INEXACT - NEWTON METHODS AND THE COMPUTATION OF SINGULAR POINTS

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ABSTRACT – The inexact-Newton method is frequently used for solving large-scale nonlinear systems of equations. In this paper we introduce a new globally convergent version of the method to the problem of finding singular points of $H(y,t) = 0$, where $H : \mathbb{R}^{m+1} \to \mathbb{R}^m$. We present numerical experiments.

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INEXACT - NEWTON METHODS AND THE COMPUTATION OF SINGULAR POINTS [*]

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Abstract. The inexact-Newton method is frequently used for solving large-scale nonlinear systems of equations. In this paper we introduce a new globally convergent version of the method to the problem of finding singular points of $H(y,t) = 0$, where $H : \mathbb{R}^{m+1} \to \mathbb{R}^m$. We present numerical experiments.

Keywords. Inexact - Newton method, global convergence, singular points, turning points.

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1 Introduction

The inexact-Newton method is one of the most successful techniques for solving nonlinear systems of equations

$$F(x) = 0, \tag{1}$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ is differentiable (we denote $J(x) \equiv F'(x)$, the Jacobian matrix of F). According to [3], at each iteration k of the inexact-Newton method, an increment $s_k \in \mathbb{R}^n$ is computed such that

$$\|J(x_k)s_k + F(x_k)\| \leq \theta_k \|F(x_k)\|, \tag{2}$$

where $x_{k+1} = x_k + s_k$, $\theta_k \in [0, \theta]$ for all $k \in N$ and $0 < \theta < 1$. The increment s_k is usually obtained by means of an iterative linear solver. So, matrix factorizations are avoided, which is an attractive feature for large problems. Many authors analyzed the inexact-Newton ideas from different points of view: affine invariancy ([23], [4]), preconditioning ([12], [13], [14]), global convergence [5], nonsmooth problems [15], etc.

In [3], the local convergence of (2) is analyzed. If x_* is a solution of (1) where $J(x_*)$ is nonsingular, local linear convergence (in the norm $\|z\|_* = \|J(x_*)z\|$) takes place and, if $\theta_k \to 0$, the convergence is q-superlinear.

In this paper, we apply the inexact-Newton method to the computation of *singular points* of an homotopic path. See [19]. This is a subject of permanent interest in physical and engineering applications, as well as in the efficient computation of solution paths of

$$H(y, t) = 0, \tag{3}$$

where $H : \mathbb{R}^{m+1} \to \mathbb{R}^m$. A singular point is a solution of (3) where the $m \times m$ Jacobian matrix $H_y(y, t)$ is singular. When the rows of $H'(y, t)$ are linearly independent (so, $H_t(y, t)$ does not belong to the range of $H_y(y, t)$), the singular point is called a *turning point.* Several methods have been proposed for computing turning points where the system (3) is enlarged and the nonsingularity of the Jacobian matrix of the expanded system is guaranteed. See [17], [16], [1]. All these methods involve some type of factorization of matrices, which is inconvenient in large problems. This motivates the use of the inexact-Newton method for these problems.

In Section 2 of this paper we introduce a very general scheme, which allows us to define a globally convergent inexact-Newton algorithm. In Section 3 we describe an

implementation of the algorithm. In Section 4 we introduce new enlarged systems whose solutions correspond to singular points of (3). In Section 5 we show numerical experiments using the globalized inexact-Newton methods for solving the enlarged systems of Section 4. Most of the experiments are taken from a collection of Melhem and Rheinboldt [16]. Conclusions are stated in Section 6.

2 Globally convergent algorithm

In this section we introduce a globally convergent algorithm for solving (1) which can be implemented with directions generated by the inexact-Newton method. Our approach is similar to the one of Eisenstat and Walker [5] and Martínez and Qi [15] but we are more general so that strategies not based on line-searches can be considered.

As usually, the idea is to consider the sum of squares of $F(x)$ as merit function:

$$f(x) = \frac{1}{2}\|F(x)\|^2, \tag{4}$$

and to define an algorithm which, essentially, reduces monotonically $f(x_k)$. The description of the algorithm follows. In this section $\|.\|$ represents the Euclidean norm.

Algorithm 2.1. Assume that $\sigma \in (0,1)$, $\gamma \in (0,1]$, $\eta_1, \eta_2 \in (0,1)$, $\eta_1 < \eta_2$ are given independently of k. $x_0 \in I\!R^n$ is an arbitrary initial approximation and $\alpha_0 = 1$. Given $x_k \in I\!R^n$, $\alpha_k \in (0,1]$, the steps for obtaining x_{k+1}, α_{k+1} are:

Step 1. Choose

$$d_k \in I\!R^n. \tag{5}$$

Step 2. If

$$f(x_k + \alpha_k d_k) < f(x_k) \tag{6}$$

compute $x_{k+1} = x_k + \alpha_k d_k$. If (6) does not hold, define $x_{k+1} = x_k$.

Step 3. If

$$f(x_{k+1}) \leq (1 - \sigma\gamma\alpha_k) f(x_k) \tag{7}$$

define $\alpha_{k+1} = 1$. Otherwise, choose

$$\alpha_{k+1} \in [\eta_1\alpha_k, \eta_2\alpha_k]. \tag{8}$$

Algorithm 2.1 is extremely general. No conditions are assumed on the directions d_k and, in fact, even the null directions $d_k \equiv 0$ are admitted. However, a simple "global convergence lemma" can still be proved.

Lemma 2.1. *Let $\{x_k\}$ be the sequence generated by Algorithm 2.1. Let us call $K_1 = \{k \in N \mid (7) \text{ holds}\}$. If K_1 is infinite and $\limsup_{k \in K_1} \alpha_k > 0$ then*

$$\lim_{k \to \infty} \|F(x_k)\| = 0. \tag{9}$$

Proof. Assume that K_2 is an infinite subset of K_1 such that

$$\alpha_k \geq \bar{\alpha} > 0$$

for all $k \in K_2$. Then

$$1 - \sigma\gamma\alpha_k \leq 1 - \sigma\gamma\bar{\alpha} \equiv r < 1$$

for all $k \in K_2$. Therefore $\{f(x_k)\}$ is a nonincreasing sequence such that $f(x_{k+1}) \leq rf(x_k)$ for all $k \in K_2$. This implies that $f(x_k) \to 0$ and, thus, (9) holds. □

In the following theorem, some conditions are imposed on the directions d_k so that a more interesting convergence result can be proved.

Theorem 2.2. *Assume that $\{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\}$ is bounded. Let $\{x_k\}$ be the sequence generated by Algorithm 2.1. Assume that there exists $M > 0$ such that for all $k = 0, 1, 2, \ldots$,*

$$\|d_k\| \leq M \tag{10}$$

and

$$\langle J(x_k)d_k, F(x_k)\rangle \leq -\frac{\gamma}{2}\|F(x_k)\|^2 . \tag{11}$$

Then

(a) Any limit point x_* of $\{x_k\}$ satisfies $F(x_*) = 0$.

(b) If a limit point x_* is an isolated solution of (1) and $\alpha_k \to 0$, then $\{x_k\}$ converges to x_*.

(c) If a limit point x_* is an isolated solution of (1) and there exists $\beta > 0$ such that $\|d_k\| \leq \beta\|F(x_k)\|$ for all $k = 0, 1, 2, \ldots$, then $\{x_k\}$ converges to x_*.

Proof. Let K_1 be as in Lemma 2.1. If K_1 is infinite and $\limsup_{k\in K_1} \alpha_k > 0$ the desired result follows from Lemma 2.1 and the continuity of F. So, the following possibilities remain to be considered: (i)

$$K_1 \text{ is finite;} \tag{12}$$

(ii)

$$K_1 \text{ is infinite but } \lim_{k\in K_1} \alpha_k = 0. \tag{13}$$

Let us consider first (ii). By the compactness of the level set of f, there exists $x_* \in \mathbb{R}^n$ and K_2, an infinite subset of K_1 such that

$$\lim_{k\in K_2} x_k = x_*.$$

Without loss of generality, assume that $\alpha_k < 1$ for all $k \in K_2$. So, by (8) and (7), we have that, for all $k \in K_2$,

$$\alpha_k \in [\eta_1\alpha_{k-1}, \eta_2\alpha_{k-1}] \tag{14}$$

and

$$f(x_{k-1} + \alpha_{k-1}d_{k-1}) > (1 - \sigma\gamma\alpha_{k-1})f(x_{k-1}). \tag{15}$$

By (13) and (14) we have that

$$\lim_{k\in K_2} \alpha_{k-1} = 0.$$

So, using (10), we see that

$$\lim_{k\in K_2} x_{k-1} = x_*.$$

Now, by (15),

$$\frac{f(x_{k-1} + \alpha_{k-1}d_{k-1}) - f(x_{k-1})}{\alpha_{k-1}} > -\sigma\gamma f(x_{k-1})$$

for all $k \in K_2$. By the Mean Value Theorem, this implies that, for all $k \in K_2$, there exists $\xi_{k-1} \in [0, 1]$ such that

$$\langle \nabla f(x_{k-1} + \xi_{k-1}\alpha_{k-1}d_{k-1}), d_{k-1}\rangle > -\sigma\gamma f(x_{k-1}). \tag{16}$$

Assume, by contradiction, that $F(x_*) \neq 0$. Then, by (11), the sequence $\{\|d_{k-1}\|, k \in K_2\}$ is bounded away from zero. So, by (10), there exists K_3, an infinite subset of K_2, and $d \neq 0$ such that

$$\lim_{k\in K_3} d_{k-1} = d.$$

Taking limits for $k \in K_3$ on both sides of (16), we obtain

$$\langle \nabla f(x_*), d \rangle \geq -\sigma\gamma f(x_*).$$

So, for large enough $k \in K_3$,

$$\langle \nabla f(x_{k-1}), d_{k-1} \rangle \geq -\frac{\sigma+1}{2}\gamma f(x_{k-1}) > -\gamma f(x_{k-1}) = -\frac{\gamma}{2}\|F(x_{k-1})\|^2. \qquad (17)$$

But $\nabla f(x) = J(x)^T F(x)$, so

$$\langle \nabla f(x_{k-1}), d_{k-1} \rangle = \langle J(x_{k-1})^T F(x_{k-1}), d_{k-1} \rangle = \langle J(x_{k-1}) d_{k-1}, F(x_{k-1}) \rangle.$$

Therefore, (17) contradicts (11). This proves that $F(x_*) = 0$. As a result, since $\{f(x_k)\}$ is monotone, we have that any other limit point of $\{x_k\}$ must be a solution of (1).

Let us now assume (i). Since K_1 is finite, there exists $k_0 \in N$ such that (7) does not hold for all $k \geq k_0$. Therefore, $\alpha_k \to 0$ and we can repeat the preceeding proof, with minor modifications, for proving that any limit point must be a solution of (1).

Let us now prove (b). Since x_* is an isolated solution of (1), there exists $\delta > 0$ such that x_* is the unique global minimizer of $\|F(x)\|$ for $\|x - x_*\| \leq \delta$. Since $\alpha_k \to 0$, by (10), we have that $\|x_{k+1} - x_k\| \to 0$. Let $\delta' \in (0, \delta)$. Let $k_0 \in N$ be such that $\|x_{k+1} - x_k\| < \delta - \delta'$ whenever $k \geq k_0$. Let $\mu > 0$ be the minimum value of $\|F(x)\|$ on the region $\delta' \leq \|x - x_*\| \leq \delta$. Let $k_1 \geq k_0$ be such that $\|x_{k_1} - x_*\| \leq \delta'$ and $\|F(x_{k_1})\| < \mu$. Since $\|F(x_{k_1+1})\| < \|F(x_{k_1})\|$, we have that $\|F(x_{k_1+1})\| < \mu$. But, since

$$\|x_{k_1+1} - x_{k_1}\| \leq \delta - \delta',$$

we also have that $\|x_{k_1+1} - x_*\| \leq \delta$. So, by the definition of μ, $\|x_{k_1+1} - x_*\| \leq \delta'$. It follows, by induction, that $\|x_k - x_*\| \leq \delta'$ and $\|F(x_k)\| < \mu$ for all $k \geq k_1$. Since x_* is the unique accumulation point of x_k in this region, it follows that $\{x_k\}$ converges to $\{x_*\}$. This proves (b).

The proof of (c) is similar. Define δ as in the proof of (b) and $\delta' \in (0, \delta)$ such that

$$\|x_{k+1} - x_k\| \leq \|d_k\| \leq \beta\|F(x_k)\| \leq \delta - \delta'$$

whenever $\|x_k - x_*\| \leq \delta'$. The proof is completed as in (b). □

Essentially, Theorem 2.2 says that, if we are able to compute search directions d_k such that the conditions (10) and (11) are satisfied at each iteration, then global

convergence to a solution of the system is ensured. If $J(x_k)$ is nonsingular, the Newton direction $d_k^N = -J(x_k)^{-1}F(x_k)$ satisfies (11) with $\gamma = 1$. More generally, if d_k satisfies

$$\|J(x_k)d_k + F(x_k)\|^2 \leq t\|F(x_k)\|^2, \tag{18}$$

with $t \in [0,1)$ we have that

$$\langle J(x_k)d_k, J(x_k)d_k\rangle + 2\langle J(x_k)d_k, F(x_k)\rangle \leq (t-1)\|F(x_k)\|^2$$

So,

$$\langle J(x_k)d_k, F(x_k)\rangle \leq \frac{t-1}{2}\|F(x_k)\|^2,$$

that is, the condition (11) is satisfied with $\gamma = 1 - t$. The condition (18) is a "squared version" of the classical criterion given in (2) to define the inexact-Newton iteration. We see, by Theorem 2.2, that when Newton's method (or the inexact Newton generalization) fails to converge, using the globalization given by Algorithm 2.1, then the generated sequence of directions d_k is unbounded. In this case, the method tends to converge to a point where the Jacobian is singular. This point is not necessarily a local minimizer, or even a stationary point of $f(x)$, as the following example shows.

Define $F(x) = (f_1(x_1, x_2),\ f_2(x_1, x_2))^T$ where

$$f_1(x_1, x_2) = -\frac{x_1^3}{3} + x_1 - x_2 + 2\,,\ f_2(x_1, x_2) = x_2.$$

This system has only one solution $x_* \approx (2.35, 0)^T$. The Jacobian is singular if $x_1 = 1$ or $x_1 = -1$. If we apply Newton's method with the globalization given by Algorithm 2.1, starting near $(-1, 0)^T$, the iterations converge to $(-1, 0)^T$, which is not a stationary point of f. The directions d_k are unbounded as we approach to $(-1, 0)^T$. In fact, Newton iterations always satisfy the linear equation $f_2(x_1, x_2) = 0$, and this region does not contain stationary points of f.

3 Implementation

In this section we describe a practical implementation of Algorithm 2.1. The idea is to choose, at each iteration, $s_k \equiv \alpha_k d_k$ as an *approximate minimizer* of

$$\psi(s) \equiv \frac{1}{2}\|J(x_k)s + F(x_k)\|^2$$

on an appropriate trust-region (see [6]) of the form $\|s\|_\infty \leq \Delta$. If 0 is not a minimizer of ψ, that is, $J(x_k)^T F(x_k) \neq 0$, we will be able to obtain s_k such that

$$\|J(x_k)s_k + F(x_k)\|^2 < \|F(x_k)\|^2$$

which implies that

$$\langle J(x_k)d_k, F(x_k)\rangle < 0.$$

independently of the value of $\alpha_k > 0$. After the computation of s_k, we test the inequalities (10) and (11). If one of them does not hold, we stop the execution (the algorithm breaks down). This necessarily happens when the problem has no solutions. The choice of the $\|.\|_\infty$ norm instead of the Euclidean norm here obeys the necessity of considering possible bounds on the variables x_i. In this case, the $\|.\|_\infty$ norm fits well with the bounds and the approximate minimizers are not difficult to find.

Algorithm 3.1

Let $\sigma \in (0,1)$, $\gamma \in (0,1]$, $\eta_1, \eta_2 \in (0,1)$, $\eta_1 < \eta_2$, $M > 0$, $tol \in (0,1)$, $max \in N$ be given independently of k and let $x_0 \in I\!R^n$ be an arbitrary initial point, $\Delta_0 = M$ and $\alpha_0 = 1$. Given $x_k \in I\!R^n$ such that $J(x_k)^T F(x_k) \neq 0$, $\Delta_k > 0$ and $\alpha_k \in (0,1]$, the steps for obtaining x_{k+1}, Δ_{k+1} and α_{k+1} are the following:

Step 1. Compute s_k as an "approximate solution" of

$$\text{Minimize } \psi(s) \equiv \frac{1}{2}\|J(x_k)s + F(x_k)\|^2 \text{ s.t. } \|s\|_\infty \leq \Delta_k. \tag{19}$$

The approximate solution of (19) is obtained applying the method described in [7] (see also [8]) stopping when

$$\|\nabla_P \psi(s_k)\| \leq tol\ \|\nabla_P \psi(0)\|, \tag{20}$$

(where $\nabla_P \psi(s)$ is the projected gradient of ψ on the box $\|s\|_\infty \leq \Delta_k$) or when the number of iterations used by the algorithm [7] exceeds max. (This guarantees that, at least $\|J(x_k)s_k + F(x_k)\| < \|F(x_k)\|$.)

Step 2. Define $d_k = s_k/\alpha_k$. If (11) and (10) hold, go to Step 3. Otherwise, stop (the algorithm breaks down, probably, by the proximity of a singular Jacobian).

Step 3. The same as Step 2 of Algorithm 2.1.

Step 4. The same as Step 3 of Algorithm 2.1.

Step 5. If $\alpha_{k+1} = 1$, define $\Delta_{k+1} = M$. Otherwise, define $\Delta_{k+1} = \|s_k\|_\infty/2$.

The parameters used in our implementation were $\sigma = 10^{-5}$, $\gamma = 10^{-4}$, $\eta_1 = \frac{1}{2}$, $\eta_2 = \frac{1}{2}$, $M = 10^{10}$, $tol = \frac{1}{10}$, $max = n$. The software used for this implementation was an adaptation of the algorithm for box constrained minimization introduced by Friedlander, Martínez and Santos [8]. The algorithm used for obtaining the approximate solution of (19) (see [7]) is an active set method that combines conjugate gradient iterations with projected and "chopped" gradient iterations in such a way that many active constraints can be added or dropped in a single iteration. The computer code was written in Fortran, using double precision, and is fairly portable.

4 Computing singular points

Given $H : \mathbb{R}^{m+1} \to \mathbb{R}^m$, $H = H(y,t)$, $H \in C^1(\mathbb{R}^{m+1})$, we say (following [17]) that (y_*, t_*) is a *singular point* of $H(y,t) = 0$ iff $H(y_*, t_*) = 0$ and $H_y(y_*, t_*)$ is singular. If rank $(H'(y_*, t_*)) = m$ we say that (y_*, t_*) is a ***turning point.*** Singular points are solutions of

$$\left.\begin{array}{l} H(y,t) = 0 \\ H_y(y,t)v = 0 \\ \|v\|^2 = 1 \end{array}\right\} \tag{21}$$

for some $v \in \mathbb{R}^m$. The system (21) has $2m+1$ equations and unknowns.

The resolution of (21) by an inexact-Newton method requires computation of second derivatives of H. However, observe that

$$H_y(y,t)v = \lim_{h \to 0} \frac{H(y+hv,t) - H(y-hv,t)}{2h}. \tag{22}$$

Therefore, it is natural to replace (21) by the system

$$\left.\begin{array}{l} H(y,t) = 0 \\ \frac{H(y+hv,t)-H(y-hv,t)}{2h} = 0 \\ \|v\|^2 = 1 \end{array}\right\} \tag{23}$$

for $h > 0$. Hopefully, the solutions of (23) for small h will be good approximations for the solutions of (21).

A second alternative is to consider, instead of (21), the system

$$\left.\begin{aligned} H(y,t) &= 0 \\ H_y(y,t)v &= 0 \\ r^T v &= 1 \end{aligned}\right\} \tag{24}$$

where $r \in \mathbb{R}^m$ does not belong to $\mathcal{R}(H_y(y,t))$ (the range of $H_y(y,t)$), which ensures that a solution of the last two equations of (24) exists. This system has been used by Moore and Spence [17] and Seydel [22]. Corresponding to (24), and using the approximation (22), we consider the system

$$\left.\begin{aligned} H(y,t) &= 0 \\ \tfrac{H(y+hv,t)-H(y-hv,t)}{2h} &= 0 \\ r^T v &= 1 \end{aligned}\right\} \tag{25}$$

The advantage of (25) over (23) is that the nonquadratic term $(\|v\|^2 - 1)^2$ in the merit function (4) has been replaced by $(r^T v - 1)^2$. However, if, by chance, we choose $r \in \mathcal{R}(H_y(y_*, t_*))$, where (y_*, t_*) is the turning point that we want to compute, the system (24) will have no solution. If the angle between r and $\mathcal{R}(H_y(y_*, t_*))$ is small, the problem of finding v satisfying $H_y(y,t)v = 0$ and $r^T v = 1$ can be very ill-conditioned, leading to unreliable results. In our experiments we used $r = v_0 = (1, \ldots, 1)^T / m^{\frac{1}{2}}$.

By direct calculation, we see that the Jacobian matrices $J_1(y,t)$ and $J_2(y,t)$ of the systems (23) and (25) are, respectively,

$$J_1(x) = \begin{bmatrix} H'(y,t) & 0 \\ \frac{H'(y+hv,t)-H'(y-hv,t)}{2h} & \frac{H_y(y+hv,t)+H_y(y-hv,t)}{2} \\ 0 & 2v^T \end{bmatrix} \tag{26}$$

and

$$J_2(x) = \begin{bmatrix} H'(y,t) & 0 \\ \frac{H'(y+hv,t)-H'(y-hv,t)}{2h} & \frac{H_y(y+hv,t)+H_y(y-hv,t)}{2} \\ 0 & r^T \end{bmatrix} \tag{27}$$

Let us emphasize that in the implementation of Algorithm 3.1 no factorizations of matrices are used. In fact we only need to provide subroutines that compute the products $J_1(y,t)w$ and $J_2(y,t)w$ for arbitrary vectors w. Due to (26) and (27), it is easy to see that fully advantage can be taken from the structure of these matrices.

5 Numerical experiments

We used six test problems described in [16] and an additional problem coming from the theory of radiative transfer (see [18], [2], [11]). We developed a specific code for each problem, using FORTRAN 77 (double precision) in a PC 486 for problems 1 to 6. The tests for problem 7 were run in a SUN Sparc Station 10.

Problem 1: A Two-bar Framework
This is the first test problem from [16] and was implemented with a slight modification in the second load vector, in order to reproduce the results of [16]. Instead of $(0.3, 0.91)$ we used $(\sqrt{0.91}, 0.3)$. As regards the limit points relative to the first load vector, we observe that $2+\frac{2}{\sqrt{3}}$ corresponds to $-\frac{16}{3\sqrt{3}}$ and $2-\frac{2}{\sqrt{3}}$ corresponds to $+\frac{16}{3\sqrt{3}}$. Problem (1.a) corresponds to the load vector $(1,0)$ and problem (1.b) corresponds to the load vector $(\sqrt{0.91}, 0.3)$.

Problem 2: The Freudenstein-Roth Function
This is the second test problem from [16] and was implemented exactly as described in such a paper.

Problem 3: An Aircraft-Stability Problem
This is the third test problem from [16] and was implemented with two worthwhile mentioning corrections, obtained from [21]: The element A_{31} is 0.0002 and, in the function $\varphi(y,u)$, the term y_4y_2 is, in fact, y_4u_2. We used five different values for the parameter $\overline{\gamma}$.

Problem 4: A Trigger Circuit
This is the fourth test problem from [16] and was implemented with two corrections, according to [20] and [22]. Instead of $-R_2^{-1}$, the element A_{17} is R_2^{-1}. The diode function is given by $g_1(u) = (5.6 \times 10^{-8})[exp(25u) - 1]$.

Problem 5: A Chemical Reaction Problem
This is the fifth test problem from [16] and was implemented with a trapezoidal rule with the following weights: $w_0 = w_n = 0.5$ and $w_i = 1$, $i = 1, \ldots, n-1$.

Problem 6: Chandrasekhar's Equation
This problem, originally introduced by Chandrasekhar [1960], has been used as a test case by many authors (see [18] [11]). We decided to replace the sixth problem from [16] (*A Shallow, Circular Arch*) by Chandrasekhar's equation because we were not able to reproduce their results, probably due to non availability of the code used in [16]. In this experiment, M is the number of points used in the numerical integration.

Problem 7: A Mildly-Nonlinear Boundary Value Problem
This is the seventh test problem from [16] and was implemented exactly as described in such a paper. Problem 7.a corresponds to $g(u) = e^u$ and Problem 7.b corresponds to $g(u) = 1 + \frac{u+\frac{u^2}{2}}{1+\frac{u^2}{100}}$. M is the number of points used in the discretization.

The results of the numerical experiments are given in Table 1. In the first column of this table we give the number of the problem considered. In the second column the initial approximation y_0, t_0 used in the experiment. In the third column we report the enlarged system considered in the experiment ((23) or (25)). In columns fourth to eigth we report the results of the experiments: obtained value for t_*, lowest singular value of H_y at the final approximation, largest singular value of H_y at this approximation, the sum of squares $f(y_*, t_*)$, number of iterations and number of function evaluations used by Algorithm 3.1, respectively.

Problem	(y_0, t_0)	Syst.	t_*	$\sigma_1(H_y)$	$\sigma_n(H_y)$	$f(y_*, t_*)$	Iter.	Eval.
1a	(3, 0), -3	(23)	-3.079205	4.86930 E-6	6.66665 E-1	9.87 E-9	9	10
		(25)	-3.079213	1.23839 E-8	6.66667 E-1	4.38 E-10	8	10
	(0, 0), 5	(23)	3.079201	5.70889 E-7	6.66666 E-1	3.72 E-10	8	9
		(25)	3.079209	6.27195 E-5	6.66646 E-1	7.23 E-9	10	14
1b	(1,1), 1	(23)	1.933818	3.94483 E-6	4.76546	1.37 E-10	4	5
		(25)	1.933836	1.30527 E-7	4.76544	9.97 E-14	5	6
	(3,1), -3	(23)	-2.307797	3.06106 E-5	2.48282	7.94 E-10	4	5
		(25)	-2.307831	1.04685 E-6	2.48281	3.73 E-10	5	6
2	(1,1), 1	(23)	5.875923 E-1	1.56757 E-6	1.89761 E1	5.18 E-9	14	22
		(25)	5.875873 E-1	5.68896 E-6	1.89762 E1	2.87 E-11	20	36
	(50, 10), -10	(23)	-6.863575 E-1	6.65021 E-5	7.73971	8.05 E-9	16	33
		(25)	-6.863527 E-1	3.45522 E-8	7.73994	1.00 E-14	24	53
3 $\bar{\gamma} = -0.05$	(-3,1,-.1,.5,-.3),0.5	(23)	5.087968 E-1	1.26152 E-5	2.20649 E2	1.56 E-10	68	139
		(25)	5.087889 E-1	2.64036 E-6	2.20615 E2	1.04 E-9	341	561
3 $\bar{\gamma} = -0.008$	(-3,-.2,-.1,.02,.1), 0.2	(23)	2.063399 E-1	5.17399 E-5	4.99307 E1	9.74 E-9	33	52
		(25)	2.065148 E-1	2.07148 E-6	4.99492	5.07 E-9	49	73
3 $\bar{\gamma} = 0.$	(-3,-.2,-.1,.02,.1), 0.2	(23)	1.872326 E-1	1.09060 E-5	5.86032 E1	1.08 E-10	37	65
		(25)	3.887898 E-1	1.62702 E-3	4.70969 E1	8.62 E-4	500	950
3 $\bar{\gamma} = 0.05$	(-2.5,-.8,.03,-.04),0.3	(23)	2.929449 E-1	4.55929 E-5	1.84044 E2	9.12 E-9	22	37
		(25)	2.929395 E-1	7.84537 E-6	1.84049 E2	2.60 E-10	61	77
3 $\bar{\gamma} = 0.1$	(-2.5,1.5,.06,-.08,.6),0.7	(23)	9.227714 E-2	3.46267 E-1	7.96651 E1	1.02 E-1	60	165
		(25)	2.789284 E-2	2.26696 E-2	1.04950 E2	1.59 E-1	105	214
4	(.05,.5,.05,.05,.15,.13),0.5	(23)	6.020924 E-1	1.26527 E-4	1.03291 E-1	8.23 E-9	98	215
		(25)	6.013642 E-1	7.28746 E-5	1.03195 E1	9.74 E-9	118	148
	(.2,.6,.2,.2,.6,9.5),0.3	(23)	3.326203 E-1	1.82771 E-5	2.08855 E1	7.58 E-9	57	93
		(25)	3.329312 E-1	1.94789 E-5	2.07835 E1	8.57 E-9	27	43
5	(1,...,1),0.2	(23)	1.375316 E-1	3.28343 E-5	1.00738	8.30 E-9	4	5
		(25)	1.375395 E-1	2.22622 E-6	1.00737	8.39 E-11	4	5
	(.5,...,.5),0.1	(23)	7.791575 E-2	8.48140 E-6	1.09061	9.50 E -11	6	11
		(25)	7.791559 E-2	4.60560 E-6	1.09061	5.49 E-10	6	14
6 $M = 8$	(.5,...,.5),0.1	(23)	1.000003	3.42256 E-6	8.88266 E-1	3.67 E-10	6	9
		(25)	1.000000	1.80806 E-8	8.88266 E-1	4.30 E-12	7	10
6 $M = 16$	(.5,...,.5),0.1	(23)	1.000000	4.48221 E-7	9.35484 E-1	4.66 E-11	9	12
		(25)	1.000004	6.43785 E-5	9.35479 E-1	3.47 E-9	7	12
6 $M = 32$	(.5,...,.5),0.1	(23)	1.000000	1.67478 E-6	9.63297 E-1	1.29 E-9	8	11
		(25)	1.000000	9.12465 E-8	9.63297 E-1	2.21 E-11	8	13
7a $M = 49$	(1,...,1),8.	(23)	6.807507	8.35879 E-7	3.07280 E1	1.93 E-9	6	7
		(25)	6.807504	9.44063 E-7	3.07280 E1	1.44 E-10	8	9
7a $M = 121$	(1,...,1),8.	(23)	6.808005	1.25211 E-6	3.14486 E1	3.39 E-10	8	9
		(25)	6.808005	1.44243 E-6	3.14486 E1	2.85 E-10	8	9
7a $M = 225$	(1,...,1),8.	(23)	6.808096	3.73244 E-6	3.14365 E1	1.03 E-9	9	10
		(25)	6.808045	1.04390 E-6	3.16927 E1	1.68 E-9	7	8
7b $M = 49$	(1,...,1),8.	(23)	7.980354	5.52905 E-7	3.07123 E1	2.90 E-11	15	30
		(25)	7.980359	1.14418 E-4	3.07123 E1	9.15 E-9	13	23
7b $M = 121$	(1,...,1),8.	(23)	7.981427	2.06899 E-5	3.14425 E1	2.76 E-10	23	52
		(25)	7.981423	1.16229 E-6	3.14425 E1	1.30 E-10	24	54
7b $M = 225$	(1,...,1),8.	(23)	7.981605	1.07876 E-4	3.16894 E1	6.04 E-9	44	76
		(25)	7.981612	8.60734 E-5	3.16894 E1	5.44 E-9	23	40

Table 1. Numerical results

We proceed to a brief analysis of the numerical experiments. The value effectivelly used for the increment h both in (23) and (25) was 10^{-4}. Such a choice is validated by the singular values of H_y at the final approximation, as can be seen in Table 1.

Except for three cases of problem 3, the convergence criterion reached by the sum of squares $f(x_k) = f(y_k, t_k)$ in the final approximation was $\|f(x_k)\| \leq 10^{-8}$. For problem 3 with $\overline{\gamma} = 0$ and using (25), the maximum number of iterations (500) was achieved. For $\overline{\gamma} = 0.1$, convergence was declared because the criterion $\|\nabla_P f(x_k)\| \leq 10^{-5} \max\{|f(x_k)|, 1\} / \max\{\|x_k\|, 1\}$ concerning the projected gradient on the box $-10 \leq y_i \leq 10$, $i = 1, \ldots, 5$, $-1 \leq t \leq 1$ was satisfied.

Comparing the performance of (23) and (25) in the experiments, none of them can be singled out as the best one. The behavior of both approaches depends not only on the initial point adopted, but also on the nonlinearity of the problem.

6 Conclusions

In this paper we introduce a globally convergent algorithm for solving nonlinear systems of equations. We prove that if a sequence of iterates can be defined satisfying certain conditions ((10) and (11)) then an approximate solution exists and can be computed by the algorithm. The method does not use line searches. In fact, its generality makes it easily implemented by means of trust-region strategies. When a solution does not exist, we prove that the algorithm eventually fails (breaks down), that is, a direction with the properties (10) and (11) cannot be computed. In the practical implementation of the general algorithm, we define a procedure that (very likely) finds directions satisfying (10) and (11), when they exist. This procedure, borrowed from the well developed area of box constrained optimization, can, of course, fail to produce the desired directions. When this occurs, we stop the execution with the diagnostic of (practical) breakdown.

We tested our method for computing singular points of homotopic curves. The results seem to be reliable. The key point of our formulation is to replace the equation which states that the null-space of the Jacobian has a nonnull vector by a finite difference equations where derivatives are not involved. The numerical experiments show that the method usually finds an accurate solution and that an empirically optimal discretization parameter can be recommended.

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