On the Nonmonotone Behavior of the Newton-Gmback Method

Emil Cătinaş

Romanian Academy, "T. Popoviciu" Institute of Numerical Analysis, P.O. Box 68–1, Cluj-Napoca, Romania, e-mail: ecatinas@ictp.acad.ro

Abstract. GMBACK is a Krylov solver for large linear systems, which is based on backward error minimization properties. The minimum backward error is guaranteed (in exact arithmetic) to decrease when the subspace dimension is increased. In this paper we consider two test problems which lead to nonlinear systems which we solve by the Newton-GMBACK. We notice that in floating point arithmetic the mentioned property does not longer hold; this leads to nonmonotone behavior of the errors, as reported in a previous paper. We also propose a remedy, which solves this drawback.

Keywords: linear/nonlinear systems, Krylov solvers, Newton method.
PACS: 02.60.Cb

NONLINEAR SYSTEMS.

The Newton method for solving a nonlinear system $F(x)=0, \quad F: D \subseteq \mathbb{R}^N \to \mathbb{R}^N$ leads to the solving of a linear system at each iteration step:

$$\begin{aligned} &F'(x_k)\, s_k = -F(x_k) \\ &x_{k+1} = x_k + s_k, \qquad k=0,1,\ldots, \quad x_0 \in D. \end{aligned}$$

Under the following conditions (which will be implicitly assumed throughout this paper) the Newton method converge locally at q-superlinear rate (see [7]):

- $\exists x^* \in \operatorname{int} D$ such that $F(x^*)=0$
- the mapping F is Fréchet differentiable on $\operatorname{int} D$, with F' continuous at x^*;
- the Jacobian $F'(x^*)$ is invertible.

When one considers approximate Jacobians at each step, $F'(x_k)+\Delta_k \in \mathbb{R}^{N\times N}$, we are lead to the quasi-Newton (QN) iterates

$$\begin{aligned} &(F'(x_k)+\Delta_k)s_k = -F(x_k) \\ &x_{k+1} = x_k + s_k, \qquad k=0,1,\ldots, \quad x_0 \in D. \end{aligned}$$

We have characterized the superlinear convergence of these iterates in the following result:

Theorem 1. *[3] Assume that the* QN *iterates converge to x^*. Then the convergence is superlinear if and only if*

$$\|\Delta_k s_k\| = o\big(\|F(x_k)\|\big), \quad \text{as } k \to \infty. \tag{1}$$

THE GMBACK METHOD

When the dimension N is large, the numerical solving of a linear system

$$Au = b, \quad A \in \mathbb{R}^{N\times N} \text{nonsingular}, b \in \mathbb{R}^N,$$

becomes a difficult task. The Krylov solvers are popular choices for accomplishing this task, since they may offer good approximations at low computational cost.

We shall consider here the GMBACK solver introduced by Kasenally in [6]. For a given subspace dimension $m \in \{1,\ldots,N\}$ and an initial approximation $u_0 \in \mathbb{R}^N$ having the residual $r_0 = b - Au_0$, it finds $u_m^{GB} \in u_0 + \mathscr{K}_m = u_0 + \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$ by the following minimization property:

$$\left\|\Delta_m^{GB}\right\|_F = \min_{u_m \in u_0+\mathscr{K}_m} \|\Delta_m\|_F \quad \text{w.r.t. } (A-\Delta_m)u_m = b.$$

Here $\|\cdot\|_F$ denotes the Frobenius norm of a matrix, $\|Z\|_F = tr(ZZ^t)^{1/2}$ while $\|\cdot\|_2$ will denote the Euclidean norm from $\mathbb{R}^N$ and its induced operator norm.

The following steps are performed for determining u_m^{GB}:

Arnoldi

- Let $r_0 = b - Ax_0$, $\beta = \|r_0\|_2$ and $v_1 = \frac{1}{\beta} r_0$;
- For $j = 1,\ldots,m$ do
  $h_{ij} = (Av_j, v_i), \quad \text{for } i = 1,\ldots,j$
  $\hat{v}_{j+1} = A\hat{v}_j - \sum_{j=1}^{i} h_{ij} v_i$
  $h_{j+1,j} = \left\|\hat{v}_{j+1}\right\|_2$
  $v_{j+1} = \frac{1}{h_{j+1,j}} \hat{v}_{j+1}$
- Form the Hessenberg matrix $\bar{H}_m \in \mathbb{R}^{(m+1)\times m}$ with the (possible) nonzero elements h_{ij} determined above, and the matrix $V_m \in \mathbb{R}^{N\times m}$ having as columns the vectors v_j: $V_m = [v_1 \ \ldots \ v_m]$.

GMBACK

- Let $\beta = \|r_0\|_2$,
  $\hat{H}_m = [-\beta e_1 \quad \bar{H}_m] \in \mathbb{R}^{(m+1)\times(m+1)}, \quad \hat{G}_m = [u_0 \quad V_m] \in \mathbb{R}^{N\times(m+1)}$,
  $P = \hat{H}_m^t \hat{H}_m \in \mathbb{R}^{(m+1)\times(m+1)} \quad \text{and} \quad Q = \hat{G}_m^t \hat{G}_m \in \mathbb{R}^{(m+1)\times(m+1)}$;
- Determine an eigenvector v_{m+1} corresponding to the smallest eigenvalue λ_{m+1}^{GB} of the generalized eigenproblem $Pv = \lambda Qv$;
- If the first component $v_{m+1}^{(1)}$ is nonzero, compute the vector $y_m^{GB} \in \mathbb{R}^m$ by scaling v_{m+1} such that

$$\begin{bmatrix} 1 \\ y_m^{GB} \end{bmatrix} = \frac{1}{v_{m+1}^{(1)}} v_{m+1};$$

- Set $u_m^{GB} = x_0 + V_m y_m^{GB}$.

We shall assume in the following analysis that u_m^{GB} exists (this may not be the case when all the eigenvectors of the smallest eigenvalue have the first component 0).

Kasenally proved that for any $u_0 \in \mathbb{R}^N$ and $m \in \{1,\ldots,N\}$, the backward error Δ_m^{GB} corresponding to the GMBACK solution satisfies

$$\left\|\Delta_m^{GB}\right\|_F = \sqrt{\lambda_{m+1}^{GB}}. \tag{2}$$

Regarding the induced operator Euclidean norm, the following inequality is known:

$$\|Z\|_2 \le \|Z\|_F, \quad \text{for all } Z \in \mathbb{R}^{N\times N}. \tag{3}$$

The eigenvalues at steps m and $m+1$ in the Arnoldi algorithm interlace as follows.

Lemma 2. *[6] Suppose that $m+1$ steps of the Arnoldi process have been taken and $h_{m+2,m+1} \neq 0$. Furthermore, assume that $\{\lambda_i^{GB}\}_{i=1,\ldots,m+1}$ and $\{\hat{\lambda}_i^{GB}\}_{i=1,\ldots,m+2}$ are, respectively, the eigenvalues of the matrix pairs (P_m, Q_m) and (P_{m+1}, Q_{m+1}) arranged in decreasing order. Then, for any $i \le m+1$,*

$$\hat{\lambda}_i^{GB} \le \lambda_i^{GB} \le \hat{\lambda}_{i+1}^{GB}.$$

THE CONVERGENCE OF THE NEWTON-GMBACK METHOD

The Newton-GMBACK iterates may be written as

$$\left(F'(y_k) - \Delta_k^{GB}\right) s_k^{GB} = -F(y_k), \tag{4}$$

and we may control the convergence of the iterates by Theorem 1 with the aid of the backward error. It is worth noting that we may use formulas (2) and (3) to evaluate the magnitude of the backward error in the Euclidean norm.

We obtain:

Theorem 3. *Assume that the Newton-GMBACK iterates are well defined and converge to x^*. If*

$$\lambda_k^{GB} \to 0, \quad as\ k \to \infty, \tag{5}$$

then they converge superlinearly.

Of course, we may also use the inexact Newton model, and control the convergence of the iterates with the aid of residuals, see [4].

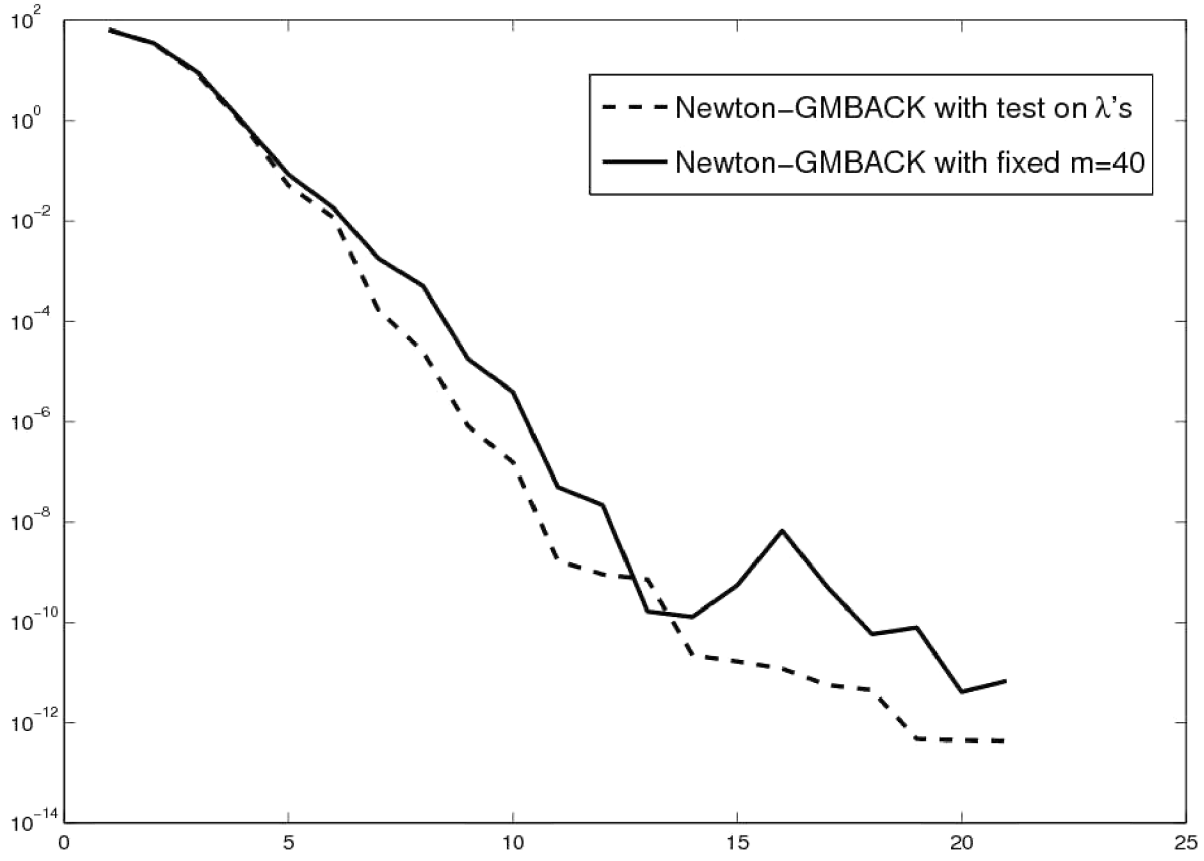

FIGURE 1. Newton-GMBACK errors for the Bratu problem.

Bratu problem

Consider the nonlinear partial differential equation

$$-\triangle u + \alpha u_x + \lambda e^u = f,$$

over the unit square of $\mathbb{R}^2$, with Dirichlet boundary conditions. As mentioned in [1], this is a standard problem, a simplified form of which is known as the Bratu problem. We have discretized by 5-point finite differences, respectively by central finite differences on a uniform mesh, obtaining a system of nonlinear equations of size $N = (n-2)^2$, where n is the number of mesh points in each direction. As in [1], we took f such that the solution of the discretized problem to be the constant unity, and $\alpha = 10$, $\lambda = 1$, the initial approximations in the inner iterations were zero. The runs were made on a HP Proliant 570 G4 server, using MATLAB 2007a.

We took $N = 16,384$ and considered first some standard iterations, with fixed subspace dimension, of size $m = 40$. We noticed that, starting from outer iteration $k = 9$, where $\|F\|$ was of magnitude 1e$-$9, lemma 2 did not hold in floating point arithmetic. As we can see in figure 1, the consequence is that the convergence of the errors of iterates is no longer monotone.

The remedy we propose is to check at each inner iteration step in GMBACK whether the size of λ is decreasing, and to stop the iterations if the size is increasing. We obtain monotone behavior of the errors, and the plot in figure 1 is relevant for the runs we made.

ACKNOWLEDGMENTS

This research has been supported by MEdC under grant 2CEx06-11-96.

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