementarity problem can be reformulated as a square system of equations with box constraints in the following way:

$$x \geq 0, y \geq 0, G(x) - y = 0, x_i y_i = 0 \quad \forall i = 1, \dots, n.$$

Similar reformulations are possible for the slightly more general class of mixed complementarity problems, and a large number of (often very difficult) test problems of this class is given in the MCPLIB collection, see [19]. Since the standard starting points for these examples are sometimes on the boundary of the feasible region, we use the strategy from [47] and project the standard starting vector x^0 of the MCPLIB on the smaller box $[\hat{l}, \hat{u}]$ with $\hat{l}_i = l_i + 0.01$ and $\hat{u}_i = u_i - 0.01$ for $i = 1, \dots, n$, whereas we use $y_i^0 := 1$ for the slack variables.

In the following tables, we present our numerical results. For each test problem, the size of the problem (n), the number of iterations (iter), the evaluations of the function F (eval), the norm of this function in the last iterate ($\|F(x)\|$), and the norm of the stopping criterion in the last iterate ($\|D^{1/2}(x)g(x)\|$) are given. Moreover, the number of iterations needed by the STRSCNE code described in [3] is presented. If a method fails to solve a problem, this is denoted by ”-”. Table 1 contains the results obtained for all examples not taken from the MCPLIB collection.

problem	n	iter	eval	$\ F(x)\ $	$\ D^{1/2}(x)g(x)\ $	strscne
H-equation, $c = 0.99$	1000	8	15	9.253655e-07	1.618650e-05	9
H-equation, $c = 0.9999$	1000	11	21	4.805774e-08	9.663247e-07	11
H-equation, $c = 1$	1000	14	29	3.564824e-07	7.302551e-06	16
7-diagonal	100000	6	7	1.079756e-07	1.265867e-06	6
reactor	10000	20	37	1.351386e-09	4.016356e-09	17
reactor	100000	33	63	1.328888e-08	4.195698e-08	24
chemical-eq.	11000	14	26	1.024321e-08	1.840348e-08	27
BVP1	800	7	12	4.219342e-10	6.250179e-10	6
BVP2	500	2	3	6.250000e-06	2.210701e-08	4
BVP3	500	3	4	3.750000e-07	7.526758e-07	6
Floudas no. 1	2	5	7	9.663381e-13	1.249890e-10	5
Floudas no. 2	5	12	13	2.790805e-10	1.348797e-09	12
Floudas no. 3	2	46	86	4.794279e-07	6.008817e-03	20
Floudas no. 4	2	4	6	1.040490e-07	1.158006e-07	5
Floudas no. 5	5	9	12	2.387465e-09	5.338527e-09	9
Floudas no. 6	8	6	9	1.466922e-07	1.214811e-07	9

Floudas no. 7	9	–	–	–	–	–
Floudas no. 8	2	7	12	1.151719e-07	9.103543e-08	5
Floudas no. 9	1	3	4	1.163838e-05	4.852898e-07	4

Table 1: Results for problem classes 1–8

Both our method and the related algorithm from [3] are able to solve all test examples with the exception of one example from the Floudas et al. collection. However, this problem is regarded as very challenging, even the solution given in [25] seems to be wrong. The behaviour of the two methods on the other examples is more or less similar, and there is no clear winner on this set of test problems.

We next present our numerical results for all test examples of dimension $n \geq 1000$ from the MCPLIB. The corresponding numerical results are contained in Table 2. The columns have the same meaning as in Table 1, in particular, we also compare our results with those obtained by using the STRSCNE code from [3].

problem	n	iter	eval	$\ \Phi(x)\ $	$\ D^{1/2}(x)g(x)\ $	strscne
bert_oc	5000	12	21	8.800055e-07	8.056348e-09	17
bishop	1645	–	–	–	–	–
bratu	5625	17	35	9.147845e-06	5.653325e-07	21
obstacle	2500	22	45	7.392367e-06	6.180783e-07	20
opt_cont31	1024	19	35	6.710511e-07	6.422693e-07	–
opt_cont127	4096	14	25	1.265241e-10	7.121115e-10	–
opt_cont255	8192	83	162	2.967351e-09	6.492866e-09	–
opt_cont511	16384	84	165	5.339209e-07	3.712466e-06	–
trafelas	2904	68	136	9.407251e-07	7.632607e-06	79

Table 2: Results for large-scale mixed complementarity problems

Algorithm 2.1 is able to solve all example with the exception of the **bishop** problem. In this case, our method compares very favourably with the STRSCNE code from [3] which produces five error messages and is able to solve only four test examples.

We stress, however, that the reformulation of the complementarity problems used for our test runs is not necessarily the best formulation. For example, if a solution x^* of the complementarity problem is degenerate, i.e., if there is at least one index such that both $x_i^* = 0$ and $G_i(x^*) = 0$, then it is easy to see that the Jacobian F' of our reformulated system is singular at the solution, hence we cannot expect quadratic convergence.

We illustrate this point using the Kojima-Shindo example. This is a complementarity problem with four variables which has two solutions, one is nondegenerate and one is degenerate. Using the standard starting point, our method converges to the degenerate solution. The iteration history is given in Table 3.

k	$\ F(x^k)\ $	$\ D_k^{1/2}g(x^k)\ $	eval	Δ_k	direction
0	2.475100e+00	1.952834e+01	2	2	proj. Newton
1	5.716714e-02	7.597381e-01	3	4	proj. Newton
2	1.918792e-02	2.054685e-01	4	8	proj. Newton
3	1.849870e-04	1.230285e-03	5	16	proj. Newton
4	8.646631e-05	8.838446e-04	6	32	proj. Newton
5	1.025541e-07	1.001342e-06	7	64	proj. Newton
6	7.995851e-09	8.182092e-08	8	128	proj. Newton

Table 3: Iteration history for the smooth reformulation of the Kojima-Shindo problem

Clearly, Table 3 shows that we do not have quadratic convergence, although the rate of convergence is still relatively fast. If we would require higher accuracy, however, we would run into singularity problems. In fact, if we iterate a bit further, we see that we get very slow convergence using Cauchy points all the time from iteration 8 on.

There exist other reformulations of the complementarity problem as a semismooth system of equations such that the corresponding merit function is continuously differentiable and such that quadratic convergence can still be expected even in the case of degenerate solutions. We refer to [15, 8] for the corresponding background. In particular, using the semismooth reformulation from [8] and applying our code to this reformulation using the Kojima-Shindo example once again, we get the iteration history from Table 4.

k	$\ \Phi(x^k)\ $	$\ D_k^{1/2}g(x^k)\ $	eval	Δ_k	direction
0	1.789473e-01	1.296482e+00	2	2	proj. Newton
1	3.737455e-02	1.221021e+00	3	4	proj. Newton
2	1.581268e-04	1.211466e-03	4	8	proj. Newton
3	1.506474e-08	1.147681e-07	6	2	trunc. Newton

Table 4: Iteration history for the semismooth reformulation of the Kojima-Shindo problem

Obviously, the method is quadratically convergent in this case. Note that we cannot apply the STRSCNE code from [3] to this semismooth reformulation since this method requires smooth functions F .

6 Final Remarks

We have introduced an interior-point trust region method for box constrained nonlinear systems of equations. The method follows the so called affine-scaling approach and generates strictly feasible iterates. It differs from other methods of this type in the choice

of the scaling matrix and the transition from the global to the local method. Moreover, the method can be applied to both continuously differentiable and semismooth systems of equations. Hence the method is applicable to a wider class of problems than, for example, the related algorithms from [2, 3, 4, 5], and this was illustrated for the class of complementarity problems. Compared to the method from the previous references, we also avoid a nonsingularity assumption that was used in these references in order to get a well-defined method.

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