On the Convergence of Newton Iterations to Non-Stationary Points

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Abstract

We study conditions under which line search Newton methods for nonlinear systems of equations and optimization fail due to the presence of singular non-stationary points. These points are not solutions of the problem and are characterized by the fact that Jacobian or Hessian matrices are singular. It is shown that, for systems of nonlinear equations, the interaction between the Newton direction and the merit function can prevent the iterates from escaping such non-stationary points. The unconstrained minimization problem is also studied, and conditions under which false convergence cannot occur are presented. Several examples illustrating failure of Newton iterations for constrained optimization are also presented. The paper also shows that a class of line search feasible interior methods cannot exhibit convergence to non-stationary points.

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1 Introduction

It is well known that a Newton method with no globalization strategy can behave quite unpredictably, but that use of a line search stabilizes the iteration so that, in most cases, it makes steady progress towards a solution. We wish to consider the question of when singularity of the Jacobian or Hessian can cause serious difficulties for line search Newton methods. If we allow the possibility of singularity, there are in principle many forms that failure could take; for example, the method may break down, the iterates might oscillate between two non-stationary points, or they could converge to a non-stationary point. Our view is that, when methods fail in practice, there is often apparent convergence to a spurious solution, or at least, negligible progress toward the solution. Therefore we consider convergence to a non-solution point to be a failure of practical interest, and in this paper we study conditions under which it can occur. We will analyze the performance of Newton methods on three classes of problems: systems of nonlinear equations, unconstrained and constrained optimization.

The difficulties studied in this paper do not take place when Newton's method is globalized by means of trust region techniques, and therefore almost no attention will be given here to trust region methods. We concentrate instead on line search methods because they are extensively used in many areas of computational mathematics (see e.g. [2]) and because they can be negatively impacted by the presence of singularity of the Jacobian or Hessian. Our view is that basic line search Newton iterations are so important that their properties must be well understood so that inefficiencies and failures can be properly diagnosed, and if necessary, corrected.

A line search Newton method for solving a system of n nonlinear equations $F(x) = 0$ in n unknowns takes the form,

$$d_k = -F'(x_k)^{-1}F(x_k) \tag{1.1a}$$

$$x_{k+1} = x_k + \alpha_k d_k, \tag{1.1b}$$

where the steplength α_k is chosen to reduce a merit function ϕ along d_k. The merit function is often taken to be

$$\phi(x) = \tfrac{1}{2}\|F(x)\|_2^2. \tag{1.2}$$

It is well known that this iteration cannot be guaranteed to converge to a solution of the nonlinear system; in particular if an iterate is near a local minimizer $\hat{x}$ of ϕ, then the iteration may converge to $\hat{x}$ even though we could have that $F(\hat{x}) \neq 0$. A reasonable expectation for a practical Newton method is, however, that it continue until it finds a *stationary point* of the merit function ϕ, i.e., a point such that $\nabla\phi(x) = 0$. For the Newton iteration (1.1) this can be mathematically guaranteed under the condition that the Jacobian $F'(x_k)$ is bounded away from singularity for all k and that the steplength α_k provides sufficient decrease in ϕ at each iteration (see e.g. [5]).

There is a well known example of the type of failure that is the subject of this paper. Powell [13] describes a nonlinear system of equations for which the iteration (1.1) with an exact line search converges to a point z that is not stationary for the merit function ϕ and where F' becomes singular. This is disturbing because there are directions of search from

z that allow us to both decrease the merit function and move toward the solution, but the algorithm is unable to generate such directions. Wächter and Biegler [15] have recently described another example of failure of a Newton iteration in the context of constrained optimization. They show that a class of interior methods can fail to generate a feasible point for a simple problem in three variables, and that the iterates do not approach a stationary point of any measure of infeasibility for the problem. In this paper we present conditions under which failures due to singularities can occur, as well as conditions that ensure that failure cannot take place. We present several examples illustrating the role of the merit function and the behavior of the search direction in various cases.

In section 2, we study the solution of nonlinear systems of equations and show that the interaction between the Newton direction d_k and the merit function in a neighborhood of singular non-stationary points can cause convergence to such points. We also demonstrate by means of an example, that although simple regularization techniques can prevent convergence to non-stationary points, regularized Newton iterations can be very inefficient if they approach such points. A trust region approach, on the other hand, performs efficiently on the same example. In section 3 we study the solution of unconstrained minimization problems and present conditions under which false convergence cannot occur. These results suggest that there is fundamental difference between unconstrained minimization problems and systems of nonlinear equations in that convergence to singular non-stationary points seems much less likely for minimization problems. In section 4 we consider constrained optimization problems. We present two examples illustrating failure of Newton iterations that are different from those described by Wächter and Biegler. We also show that a class of feasible interior methods cannot converge to non-stationary points if an appropriate merit function is used.

In this paper we do not propose remedies to the inefficiencies of line search Newton methods that we discuss. As is well known, trust region techniques provide one mechanism for overcoming the difficulties. We limit our analysis to basic line search Newton iterations of the type that is commonly used in scientific and engineering applications.

All the numerical experiments were performed on a Sun Ultra 5 with 384 MB of memory using double precision IEEE arithmetic. The implementations were done in Matlab except when indicated otherwise.

Notation. Throughout the paper $\|\cdot\|$ denotes the Euclidean norm of a vector, $\mathcal{R}(A)$ the range space of the matrix A, and `macheps` the machine unit roundoff error.

2 Systems of Nonlinear Equations

In this section we consider the solution of a nonlinear system of equations

$$F(x) = 0, \tag{2.1}$$

where F is a twice continuously differentiable mapping from $I\!R^n$ to $I\!R^n$. We are interested in studying the convergence of the line search Newton iteration (1.1) to points that are neither solutions of (2.1) nor stationary points for the merit function (1.2).

Definition 2.1 *A point* $z \in I\!R^n$ *is a* singular non-stationary point *for problem* (2.1)*, with respect to the merit function* ϕ*, if*

$$F'(z) \text{ is singular} \quad \text{and} \quad \nabla\phi(z) \neq 0 \quad (\text{which implies that } F(z) \neq 0). \tag{2.2}$$

As mentioned in the introduction, it is well known that the line search Newton iteration can converge to singular non-stationary points.

Example 1 (Powell [13]) Consider the problem of finding a solution of the nonlinear system

$$F(x, y) \equiv \begin{pmatrix} x \\ 10x/(x+0.1) + 2y^2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{2.3}$$

The unique solution is $(x_*, y_*) = (0, 0)$. Let us try to solve the problem using the Newton iteration (1.1) where α_k is chosen to minimize ϕ along d_k. It has been proved in [13] that, starting from

$$(x_0, y_0) = (3, 1), \tag{2.4}$$

the iterates converge to the point $z \approx (1.8016, 0.0000)$. That z is not a stationary point for ϕ is apparent from Figure 1 where we plot ϕ in the region of interest. More specifically, the directional derivative of ϕ at z in the direction $(x_*, y_*) - z$ is negative. Note also that F' is singular at z, as it is all along the x axis. Therefore the Newton iteration converged to a singular non-stationary point for this problem. □

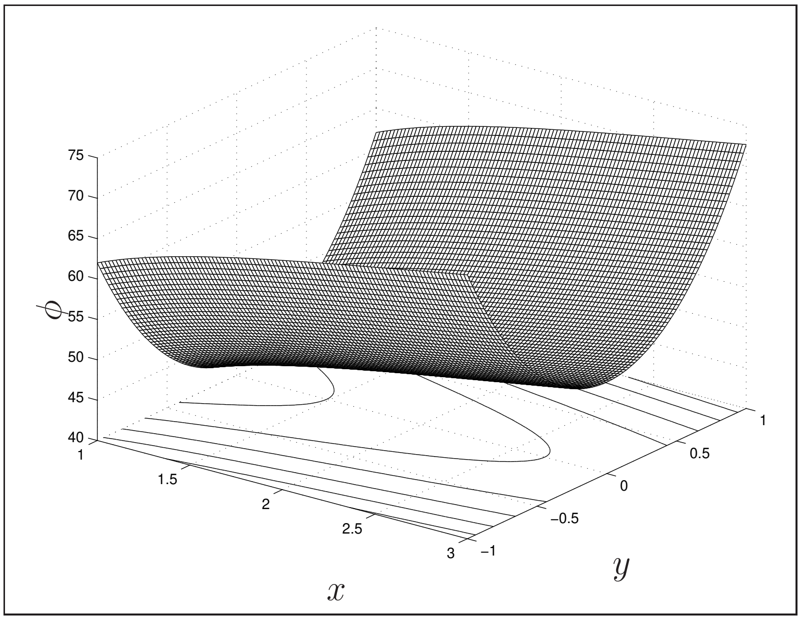

Figure 1: Plot of $\phi(x, y) = \frac{1}{2}\|F(x, y)\|^2$ for Example 1.

Nonlinear systems of equations typically contain many singular non-stationary points, but the Newton iteration is often not attracted to them. The goal of this section is to try to understand why the Newton iterates converge to some of these points, but not to others.

To motivate the analysis that follows, let us refer again to Figure 1. The whole half-line

$$\ell = \{(x, y) : y = 0,\ x > 0\} \tag{2.5}$$

consists of singular non-stationary points, and choosing certain initial guesses (x_0, y_0), the iteration converges to different points on ℓ. An examination of the numerical test mentioned in Example 1 shows that, as the iterates approach the singular half-line ℓ, the Newton directions d_k become increasingly longer and ever more perpendicular to the half line ℓ, but due to the (local) convexity of the merit function ϕ along these directions, the line search forces the iterates to approach ℓ. Without this convexity property the iterates would move away from the singular half-line. This suggests that the interaction between the Newton direction and the merit function plays a crucial role in provoking convergence to a singular non-stationary point. This phenomenon is described in Theorem 2.2 below. Before presenting this result, we introduce some notation and assumptions.

Let $z \in I\!R^n$ be a singular non-stationary point, i.e., a point that satisfies (2.2). Suppose, in addition, that

$$\begin{aligned} \operatorname{rank}(F'(z)) &= n-1, \quad \text{and} && (2.6\text{a}) \\ F(z) &\notin \mathcal{R}(F'(z)). && (2.6\text{b}) \end{aligned}$$

Later on we will see that the rank assumption (2.6a) can be generalized to allow any degree of rank-deficiency, but that the range assumption (2.6b) is necessary to establish Theorem 2.2.

We define the singular value decompositions

$$F'(x_k) = U_k \Sigma_k V_k^T, \qquad F'(z) = U \Sigma V^T, \tag{2.7}$$

and denote the columns of U_k and V_k by $u_1^k, \ldots, u_n^k$, and $v_1^k, \ldots, v_n^k$, respectively, and the singular values by $\sigma_1^k \geq \cdots \geq \sigma_n^k$. A similar notation (without the superscript k) will be used for the singular vectors and values of $F'(z)$. From assumption (2.6a) we have that $\sigma_1 \geq \cdots \geq \sigma_{n-1} > \sigma_n = 0$ and that v_n spans the null space of $F'(z)$.

The following result shows that, if in a neighborhood of a singular non-stationary point z, the merit function satisfies a (local) convexity condition along the Newton directions d_k, then the total displacements $x_{k+1} - x_k$ become arbitrarily small near z. The convexity assumption will be phrased in terms of the second directional derivative of ϕ along a vector v, which we write as $D^2\phi(x; v)$.

Theorem 2.2 *Consider the Newton iteration* (1.1) *where* α_k *is the first local minimizer of the merit function* $\phi(x) = \frac{1}{2}\|F(x)\|^2$. *Let* z *be a singular non-stationary point of problem* (2.1) *satisfying* (2.6).

(i) If

$$D^2\phi(z; v_n) = \sum_{i=1}^{n} F_i(z)\, v_n^T \nabla^2 F_i(z) v_n > 0, \tag{2.8}$$

then for any $\varepsilon > 0$, there is a $\delta > 0$ such that, if $\|x_k - z\| \le \delta$ and $F'(x_k)$ is nonsingular, we have that $\|x_{k+1} - x_k\| \le \varepsilon$.

(ii) On the other hand, if $D^2\phi(z; v_n) < 0$, then for all sufficiently small $\delta > 0$, there exists a constant $T > 0$ such that, if $\|x_k - z\| \le \delta$ and $F'(x_k)$ is nonsingular, then $\|x_{k+1} - x_k\| \ge T$.

Proof. Using the singular value decomposition (2.7) of $F'(x_k)$, the Newton direction can be written as

$$d_k = -\left[F'(x_k)\right]^{-1} F(x_k) = -\sum_{i=1}^{n} \frac{(u_i^k)^T F(x_k)}{\sigma_i^k} v_i^k. \tag{2.9}$$

Since by (2.6*a*)

$$\mathcal{R}(F'(z)) = \text{span}\{u_1, \dots, u_{n-1}\},$$

assumption (2.6*b*) implies that $F(z)^T u_n \neq 0$. Therefore $(u_n^k)^T F(x_k)$ is bounded away from zero for all x_k in a neighborhood of z. By continuity of singular values, σ_n^k approaches zero as x_k approaches z, while the other singular values remain bounded away from zero. These facts and (2.9) imply that the norm of d_k becomes arbitrarily large, and its direction arbitrarily parallel to v_n, as x_k approaches z. That is,

$$\lim_{x_k \to z} \|d_k\| = \infty \quad \text{and} \quad \lim_{x_k \to z} \frac{d_k}{\|d_k\|} = v_n. \tag{2.10}$$

To estimate the steplength α_k we define the function

$$h_k(\tau) = \phi(x_k + \tau d_k / \|d_k\|), \tag{2.11}$$

which is the restriction of the merit function ϕ along the normalized Newton direction. We compute the steplength of the Newton iteration by finding the first local minimizer of the function $h_k(\cdot)$, obtaining, say τ_k. Note, however, that τ_k is not the steplength parameter α_k in (1.1*b*) since h_k is defined in terms of the normalized Newton direction, but it is related to α_k by

$$\alpha_k = \frac{\tau_k}{\|d_k\|}.$$

It follows that the total displacement of the Newton iteration is

$$\|x_{k+1} - x_k\| = \alpha_k \|d_k\| = \tau_k, \tag{2.12}$$

and our goal is therefore to estimate the magnitude of τ_k.

By differentiating ϕ, we have

$$\nabla\phi(x) = F'(x)^T F(x) \tag{2.13a}$$

$$\nabla^2\phi(x) = F'(x)^T F'(x) + \sum_{i=1}^{n} F_i(x) \nabla^2 F_i(x). \tag{2.13b}$$

Recalling (2.11), (2.13a) and the first equality in (2.9), we obtain

$$\begin{aligned} h_k'(0) &= (d_k)^T F'(x_k)^T F(x_k)/\|d_k\| \\ &= -\|F(x_k)\|^2/\|d_k\| < 0. \end{aligned} \tag{2.14}$$

It also follows from (2.11), that the second derivative of $h_k(\cdot)$ is given by

$$h_k''(\tau) = \left(\frac{d_k}{\|d_k\|}\right)^T \nabla^2\phi\left(x_k + \tau\frac{d_k}{\|d_k\|}\right)\left(\frac{d_k}{\|d_k\|}\right). \tag{2.15}$$

Case (i) Let us assume that $\rho \equiv D^2\phi(z; v_n) > 0$. We write (2.15) as

$$h_k''(\tau) = \psi(d_k/\|d_k\|, x_k, \tau), \tag{2.16}$$

where the function ψ is defined as

$$\psi(w, x, \tau) = w^T\nabla^2\phi(x + \tau w)w. \tag{2.17}$$

Note that ψ is a continuous function in a neighborhood of (z, v_n, τ).

Recalling (2.13b), and the fact that v_n is a null vector of $F'(z)$, it follows that

$$\begin{aligned} \rho = D^2\phi(z; v_n) &= v_n^T\nabla^2\phi(z)v_n \\ &= \sum_{i=1}^{n} F_i(z)\, v_n^T\nabla^2 F_i(z)v_n \\ &= \psi(v_n, z, 0). \end{aligned} \tag{2.18}$$

By (2.18), (2.16), the second relation in (2.10), and continuity of the function ψ, we know that there exist positive values δ_1 and T such that if $\|x_k - z\| < \delta_1$ and $\tau \le T$ then

$$h_k''(\tau) \ge \tfrac{1}{2}\rho > 0. \tag{2.19}$$

Additionally, by the first relation in (2.10), the continuity of F, and (2.14),

$$\lim_{x_k \to z} h_k'(0) = 0, \tag{2.20}$$

which implies there exists $\delta_2 \le \delta_1$ such that for all $\|x_k - z\| < \delta_2$,

$$|h_k'(0)| < \tfrac{1}{4}\rho T. \tag{2.21}$$

We will now combine (2.19), (2.20) and (2.21) to show that τ_k becomes arbitrarily small as x_k approaches z. A Taylor expansion and (2.19) give

$$\begin{aligned} h_k(\tau) &\ge h_k(0) + \tau h_k'(0) + \tfrac{1}{4}\rho\tau^2 \\ &\ge h_k(0) + \tau\left[h_k'(0) + \tfrac{1}{4}\rho\tau\right], \end{aligned} \tag{2.22}$$

for $\|x_k - z\| < \delta_2$ and $\tau \le T$. Note that the term inside the square brackets is non-negative for $\tau \ge -4h_k'(0)/\rho$. Thus inequality (2.22) implies that for such x_k, there must be a local minimizer of $h_k(\cdot)$ in the interval $(0, -4h_k'(0)/\rho)$ and, by (2.21), this interval is contained in $(0, T)$. Thus, the first local minimizer τ_k of $h_k(\cdot)$ satisfies

$$\tau_k < \frac{-4h_k'(0)}{\rho}.$$

Therefore, by (2.20), for any $\varepsilon > 0$ there exists $\delta \in (0, \delta_2)$ such that if $\|x_k - z\| \le \delta$ then $\|x_{k+1} - x_k\| = \tau_k < \varepsilon$.

Case (ii) Let us assume now that $\rho \equiv D^2\phi(z; v_n) < 0$. The continuity of the function ψ defined by (2.17) implies that there exist constants $\delta_2 > 0$ and $T > 0$ such that if $\|x_k - z\| < \delta_2$ and $\tau \le T$, then

$$h_k''(\tau) \le \tfrac{1}{2}\rho. \tag{2.23}$$

A Taylor expansion, (2.23) and the fact that $h_k'(0) < 0$ give that

$$h_k'(\tau) \le h_k'(0) + \tfrac{1}{2}\rho \le \tfrac{1}{2}\rho < 0 \tag{2.24}$$

for $\|x_k - z\| < \delta_2$ and $\tau \in [0, T]$. Therefore, the minimizers of h_k lie in the interval $[T, +\infty)$, and hence $\|x_{k+1} - x_k\| \ge T$. $\square$

We should note that the convexity assumption (2.8) implies, not only that ϕ is convex at z along the null direction v_n, but that along that direction ϕ actually has a one-dimensional minimizer at z. This follows from the fact that $D\phi(z; v_n) = v_n^T F'(z)^T F(z) = 0$ and from (2.8). Therefore when x is close to z and the Newton direction is closely aligned with v_n, the first one-dimensional minimizer of ϕ along the Newton direction will be close to z. This is the mechanism that prevents the iterates from immediately running away from a singular non-stationary stationary point.

Theorem 2.2 implies that singularities of the Jacobian are likely to cause problems for Newton's method in a significant proportion of cases, in view of the condition (2.8). However, this argument does not necessarily imply *convergence* to a non-stationary point. All that Theorem 2.2 states is that if the iterates fall sufficiently close to such a singular non-stationary point z, the displacements will be arbitrarily small. Mathematically, this means that an arbitrarily large number of iterations can be made in a neighborhood of a singular non-stationary point. This has important practical implications, as most implementations of Newton's method will terminate in this situation, either because of an explicit stopping test of the form $\|x_{k+1} - x_k\| < \varepsilon$, or because in finite precision we will have $\phi(x_k + \alpha_k d_k) = \phi(x_k)$, which will cause a failure in the line search procedure. It is clear that the conditions of Theorem 2.2 can lead to convergence to a singular non-stationary point in some cases, but whether it always does is an open question.

The assumption that the line search computes the first local minimizer of the merit function ϕ, can be replaced, for example, by a line search that finds a steplength belonging to the first interval of steplengths satisfying the Wolfe conditions

$$\phi(x_k + \alpha_k d_k) \le \phi(x_k) + \eta\, \alpha_k \nabla\phi(x_k)^T d_k \tag{2.25a}$$

$$\nabla\phi(x_k + \alpha_k d_k)^T d_k \ge \beta\, \nabla\phi(x_k)^T d_k, \tag{2.25b}$$

where η and β are constants that satisfy $0 < \eta < \beta < 1$; see e.g. [12]. Let us consider how the proof can be extended to cover this case. In case (i) little change is needed since all such points lie in the interval $(0, -4h_k'(0)/\rho)$ specified in the proof. In case (ii), the Wolfe condition (2.25b), which can be written as $h_k'(\tau_k) \geq \beta h_k'(0)$, does not hold for all $\tau \in [0, T]$ by virtue of the first inequality in (2.24). Therefore, all the acceptable points will lie in the interval $[T, +\infty)$.

This analysis will not apply, however, to a line search that backtracks from the unit steplength because, since the lengths of the Newton directions tend to infinity, the steplength $\alpha_k = 1$ would result in trial points of increasingly large magnitude. To extend Theorem 2.2 to a backtracking line search would require a stronger assumption, for example, that the merit function is unimodal along the sequence of rays $\{x_k + \alpha d_k;\ \alpha > 0\}$.

Example 1-Revisited The Jacobian of the function (2.3),

$$F'(x, y) = \begin{bmatrix} 1 & 0 \\ 1/(x + 0.1)^2 & 4y \end{bmatrix},$$

is singular on the half-line (2.5), and we can define $v_n = (0, 1)^T$. It is easy to show that for any point z on the half-line ℓ, the rank and range conditions (2.6) hold and $D^2\phi(z, v_n) > 0$. Thus Theorem 2.2 applies to this example and predicts that the lengths of the Newton displacements tend to zero in a neighborhood of the half line ℓ.

Figure 2 plots the estimated length of the Newton displacements for problem (2.3) for all values of (x, y) in a grid over the region $[1, 3] \times [-1, 1]$. We estimate the length of the Newton displacement, which by (2.12) is the steplength τ_k to the first local minimizer of h_k, by means of the length of the one-dimensional Newton step on h_k, which is given by $-h_k'(0)/h_k''(0)$. This estimate is increasingly accurate as x approaches the singular half-line. In Figure 2 we plot $\xi(x_k, y_k) = -h_k'(0)/h_k''(0)$, for all (x_k, y_k) on the grid. The function ξ is not defined on the half-line $y = 0$, but as expected its limit is zero as one approaches that half-line. $\square$

The assumption that $F'(z)$ has rank $n - 1$ was made for simplicity, and the proof of Theorem 2.2 can easily be extended to the case in which $F'(z)$ is singular with an arbitrary rank deficiency. We now restate the theorem including all the generalizations discussed so far.

Theorem 2.3 *Consider the Newton iteration* (1.1) *where α_k is either the first local minimizer of the merit function $\phi(x) = \frac{1}{2}\|F(x)\|^2$ or belongs to the first interval of steplengths satisfying the Wolfe conditions* (2.25). *Let z be a singular non-stationary point of problem* (2.1) *satisfying* (2.6b). *If the matrix*

$$\sum_{i=1}^{n} F_i(z)\, \nabla^2 F_i(z) \tag{2.26}$$

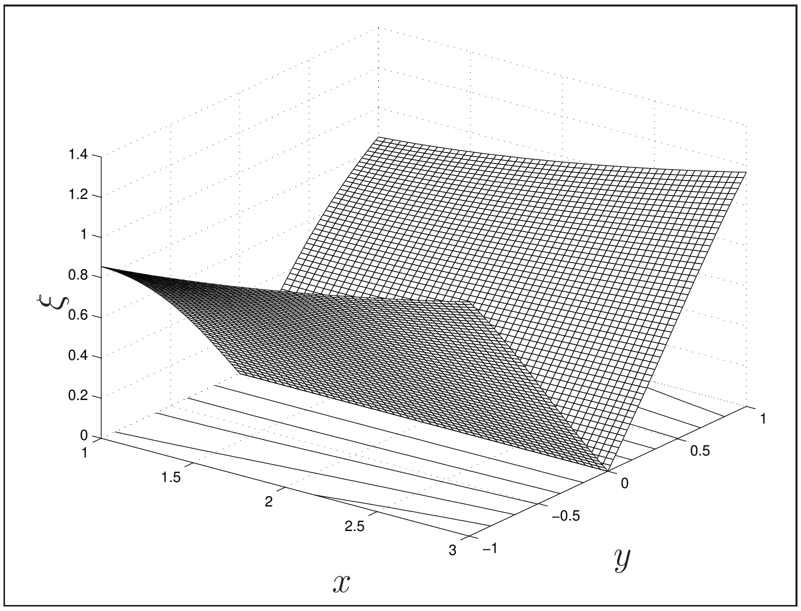

Figure 2: Estimated lengths of the Newton steps on Example 1.

is positive definite on the null space of $F'(z)$, then for any $\varepsilon > 0$, there is a $\delta > 0$ such that, if $\|x_k - z\| \le \delta$ and $F'(x_k)$ is nonsingular, we have that $\|x_{k+1} - x_k\| \le \varepsilon$. On the other hand, if the matrix (2.26) is negative definite on the null space of $F'(z)$, then for all δ sufficiently small, there exists a constant $T > 0$ such that if $\|x_k - z\| \le \delta$ then $\|x_{k+1} - x_k\| \ge T$.

We conclude this section by showing that the range assumption (2.6*b*) is necessary in Theorem 2.2 (or Theorem 2.3). Specifically, we will now show that if

$$F(z) \in \mathcal{R}(F'(z)),$$

and if all the other conditions of Theorem 2.2 (or Theorem 2.3) hold, there are problems for which the conclusions of this theorem are valid, and others for which they are not.

Let us examine the problem

$$F(x,y) = (x^2 + y^2,\ y^2)^T = 0.$$

The point $z = (2,0)$ is a singular non-stationary point at which the conditions (2.6*a*) and (2.8) hold, but (2.6*b*) is violated. Consider the starting point (x_0, y_0) with $y_0 \neq 0$. It is easy to see that the Newton step d_0 points directly to the solution $(0,0)$, and that $\phi = \frac{1}{2}\|F\|^2$ decreases monotonically along d_0, from (x_0, y_0) to the solution. Thus, with either an exact or backtracking line search, the total displacement $\|(x_1, y_1) - (x_0, y_0)\|$ will be bounded below, regardless of how close is (x_0, y_0) to $(2,0)$. Therefore, in this example, the conclusion (i) of Theorem 2.2 does not hold.

In the following example, on the other hand, the range assumption (2.6*b*) is violated, but conclusion (i) of Theorem 2.2 is still valid.

Example 2 The only solution of the system of equations

$$F(x,y) = (x + y^2,\ 2(x-1)y)^T = 0, \tag{2.27}$$

is $(0,0)$. Let us define the line

$$\mathcal{T} = \{(1,y) : y \in I\!R\}.$$

We will show that if the starting point (x_0, y_0) belongs to the set $\mathcal{T} \setminus \{(1,0)\}$, then the iterates generated by Newton's method are confined to $\mathcal{T}$. (The point $(1,0)$ is excluded as initial point because the Jacobian is singular at this point.)

Let $(1, y_k)$ be an iterate in $\mathcal{T} \setminus \{(1,0)\}$. Since the Newton direction is given by

$$d_k = -\left[F'(1,y_k)\right]^{-1} F(1,y_k) = \frac{1}{4y_k^2}\begin{bmatrix} 0 & -2y_k \\ -2y_k & 1 \end{bmatrix}\begin{pmatrix} 1+y_k^2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{1+y_k^2}{2y_k} \end{pmatrix}, \tag{2.28}$$

the next iterate $(x_{k+1}, y_{k+1}) = (x_k, y_k) + \alpha_k d_k$ also belongs to $\mathcal{T}$. Note that on $\mathcal{T}$, the merit function takes the form

$$\phi(1,y) = \tfrac{1}{2}\|F(1,y)\|^2 = \tfrac{1}{2}(1+y^2)^2, \tag{2.29}$$

and that

$$\nabla\phi(1,y) = F'(1,y)^T F(1,y) = (1+y^2)\begin{pmatrix} 1 \\ 2y \end{pmatrix},$$

which implies that

$$\|\nabla\phi(1,y)\| = (1+y^2)\sqrt{1+4y^2} \geq 1 \tag{2.30}$$

for all y. The line $\mathcal{T}$ therefore is not only disjoint from the solution set $\{(0,0)\}$ of (2.27), but contains *no* stationary points for $\phi = \frac{1}{2}\|F\|^2$.

Denoting by $(d_y)_k$ the second element of d_k, we observe from (2.28) that $\operatorname{sign}((d_y)_k) = -\operatorname{sign}(y_k)$, so that d always points in the direction of the singular non-stationary point $z = (1,0)$. Therefore, a backtracking line search or a line search that enforces the Wolfe conditions (2.25) would force the iterates to converge to z. (Note, from (2.29) that an exact line search would immediately lead to z.)

Thus, in this case, the length of the displacements tends to zero near z, so that the conclusion (i) of Theorem 2.2 holds. Note that the assumptions (2.6a) and (2.8) are satisfied at z but (2.6b) is violated.

2.1 Regularized Newton Method

In many practical implementations of Newton's method for systems of nonlinear equations, a modification is introduced if the Jacobian matrix is singular or nearly singular. One of these mechanisms consists of introducing a trust region to control the size and quality of the step. A more common modification, found in many areas of application, consists of introducing a (fixed) regularization parameter whose objective is to ensure that the iteration matrix of the line search Newton method is not close to singular.

One could speculate that singular non-stationary points of the type described above do not pose real difficulties in practice since the modified iteration will not converge to them. This is indeed the case when trust region techniques are employed. However, as we now show by means of an example, if the modification takes the form of a regularization using a fixed parameter, the line search iteration can be very inefficient in the presence of singular non-stationary points.

Suppose that the standard Newton equations (1.1a) are replaced by

$$(F'(x_k)^T F'(x_k) + \rho I)d = -F'(x_k)^T F(x_k), \tag{2.31}$$

where $\rho \geq 0$ is chosen so that the eigenvalues of the matrix on the left hand side are greater than a certain threshold value; see for example [5, section 6.5]. A problematic aspect of this approach is the selection of the threshold value, and hence ρ. To illustrate this, we applied this modified Newton iteration to problem (2.3), using a backtracking line search on the merit function $\phi = \frac{1}{2}\|F\|^2$. The starting point was $(x_0, y_0) = (1.7, 0.1)$, which is near, but not extremely close to the singular line $y = 0$.

The regularization was performed as follows. We first choose a fixed value of ρ, and if the eigenvalues of the matrix $(F_k')^T F_k'$ are larger than or equal to ρ, then the step is computed by the standard Newton iteration (1.1a); otherwise the step is computed by (2.31). The results are given in Table 1 for various values of the parameter ρ. We report the total number of iterations performed (iter), the number of iterations in which the step was computed by (2.31) (# reg), and the final values of $\|F\|$ and $\|\nabla\phi\|$. We terminated the iteration when $\|F_k\| < 10^{-6}$, or when the line search could not produce a lower value of the merit function after 100 trials. We also imposed a limit of 1000 iterations. This example indicates that

ρ	iter	# reg	final $\|F\|$	final $\|\nabla\phi\|$
0	25#	0	9.585e+00	4.662e+00
$\sqrt{\texttt{macheps}}$	1000*	495	9.585e+00	4.662e+00
1e-4	1000*	452	9.563e+00	4.774e+00
1e-2	1000*	940	1.629e-04	9.034e-07
1e-1	1000*	994	1.392e-03	1.492e-05

Table 1: Regularized Newton method (2.31) on Example 1. (#) Line search failed, (*) maximum number of iterations reached; `macheps` $= 2.22 \times 10^{-16}$.

singular non-stationary points can be troublesome for a line search Newton iteration, even for a large value of the regularization parameter, such as $\rho = 0.1$. We note that in these runs the largest eigenvalue of $(F_k')^T F_k'$ was of order 100, so that the regularization value $\rho = 0.1$ is not numerically insignificant with respect to this large eigenvalue.

A regularization based on the singular value decomposition does not perform any better in this example. We implemented it as follows. At the current iterate x_k, we compute the singular value decomposition (2.7) of $F'(x_k)$, and based on it, we define the modification

$$U_k \bar{\Sigma}_k V_k^T,$$

where the diagonal entries of $\bar{\Sigma}_k$ are given by

$$\bar{\sigma_i} = \max(\sigma_i,\ \rho) \qquad i = 1, \ldots, n.$$

and $\rho > 0$ is the regularization parameter. The modified Newton direction is defined as

$$d_k = -V_k \bar{\Sigma}_k^{-1} U_k^T F_k.$$

Applying this method with the same initial point and backtracking line search as before, we observed that, for $\rho = 0.1$, the distance to the solution is still $\|x_k - x_*\| = O(10^{-2})$ after 1000 iterations. In 963 of these iterations the modification occurred. Smaller values of ρ gave similar, or worse performance.

Given that regularization techniques were so unsuccessful on this problem, it is interesting to ask how a trust region method would perform on this problem. From the point of view of global convergence theory, trust region methods are not affected by singular non-stationary points, but we would like to observe their behavior on Example 1. To this end, we consider the Levenberg-Morrison-Marquardt trust region method (see e.g. [4]) that computes a step d by solving the subproblem

$$\min_d \|F_k + F_k' d\|^2 \qquad \text{subject to} \quad \|d\| \leq \Delta_k,$$

where Δ_k is the trust region radius. It is well known that the solution of this problem has the form (2.31), for some value $\rho \geq 0$.

We solved problem (2.3) using the Fortran code LMDER from the MINPACK package [11] which implements the Levenberg-Morrison-Marquardt method, using again the starting point $(1.7, 0.1)$. In Table 2 we report whether the step reduced the merit function $\|F\|$ sufficiently and was accepted, or whether it was rejected; the value of the merit function; and the "Levenberg-Marquardt" parameter chosen by the algorithm, which is the value of ρ in (2.31). We also report the eigenvalues of $(F_k')^T F_k'$. The iteration was stopped when $\|F_k\| \leq 10^{-6}$. The Levenberg-Morrison-Marquardt method was very efficient in this example, taking only 12 iterations to solve the problem to the prescribed accuracy. Note that the parameter ρ varied significantly, taking values within the wide range $[0, 401]$. Also observe that once the iterates reached a neighborhood of the solution, pure Newton steps (with $\rho = 0$) were taken during the last 4 iterations. (We note that the value of ρ reported in the table is that used to obtain the function value in the next line; in particular $\rho = 4.010$e-02 gave rise to a successful step with the new function value 2.319.)

It is also clear that this toy problem can be solved by taking a few steepest descent steps on the squared residual, and then reverting to Newton's method. However, it is quite likely that a realistic difficult problem of this type might also have severe ill-conditioning that could cause these steepest descent steps to make very slow progress.

3 Unconstrained Minimization

We have seen in the previous section that a line search Newton iteration for solving systems of nonlinear equations can be attracted to singular non-stationary points. We now study

iter		$\|F\|$	ρ	eigenvalues of $(F_k')^T F_k'$	
0		9.615e+00	2.743e+00	1.111e+00	1.439e-01
1	Rejected	1.110e+01	1.689e+01	7.713e-01	2.764e+01
2	Accepted	9.492e+00	1.984e+01	1.216e+00	1.896e-01
3	Accepted	9.322e+00	1.984e+01	1.408e+00	1.179e-01
4	Accepted	9.030e+00	1.256e+01	5.041e-02	2.163e+00
5	Accepted	6.419e+00	7.030e-03	1.629e-03	1.726e+02
6	Rejected	2.014e+01	4.010e+02	1.536e-02	1.872e+03
7	Accepted	2.319e+00	1.983e-04	7.250e-05	3.540e+03
8	Accepted	6.773e-01	0.000e+00	3.358e-05	1.327e+04
9	Accepted	1.784e-05	0.000e+00	1.427e-08	1.000e+04
10	Accepted	4.461e-06	0.000e+00	3.569e-09	1.000e+04
11	Accepted	1.115e-06	0.000e+00	8.923e-10	1.000e+04
12	Accepted	2.788e-07			

Table 2: Levenberg-Morrison-Marquardt trust region method on Example 1.

whether a similar phenomenon can take place when solving an unconstrained minimization problem,

$$\min\ f(x), \tag{3.1}$$

where $f : I\!R^n \to I\!R$ is a smooth function. We will consider the Newton iteration

$$\begin{aligned} \nabla^2 f(x_k) d_k &= -\nabla f(x_k) && (3.2a) \\ x_{k+1} &= x_k + \alpha_k d_k, && (3.2b) \end{aligned}$$

where α_k is a steplength chosen to satisfy the Wolfe conditions

$$\begin{aligned} f(x_k + \alpha_k d_k) &\leq f(x_k) + \eta\, \alpha_k \nabla f(x_k)^T d_k && (3.3a) \\ \nabla f(x_k + \alpha_k d_k)^T d_k &\geq \beta\, \nabla f(x_k)^T d_k, && (3.3b) \end{aligned}$$

where the constants η and β satisfy $0 < \eta < \beta < 1$.

We would like to know whether this iteration can converge to a singular non-stationary point z, which we define as follows.

Definition 3.1 *A point $z \in I\!R^n$ is called a* singular non-stationary point *for the unconstrained optimization problem* (3.1) *if*

$$\nabla f(z) \neq 0, \qquad \textit{and} \qquad \nabla^2 f(z) \textit{ is positive semi-definite and singular.}$$

We begin by introducing some notation. We denote the eigenpairs of $\nabla^2 f(x_k)$ by

$$\lambda_1^k \geq \cdots \geq \lambda_n^k \quad \text{and} \quad v_1^k, \ldots, v_n^k, \tag{3.4}$$

and let

$$\lambda_1 \geq \cdots \geq \lambda_n \quad \text{and} \quad v_1, \ldots, v_n$$

denote the eigenpairs of $\nabla^2 f(z)$. We assume that the eigenvectors always form an orthonormal set.

The question of whether the Newton iteration (3.2) can converge to a singular non-stationary point was posed by Fletcher [7, p. 121] while comparing the convergence properties of algorithms for nonlinear equations and optimization. However, to the best of our knowledge, this question has not been investigated. Fletcher states (using our notation):

> [I]f $F'(x_k)$ loses rank in the limit, then convergence [of Newton's method for systems of equations] to a non-stationary point can occur [13]. The situation may therefore be more severe than with Newton's method for minimization, for which no such example (with $x_k \to z$, $\nabla f(z) \neq 0$, $\{\nabla^2 f(x_k)\}$ positive definite and $\nabla^2 f(z)$ singular) has been developed to my knowledge.

We now establish a result showing that, in many cases, the Newton iteration cannot converge to a singular non-stationary point.

Theorem 3.2 *Suppose that f is twice continuously differentiable, and that $\nabla^2 f(x_k)$ is positive definite for all k so that the Newton iteration* (3.2)–(3.3) *is well defined. Assume that $z \in I\!R^n$ is a singular non-stationary point of problem* (3.1), *with* $\text{rank}(\nabla^2 f(z)) = n-1$, *and that $\nabla f(z) \notin \mathcal{R}(\nabla^2 f(z))$. Then, the iterates $\{x_k\}$ are bounded away from z.*

Proof. As in the previous section, it will be useful to work with a merit function based on a normalized direction, and therefore we define

$$h_k(\tau) = f(x_k + \tau d_k/\|d_k\|). \tag{3.5}$$

Then

$$h_k'(0) = \nabla f_k^T d_k/\|d_k\|, \qquad h_k''(\tau) = d_k^T \nabla^2 f(x_k + \tau \frac{d_k}{\|d_k\|}) d_k/\|d_k\|^2. \tag{3.6}$$

Note from (3.2*b*) that the total displacement is

$$\tau_k = \alpha_k \|d_k\| = \|x_{k+1} - x_k\|. \tag{3.7}$$

We can write the curvature condition (3.3*b*) as

$$h_k'(\tau_k) \geq \beta h_k'(0).$$

This expression and the mean value theorem give

$$h_k'(\tau_k) = h_k'(0) + \tau_k h_k''(\xi_k) \geq \beta h_k'(0), \tag{3.8}$$

for some scalar $\xi_k \in (0, \tau_k)$. Let us assume that x_k is not a stationary point, so that $h_k'(0) < 0$. This fact, inequality (3.8), and the assumption $\beta < 1$, imply that $h_k''(\xi_k) > 0$. Therefore

$$\tau_k \geq \frac{(\beta - 1) h_k'(0)}{h_k''(\xi_k)}. \tag{3.9}$$

Using (3.2) and (3.4) we have that

$$d_k = -\sum_{i=1}^{n-1} \frac{(\nabla f_k^T v_i^k)}{\lambda_i^k} v_i^k - \frac{(\nabla f_k^T v_n^k)}{\lambda_n^k} v_n^k,$$

and recalling (3.6), we obtain

$$h_k'(0) = -\frac{\sum_{i=1}^{n-1} (\nabla f_k^T v_i^k)^2/\lambda_i^k + (\nabla f_k^T v_n^k)^2/\lambda_n^k}{\sqrt{\sum_{i=1}^{n-1} \left(\nabla f_k^T v_i^k/\lambda_i^k\right)^2 + \left(\nabla f_k^T v_n^k/\lambda_n^k\right)^2}}. \tag{3.10}$$

With the purpose of finding a contradiction, assume that there is a subsequence $\{x_{k_i}\}$ of the iterates that converges to a singular non-stationary point z. Since $\nabla f(z) \notin \mathcal{R}(\nabla^2 f(z))$, we have that

$$\nabla f(z)^T v_n \neq 0, \tag{3.11}$$

and thus $\{\nabla f_{k_i}^T v_n^{k_i}\}$ does not tend to zero as $i \to \infty$. Therefore, as $\lambda_n^{k_i} \to \lambda_n = 0$, we have that

$$|\nabla f_{k_i}^T v_n^{k_i}|/\lambda_n^{k_i} \to +\infty.$$

Using this limit and (3.11) in (3.10), and since the other terms in the summations in (3.10) are bounded, we obtain

$$h_{k_i}'(0) \to -|\nabla f(z)^T v_n| \neq 0,$$

which shows that $\{h_{k_i}'(0)\}$ is bounded away from zero.

Recalling that $\{f(x_k)\}$ is decreasing, the first Wolfe condition (3.3a), the first equality in (3.6) and (3.7), we deduce that

$$\begin{aligned} f(x_{k_i}) - f(x_{k_{i+1}}) &\geq f(x_{k_i}) - f(x_{k_i+1}) \\ &\geq -\eta\, \alpha_{k_i} \nabla f(x_{k_i})^T d_{k_i} \\ &= -\eta\, \tau_{k_i} h_{k_i}'(0). \end{aligned} \tag{3.12}$$

Now, $f(x_{k_i}) - f(x_{k_{i+1}}) \to 0$, as $\{f(x_{k_i})\}$ is convergent. Recalling that $\{h_{k_i}'(0)\}$ is bounded away from zero, relation (3.12) implies that $\tau_{k_i} \to 0$. Also, since $\nabla^2 f$ is continuous, by (3.6) we have that $\{h_{k_i}''(0)\}$ is bounded. All these facts contradict (3.9), as they imply that, for the subsequence $\{x_{k_i}\}$, the right hand side of (3.9) is bounded away from zero while the left hand side tends to zero. □

What this result tells us is that, when $\text{rank}(\nabla^2 f(z)) = n-1$, Newton's method for minimization cannot converge to the singular non-stationary point z, except (possibly) in the fairly special case when $\nabla f(z) \in \mathcal{R}(\nabla^2 f(z))$. We have not been able to find an example of such false convergence when $\nabla f(z) \in \mathcal{R}(\nabla^2 f(z))$, nor have we investigated the case when the rank of $\nabla^2 f(x)$ is less than $n-1$. Therefore the question of whether Lemma 3.2 can be proved under weaker assumptions must be considered open. It is clear, though, that as Fletcher observes, convergence to a singular non-stationary point appears much less likely in this case than in the case of a general nonlinear system.

The assumption that $\nabla^2 f(x_k)$ is positive definite for all k may appear to be restrictive, given that $\nabla^2 f(z)$ is assumed to be singular. We make this assumption because a practical line search Newton method would modify the Hessian if its eigenvalues are not sufficiently positive, and this modification makes it even less likely that the iterates will converge to z. Thus, we are showing that even in an unfavorable situation, convergence to a singular non-sationary point cannot take place.

If we ask what it is about the case of minimization that makes such failure less likely than for nonlinear systems of equations, we observe that the Newton iteration (3.2) is special in two ways. First, it is a special case of a Newton iteration for nonlinear systems in which the Jacobian is always symmetric. Second, the line search is performed on the objective function f rather than the norm of the nonlinear system (i.e., the norm of the gradient in the unconstrained minimization case). It appears that this second factor is crucial, since in the case of minimization the step along the Newton direction minimizes the objective based on first and second derivative of the objective function, but when we do a line search on the norm of the nonlinear system we do not have (with Newton's method) access to the second derivative of that function.

4 Constrained Optimization

We now study whether convergence to singular non-stationary points can also take place in the context of constrained optimization. We will consider problems of the form

$$\min f(x) \quad \text{subject to} \quad g(x) \geq 0, \tag{4.1}$$

where $f : I\!R^n \mapsto I\!R$ and $g : I\!R^n \mapsto I\!R^m$ are smooth functions. We will restrict our attention to the behavior of interior point methods, which solve a sequence of barrier problems of the form

$$\min_x \ \psi_\mu(x) \equiv f(x) - \mu \sum_{i=1}^m \ln g_i(x), \tag{4.2}$$

where $\mu > 0$ is the barrier parameter. To facilitate the analysis, we will study algorithms that decrease μ only after the optimality conditions of the barrier problem have been satisfied to some accuracy—as opposed to algorithms that redefine μ at every iteration.

An optimization algorithm can fail to solve a problem because it never achieves feasibility, or if it does, because it cannot attain optimality. We will begin by considering the latter case, and in section 4.3 we will study failures to achieve feasibility.

4.1 Failure in the Feasible Case

The following example shows that a line search interior method in which the merit function is the norm of the perturbed KKT error, can converge to a singular non-stationary point even if all the iterates are feasible.

Example 3 Consider the one-variable problem

$$\min \tfrac{1}{3}(x-1)^3 + x \quad \text{subject to} \quad x \geq 0, \tag{4.3}$$

whose only optimal solution is $x_* = 0$. We use a primal-dual line search interior method to solve this problem. This amounts [1, 6, 9, 14] to applying the Newton iteration (1.1) to the perturbed KKT conditions for (4.3), which are given by

$$F_\mu(x, \lambda) = \begin{pmatrix} (x-1)^2 + 1 - \lambda \\ x\lambda - \mu \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{4.4}$$

where λ is the Lagrange multiplier. Let us choose the barrier parameter as $\mu = 0.01$. After some algebraic manipulations one can show that the system (4.4) has only one solution, which is approximately $(5 \times 10^{-3}, 1.99)$, and which satisfies the non-negativity bounds

$$x, \lambda > 0. \tag{4.5}$$

Moreover, one can also show that this solution is the only stationary point of the merit function

$$\phi_\mu(x, \lambda) = \tfrac{1}{2}\|F_\mu(x, \lambda)\|^2. \tag{4.6}$$

It would therefore appear that this merit function is appropriate for this problem; see [9, section 5.1], [6].

We applied Newton's method to (4.4) with μ fixed at 0.01. The steplength α_k was computed by means of a backtracking line search on (4.6), starting always with the steplength of 1 and keeping the iterates interior by means of a fraction to the boundary rule of the form $(x_{k+1}, \lambda_{k+1}) \geq (1-\tau)(x_k, \lambda_k)$ with τ set to a small positive number. The initial point is chosen as $(x_0, \lambda_0) = (5, 1)$, which is feasible. Table 3 reports the output of the run.

As the table indicates, the search directions tend to become orthogonal to $\nabla\phi_\mu$, and the steplengths α_k and total displacements $x_{k+1} - x_k$ tend to zero. We should note that the backtracking line search based on the merit function (4.6) automatically ensured that the iterates remained well inside the positivity constraints (4.5), so that bounds (4.5) did not need to be enforced explicitly. The algorithm terminated at iteration 15 when the line search procedure failed to reduce the value of ϕ_μ. The final iterate is, to five digits, $z = $ (9.6364e-01, 7.0085e-02).

Note that the behavior of the iteration is very similar to that observed for the nonlinear system of equations described in Example 1. In fact, since the merit function is given by (4.6), we can view the use of the interior method as the application of a standard line search Newton method to the nonlinear system (4.4). In this light, the point z can be considered as a singular non-stationary point (see (2.2)) since $F'_\mu(z)$ is numerically singular, and since z is neither a solution of (4.4) nor a stationary point of the merit function. It is also easy to verify that the conditions (2.6) and (2.8) are satisfied by the function F_μ at the limit point $z = $ (9.6364e-01, 7.0085e-02), so that by Theorem 2.2 it is not surprising that the algorithm grinds to a halt here.

In summary, the iteration was unable to sufficiently reduce the optimality conditions of the barrier problem, as measured by the norm of the KKT error, ϕ_μ. If the interior method

k	x_k	λ_k	α_k	$\cos(\nabla\phi_\mu, d_k)$	ϕ_μ	$\|\nabla\phi_\mu\|$
0	5.0000e+00	1.0000e+00	1.00e+00	-9.79e-01	1.40e+02	1.33e+02
1	2.9271e+00	4.1659e-01	1.00e+00	-9.69e-01	9.96e+00	1.71e+01
2	1.7485e+00	1.7115e-01	1.00e+00	-8.94e-01	1.01e+00	2.31e+00
3	7.7378e-01	1.0113e-01	6.25e-02	-2.80e-01	4.54e-01	9.92e-01
4	9.7547e-01	6.9258e-02	2.44e-04	-2.20e-02	4.35e-01	8.76e-01
5	9.6445e-01	7.0026e-02	1.91e-06	-1.50e-03	4.35e-01	8.78e-01
6	9.6319e-01	7.0117e-02	4.77e-07	-8.29e-04	4.35e-01	8.78e-01
7	9.6375e-01	7.0076e-02	2.98e-08	-2.20e-04	4.35e-01	8.78e-01
8	9.6362e-01	7.0086e-02	4.66e-10	-2.67e-05	4.35e-01	8.78e-01
9	9.6364e-01	7.0084e-02	1.46e-11	-5.21e-06	4.35e-01	8.78e-01
10	9.6364e-01	7.0085e-02	7.11e-15	-1.13e-07	4.35e-01	8.78e-01
11	9.6364e-01	7.0085e-02	3.47e-18	-2.19e-09	4.35e-01	8.78e-01
12	9.6364e-01	7.0085e-02		-6.93e-10	4.35e-01	8.78e-01

Table 3: Primal dual interior method with merit function (4.6) on Example (4.3).

required a higher accuracy in this optimality measure, then the algorithm would fail by converging to the singular non-stationary point z of the barrier problem. □

Let us discuss the significance of Example 3. The fact that the primal-dual iteration can fail (for a fixed value of μ) does not follow from Example 1, since a primal-dual system such as (4.4) always contains one or more equations involving products of variables, namely the perturbed complementarity conditions. This is not the case in the system (2.3), and therefore, it is not clear from the discussion in section 1 that convergence to stationary points can be proved for systems of the primal-dual form. As was the case with Example 1, the failure of Newton's method in Example 3 can be remedied if one is willing to use a trust region method. In the next subsection we consider an approach that will get around this problem by using a different merit function.

4.2 Globally Convergent Feasible Methods.

We now address the question of whether failures of the type just described can occur with methods that enforce descent on other, more appropriate, merit functions. If all the iterates are feasible, the merit function can be chosen simply as the barrier function (4.2). It turns out that, for this choice of merit function, a feasible interior method cannot converge to singular non-stationary points if certain precautions are taken to control the Hessian approximation. To see this, we describe the interior point iteration in more detail.

The perturbed KKT conditions for problem (4.1) are given by

$$\nabla f(x) - A(x)\lambda = 0 \tag{4.7a}$$

$$G(x)\lambda - \mu e = 0, \tag{4.7b}$$

where $\lambda \in I\!R^m$ are the Lagrange multipliers estimates, $A(x)^T$ is the Jacobian of $g(x)$, $G(x)$ is a diagonal matrix with diagonal elements $G(x)_{ii} = g_i(x)$, and e is the m-vector of all ones. The search direction of a feasible primal-dual interior method is obtained by applying Newton's method to (4.7) at the current iterate (x_k, λ_k), giving

$$\begin{bmatrix} \nabla^2 \mathcal{L}_k & -A_k \\ \Lambda_k A_k^T & G_k \end{bmatrix} \begin{pmatrix} d_x \\ d_\lambda \end{pmatrix} = - \begin{pmatrix} \nabla f_k - A_k \lambda_k \\ G_k \lambda_k - \mu e \end{pmatrix}, \tag{4.8}$$

where

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i=1}^{m} \lambda_i g_i(x)$$

is the Lagrangian of the nonlinear program (4.1) and Λ_k is a diagonal matrix satisfying $\Lambda_k e = \lambda_k$.

Assume that the steplength α_k is determined by a line search that satisfies the Wolfe conditions (3.3) on the barrier function ψ_μ, given by (4.2).

The matrix G_k is positive definite for all k since we assume that all iterates are strictly feasible with respect to the constraint $g(x) \geq 0$. Therefore we can rewrite (4.8) as

$$\left[\nabla^2 \mathcal{L}_k + A_k G_k^{-1} \Lambda_k A_k^T\right] d_x = -\nabla f_k + \mu A_k G_k^{-1} e = -\nabla \psi_\mu(x_k) \tag{4.9a}$$

$$d_\lambda = -\lambda_k + G_k^{-1}(\mu e - \Lambda_k A_k^T d_x). \tag{4.9b}$$

If the coefficient matrix in (4.9a) is positive definite, then the search direction can be shown to be a descent direction for a variety of merit functions including ψ_μ; otherwise, there are practical ways to modify it so that its eigenvalues are bounded above and away from zero for all k [8, 9, 14]. We will assume here that such a matrix modification is performed.

This approach is thus similar to that used in unconstrained optimization, where global convergence can be proved under standard assumptions [5, 12] if the modified Hessian approximations have eigenvalues bounded above and away from zero. The only difficulty in applying that standard analysis to this case is that the unboundedness in the derivatives in ψ_μ might cause steps to become arbitrarily short. However, it can be shown (see [3]) that this cannot occur by noting that all iterates must remain in a level set where ψ_μ is well-behaved, and the line segment between successive iterates can go outside this set only if the step has a significant length.

We can conclude therefore that failures like that in Example 3 cannot occur in a feasible primal dual method using ψ_μ as a merit function provided that the Hessian is modified if necessary to guarantee a descent direction. Thus rank deficiency in the Jacobian does not cause difficulties under these conditions. It is reasonable to consider whether the difference between the situation here and Example 3 is due to a different merit function, or to the change in the Newton step caused by the Hessian modification. Clearly, both are important, but it should be noted that if the Hessian is positive definite everywhere, the modification is not required.

We now consider the possibility of failure of algorithms that do not stay feasible.

4.3 Failure To Achieve Feasibility

As we mentioned at the beginning of this section, an interior method can fail because it cannot attain feasibility. Wächter and Biegler [15] describe a problem for which a general class of interior methods is unable to generate a feasible point, even in the limit. An instance of their problem is given by

$$
\begin{aligned}
& && \min \; f(x) && && (4.10a)\\
&\text{subject to} && (x_1)^2 - x_2 - 1 &&= 0 && (4.10b)\\
& && x_1 - x_3 - 2 &&= 0 && (4.10c)\\
& && x_2 \geq 0, \; x_3 &&\geq 0, && (4.10d)
\end{aligned}
$$

where the objective $f(x)$ is any smooth function. They show that, for a large choice of starting points, the iterates remain bounded away from the feasible region and from any stationary point of the norm of the constraints. This failure of the iteration takes place regardless of the choice of merit function, and with any iteration that imposes the linearized equality constraints

$$h(x_k) + h'(x_k)d = 0, \tag{4.11}$$

where $h(x) = 0$ denotes the equality constraints (4.10b)–(4.10c). What occurs with a typical implementation is that steps towards satisfaction of (4.11) are blocked by the bounds, forcing the step to be truncated. The iterates converge to a point on the edge of the bounds where the gradients of all active constraints are dependent. The presence of the bounds plays a key role in blocking progress toward feasibility.

We now describe an example of a different kind, in which a class of of Newton methods cannot attain feasibility, regardless of the choice of merit function and of the step selection strategy. In this example the failure is of a different nature than that of problem (4.10), because the bounds on the variables play no role.

Example 4 Consider the problem

$$
\begin{aligned}
& && \min \; f(x,y,z) && && (4.12a)\\
&\text{subject to} && x + y^2 &&= 0 && (4.12b)\\
& && 2(x-1)y &&= 0 && (4.12c)\\
& && z &&\geq -1 && (4.12d)
\end{aligned}
$$

where $f : \mathbb{R}^3 \to \mathbb{R}$ is any smooth function. Notice that the equalities (4.12*b*)–(4.12*c*) are those in the system of equations (2.27) from Example 2. The feasible region for problem (4.12) is the half line $\{(x,y,z) : x = y = 0, z \geq -1\}$. We will show that, for a range of infeasible initial points (x_0, y_0, z_0), any line search algorithm whose search direction d satisfies the linearization of the constraints (4.12*b*)–(4.12*c*) will never achieve feasibility (even asymptotically) nor converge to a stationary point of constraint violation.

Defining $F(x,y,z) = (x + y^2, 2(x-1)y)^T$, we can now reason as in Example 2 (except for the presence of the variable z, which plays no role). Consider the plane

$$\mathcal{P} = \{(1, y, z) : y, z \in \mathbb{R}\},$$

which is disjoint from the feasible region. If $(x_k, y_k, z_k) \in \mathcal{P}$, with $y_k \neq 0$, and the search direction d satisfies $F_k + F_k' d = 0$, then it follows from (2.28) that d has the form

$$d = (0, -\frac{1+y_k^2}{2y_k}, d_z) \qquad d_z \in I\!R.$$

This implies that $(x_{k+1}, y_{k+1}, z_{k+1}) = (x_k, y_k, z_k) + \alpha d$ will also belong to $\mathcal{P}$ for any positive steplength α, and therefore the iterates will never become feasible. Moreover, the gradient of the constraint violation $\phi(x, y, z) = \frac{1}{2}\|F(x, y, z)\|^2$ is bounded away from zero on $\mathcal{P}$, as from (2.30) we have that $\|\nabla\phi(1, y, z)\| \geq 1$ for all $y, z \in I\!R$. $\square$

The examples and analysis in this section show that failure of a feasible primal-dual iteration can occur with a KKT-based merit function of the form (4.6), but, under certain conditions, failure will not occur with the barrier function (4.2) as a merit function. With a method that generates infeasible iterates failure can take place in the neighborhood of a point where that active constraints are dependent. This can occur because of the effect of bounds or inequality constraints as in the example of Wächter and Biegler or without involvement from bounds as in Example 4, which displays essentially the same type of failure that occurs in Examples 1 and 2.

5 Final Remarks

We have provided new results about the behavior of standard line search Newton iterations in the vicinity of singular non-stationary points. Newton iterations of this kind are extensively used in many areas of computational mathematics to solve nonlinear systems of equations, and have recently received much attention in the context of interior methods for constrained optimization. Our results show that in some cases singular non-stationary points can be problematic, but in other cases they are not.

The failures and inefficiencies discussed in this paper can be avoided by means of trust region techniques (see [10] for a survey or [4] for an extensive treatment of the subject) or by a modification of line search methods (see e.g. [16] for a recent modification that includes a feasibility restoration phase). We have not discussed these, more robust, techniques in this paper. Instead we have focused exclusively on the behavior of simple line search Newton iterations, which are still more widely used in practice than trust region implementations, and whose properties must be well understood.

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