ON AFFINE-SCALING INTERIOR-POINT NEWTON METHODS FOR NONLINEAR MINIMIZATION WITH BOUND CONSTRAINTS

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September 14, 2004 (revised June 29, 2005)

Abstract. A class of new affine-scaling interior-point Newton-type methods are considered for the solution of optimization problems with bound constraints. The methods are shown to be locally quadratically convergent under the strong second order sufficiency condition without assuming strict complementarity of the solution. The new methods differ from previous ones by Coleman and Li [*Mathematical Programming*, 67 (1994), pp. 189–224] and Heinkenschloss, Ulbrich, and Ulbrich [*Mathematical Programming*, 86 (1999), pp. 615–635] mainly in the choice of the scaling matrix. The scaling matrices used here have stronger smoothness properties and allow the application of standard results from nonsmooth analysis in order to obtain a relatively short and elegant local convergence result. An important tool for the definition of the new scaling matrices is the correct identification of the degenerate indices. Some illustrative numerical results with a comparison of the different scaling techniques are also included.

Key Words. Newton's method, affine scaling, interior-point method, quadratic convergence, identification of active constraints.

1 Introduction

We consider the nonlinear minimization problem with bound constraints

$$\text{minimize } f(x) \quad \text{subject to} \quad x \in \mathcal{B} := \{x \in \mathbb{R}^n : l_i \leq x_i \leq u_i \quad \forall i = 1, \ldots, n\}, \tag{P}$$

where l_i and u_i denote the lower and upper bounds, respectively, and $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ is the objective function. Throughout this text, we assume that $l_i < u_i$ for all $i = 1, \ldots, n$ and that f is twice continuously differentiable with a locally Lipschitz continuous Hessian in an open neighbourhood of the feasible set $\mathcal{B}$. Moreover, we assume that all bounds l_i and u_i are finite, but this is mainly a notational assumption since it simplifies many formulas in our analysis like the definitions of the scaling matrices that will be introduced later. However, it is not difficult to see that all results remain true with a suitable redefinition of these scaling matrices if either l_i or u_i or both are infinite for some indices $i \in \{1, \ldots, n\}$.

The optimization problem (P) has attracted quite a few researchers during the last 15 years, and a number of different methods for its solution may be found in [4, 5, 9, 10, 15, 16, 20, 23, 24, 25, 31]. The approach we follow in this work is typically called the affine-scaling interior-point Newton method. Following an observation by Coleman and Li [7, 8], these methods exploit the fact that the first order optimality conditions of (P) may be rewritten as a (bound constrained) nonlinear system of equations

$$G(x) = 0, \quad x \in \mathcal{B}, \tag{1}$$

where $G : \mathbb{R}^n \to \mathbb{R}^n$ is defined by

$$G(x) := D(x)\nabla f(x)$$

for a certain scaling matrix $D(x)$, i.e.,

$$D(x) = \operatorname{diag}\big(d_1(x), \ldots, d_n(x)\big)$$

is a diagonal matrix with suitable components $d_i(x)$, see Section 2 for further details. Following [21], we call

$$d_i(x) := d_i^{CL}(x) := \begin{cases} x_i - l_i & \text{if } [\nabla f(x)]_i > 0, \\ u_i - x_i & \text{if } [\nabla f(x)]_i < 0, \\ \min\{x_i - l_i, u_i - x_i\} & \text{if } [\nabla f(x)]_i = 0 \end{cases} \tag{2}$$

the Coleman-Li scaling (the actual scaling used in [7, 8] is slightly different when $[\nabla f(x)]_i = 0$). The corresponding method was shown to be locally quadratically convergent in [7, 8] under certain assumptions including *strict complementarity* of the solution x^* of problem (P), i.e., under the assumption that, for all indices $i \in \{1, \ldots, n\}$, we have

$$x_i^* \in \{l_i, u_i\} \Longrightarrow [\nabla f(x^*)]_i \neq 0.$$

In order to avoid this strict complementarity condition, Heinkenschloss et al. [21] use a different scaling matrix defined by

$$d_i(x) := d_i^{HUU}(x) := \begin{cases} d_i^{CL}(x) & \text{if } |[\nabla f(x)]_i| < \min\left\{x_i - l_i, u_i - x_i\right\}^p \\ & \text{or } \min\left\{x_i - l_i, u_i - x_i\right\} < |[\nabla f(x)]_i|^p, \\ 1 & \text{otherwise} \end{cases} \tag{3}$$

for some constant $p > 1$. Extensions of these methods (sometimes to infinite-dimensional problems arising from optimal control) may be found in [11, 29, 30], for example. In particular, [29, 30] consider other scaling matrices suitable for infinite-dimensional problems. The class of affine-scaling interior-point Newton methods has recently also been applied quite successfully to the solution of nonlinear systems of equations with box constraints, see [1, 2, 3].

Here we introduce a new class of affine-scaling methods for the solution of the box constrained optimization problem (P). This new class differs from the previous works mainly by using a different scaling $D(x)$. To this end, we note that both the Coleman-Li matrix $D(x) = D^{CL}(x)$ and the Heinkenschloss et al. scaling $D(x) = D^{HUU}(x)$ are, in general, discontinuous even at a solution x^*. This makes it relatively difficult to predict the behaviour of Newton's method. Hence we suggest another scaling matrix which is continuous (in fact, Lipschitz continuous) around a solution of problem (P). It turns out that the use of locally Lipschitz continuous scaling matrices simplifies the algorithm to some extend and, in particular, allows a relatively short and straightforward convergence proof; in particular, it is not necessary to introduce a second scaling as in Heinkenschloss et al. [21] in order to get uniformly bounded (generalized) Jacobians. Of central importance for our new scaling matrix, however, is the fact that we are able to identify the degenerate indices correctly, where an index i is called *degenerate* at a solution x^* of problem (P) if both $x_i^* \in \{l_i, u_i\}$ and $[\nabla f(x^*)]_i = 0$.

The paper is organized as follows: In Section 2 we start with a negative result showing that for a whole class of scaling matrices $D(x)$, the (generalized) Jacobian of G is singular at a solution x^* of (P) whenever strict complementarity is not satisfied at x^*. This result will later be used in order to motivate the definition of our new scaling matrix. In particular, it turns out that we need to identify the degenerate indices correctly. A suitable technique for doing this is therefore presented in Section 3. Exploiting this technique, we then define our scaling matrices in Section 4, state some of its properties and give a formal description of the affine-scaling interior-point Newton method for the solution of the bound constrained optimization problem (P). The local quadratic convergence of this method under the strong second order sufficiency condition is shown in Section 5. Note that strict complementarity is not assumed in our convergence theory. Some numerical results and a short comparison with the Coleman-Li and Heinkenschloss et al. scaling matrices are given in Section 6. We then close with some final remarks in Section 7.

Notation: For a vector $x \in \mathbb{R}^n$, we denote by x_i and, sometimes, by $[x]_i$ its ith component. If $F : \mathbb{R}^n \to \mathbb{R}^m$ is a vector-valued mapping, F_i is used for its ith component function. In the differentiable case, $F'(x)$ denotes the Jacobian of F at a point $x \in \mathbb{R}^n$, whereas $\nabla F(x)$ is the transposed Jacobian. In particular, if $m = 1$, the gradient $\nabla F(x)$ is

viewed as a column vector. Throughout this text, $\|\cdot\|$ denotes the Euclidean vector norm or the corresponding matrix norm. Furthermore, $P_{\mathcal{B}}(x)$ is the (Euclidean) projection of a vector $x \in \mathbb{R}^n$ onto the feasible set $\mathcal{B}$. Note that this projection can be calculated quite easily since we are dealing with box constraints only. Finally, given a matrix $A \in \mathbb{R}^{n\times n}$, we write A_i for the ith column of this matrix.

2 Singularity Problems of Affine-Scaling Methods

A careful convergence analysis in Heinkenschloss et al. [21] shows that the affine-scaling interior-point Newton method using the Coleman-Li scaling matrices from (2) is, in general, not quadratically convergent if strict complementarity does not hold at a local minimum x^*. The aim of this section is to give another reason for the failure of a whole class of affine-scaling methods in the absense of strict complementarity. In subsequent sections, this result will be used in order to motivate our new choice of the scaling matrix $D(x)$.

We first recall a simple optimality condition for the optimization problem (P).

Theorem 2.1 *Let x^* be a local minimum of the optimization problem* (P). *Then*

$$[\nabla f(x^*)]_i \begin{cases} = 0 & \text{if } \ l_i < x_i^* < u_i, \\ \geq 0 & \text{if } \ x_i^* = l_i, \\ \leq 0 & \text{if } \ x_i^* = u_i. \end{cases} \tag{4}$$

As noted in the introduction, the first order necessary optimality condition (4) is equivalent to the nonlinear system of equations (1) using the Coleman-Li scaling matrix. This equivalence can be extended to more general scaling matrices. More precisely, we have the following result, cf. Heinkenschloss et al. [21].

Lemma 2.2 *Let $x^* \in \mathcal{B}$. Then x^* satisfies the first order optimality conditions* (4) *if and only if it is a solution of the nonlinear system of equations*

$$G(x) := D(x)\nabla f(x) = 0, \tag{5}$$

where $D(x) := \mathrm{diag}\big(d_1(x), \ldots, d_n(x)\big)$ is any scaling matrix having the following properties on the feasible set $\mathcal{B}$:

$$d_i(x) \begin{cases} = 0 & \text{if } x_i = l_i \text{ and } [\nabla f(x)]_i > 0, \\ = 0 & \text{if } x_i = u_i \text{ and } [\nabla f(x)]_i < 0, \\ \geq 0 & \text{if } x_i \in \{l_i, u_i\} \text{ and } [\nabla f(x)]_i = 0, \\ > 0 & \text{else.} \end{cases} \tag{6}$$

Motivated by Lemma 2.2, some methods for solving the bound constrained optimization problem (P) apply a Newton-type method to the corresponding nonlinear system (5) (taking into account explicitly the simple bound constraints $x \in \mathcal{B}$). Unfortunately, it turns out that the (generalized) Jacobian of the mapping G is singular under fairly mild assumptions

if strict complementarity does not hold. This is the main result we want to show in this section.

To this end, we assume that $D(x)$ is at least locally Lipschitz continuous around a local minimum x^* of problem (P). Then the mapping G is also locally Lipschitz. Hence we can compute its generalized Jacobian in the sense of Clarke [6]. For simplicity, we restate the definition of this generalized Jacobian.

Definition 2.3 Let $F : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ be locally Lipschitz continuous in $x^* \in \mathbb{R}^n$ and $D_F := \{x \in \mathbb{R}^n | F \text{ differentiable in } x\}$ the set of differentiable points of F. Then the set

$$\partial_B F(x^*) := \left\{V \in \mathbb{R}^{m\times n} | \exists\, \{x_k\} \subseteq D_F \text{ with } x_k \to x^* \text{ and } F'(x_k) \to V\right\}$$

is called the *B-subdifferential* of F in x^*, and its convex hull

$$\partial F(x^*) := \text{conv}\partial_B F(x^*)$$

is the *generalized Jacobian* of F in x^*. If $m = 1$, the set $\partial F(x^*)$ is called the *generalized gradient* of F in x^*.

By calculating the generalized Jacobian of the mapping G, we obtain the following negative result, where, in addition to our previous assumptions, we also assume that the scaling matrix $D(x) = \text{diag}\left(d_1(x), \ldots, d_n(x)\right)$ has the property that

$$d_i(x) = 0 \quad \text{if } x_i \in \{l_i, u_i\}. \tag{7}$$

This is a rather natural condition since the components $d_i(x)$ usually represent an estimate for the distance of the component x_i to the boundary of the feasible set $\mathcal{B}$.

Theorem 2.4 *Let x^* be a local minimum of (P) such that strict complementarity does not hold. Suppose further that $D(x) = \text{diag}\left(d_1(x), \ldots, d_n(x)\right)$ is locally Lipschitz continuous and satisfies* (6) *and* (7)*. Then:*

(a) The ith component function G_i is differentiable with gradient $\nabla G_i(x^*) = 0$ for every index i where strict complementarity is violated.

(b) All elements of the generalized Jacobian $\partial G(x^*)$ are singular.

Proof. Recall that $G(x) := D(x)\nabla f(x)$ is locally Lipschitz continuous. Using the product rule from [6, Proposition 2.3.13] for the ith component $G_i(x) = d_i(x)[\nabla f(x)]_i$, it follows that

$$\partial G_i(x^*) \subseteq [\nabla f(x^*)]_i \partial d_i(x^*) + d_i(x^*)\partial[\nabla f(x^*)]_i.$$

Since strict complementarity does not hold at x^*, there is an index i_0 such that both $x^*_{i_0} \in \{l_{i_0}, u_{i_0}\}$ and $[\nabla f(x^*)]_{i_0} = 0$. For this particular component, we therefore get

$$\partial G_{i_0}(x^*) \subseteq \underbrace{[\nabla f(x^*)]_{i_0}}_{=0} \partial d_{i_0}(x^*) + \underbrace{d_{i_0}(x^*)}_{=0 \text{ by } (7)} \partial[\nabla f(x^*)]_{i_0} = \{0\}.$$

Since the generalized gradient $\partial G_{i_0}(x^*)$ is nonempty (see [6, Proposition 2.6.2]), it follows that $\partial G_{i_0}(x^*) = \{0\}$. But then [6, Proposition 2.2.4] implies that G_{i_0} is differentiable in x^*, and its gradient is given by $\nabla G_{i_0}(x^*) = 0$. However, since we have

$$\partial G(x^*) \subseteq \left\{ (g_1, \ldots, g_n)^T \,\middle|\, g_1 \in \partial G_1(x^*), \ldots, g_n \in \partial G_n(x^*) \right\}$$

due to [6, Proposition 2.6.2], it follows that each element $V \in \partial G(x^*)$ has a zero row and is therefore singular. This completes the proof of both statements. □

The previous proof shows that Theorem 2.4 actually holds under much weaker conditions. In fact, the local Lipschitz continuity of the scaling matrix $D(x)$ has been exploited only in the degenerate components. The other components, where strict complementarity is satisfied, are not really important. The only difficulty which arises without assuming local Lipschitz continuity of all components $d_i(x)$ is that we have to use an extended definition for a generalized Jacobian for non-Lipschitzian functions. However, whatever this extended definition might be, if we require that the ith row of such a more general Jacobian is equal to the gradient of the ith component function $G_i(x)$ whenever this function is differentiable at the current point (and this is a very natural condition), then it follows that Theorem 2.4 still holds. Moreover, the proof of Theorem 2.4 clearly shows that the statement also holds if property (7) is only satisfied at the local minimum x^* of problem (P).

We note that both the Coleman-Li scaling $d_i^{CL}(x)$ as well as the Heinkenschloss et al. scaling $d_i^{HUU}(x)$ satisfy (6). Moreover, $d_i^{CL}(x)$ has the property (7) which turned out to be quite negative in the discussion by Heinkenschloss et al. [21]. Here we introduce another scaling matrix $D^{MIN}(x) = \operatorname{diag}\big(d_1^{MIN}(x), \ldots, d_n^{MIN}(x)\big)$ defined by

$$d_i^{MIN}(x) := \min\left\{ x_i - l_i + \gamma \max\{0, -[\nabla f(x)]_i\}, u_i - x_i + \gamma \max\{0, [\nabla f(x)]_i\} \right\} \quad \forall i = 1, \ldots, n \tag{8}$$

for some constant $\gamma > 0$. This scaling matrix will play an important role in this work, and it has the advantage of being locally Lipschitz continuous. Moreover, it is easy to see that it satisfies (6). Furthermore, (7) also holds at a local minimum x^* of problem (P). Therefore, we obtain the following result as a direct consequence of Theorem 2.4 (and the previous notes).

Corollary 2.5 *Let x^* be a local minimum of (P) such that strict complementarity does not hold. Suppose further that $D(x) = D^{MIN}(x)$ denotes the scaling matrix with its components defined by* (8)*. Then all elements of the generalized Jacobian $\partial G^{MIN}(x^*)$ are singular.*

We note that we cannot apply Theorem 2.4 directly to the Coleman-Li scaling since $D^{CL}(x)$ is, in general, discontinuous (and therefore not locally Lipschitz continuous). Nevertheless, a related singularity problem was also observed for this scaling in Heinkenschloss et al. [21, pp. 621–622]. In fact, this observation was the main motivation to introduce another scaling matrix. However, the Heinkenschloss et al. scaling is also discontinuous in general, even around a local minimum x^* (namely in those components where $[\nabla f(x^*)]_i = 0$). Since

the behaviour of Newton's method is usually less predictable for discontinuous functions than for smooth ones, we prefer to work with scaling matrices which are at least locally Lipschitz continuous around a local minimum x^*. Hence the scaling matrix from (8) is a natural candidate, but in view of Corollary 2.5, it has to be modified in order to avoid the strict complemementarity assumption.

3 Identification of Active and Degenerate Indices

The analysis from our previous section shows that it is quite important for fast local convergence to identify the degenerate indices in a local minimum of problem (P). The aim of this section is therefore to describe a simple and computationally efficient technique for the identification of these indices. To this end, we begin with the following definition.

Definition 3.1 Let $x \in \mathcal{B}$ and the index set $I := \{1, \ldots, n\}$ be given. Then we call

$$I_0(x) := \big\{ i \in I | x_i \in \{l_i, u_i\} \big\}$$

the *set of active indices* and

$$I_{00}(x) := \big\{ i \in I_0(x) | [\nabla f(x)]_i = 0 \big\}$$

the *set of degenerate indices*.

In order to identify the index set $I_{00}(x^*)$ exactly in a neighbourhood of a local minimum x^* of (P), we use an idea from Facchinei et al. [14] and specialize or modify their results to our situation. The fundamental definition from [14] is the following one.

Definition 3.2 A function $\rho : \mathbb{R}^n \longrightarrow \mathbb{R}_+$ is called an *identification function* for (P) if, for an isolated $x^* \in \mathcal{B}$ satisfying (4), the following properties hold:

(i) ρ is continuous in x^*,

(ii) $\rho(x^*) = 0$,

(iii) $\lim_{x \to x^*,\, x \neq x^*} \frac{\rho(x)}{\|x - x^*\|} = +\infty$.

Note that, in Definition 3.2, we call a vector x^* satisfying (4) *isolated* if there is a whole neighbourhood around this point such that x^* is the only vector satisfying the first order optimality conditions (4) in this neighbourhood. In our local convergence analysis to be presented in Section 5, this local uniqueness condition is a consequence of another assumption (strong second order sufficiency condition) and, therefore, not as restrictive as it might appear in the beginning.

Later in this section, we will give two examples of suitable identification functions. For the moment, however, we assume that we have such an identification function ρ. Using this identification function ρ, we define an estimate of the active indices $I_0(x)$ by

$$A_0(x) := \big\{ i \in I | x_i - l_i \leq \rho(x) \text{ or } u_i - x_i \leq \rho(x) \big\} = \big\{ i \in I | \min\{x_i - l_i, u_i - x_i\} \leq \rho(x) \big\}. \tag{9}$$

Then we have the following result which shows that $A_0(x)$ is equal to the set $I_0(x^*)$ in a sufficiently small neighbourhood of a solution x^* of (P), i.e., we are able to identify the set of active indices correctly.

Theorem 3.3 *Let ρ be an identification function for problem (P) and $x^* \in \mathcal{B}$ be an isolated vector satisfying (4). Then there exists an $\epsilon > 0$ such that*

$$A_0(x) = I_0(x^*)$$

holds for all $x \in B_\epsilon(x^*)$.

Proof. The proof is similar to [14, Theorem 2.3] and is presented here for the sake of completeness.

First let $i \in I_0(x^*)$. Then we either have $x_i^* = l_i$ or $x_i^* = u_i$. Consider the case $x_i^* = l_i$ and define $g_i(x) := x_i - l_i$ (the argument is similar if $x_i^* = u_i$). Since $g_i(x^*) = 0$ and g_i is Lipschitz continuous with constant $L = 1$, we get

$$g_i(x) \leq g_i(x^*) + \|x - x^*\| = \|x - x^*\|$$

for all $x \in \mathbb{R}^n$. Using the definition of an identification function, we therefore obtain

$$x_i - l_i = g_i(x) \leq \|x - x^*\| \leq \rho(x) \quad \forall x \in B_{\epsilon_1}(x^*)$$

for some $\epsilon_1 > 0$ sufficiently small. Hence we have $i \in A_0(x)$ for all $x \in B_{\epsilon_1}(x^*)$.

Conversely, take an arbitrary index $i \notin I_0(x^*)$. Then we have $l_i < x_i^* < u_i$. Using $\rho(x^*) = 0$ and a continuity argument, it follows that $\rho(x) < \min\{x_i - l_i, u_i - x_i\}$ for all $x \in B_{\epsilon_2}(x^*)$ for some $\epsilon_2 > 0$ sufficiently small (note that the choice of ϵ_2 depends on the index i, but since there are only finitely many $i \in \{1, \ldots, n\}$, we may choose $\epsilon_2 > 0$ independent of i). Hence $i \notin I_0(x^*)$ implies $i \notin A_0(x)$ for all $x \in B_{\epsilon_2}(x^*)$, and this is equivalent to $A_0(x) \subseteq I_0(x^*)$ for all $x \in B_{\epsilon_2}(x^*)$.

Using $\epsilon := \min\{\epsilon_1, \epsilon_2\}$, we therefore obtain the desired result. □

Now we are able to estimate the active constraints exactly, but since we want to identify the degenerate ones, we also use the set

$$A_+(x) := \{ i \in A_0(x) | \lambda_i(x) > \rho(x) \} \tag{10}$$

where $\lambda(x)$ is a *multiplier function*, i.e., $\lambda(x)$ is continuously differentiable (local Lipschitz continuity would be enough for our purpose) and has the property that

$$\lambda(x^*) = \lambda^*$$

for any vector x^* satisfying (4) and the corresponding (unique) Lagrange multiplier λ^* for problem (P). The interested reader is referred to [13, 12] for some suitable examples of multiplier functions. Note that these multiplier functions can be evaluated quite easily in the case of bound constrained optimization problems.

Theorem 3.4 *Let ρ be an identification function for problem (P) and $x^* \in \mathcal{B}$ be an isolated vector satisfying* (4)*. Then there exists an $\epsilon > 0$ such that*

$$A_+(x) = I_0(x^*) \backslash I_{00}(x^*)$$

holds for all $x \in B_\epsilon(x^*)$.

Proof. The technique of proof is taken from [14, Theorem 2.4] and included here for the sake of clarity.

First consider an index $i \in I_0(x^*) \setminus I_{00}(x^*)$. Since $i \in I_0(x^*)$, Theorem 3.3 shows that $i \in A_0(x)$ for all x sufficiently close to x^*. Furthermore, since $i \notin I_{00}(x^*)$ and $I_{00}(x^*)$ may be rewritten as $I_{00}(x^*) = \{i \in I_0(x^*) | \lambda_i^* = 0\}$ in terms of the multipliers λ_i^*, we have $\lambda_i(x^*) = \lambda_i^* > 0$, whereas $\rho(x^*) = 0$ holds. By continuity, this implies $\lambda_i(x) > \rho(x)$ for all $x \in B_{\epsilon_1}(x^*)$ for a suitable constant $\epsilon_1 > 0$, so that $i \in A_+(x)$.

To prove the converse inclusion, suppose that $i \in I_{00}(x^*)$. Then $\lambda_i(x^*) = \lambda_i^* = 0$. Moreover, since the multiplier function is continuously differentiable and, therefore, locally Lipschitz continuous around x^*, there is a constant $c > 0$ such that

$$\lambda_i(x) \leq |\lambda_i(x) - \lambda_i(x^*)| \leq \|\lambda(x) - \lambda(x^*)\| \leq c\|x - x^*\| \leq \rho(x)$$

for all x sufficiently close to x^*. Hence we have $i \notin A_+(x)$ for all these x. Hence $A_+(x) \subseteq I_0(x^*) \setminus I_{00}(x^*)$ for all $x \in B_{\epsilon_2}(x^*)$ and a suitable constant $\epsilon_2 > 0$.

Consequently, the statement holds with $\epsilon := \min\{\epsilon_1, \epsilon_2\}$. □

Using Theorems 3.3 and 3.4, it follows that

$$A_{00}(x) := A_0(x) \backslash A_+(x) \tag{11}$$

is an exact estimation of the set of degenerate indices in the sense that an $\epsilon > 0$ exists such that

$$A_{00}(x) = I_{00}(x^*) \tag{12}$$

holds for all $x \in B_\epsilon(x^*)$, where x^* is any isolated vector satisfying the optimality conditions (4).

Hence we have reached our goal provided that we have an identification function ρ. In the remaining part of this section, we therefore introduce two suitable mappings which turn out to be identification functions under certain assumptions. The main assumption that will be used here is the strong second order sufficiency condition which we restate in the following definition. We note that weaker conditions are possible for the definition of identification functions, however, the strong second order sufficiency condition will also be used in our local convergence analysis of Section 5, so this condition is needed in any case.

Definition 3.5 A point $x^* \in \mathcal{B}$ with (4) is said to satisfy the *strong second order sufficiency condition* (SSOSC for short) if

$$d^T \nabla^2 f(x^*) d > 0$$

holds for all nonzero $d \in T(x^*) := \{z \in \mathbb{R}^n | z_i = 0 \ \forall i \in I_0(x^*) \backslash I_{00}(x^*)\}$.

Note that SSOSC is equivalent to saying that the submatrix $\nabla^2 f(x^*)_{\bar{J}\bar{J}}$ is positive definite, where

$$J := I_0(x^*) \setminus I_{00}(x^*) \quad \text{and} \quad \bar{J} := \{1, \ldots, n\} \setminus J. \tag{13}$$

We therefore get the following consequence from the definition of SSOSC.

Lemma 3.6 *Let $x^* \in \mathcal{B}$ be a point satisfying* (4) *and SSOSC. Then the vectors*

$$e_i \ \ (i \in J) \quad \textit{and} \quad [\nabla^2 f(x^*)]_i \ \ (i \in \bar{J})$$

are linearly independent, where the index sets J and $\bar{J}$ are defined in (13)*, and e_i denotes the ith unit vector in $\mathbb{R}^n$.*

Proof. Consider an arbitrary linear combination

$$\sum_{i \in J} \alpha_i e_i + \sum_{i \in \bar{J}} \alpha_i [\nabla^2 f(x^*)]_i = 0. \tag{14}$$

Without loss of generality, we may assume that $J = \{1, \ldots, r\}$ with $r := |J|$. Then we can rewrite (14) as

$$M\alpha = 0 \quad \text{with} \quad M := \begin{pmatrix} I_r & \nabla^2 f(x^*)_{J\bar{J}} \\ 0 & \nabla^2 f(x^*)_{\bar{J}\bar{J}} \end{pmatrix},$$

where $\alpha := (\alpha_1, \ldots, \alpha_n)^T$. In view of our assumption, however, the block matrix $\nabla^2 f(x^*)_{\bar{J}\bar{J}}$ is positive definite and, therefore, nonsingular. This implies that the matrix M is also nonsingular. Consequently, we obtain $\alpha = 0$, thus giving the desired result. □

We now present our first identification function.

Theorem 3.7 *Let $x^* \in \mathcal{B}$ be a point satisfying* (4) *and SSOSC. Define*

$$\rho_1(x) := \sqrt{\|\phi_1(x)\|}$$

with

$$\phi_1(x) := x - P_{\mathcal{B}}\big(x - \nabla f(x)\big).$$

Then ρ_1 is an identification function for problem (P).

Proof. It is obvious or well-known that ρ_1 satisfies the two conditions (i) and (ii) of Definition 3.2. In order to verify requirement (iii), we note that SSOSC and [17, Proposition 6.2.4] imply that there is a constant $\gamma > 0$ such that

$$\|x - x^*\| \leq \gamma \|\phi_1(x)\| \tag{15}$$

holds for all x in a sufficiently small neighbourhood of x^*. More precisely, note that our mapping ϕ_1 is identical to what is called the natural residual in [17], and that SSOSC implies (for box constrained optimization problems) strong regularity in the sense of Robinson (see [28]). However, strong regularity implies semistability (see [17, p. 434]), and therefore [17, Proposition 6.2.4] can be applied.

As a consequence of (15), we get

$$\frac{\rho_1(x)}{\|x - x^*\|} = \frac{\sqrt{\|\phi_1(x)\|}}{\|x - x^*\|} \geq \frac{\sqrt{\|\phi_1(x)\|}}{\gamma \|\phi_1(x)\|} = \frac{1}{\gamma \sqrt{\|\phi_1(x)\|}} \to +\infty$$

for $x \to x^*, x \neq x^*$. Hence ρ_1 is an identification function. □

Our second identification function is given by

$$\rho_2(x) := \sqrt{\|\phi_2(x)\|}, \tag{16}$$

where the components $\phi_i^{(2)}$ of ϕ_2 are defined by

$$\phi_i^{(2)}(x) := 2x_i - l_i - u_i - |x_i - l_i - [\nabla f(x)]_i| + |x_i - u_i - [\nabla f(x)]_i|, \quad i = 1, \ldots, n. \tag{17}$$

It turns out, however, that ρ_2 is not much different from ρ_1. In fact, an elementary calculation shows that $\phi_2 = 2\phi_1$. Hence we immediately obtain the following result from Theorem 3.7.

Theorem 3.8 *Let $x^* \in \mathcal{B}$ be a point satisfying* (4) *and SSOSC. Let ρ_2 be defined as in* (16), (17). *Then ρ_2 is an identification function for problem (P).*

We close this section by noting that both Theorems 3.7 and 3.8 hold under weaker assumptions. In fact, the central result used in order to prove Theorem 3.7 was Proposition 6.2.4 from [17], and this result holds for any isolated vector x^* satisfying (4) and a condition called *semistability* in [17]. We refer the interested reader to [17] for further details on semistability.

4 Affine-Scaling Interior-Point Newton Method

In this section, we present our affine-scaling interior-point Newton method for the solution of the bound constrained optimization problem (P). Basically, it is a Newton-type method applied to the reformulation (5) of the optimality conditions (4) for a suitable scaling

matrix $D(x)$. The condition $x \in \mathcal{B}$ is guaranteed by generating strictly feasible iterates only. This, in turn, is done by incorporating a projection step as described, for example, in [21], although other choices would also be possible, see, e.g., [22].

In order to state our choice of the scaling matrix, we assume that we have an identification function ρ which allows us to define a set $A_{00}(x)$ via (11) which then identifies the set of degenerate indices $I_{00}(x^*)$ in a neighbourhood of a local minimum x^* of problem (P). Examples of suitable functions ρ having this property under the SSOSC assumption were given in Section 3.

Now, having a suitable identification function and a corresponding set $A_{00}(x)$, we define our scaling matrix by

$$D(x) = \operatorname{diag}\big(d_1(x), \ldots, d_n(x)\big) \quad \text{with} \quad d_i(x) := \begin{cases} 1, & \text{if } i \in A_{00}(x), \\ d_i^{MIN}(x) & \text{if } i \notin A_{00}(x), \end{cases} \tag{18}$$

where the components $d_i^{MIN}(x)$ are given in (8). Eventually, this definition differs from the one in (8) only in the degenerate indices. Then it is easy to see that $D(x)$ has the property (6). Moreover, we will see below that it is locally Lipschitzian around a local minimum x^* of (P) under suitable assumptions. However, it does not have the natural property from (7). On the other hand, in view of Corollary 2.5, we know that this property must be violated in order to have a chance to get nonsingular (generalized) Jacobians in the absense of strict complementarity.

We summarize these obervations and some related properties in the following result, where the notion of a strongly semismooth function is used. We do not restate the definition and the properties of (strongly) semismooth functions here, but refer the interested reader to the papers [26, 27] and the corresponding discussion in the recent book [18] for more details.

Lemma 4.1 *Let x^* be an isolated vector satisfying (4) and suppose that $A_{00}(x) = I_{00}(x^*)$ holds in a neighbourhood of x^*. Then the scaling matrix $D(x)$ defined in (18) is locally Lipschitz continuous and strongly semismooth in a neighbourhood of x^*.*

Proof. Note that $D(x)$ is locally Lipschitz and strongly semismooth if and only if each component function $d_i(x)$ is locally Lipschitz and strongly semismooth. Therefore, the local Lipschitz property follows simply from the fact that the set $A_{00}(x)$ does not change locally. Similarly, this also implies the strong semismoothness of each $d_i(x)$ since the min- and max-functions and the composition of strongly semismooth functions are known to be strongly semismooth, see [19]. □

We note that the scaling matrix $D(x)$ is not necessarily Lipschitz continuous if we are far away from a local minimum x^* of (P). In fact, in this case the function might even become discontinuous. However, since we are only interested in the local analysis, Lemma 4.1 states a desirable property of our scaling matrix $D(x)$ around a local minimum x^* of (P). In general, this property holds neither for the Coleman-Li scaling $D^{CL}(x)$ nor for the Heinkenschloss et al. matrix $D^{HUU}(x)$.

Having defined our scaling matrix $D(x)$, we now want to apply a Newton-type method to the corresponding function $G(x) = D(x)\nabla f(x)$. The problem is that this mapping is not differentiable everywhere. As a suitable replacement of the Jacobian, we take

$$M(x) := D(x)\nabla^2 f(x) + S(x) \tag{19}$$

where $S(x) := \operatorname{diag}\big(s_1(x), \ldots, s_n(x)\big)$ is a diagonal matrix with $s_i(x) \approx d_i'(x)[\nabla f(x)]_i$ ($d_i'(x)$ being the partial derivative of the mapping d_i with respect to the component x_i) being given by

$$s_i(x) := \begin{cases} 0, & \text{if } i \in A_{00}(x), \\ \delta_i[\nabla f(x)]_i \text{ for an arbitrary } \delta_i \in \partial d_i(x), & \text{if } i \notin A_{00}(x). \end{cases} \tag{20}$$

Note that the entry $s_i(x)$ of the matrix $S(x)$ corresponds to the exact derivative of the mapping $d_i(x)[\nabla f(x)]_i$ at a continuously differentiable point. In general, we have the following simple but important result.

Theorem 4.2 *Let x^* be an isolated vector satisfying* (4) *and suppose that $A_{00}(x) = I_{00}(x^*)$ holds in a neighbourhood of x^*. Then the function $G(x) := D(x)\nabla f(x)$ with $D(x)$ being defined by* (18) *is strongly semismooth in a neighbourhood of x^*. Moreover, every element $M(x) \in \partial_B G(x)$ has a representation of the form* (19) *with $S(x)$ being the matrix from* (20).

Proof. Since the product of two strongly semismooth functions in again strongly semismooth, the first statement follows from Lemma 4.1 together with our general smoothness assumption on the mapping f. The remaining statements follow directly from the definition of the B-subdifferential, see Definition 2.3 (note, however, that, usually, (19), (20) contain more elements than those belonging to $\partial_B G(x)$). □

We are now in the position to state our Newton-type method for the solution of the bound constrained optimization problem (P).

Algorithm 4.3 (Projected Affine-Scaling Interior-Point Newton Method)

(S.0) Choose $x^0 \in \operatorname{int}(\mathcal{B}), \sigma \in (0,1)$, and set $k := 0$.

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

(S.2) Compute $M(x^k) := D(x^k)\nabla^2 f(x^k) + S(x^k)$ with $D(x^k)$ and $S(x^k)$ being given by (18) and (20), respectively.

(S.3) Let $d^k \in \mathbb{R}^n$ be a solution of the linear system $M(x^k)d = -G(x^k)$.

(S.4) Compute $\sigma_k := \max\big\{\sigma, 1 - \|P_{\mathcal{B}}(x^k + d^k) - x^k\|\big\}$.

(S.5) Set $x^{k+1} := x^k + \sigma_k\big(P_{\mathcal{B}}(x^k + d^k) - x^k\big)$.

(S.6) Set $k \leftarrow k+1$, and go to (S.1).

Note that steps (S.4) and (S.5) obviously guarantee the strict feasibility of all iterates x^k.

There are two differences between Algorithm 4.3 and the corresponding method from Heinkenschloss et al. [21]: First, we use a different way to compute the entries $d_i(x)$ and $s_i(x)$ by using the identification results from Section 3. Second, we do not use a further scaling of the matrices $M(x)$ as done in [21]. This further scaling was important in [21] in order to carry out a local convergence analysis.

In particular, the exact identification result incorporated in our method turns out to be quite helpful also in order to simplify the local convergence analysis. This will be done in the following section.

5 Local Convergence Analysis

The aim of this section is to show that Algorithm 4.3 is locally quadratically convergent under the SSOSC assumption; in particular, we do not need the strict complementarity condition. Hence the local convergence result is identical to the one shown in Heinkenschloss et al. [21] for their algorithm. However, our method of proof is completely different. Rather than using relatively lengthy and technical calculations, we heavily apply standard results from nonsmooth analysis and, in this way, obtain a relatively simple proof for local quadratic convergence.

Throughout this section, we assume implicitly that we have chosen an identification function such that the corresponding index set $A_{00}(x)$ has the exact identification property (12) under the SSOSC assumption. Suitable candidates for such an identification function were given in Section 3.

We begin with the following result.

Theorem 5.1 *Let $x^* \in \mathcal{B}$ be a vector satisfying (4) and SSOSC. Then the mapping G is differentiable at x^* with $G'(x^*) = M(x^*)$ being nonsingular. Moreover, there is a neighbourhood of x^* and a constant $c > 0$ such that $M(x)$ is nonsingular with*

$$\|M(x)^{-1}\| \leq c$$

for all x in this neighbourhood.

Proof. Taking into account the definition of $M(x^*)$ in (19), (20), it follows after some elementary calculations that the ith column vector A_i of $A := M(x^*)^T$ is given by

$$A_i = \begin{cases} [\nabla f(x^*)]_i e_i, & \text{if } x_i^* = l_i \text{ and } [\nabla f(x^*)]_i > 0, \\ -[\nabla f(x^*)]_i e_i, & \text{if } x_i^* = u_i \text{ and } [\nabla f(x^*)]_i < 0, \\ [\nabla^2 f(x^*)]_i, & \text{if } i \in I_{00}(x^*), \\ d_i(x^*)[\nabla^2 f(x^*)]_i, & \text{if } i \notin I_0(x^*). \end{cases}$$

In particular, each column A_i is single-valued. Consequently, G is differentiable in x^* with $\partial_B G(x^*) = \{M(x^*)\}$, cf. [6, Proposition 2.2.4].

Now consider the equation $A\alpha = 0$ for some $\alpha \in \mathbb{R}^n$. In view of the above representation of the columns of A, this may be rewritten as

$$\begin{aligned} 0 \;=\; & \sum_{i:x_i^*=l_i,[\nabla f(x^*)]_i>0} \alpha_i [\nabla f(x^*)]_i e_i - \sum_{i:x_i^*=u_i,[\nabla f(x^*)]_i<0} \alpha_i [\nabla f(x^*)]_i e_i + \ldots \\ & \ldots \sum_{i\in I_{00}(x^*)} \alpha_i [\nabla^2 f(x^*)]_i + \sum_{i\notin I_0(x^*)} \alpha_i d_i(x^*) [\nabla^2 f(x^*)]_i. \end{aligned}$$

Furthermore, using SSOSC and Lemma 3.6, we obtain

$$\begin{aligned} \alpha_i [\nabla f(x^*)]_i &= 0 \quad \forall i : x_i^* = l_i, [\nabla f(x^*)]_i > 0, \\ -\alpha_i [\nabla f(x^*)]_i &= 0 \quad \forall i : x_i^* = u_i, [\nabla f(x^*)]_i < 0, \\ \alpha_i &= 0 \quad \forall i \in I_{00}(x^*), \\ \alpha_i d_i(x^*) &= 0 \quad \forall i \notin I_0(x^*). \end{aligned}$$

Since $d_i(x^*) > 0$ for all $i \notin I_0(x^*)$, we get $\alpha = 0$. Consequently, the matrix A and, therefore, $M(x^*)$ itself is nonsingular.

Using this nonsingularity as well as $\partial_B G(x^*) = \{M(x^*)\}$ and Theorem 4.2, it follows from [26, Lemma 2.6] that there is a constant $c > 0$ and a neighbourhood of x^* such that $M(x)$ is nonsingular with $\|M(x)^{-1}\| \leq c$ for all x in this neighbourhood. □

We are now in the position to prove our main local convergence result.

Theorem 5.2 *Let $x^* \in \mathcal{B}$ be a vector satisfying* (4) *and SSOSC. Then there is a neighbourhood of x^* such that, for any starting point $x^0 \in int(\mathcal{B})$ from this neighbourhood, Algorithm 4.3 is well-defined and generates a sequence $\{x^k\}$ which converges to x^* with a quadratic rate of convergence.*

Proof. The proof is more or less standard, and we state it here only for the sake of completeness.

In view of Theorem 5.1, there are constants $\varepsilon_1 > 0$ and $c > 0$ such that

$$\|M(x)^{-1}\| \leq c \quad \forall x \in B_{\varepsilon_1}(x^*). \tag{21}$$

Furthermore, Theorem 4.2 and standard properties of (strongly) semismooth functions (see, for example, [18, Theorem 7.4.3]) imply that there is a constant $\varepsilon_2 > 0$ such that

$$\|G(x) - G(x^*) - M(x)(x - x^*)\| \leq \frac{1}{4c}\|x - x^*\| \quad \forall x \in B_{\varepsilon_2}(x^*). \tag{22}$$

Using the definition of σ_k in (S.4) of Algorithm 4.3, we also see that there is an $\varepsilon_3 > 0$ such that

$$\sigma_k \geq \frac{3}{4} \quad \forall x^k \in B_{\varepsilon_3}(x^*) \tag{23}$$

(to this end, note that $\|P_{\mathcal{B}}(x^k + d^k) - x^k\| = \|P_{\mathcal{B}}(x^k + d^k) - P_{\mathcal{B}}(x^k)\| \leq \|d^k\|$ is very small in a neighbourhood of the solution x^* since then $G(x^k)$ is small and, therefore, the same holds for d^k in view of the nonsingularity of $M(x^k)$). Now choose $x^0 \in \operatorname{int}(\mathcal{B}) \cap B_\varepsilon(x^*)$ with $\varepsilon := \min\{\varepsilon_1, \varepsilon_2, \varepsilon_3\}$. Then $M(x^0)$ is nonsingular, d^0 from (S.3) of Algorithm 4.3 exists, and we obtain

$$\begin{aligned} \|x^0 + d^0 - x^*\| &\leq \|x^0 - x^* - M(x^0)^{-1}G(x^0)\| \\ &\leq \|M(x^0)^{-1}\| \, \|G(x^0) - G(x^*) - M(x^0)(x^0 - x^*)\| \\ &\leq \frac{1}{4}\|x^0 - x^*\| \end{aligned}$$

from (21) and (22). The definition of x^1 in Algorithm 4.3 together with (23) and the nonexpansiveness of the projection operator then implies

$$\begin{aligned} \|x^1 - x^*\| &= \big\|x^0 + \sigma_0\big(P_{\mathcal{B}}(x^0 + d^0) - x^0\big) - x^*\big\| \\ &= \big\|\sigma_0\big(P_{\mathcal{B}}(x^0 + d^0) - x^*\big) + (1 - \sigma_0)(x^0 - x^*)\big\| \\ &\leq \sigma_0\big\|P_{\mathcal{B}}(x^0 + d^0) - P_{\mathcal{B}}(x^*)\big\| + (1 - \sigma_0)\|x^0 - x^*\| \\ &\leq \|x^0 + d^0 - x^*\| + \frac{1}{4}\|x^0 - x^*\| \\ &\leq \frac{1}{2}\|x^0 - x^*\|. \end{aligned} \tag{24}$$

In particular, x^1 is also in the ball with radius ε around x^*. By induction, it follows that $\{x^k\} \subseteq \operatorname{int}(\mathcal{B})$ is well-defined and satisfies

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

Hence the sequence $\{x^k\}$ converges (at least linearly) to x^*.

In order to verify the local quadratic rate of convergence, we recall that the strong semismoothness of G (see Theorem 4.2) implies that

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

see [18, Theorem 7.4.3]. Using (21), we therefore get

$$\begin{aligned} \|x^k + d^k - x^*\| &= \|x^k - x^* - M(x^k)^{-1}G(x^k)\| \\ &\leq \|M(x^k)^{-1}\| \, \|G(x^k) - G(x^*) - M(x^k)(x^k - x^*)\| \\ &= O(\|x^k - x^*\|^2). \end{aligned}$$

Following (24), this implies

$$\begin{aligned} \|x^{k+1} - x^*\| &\leq \sigma_k\|P_{\mathcal{B}}(x^k + d^k) - P_{\mathcal{B}}(x^*)\| + (1 - \sigma_k)\|x^k - x^*\| \\ &\leq \|x^k + d^k - x^*\| + (1 - \sigma_k)\|x^k - x^*\| \\ &= O(\|x^k - x^*\|^2) + (1 - \sigma_k)\|x^k - x^*\|. \end{aligned}$$

Exploiting once again the local Lipschitz continuity of the mapping G around x^* (see Theorem 4.2), we get from (S.3) of Algorithm 4.3 together with (21)

$$\begin{aligned} 1-\sigma_k &= \|P_{\mathcal{B}}(x^k+d^k)-x^k\| \\ &\leq \|d^k\| \\ &= O(\|G(x^k)\|) \\ &= O(\|G(x^k)-G(x^*)\|) \\ &= O(\|x^k-x^*\|). \end{aligned}$$

Altogether, we therefore have $\|x^{k+1}-x^*\| = O(\|x^k-x^*\|^2)$. □

6 Numerical Examples

In this section, we want to illustrate the local behaviour of the different scaling strategies using two standard test problems. To this end, we implemented Algorithm 4.3 in MATLAB using $\sigma = 0.9995$ and the termination criterion $\|G(x)\| \leq 10^{-25}$. This is a relatively small tolerance, however, since we compare the pure local behaviour of some methods only, we prefer to have a small tolerance in order to see some interesting effects.

We then consider the following three methods which differ in the choice of the matrix $M(x) = D(x)\nabla^2 f(x) + S(x)$ from (19):

- Coleman-Li [7, 8]: Here $d_i(x) = d_i^{CL}(x)$ is defined by (2) and $s_i(x) := s_i^{CL}(x) := |[\nabla f(x)]_i|$ for all $i = 1, \ldots, n$;
- Heinkenschloss et al. [21]: Here we take $d_i(x) = d_i^{HUU}(x)$ from (3) and

$$s_i(x) := s_i^{HUU}(x) := \begin{cases} |[\nabla f(x)]_i| & \text{if } |[\nabla f(x)]_i| < \min\{x_i - l_i, u_i - x_i\}^p \text{ or} \\ & \min\{x_i - l_i, u_i - x_i\} < |[\nabla f(x)]_i|^p \\ 0 & \text{else} \end{cases}$$

  with $p = 2$;
- new method: Here $d_i(x)$ and $s_i(x)$ are defined by (18) (using $\gamma = 10^{-3}$) and (20), respectively. In order to define the index set $A_{00}(x)$ for these choices of $d_i(x)$ and $s_i(x)$, we use the identification function ρ_2 from (16), (17) and take a suitable multiplier function $\lambda(x)$ from [12, Proposition 5] (using the parameters $\gamma_1 = \gamma_2 := 0.1$ in that reference).

Note that Heinkenschloss et al. [21] use a further scaling of the matrix $M(x)$ in order to verify theoretically the uniform nonsingularity of certain Jacobian-type matrices, but that this additional scaling is not necessary for the algorithm since it can be cancelled on both sides of the corresponding linear systems to be solved in their method, see [21, Algorithm 1]. Hence our implementation is equivalent to their method.

Our first test example is the famous Rosenbrock-function

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2.$$

This function has a unique global minimum at $x^* := (1, 1)^T$. Therefore we use $l := (0, 0)^T$ and $u := (1, 1)^T$ to obtain the degenerate set $I_{00}(x^*) = \{1, 2\}$. Since we are interested in the local convergence properties, we change the standard starting point to $x^0 := (0.999, 0.999)^T$. Table 1 contains the corresponding numerical results for the Coleman-Li scaling. For each iteration k, we report the size of the stopping criterion $\|G(x^k)\|$ as well as the distance of the current iterate (and its components) to the known solution.

k	$\|G(x^k)\|$	$\|x_1^k - x_1^*\|$	$\|x_2^k - x_2^*\|$	$\|x_k - x^*\|$
0	3.994004e-01	1.000000e-03	1.000000e-03	1.414214e-03
1	3.967247e-04	9.945479e-04	1.987114e-03	2.222104e-03
2	5.463162e-07	5.425928e-04	1.085095e-03	1.213194e-03
3	1.296976e-07	2.714348e-04	5.429716e-04	6.070379e-04
4	3.162359e-08	1.357598e-04	2.716074e-04	3.036467e-04
5	7.809617e-09	6.789056e-05	1.358342e-04	1.518554e-04
6	1.940620e-09	3.394796e-05	6.792478e-05	7.593576e-05
7	4.836979e-10	1.697465e-05	3.396431e-05	3.796989e-05
8	1.207434e-10	8.487491e-06	1.698263e-05	1.898545e-05
9	3.016327e-11	4.243788e-06	8.491436e-06	9.492851e-06
⋮	⋮	⋮	⋮	⋮
31	1.659987e-24	1.011746e-12	2.024603e-12	2.263326e-12
32	4.003273e-25	5.058176e-13	1.012301e-12	1.131638e-12
33	1.000818e-25	2.529088e-13	5.061507e-13	5.658192e-13
34	2.359936e-26	1.264544e-13	2.531308e-13	2.829593e-13

Table 1: Numerical results for the Rosenbrock function using the Coleman-Li scaling

The results in Table 1 indicate a relatively slow (linear) rate of convergence. The situation is significantly better for the Heinkenschloss et al. method, and the corresponding results are given in Table 2, where we include one further column which gives the index set

$$\tilde{A}_{00}(x) := \left\{ i \,\middle|\, |[\nabla f(x)]_i| < \min\{x_i - l_i, u_i - x_i\}^p \text{ or } \min\{x_i - l_i, u_i - x_i\} < |[\nabla f(x)]_i|^p \right\}$$

which, in view of the definition of their scaling matrices in (3), may be viewed as the counterpart of our index set $A_{00}(x)$.

k	$\|G(x^k)\|$	$\|(x^k)_1 - x_1^*\|$	$\|(x^k)_2 - x_2^*\|$	$\|x^k - x^*\|$	$\tilde{A}_{00}(x^k)$
0	3.994004e-01	1.000000e-03	1.000000e-03	1.414214e-03	$\emptyset$
1	2.394061e-03	9.945479e-04	1.987114e-03	2.222104e-03	$\{1, 2\}$

2	2.644000e-04	4.972739e-07	1.587753e-06	1.663803e-06	$\{1,2\}$
3	4.481673e-10	5.981726e-11	1.208688e-10	1.348605e-10	$\{1,2\}$
4	0	0	0	0	$\{1,2\}$

Table 2: Numerical results for the Rosenbrock function using the Heinkenschloss et al. scaling

Table 2 clearly shows the local quadratic convergence of the Heinkenschloss et al. method. The same is true for our scaling technique, and the corresponding numerical results are given in Table 3. In fact, we need one iteration less than the Heinkenschloss et al. method. According to our experience, this is mainly due to the fact that our identification technique for the degenerate indices $I_{00}(x^*)$ is more effective. In fact, comparing the results in Tables 2 and 3, we see that we are able to identify the correct set from the very beginning, whereas this is not true for the Heinkenschloss et al. scaling.

k	$\|G(x^k)\|$	$\|(x^k)_1 - x_1^*\|$	$\|(x^k)_2 - x_2^*\|$	$\|x^k - x^*\|$	$A_{00}(x^k)$
0	4.481984e-01	1.000000e-03	1.000000e-03	1.414214e-03	$\{1,2\}$
1	2.245015e-04	5.000000e-07	5.000000e-07	7.071068e-07	$\{1,2\}$
2	1.587703e-10	3.536060e-13	3.536060e-13	5.000744e-13	$\{1,2\}$
3	0	0	0	0	$\{1,2\}$

Table 3: Numerical results for the Rosenbrock function using the new scaling

To illustrate this point further, we take the Wood-function

$$f(x) := 100(x_2 - x_1^2) + (1 - x_1)^2 + 90(x_4 - x_3)^2 + (1 - x_3)^2 + 10(x_2 + x_4 - 2)^2 + 0.1(x_2 - x_4)^2$$

as our second test problem. It has an unconstrained minimum in $x^* := (1, 1, 1, 1)^T$, and we use the bounds $l := (1, 1, 1, 0.99)^T$ and $u := (3, 3, 3, 3)^T$. Hence $I_{00}(x^*) = \{1, 2, 3\}$ is the degenerate set. Note, however, that also the fourth component is almost degenerate. As a very good local starting point, we take $x^0 := 1.001 \cdot (1, 1, 1, 1)^T$. The corresponding numerical results using the Coleman-Li scaling are given in Table 4.

k	$\|G(x^k)\|$	$\|x^k - x^*\|$
0	4.255314e-01	2.000000e-03
1	3.088548e-04	2.021504e-03
2	7.816318e-05	1.012668e-03
3	1.964852e-05	5.069441e-04
4	4.925803e-06	2.536260e-04
5	1.233169e-06	1.268516e-04
6	3.085074e-07	6.343543e-05
7	7.715390e-08	3.172013e-05

8	1.929178e-08	1.586067e-05
9	4.823369e-09	7.930485e-06
⋮	⋮	⋮
34	5.684342e-14	2.366777e-13
35	5.684342e-14	1.182266e-13
36	5.684342e-14	5.933163e-14
37	2.327831e-26	2.994722e-14

Table 4: Numerical results for the Wood function using the Coleman-Li scaling

Again, we see that the convergence of the Coleman-Li method is rather slow. On the other hand, we get much faster convergence for the Heinkenschloss et al. scaling, as documented in Table 5. However, we also see that the estimation $\tilde{A}_{00}(x^k)$ of the degenerate index set $I_{00}(x^*)$ is sometimes incorrect even very close to the solution.

k	$\|G(x^k)\|$	$\|x^k - x^*\|$	$\tilde{A}_{00}(x^k)$
0	4.255314e-01	2.000000e-03	$\{\}$
1	2.428585e-04	2.021504e-03	$\{2\}$
2	6.143252e-05	1.012668e-03	$\{2\}$
3	1.543420e-05	5.069441e-04	$\{2\}$
4	3.868204e-06	2.536260e-04	$\{1,2,3\}$
5	8.814318e-03	1.268516e-04	$\{1,2,3\}$
6	2.824142e-06	2.268045e-08	$\{1,2,3\}$
7	3.067384e-13	5.874748e-16	$\{1,2,3\}$
8	5.684342e-14	1.110223e-16	$\{1,2\}$
9	0	0	$\{1,2,3\}$

Table 5: Numerical results for the Wood function using the Heinkenschloss et al. scaling

The situation is significantly better when using our new scaling technique. Table 6 gives the results obtained with our method. Although the fourth index is initially viewed as being degenerate (as is to be expected), our technique eventually finds the correct index set and converges much faster than the Heinkenschloss et al. method.

k	$\|G(x^k)\|$	$\|x^k - x^*\|$	$A_{00}(x^k)$
0	5.823476e-01	2.000000e-03	$\{1,2,3,4\}$
1	1.391926e-03	9.067386e-06	$\{1,2,3,4\}$
2	2.574718e-08	1.609195e-10	$\{1,2,3\}$
3	0	0	$\{1,2,3\}$

Table 6: Numerical results for the Wood function using the new scaling

7 Final Remarks

We have introduced a new scaling technique for the solution of bound constrained optimization problems by affine-scaling interior-point Newton methods. Using this scaling technique, the strict complementarity condition is not needed in order to prove local quadratic convergence. Moreover, this new scaling allows a much simpler local convergence proof by using standard results from nonsmooth analysis.

The analysis carried out in this paper is completely local. We believe, however, that a globalization using either line search or trust-region techniques are possible, but leave this topic as part of our future research since the globalization was not the main intention of this work. It should be noted, however, that a standard globalization technique may not work in our framework since our scaling matrix fails to have some properties that are commonly used in, say, trust-region globalizations like in [7, 8].

Acknowledgement. The authors would like to thank one of the referees for some very detailed comments on a previous version of this paper.

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