A globally convergent Newton-GMRES method for large sparse systems of nonlinear equations

Heng-Bin An, Zhong-Zhi Bai

State Key Laboratory of Scientific/Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, PO Box 2719, Beijing 100080, PR China

Abstract

The inexact Newton with backtracking (INB) method is a powerful tool for solving large sparse systems of nonlinear equations. In particular, if the generalized minimal residual (GMRES) method is used to solve the Newton equations, then the Newton-GMRES with backtracking (NGB) method is obtained. In this paper, we present a new class of globally convergent Newton-GMRES methods. In these methods, the typical backtracking strategy is augmented with a new strategy that is invoked when the inexact Newton direction is not satisfactory. Global convergence properties of the proposed methods are established and numerical results are provided, showing that the new method, called the Newton-GMRES with quasi-conjugate-gradient backtracking (NGQCGB), is very robust and effective.

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1. Introduction

Consider the solution of large sparse systems of nonlinear equations

\[ F(x) = 0, \]

where \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is a continuously differentiable function. The most popular solver for the nonlinear system (1) is the well-known Newton method. As it is known, the Newton method has quadratic convergence speed if the mapping \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is continuously differentiable and if a good initial guess \( x_0 \) is easily available. However, at each iteration step it needs the exact solution of the corresponding Newton equation, which is very costly in actual applications, in particular, when the problem size \( n \) is very large. To avoid this disadvantage of the Newton method, the following inexact Newton (IN) method was established and studied in [11]; see also [5,6].
Method 1.1 (Inexact Newton method [11]). Given an initial guess $x_0 \in \mathbb{R}^n$. For $k = 0, 1, 2, \ldots$ until $\{x_k\}$ convergence. Find some $\bar{\eta}_k \in [0, 1)$ and $\bar{s}_k \in \mathbb{R}^n$ such that
\[
\|F(x_k) + F'(x_k)\bar{s}_k\| \leq \bar{\eta}_k \|F(x_k)\|,
\]
and compute
\[
x_{k+1} = x_k + \bar{s}_k.
\]

In the above inexact Newton method, $F'(x_k)$ denotes the Jacobian matrix of $F(x)$ at the current iterate $x_k$, $\bar{\eta}_k$ is the forcing term that controls the level of accuracy of the inner iteration for inexactly solving the Newton equation, the obtained $\bar{s}_k$ satisfying (2) is an inexact Newton step at level $\bar{\eta}_k$, and (2) is the so-called inexact Newton condition.

Evidently, at each iteration step of the inexact Newton method we only need to solve the Newton equation approximately by an efficient iteration solver for systems of linear equations such as the classical splitting methods [4,3,2] or the modern Krylov subspace methods [23]. This makes the above inexact Newton method more practical and effective.

According to the inner iteration solvers, if the problem size $n$ is very large, and the Jacobian matrix $F'(x)$ is sparse but nonsymmetric, the Krylov subspace iteration method GMRES [24] is a powerful algorithm for computing an inexact Newton step $\bar{s}_k$ in (2). This then leads to a special inexact Newton method, called as the Newton-GMRES method, for solving the system of nonlinear equations (1). See [7–10]. An important feature of the Newton-GMRES method is that it only requires the action of the Jacobian matrix $F'(x)$ on a vector $v$, and $F'(x)v$ can be accurately approximated by the difference quotient
\[
F'(x)v \approx \frac{F(x + \epsilon v) - F(x)}{\epsilon},
\]
where $\epsilon$ is a prescribed difference step-size. Therefore, in this manner the Newton-GMRES method could avoid direct computations of the Jacobian matrices $F'(x_k)$, and then results in a “matrix-free” iteration process [19].

The inexact Newton methods only have local convergence property. However, iterative methods with global convergence behavior are more practical and efficient for solving systems of nonlinear equations. Embedding these methods in a globalization strategy, e.g., the linesearching or trust region techniques, many researchers have modified the inexact Newton methods and obtained globally convergent ones. For details, see [7–10], [14,15,22] and references therein. The inexact Newton backtracking (INB) method studied in [14,15] is one of such typical examples. In this method, the backtracking procedure is performed along the current inexact Newton step $\bar{s}_k$ so that a “sufficient decrease” step can be obtained. In particular, when the INB method is concretized to the Newton-GMRES method, the Newton-GMRES with backtracking (NGB) method can be naturally obtained, which was studied in-depth in [7,22]. Both theoretical analysis and numerical experiments have shown that INB and its special case NGB are very robust and effective for solving large sparse systems of nonlinear equations.

It may happen that the NGB methods stagnate for some iterations or even fail. In fact, when the Newton direction is a poor direction, a large number of backtracks are needed to get the desired reduction or a satisfactory step cannot be computed in practice and the backtracking strategy breaks down [15,25]. Therefore, the authors of [7] recently presented a Newton-GMRES with equality curve backtracking (NGECB) method that is based on the NGB method. Unlike the NGB, the global convergence strategy in the NGECB method consists of two parts: first, a backtracking strategy along the inexact Newton step is applied. More precisely, a maximum number $N_b$ of backtracks is fixed in advance. Then, if within $N_b$ backtracks a satisfactory step is obtained, the NGECB method will proceed as usual; otherwise, an alternative strategy that backtracks along an equality curve will be used to find another new step. The alternative strategy used in [7] is a backtracking procedure along a piecewise linear curve that involves $\bar{s}_k$ and an alternative direction computed using the information provided by GMRES. Because of its special property, this alternative strategy is called the equality curve backtracking (ECB) strategy in [7].

We tried to replace the ECB strategy in NGECB method with a new efficient strategy, and hence, obtained a new method. This new alternative strategy, called as quasi-conjugate-gradient backtracking (QCGB) strategy, involves the known information such as the projection of the gradient $g_k = F'(x_k)^T F(x_k)$ of the merit function $f_2(x) = \frac{1}{2} \|F(x)\|^2$.\n
on a proper subspace and the last nonlinear step \( \Delta_{k-1} = x_k - x_{k-1} \). The obtained method is called the Newton-GMRES with quasi-conjugate-gradient backtracking (NGQCGB) method. We establish the global convergence theory of this NGQCGB method, and use many typical nonlinear problems to examine its numerical behavior. Numerical computations show that the NGQCGB method is more robust and effective than both NGB and NGECB methods.

The paper is organized as follows. In Section 2 we state some necessary notations and describe the NGECB method for the sake of completeness; In Section 3 we introduce the NGQCGB method assuming that neither restarting nor preconditioning is employed; Its global convergence is proved in Section 4; The NGQCGB method is extended to obtain the restarting and the preconditioning variants in Section 5; The feasibility and effectiveness of the NGQCGB method are investigated by solving ten typical nonlinear problems in Section 6; Finally, in Section 7, we end the paper with a brief conclusion.

2. Preliminaries

Throughout this paper, we use \( \| \cdot \| \) to denote the Euclidean norm for both matrices and vectors. For convenience of discussion, we introduce a function that is associated with the nonlinear function \( F(x) \): \( f_2(x) = \frac{1}{2} \| F(x) \|^2 \). Clearly, for a point \( x^* \in \mathbb{R}^n \) satisfying that \( F'(x^*) \) is nonsingular, we have

\[ F(x^*) = 0 \iff f_2(x^*) = 0. \]

The gradient of \( f_2(x) \) is denoted by \( g(x) \). Also, we will use \( g_k \) to denote the gradient of \( f_2 \) at \( x_k \), i.e., \( g_k = g(x_k) \). It is easy to see that \( g(x) = F'(x)^T F(x) \). We use \( e_i \) to denote the \( i \)-th unit vector in a real vector space, with its dimension inferred from the context; and \( N_\delta(x) \) to represent the closed ball with center \( x \) and radius \( \delta \). For a nonlinear iteration method, the term *nonlinear iteration* is employed to denote the iteration from \( x_k \) to \( x_{k+1} \), and the term *breakdown* means that the next iterate \( x_{k+1} \) cannot be determined by the method.

In the following, for reference, we give the general paradigm for the NGECB method [7]. For further details on algorithmic descriptions of the inexact Newton-GMRES method, the INB method and the NGB method, we refer to [7–10] and [14,15] for details.

**Method 2.1 (The NGECB method [7]).**

1. Given \( x_0 \in \mathbb{R}^n \), \( \epsilon_0 > 0 \), \( \eta_{\text{max}} \in [0, 1) \), \( \alpha \in (0, 1) \), \( 0 < \theta_l < \theta_u < 1 \) and a positive integer \( N_b \geq 0 \). Set \( k := 0 \).
2. While \( \| F(x_k) \| > \epsilon_0 \) do:
   2.1. Choose \( \bar{\eta}_k \in [0, \eta_{\text{max}}] \).
   2.2. Apply GMRES to the \( k \)th Newton equation\(^1\) and obtain \( \bar{s}_k := s_k^m \) such that
      \[ \| F(x_k) + F'(x_k)\bar{s}_k \| \leq \bar{\eta}_k \| F(x_k) \|. \]
   2.3. Apply the backtracking loop along \( \bar{s}_k \) and perform at most \( N_b \) repetitions:
      (a) Set \( s_k := \bar{s}_k \), \( \eta_k := \bar{\eta}_k \).
      (b) While \( \| F(x_k + s_k) \| \geq [1 - \alpha(1 - \eta_k)]\| F(x_k) \| \) do:
         • Choose \( \theta \in [\theta_l, \theta_u] \).
         • Update \( s_k := \theta s_k \) and \( \eta_k := 1 - (1 - \eta_k) \).
   2.4. If \( s_k \) satisfies the sufficient descent condition
      \[ \| F(x_k + s_k) \| \leq [1 - \alpha(1 - \eta_k)]\| F(x_k) \|, \]
      then set \( \Delta_k := s_k \), and go to step 2.6.
   2.5. Perform the *equality curve backtracking* (ECB) strategy:

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\(^1\) The \( k \)th Newton equation is \( F'(x_k)x_k = -F(x_k) \). Here, an initial guess \( s_k^0 \) for the GMRES method needs to be specified. The GMRES method starts with \( X_0 = -F(x_k) - F'(x_k)x_k^0 \), \( \beta_0 = \| x_k^0 \| \) and \( u_1 = r_k^0 / \beta_k \), then it proceeds with the Arnoldi process to obtain an orthogonal basis \( V_m = [v_1, v_2, \ldots, v_m] \) of the Krylov subspace \( K_m(F'(x_k), r_k^0) \) (see (5)). During the process, an upper Hessenberg matrix \( H_m \in \mathbb{R}^{(m+1)\times m} \) satisfying \( F'(x_k)V_m = V_m + H_m \) is built. The GMRES is terminated once \( \| r_k^m \| \leq \bar{\eta}_k \| F(x_k) \| \), where \( \| r_k^m \| := \| F'(x_k)x_k^m + F(x_k) \| = \| \beta_k e_1 - H_m y_m \| \) and \( y_m \in \mathbb{R}^m \) is the solution of the least-squares problem \( \min_{y \in \mathbb{R}^m} \| \beta_k e_1 - H_m y \\| \). Finally, \( s_k^m \) is defined as \( s_k^m = s_k^0 + V_m y_m \).
(a) Form a piecewise curve $\sigma_k(\eta)$ such that
$$\| F(x_k) + F'(x_k)\sigma_k(\eta) \| = \eta \| F(x_k) \|. \quad (4)$$

(b) Perform backtracking along $\sigma_k(\eta)$ to get a step $\sigma_k(\eta_k)$ such that
$$\| F(x_k + \sigma_k(\eta_k)) \| \leq [1 - \alpha(1 - \eta_k)] \| F(x_k) \|. \quad (5)$$

(c) Set $\Delta_k := \sigma_k(\eta_k)$.

2.6. Set $x_{k+1} := x_k + \Delta_k$.

2.7. Set $k := k + 1$.

In this method, the maximum number of backtracks along $\tilde{s}_k$ is limited to a prescribed number $N_b$. If a satisfactory step $s_k$ can be obtained within $N_b$ steps, then in [7] $\Delta_k := s_k$ is set, and the next nonlinear iterate is defined by $x_{k+1} := x_k + \Delta_k$; otherwise, an alternative procedure, the ECB-strategy, is applied to find a different new direction $\Delta_k$ (see step 2.5) which satisfies the sufficient descent condition, and the next nonlinear iterate is then defined by $x_{k+1} := x_k + \Delta_k$ with $\Delta_k$ provided by the ECB strategy.

We remark that in step 2.5, the curve $\sigma_k(\eta)$ is constructed by connecting 0, a point $z$ that is computed using information provided by GMRES, and $\tilde{s}_k$. It has the property that for each point on $\sigma_k(\eta)$, the equality constraint (4) holds, or in other words, the inexact Newton condition (2) holds with equality. Therefore, this strategy is called the equality curve backtracking (ECB) strategy. For more details about the construction of $\sigma_k(\eta)$, we refer to [7]; and for other types of equality curve methods, we refer to [14].

3. Establishment of the NGQCGB method

The main feature of the NGECB method is that the NGB method is augmented with an alternative strategy, i.e., a backtracking procedure along a new curve. The role of the alternative strategy is to overcome failures of the backtracking strategy due to poor inexact Newton steps. In fact, it provides a new step giving a sufficient decrease of the merit function. In [7], at the iteration step $k$, if the inexact Newton step is not satisfactory, we employ an alternative direction obtained by using the current available information: the projection of the gradient on the Krylov subspace and the nonlinear iteration step, to compute a good step. This motivates us to design the new Newton-GMRES with quasi-conjugate-gradient backtracking (NGQCGB) method for solving the large sparse system of nonlinear equations (1).

More specifically, in the NGQCGB method, the ECB strategy in the NGECB method is replaced by a new backtracking procedure along a direction $d_k$ located in the subspace spanned by the last nonlinear iteration step $\Delta_{k-1} = x_k - x_{k-1}$ and by the projection $\tilde{g}_k$ of the gradient $g_k = F'(x_k)^T F(x_k)$ onto the current Krylov subspace
$$K_m(F'(x_k), r_0^0) := \text{span}\{r_0^0, F'(x_k)r_0^0, \ldots, (F'(x_k))^{m-1}r_0^0\}. \quad (5)$$

We remark that the information about $\Delta_{k-1}$ is not used in the NGECB method.

Evidently, we need to show that the projection of the gradient $\tilde{g}_k$ can be efficiently computed. In what follows we will refer to the new strategy as the quasi-conjugate-gradient backtracking (QCGB) strategy.

At the $k$th iteration step of the NGQCGB method, we assume that the Jacobian matrix $F'(x_k)$ is nonsingular, neither restarting nor preconditioning is employed in GMRES and at most $m_{\text{max}}$ GMRES iterations are performed. Moreover, we assume that GMRES is started with the initial guess $z_0^0 = 0$. Let $V_m = \{v_1, v_2, \ldots, v_m\}$ be the orthonormal basis of the Krylov subspace $K_m(F'(x_k), r_0^0)$ computed by the GMRES. We remark that
$$r_k^0 = -F(x_k), \quad \beta_k = \| r_k^0 \| = \| F(x_k) \|, \quad \text{and} \quad v_1 = \frac{r_k^0}{\beta_k}.$$ 

Then, the GMRES computes an upper Hessenberg matrix $\overline{H}_m \in \mathbb{R}^{(m+1) \times m}$ such that [24]
$$F'(x_k)V_m = V_{m+1}\overline{H}_m. \quad (6)$$ 

As
$$g_k = F'(x_k)^T F(x_k),$$
it is known that the projection of \( g_k \) onto \( \mathcal{K}_m(F'(x_k), r^0_k) \) is given by
\[
\tilde{g}_k = V_m V_m^T g_k = V_m V_m^T F'(x_k)^T F(x_k).
\]
Noticing that
\[
F(x_k) = -r_k^0 - F'(x_k)s_k^0 = -\beta_k v_1,
\]
we have
\[
\tilde{g}_k = V_m (F'(x_k)V_m)^T F(x_k) = V_m (V_{m+1} H_m)^T F(x_k) = -\beta_k V_m H_m^T V_{m+1} v_1 = -\beta_k V_m H_m^T e_1.
\]
Therefore, \( \tilde{g}_k \) can be cheaply obtained from the information provided by GMRES applied to the Newton equation.

Recalling that the inexact Newton step has the form \( \tilde{s}_k = V_m y_m \), where \( y_m \) is the solution of the least-squares problem \( \min_{y \in \mathbb{R}^m} \| \beta_k e_1 - H_m y \| \), we have
\[
y_m = \beta_k (H_m^T H_m)^{-1} H_m^T e_1.
\]
In order to have a nonzero \( \tilde{s}_k \), we must have \( y_m \neq 0 \) for \( m \) is large enough. It then follows that \( H_m^T e_1 \neq 0 \) and, consequently, \( \tilde{g}_k \neq 0 \).

Now, we show how the new direction \( d_k \) used in the QCGB strategy of our new NGQCGB method can be cheaply built. To this end, we introduce the quadratic merit function
\[
\varphi_k(d) = g_k^T d + \frac{1}{2} d^T B_k d,
\]
and set
\[
\Omega_k := \text{span}\{\tilde{g}_k, \Delta_{k-1}\}, \quad \Delta_{k-1} := x_k - x_{k-1}.
\]
Let \( d_k \) be the minimizer of \( \varphi_k \) within the subspace \( \Omega_k \), i.e.,
\[
d_k = \arg \min_{d \in \Omega_k} \varphi_k(d),
\]
or equivalently,
\[
d_k = \arg \min_{d \in \Omega_k} \| F(x_k) + F'(x_k) d \|.
\]
The step \( d_k \) can be computed according to the following strategy:

(i) \( \tilde{g}_k \) and \( \Delta_{k-1} \) are collinear. In this case, by recalling that \( \tilde{g}_k \neq 0 \) we let \( d = t \tilde{g}_k \quad (t \in \mathbb{R}) \). Therefore, the optimization problem (8) reduces to
\[
\min_{t \in \mathbb{R}} t \tilde{g}_k^T \tilde{g}_k + \frac{1}{2} t^2 \tilde{g}_k^T B_k \tilde{g}_k,
\]
and its unique solution is
\[
t_k = \frac{\| V_m^T \tilde{g}_k \|^2}{\tilde{g}_k^T B_k \tilde{g}_k} = -\frac{\| V_m^T \tilde{g}_k \|^2}{\| F'(x_k) \tilde{g}_k \|^2}.
\]
Since \( V_m^T \tilde{g}_k = V_m^T g_k \) and \( V_m^T g_k = \tilde{g}_k \), it follows that \( \| V_m^T \tilde{g}_k \| = \| \tilde{g}_k \| \). Therefore, \( \| V_m^T \tilde{g}_k \| = \| \tilde{g}_k \| \) and
\[
d_k = t_k \tilde{g}_k = -\frac{\| \tilde{g}_k \|^2}{\| F'(x_k) \tilde{g}_k \|^2} \tilde{g}_k.
\]

(ii) \( \tilde{g}_k \) and \( \Delta_{k-1} \) are not collinear. In this case, we let
\[
d = \mu \tilde{g}_k + \nu \Delta_{k-1}, \quad \text{with} \quad \mu, \nu \in \mathbb{R}.
\]
Denote by \( \tilde{y}_k = B_k \Delta_{k-1} \) and \( w_k = \tilde{g}_k^T B_k \tilde{g}_k \). Then the optimization problem (8) becomes to
\[
\min_{(\mu, \nu) \in \mathbb{R}^2} \left( \tilde{g}_k^T \tilde{g}_k, \tilde{g}_k^T \Delta_{k-1} \right) \begin{pmatrix} \mu \\ \nu \end{pmatrix} + \frac{1}{2} (\mu, \nu) \begin{pmatrix} w_k \\ \tilde{g}_k^T \tilde{y}_k \end{pmatrix} \begin{pmatrix} \mu \\ \nu \end{pmatrix}.
\]
Because \( F'(x_k) \) is nonsingular, we can immediately demonstrate that the matrix
\[
A_k := \begin{pmatrix} w_k & \tilde{g}_k^T \tilde{y}_k \\ \tilde{g}_k^T \tilde{y}_k & \Delta_{k-1}^T \tilde{y}_k \end{pmatrix}
\]
is symmetric positive definite. Hence, \( D_k := \det(A_k) > 0 \). The unique solution of (11) is
\[
\begin{pmatrix} \mu_k \\ v_k \end{pmatrix} = - \begin{pmatrix} w_k & \tilde{g}_k^T \tilde{y}_k \\ \tilde{g}_k^T \tilde{y}_k & \Delta_{k-1}^T \tilde{y}_k \end{pmatrix}^{-1} \begin{pmatrix} \tilde{g}_k^T \tilde{y}_k \\ \Delta_{k-1}^T \tilde{y}_k \end{pmatrix} = - \frac{1}{D_k} \begin{pmatrix} \tilde{g}_k^T \tilde{y}_k \Delta_{k-1}^T - \tilde{y}_k \Delta_{k-1}^T \tilde{y}_k \\ \tilde{g}_k^T \tilde{y}_k \Delta_{k-1}^T - \Delta_{k-1}^T \tilde{y}_k \end{pmatrix}.
\]
It then follows that the solution of (8) is
\[
d_k = \frac{1}{D_k} \left( (\tilde{g}_k^T \tilde{y}_k \Delta_{k-1} - \Delta_{k-1}^T \tilde{y}_k \| \tilde{g}_k \|^2) \tilde{g}_k + (\tilde{g}_k^T \tilde{y}_k \| \tilde{g}_k \|^2 - w_k \tilde{g}_k^T \Delta_{k-1}) \Delta_{k-1} \right).
\]
(12)

Note that the above two cases show that \( d_k \) satisfies (8) or (9) is unique. Besides, as proved by the following Proposition 3.1, \( d_k \) is a descent direction for \( f_2 \) at \( x_k \).

**Lemma 3.1.** Assume that \( F : \mathbb{R}^n \to \mathbb{R}^n \) is continuously differentiable. Then \( p \in \mathbb{R}^n \) is a descent direction of \( f_2 \) at \( x \) if and only if there exists a \( \lambda \in (0, 1] \) such that
\[
\| F(x) + F'(x)(\lambda p) \| < \| F(x) \|.
\]

**Proof.** After direct computations we have
\[
\begin{align*}
\| F(x) + F'(x)(\lambda p) \|^2 - \| F(x) \|^2 &= 2\lambda \langle F(x), F'(x)p \rangle + \| F'(x)(\lambda p) \|^2 \\
&= 2\lambda \langle F(x), F'(x)p \rangle + \lambda^2 \| F'(x)p \|^2 \\
&= \lambda (2 \| F(x)p \|^2 + \lambda \| F'(x)p \|^2).
\end{align*}
\]
Hence, \( p \in \mathbb{R}^n \) is a descent direction of \( f_2 \) at \( x \) if and only if there exists a sufficiently small \( \lambda \in (0, 1] \) such that
\[
\| F(x) + F'(x)(\lambda p) \| < \| F(x) \|.
\]

**Proposition 3.1.** The vector \( d_k \) given in (12) is a descent direction for \( f_2 \) at \( x_k \).

**Proof.** Because \( -\tilde{g}_k \in \Omega_k \) is a descent direction of \( f_2 \) at \( x_k \), by Lemma 3.1, there exists a \( \lambda_0 \in (0, 1] \) such that
\[
\| F(x_k) - F'(x_k)\lambda_0 \tilde{g}_k \| < \| F(x_k) \|.
\]
Therefore, by (9) we have
\[
\| F(x_k) + F'(x_k)d_k \| = \min_{d \in \Omega_k} \| F(x_k) + F'(x_k)d \| \leq \min_{t \in \mathbb{R}} \| F(x_k) - F'(x_k)(t \tilde{g}_k) \|
\leq \| F(x_k) - F'(x_k)(\lambda_0 \tilde{g}_k) \| < \| F(x_k) \|.
\]
(13)

By Lemma 3.1 again, we know that \( d_k \) is a descent direction for \( f_2 \) at \( x_k \).

Now, we are ready to describe the NGQCGB method.

**Method 3.1 (The NGQCGB method).**

1. Given \( x_0 \in \mathbb{R}^n, \varepsilon_0 > 0, \eta_{\text{max}} \in [0, 1) \), \( 0 < \alpha < \beta < 1, 0 < \theta_l < \theta_u < 1 \), and a positive integer \( N_b \). Set \( k := 0 \) and \( \Delta_{-1} := 0 \).
2. While \( \| F(x_k) \| > \varepsilon_0 \) do:
   2.1. Choose \( \tilde{\eta}_k \in [0, \eta_{\text{max}}] \).
2.2. Apply GMRES to the $k$th Newton equation (see step 2.2 in the NGECB method 2.1) and obtain $\tilde{s}_k := s_k^m$ such that
\[
\| F(x_k) + F'(x_k)\tilde{s}_k \| \leq \tilde{\eta}_k \| F(x_k) \|.
\]
2.3. Apply the backtracking loop along $\tilde{s}_k$ (see step 2.3 in the NGECB method 2.1) and perform at most $N_b$ repetitions, so that a step $s_k$ is obtained.

2.4. If $s_k$ satisfies the sufficient descent condition
\[
\| F(x_k + s_k) \| \leq [1 - \alpha(1 - \eta_k)] \| F(x_k) \|,
\]
then set $\Delta_k := s_k$, and go to step 2.6.

2.5. Perform QCGB strategy (see step 2.5 in the NGECB method 2.1):
(a) If $\tilde{g}_k$ and $\Delta_k - 1$ are collinear, then compute $d_k$ by (10); else compute $d_k$ by (12).
(b) Set $\Delta_k := d_k$.
(c) If
\[
\begin{cases}
  f_2(x_k + \Delta_k) & \leq f_2(x_k) + \alpha g(x_k)^T \Delta_k, \\
  g(x_k + \Delta_k)^T \Delta_k & \geq \beta g(x_k)^T \Delta_k,
\end{cases}
\]
then go to step 2.6.
(d) Choose $\theta \in [\theta_l, \theta_u]$ and update $\Delta_k := \theta \Delta_k$. Go to step (c).

2.6. Set $x_{k+1} := x_k + \Delta_k$.

2.7. Set $k := k + 1$.

We remark that (14) is the Goldstein–Armijo condition, which is often used in linesearch strategies (see [12, 26]). Because Proposition 3.1 shows that $d_k$ determined by either (10) or (12) is a descent direction of $f_2$ at $x_k$, the existence of an $x_{k+1}$ that satisfies the Goldstein–Armijo condition (14) is guaranteed (see [12]). The QCGB strategy then determines the nonlinear iteration step $\Delta_k$ by backtracking along the direction $d_k$ until the Goldstein–Armijo condition (14) is satisfied.

Note that, in the above method, if the QCGB strategy is employed at the $k$th iteration, then we have
\[
x_{k+1} = x_k + \Delta_k, \quad \text{with} \quad \Delta_k = \tilde{\mu}_k \tilde{g}_k + \tilde{v}_k \Delta_k - 1,
\]
for some $\tilde{\mu}_k, \tilde{v}_k \in \mathbb{R}^1$. This formula is very similar to the conjugate gradient method [26] applied to the problem $\min f_2(x)$, the only difference is that $g_k$ in the conjugate gradient method [26] is replaced by $\tilde{g}_k$ in (15). This is why we call the alternative backtracking strategy defined by step 2.5 in Method 3.1 as the quasi-conjugate-gradient backtracking strategy.

In addition, we should point out that our NGQCGB method also admits matrix-free implementation. In fact, the computation of $d_k$ only depends on $F'(x_k)\tilde{g}_k$ and $F'(x_k)\Delta_k - 1$ due to the validity of the following identities:

(a) $\tilde{g}_k^T \tilde{y}_k = \tilde{g}_k^T B_k \Delta_k - 1 = (F'(x_k)\tilde{g}_k)^T (F'(x_k)\Delta_k - 1)$;
(b) $g_k^T \Delta_k - 1 = F(x_k)^T (F'(x_k)\Delta_k - 1)$;
(c) $\Delta_k^T \tilde{y}_k = \Delta_k^T B_k \Delta_k - 1 = \| F'(x_k)\Delta_k - 1 \|^2$; and
(d) $w_k = \tilde{g}_k^T B_k \tilde{g}_k = \| F'(x_k)\tilde{g}_k \|^2$.

In particular, from (7) we can get
\[
F'(x_k)\tilde{g}_k = -\beta_k (F'(x_k)V_m) \tilde{H}_m^T e_1.
\]
As $F'(x_k)V_m$ is readily available in the GMRES process, $F'(x_k)\tilde{g}_k$ can be computed with little workload. Therefore, we only need to compute $F'(x_k)\Delta_k - 1$ approximately by making use of the formula (3) without explicitly forming the Jacobian matrix $F'(x_k)$.

4. Convergence of the NGQCGB method

In this section, we will prove the global convergence of the new NGQCGB method. To this end, we first make the following two basic assumptions:
\textbf{A1.} \( f_2(x) = \frac{1}{2} \| F(x) \|^2 \) is continuously differentiable on the level set \( L = \{ x \mid f_2(x) \leq f_2(x_0) \} \)

for a given point \( x_0 \in \mathbb{R}^n \), and there exists a constant \( \gamma > 0 \) such that \( \| g(x) - g(y) \| \leq \gamma \| x - y \|, \forall x, y \in L; \)

\textbf{A2.} For an NGQCGB iteration sequence \( \{ x_k \} \), it holds that

\[
\| F(x_k) + F'(x_k) \tilde{s}_k \| \leq \eta_{\text{max}} \| F(x_k) \|, \quad k = 0, 1, 2, \ldots .
\]

According to Lemma 3.1, Assumption A2 guarantees that when \( \eta_{\text{max}} < 1 \) \( \tilde{s}_k \) is a descent direction of \( f_2 \) at the current iterate \( x_k \).

Now, we will establish some relationship between the NGQCGB method and the GIN (global inexact Newton) method in \cite{14}. It follows from (13) that

\[
\tilde{\eta}_k := \frac{\| F(x_k) + F'(x_k) d_k \|}{\| F(x_k) \|} \in [0, 1).
\]

Define

\[
\tau(\eta) = \left( \frac{\eta^2 - \tilde{\eta}_k^2}{1 - \tilde{\eta}_k^2} \right)^{\frac{1}{2}}, \quad \eta \in [\tilde{\eta}_k, 1]
\]

and

\[
E_k(\eta) = [1 - \tau(\eta)] d_k, \quad \eta \in [\tilde{\eta}_k, 1].
\]

Then we have the following result.

\textbf{Proposition 4.1.} \textit{The curve} \( E_k(\eta) \) \textit{defined by (18) satisfies}

\[
\| F(x_k) + F'(x_k) E_k(\eta) \| = \eta \| F(x_k) \|, \quad \eta \in [\tilde{\eta}_k, 1].
\]

\textbf{Proof.} From the definition of \( d_k \), it follows that \( F(x_k) + F'(x_k) d_k \) is orthogonal to the subspace \( F'(x_k) \Omega_k \). Therefore,

\[
\{ F'(x_k) d_k, F(x_k) + F'(x_k) d_k \} = 0.
\]

By (20) and (16), we have

\[
\{ F(x_k), F(x_k) + F'(x_k) d_k \} = \| F(x_k) + F'(x_k) d_k \|^2 = \tilde{\eta}_k^2 \| F(x_k) \|^2.
\]

Thus, by (18), (21) and (17), we obtain

\[
\| F(x_k) + F'(x_k) E_k(\eta) \|^2 \\
= \| F(x_k) + F'(x_k) [1 - \tau(\eta)] d_k \|^2 \\
= \| \tau(\eta) F(x_k) + [1 - \tau(\eta)] [F(x_k) + F'(x_k) d_k] \|^2 \\
= \| \tau(\eta) F(x_k) \|^2 + 2 \tau(\eta) [1 - \tau(\eta)] \| F(x_k), F(x_k) + F'(x_k) d_k \| + \| [1 - \tau(\eta)] [F(x_k) + F'(x_k) d_k] \|^2 \\
= \tau(\eta)^2 \| F(x_k) \|^2 + 2 \tau(\eta) [1 - \tau(\eta)] \tilde{\eta}_k^2 \| F(x_k) \|^2 + [1 - \tau(\eta)]^2 \tilde{\eta}_k^2 \| F(x_k) \|^2 \\
= \eta^2 \| F(x_k) \|^2.
\]

This shows that (19) holds. \( \square \)

Because

\[
E_k(\tilde{\eta}_k) = d_k \quad \text{and} \quad E_k(1) = 0,
\]

Because
we know that the backtracking procedure along \( d_k \) in the QCGB strategy is substantially a backtracking procedure along the parametrized curve \( E_k(\eta) \). If \( \Delta_k = \theta_k d_k \) is computed by the QCGB strategy with \( \theta_k \in (0, 1] \), then there exists a unique \( x_k \in [\bar{x}_k, 1) \) such that \( \Delta_k = E_k(\eta_k) \).\(^2\) For this \( \eta_k \), by making use of (19) we get
\[
\| F(x_k) + F'(x_k)\Delta_k \| = \eta_k \| F(x_k) \| .
\]

Since this \( \Delta_k \) also satisfies (14), Proposition 2.1 in [14] immediately leads to
\[
\| F(x_k + \Delta_k) \| \leq [1 - \alpha(1 - \eta_k)] \| F(x_k) \| .
\]

The above investigation shows that the NGQCG method actually belongs to the following general paradigm, which is the GIN method in [14].

1. Let \( x_0 \in \mathbb{R}^n \) and \( \alpha \in (0, 1) \) be given;
2. For \( k = 0, 1, 2, \ldots \) until \( \{x_k\} \) convergence,
   2.1. Find some \( \eta_k \in (0, 1) \) and \( \Delta_k := \Delta_k(\eta_k) \) such that
   \[
   \| F(x_k) + F'(x_k)\Delta_k \| \leq \eta_k \| F(x_k) \| ,
   \]
   and
   \[
   \| F(x_k + \Delta_k) \| \leq [1 - \alpha(1 - \eta_k)] \| F(x_k) \| .
   \]
   2.2. Set \( x_{k+1} := x_k + \Delta_k \).

We remark that in the NGQCG method, \( \Delta_k \) is determined either by the backtracking loop strategy along
\[
\sigma_k(\eta) = \frac{1 - \eta}{1 - \eta_k} \bar{s}_k, \quad \eta \in [\bar{\eta}_k, 1],
\]

or by the QCGB strategy along \( E_k(\eta) \) (\( \bar{\eta}_k \leq \eta \leq 1 \)). The following two lemmas are necessary for us to analyze the convergence property of the NGQCG method.

**Lemma 4.1.** [10, Corollary 3.5] Let \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \) be continuously differentiable such that \( F(x) \neq 0 \) and \( F'(x) \) is nonsingular for \( x \in \mathbb{R}^n \). Consider the subspace \( \mathcal{K} = \text{span}(V) \subset \mathbb{R}^n \), where the columns of \( V \) form an orthogonal set of vectors. If there exists a \( p \in \mathcal{K} \) such that
\[
\| F(x) + F'(x)p \| \leq \eta \| F(x) \| ,
\]
with \( \eta \in (0, 1) \), then
\[
\| V^T g(x) \| \geq \frac{1 - \eta}{\kappa(F'(x))(1 + \eta)} \| g(x) \| ,
\]
where \( \kappa(F'(x)) \) is the Euclidean condition number of the matrix \( F'(x) \).

**Lemma 4.2.** [14, Theorem 3.5] Let \( \{x_k\} \subset \mathbb{R}^n \) be a vector sequence satisfying both (22) and (23), \( \Gamma \) a constant independent of \( k \), and \( x^* \in \mathbb{R}^n \) be its limit point, such that
\[
\| \Delta_k \| \leq \Gamma(1 - \eta_k) \| F(x_k) \| 
\]
whenever \( x_k \) is sufficiently near \( x^* \) and \( k \) is sufficiently large. Then \( x_k \rightarrow x^* \ (k \rightarrow +\infty) \).

In Lemma 4.2 and the remainder of this section, we say that \( x^* \in \mathbb{R}^n \) is a limit point of a sequence \( \{x_k\} \subset \mathbb{R}^n \) if there exists an infinite subsequence \( \{x_{k_i}\} \) of \( \{x_k\} \) such that \( x_{k_i} \rightarrow x^* \ (i \rightarrow +\infty) \).

Now, we investigate some useful properties of the NGQCG method. Note that if \( F(x_k) = 0 \) for some \( k \), then the NGQCG iteration terminates immediately as we have already got a solution of the system of nonlinear equations (1). Hence, from now on, we make the following assumption:

\(^2\) Note that \( \eta_k \) determined in the backtracking loop along \( \bar{s}_k \) is not used when the QCGB strategy is implemented. Hence, we use the notation \( \eta_k \) without causing confusion.
A3. The NGQCGB iteration does not break down with $\varepsilon_0 = 0$, and generates an infinite iteration sequence $\{x_k\} \subset \mathbb{R}^n$; furthermore, $\{x_k\}$ has a limit point $x^* \in \mathbb{R}^n$ such that $F'(x^*)$ is invertible.

Based on the above assumption, we will use the following notations:

- $\zeta = \|F'(x^*)^{-1}\|$
- $\delta > 0$ is a sufficiently small number such that $F'(x)$ is invertible and $\|F'(x)^{-1}\| \leq 2\zeta$ whenever $x \in N_\delta(x^*$),
- $\bar{\zeta} := \sup_{x \in N_\delta(x^*)} \|F'(x)\|$
- $\kappa(F'(x))$ is the Euclidean condition number of the matrix $F'(x)$ for $x \in N_\delta(x^*)$.

With Assumption A3 and the above notations, we will prove that $x_k \to x^*$ whenever $k \to +\infty$ and $F(x^*) = 0$. First, we prove that the acute angle between $F(x_k)$ and $F'(x_k)d_k$ is uniformly bounded away from $\frac{\pi}{2}$ for $x_k$ sufficiently near $x^*$.

**Lemma 4.3.** If Assumption A3 holds, then there exists a $\lambda > 0$ independent of $k$ such that

$$\frac{|\langle F(x_k), F'(x_k)d_k \rangle|}{\|F(x_k)\| \|F'(x_k)d_k\|} \geq \lambda$$

whenever $x_k \in N_\delta(x^*)$.

**Proof.** For $x_k \in N_\delta(x^*)$, using Assumption A2 and Lemma 4.1 we have

$$\frac{\|V_m^T g_k\|}{\|g_k\|} \geq \frac{1 - \eta_{\max}}{\kappa(F'(x_k))(1 + \eta_{\max})},$$

where $V_m$ is the orthogonal basis of the Krylov subspace $K_m(F'(x_k), r_k^0)$ (see (5)). Since $F'(x_k)$ is nonsingular and $g_k \neq 0$, we have $F'(x_k)g_k \neq 0$ and, hence,

$$\max_{z \in \Omega_k \setminus \{0\}} \frac{|F(x_k)^T F'(x_k)z|}{\|F(x_k)\| \|F'(x_k)z\|} \geq \frac{|F(x_k)^T F'(x_k)g_k|}{\|F(x_k)\| \|F'(x_k)g_k\|} = \frac{|g_k^T V_m V_m^T g_k|}{\|F(x_k)\| \|F'(x_k)\|} = \frac{|g_k^T V_m^2 g_k|}{\|V_m^T g_k\|} = \frac{1 - \eta_{\max}}{\kappa(F'(x_k)) \|g_k\|} \geq \frac{1 - \eta_{\max}}{\kappa(F'(x_k)) \|g_k\|} \geq \frac{1 - \eta_{\max}}{\frac{3}{2} \pi^2 (1 + \eta_{\max})} \equiv \lambda.$$

Therefore, by the definition of $d_k$ and following the proof of Theorem 8.4 of [14], we have

$$\|F(x_k) + F'(x_k)d_k\| = \min_{z \in \Omega_k} \|F(x_k) + F'(x_k)z\|$$

$$= \min_{z \in \Omega_k \setminus \{0\}} \|F(x_k) + F'(x_k)z\|$$

$$= \min_{z \in \Omega_k \setminus \{0\}} \min_{\mu \in \mathbb{R}} \|F(x_k) + F'(x_k)(\mu z)\|$$

$$= \min_{z \in \Omega_k \setminus \{0\}} \left( \|F(x_k)\|^2 - \frac{|F(x_k)^T F'(x_k)z|^2}{\|F'(x_k)z\|^2} \right)^{\frac{1}{2}}$$

$$= \left(1 - \max_{z \in \Omega_k \setminus \{0\}} \frac{|F(x_k)^T F'(x_k)z|^2}{\|F(x_k)\|^2 \|F'(x_k)z\|^2} \right)^{\frac{1}{2}} \|F(x_k)\|$$

$$\leq \sqrt{1 - \lambda^2} \|F(x_k)\|.$$
This inequality implies that
\[ \lambda^2 \| F(x_k) \|^2 + 2 \langle F(x_k), F'(x_k) dk \rangle + \| F'(x_k) dk \|^2 \leq 0. \]

Hence, \[
\left| \langle F(x_k), F'(x_k) dk \rangle \right| \| F(x_k) \| \| F'(x_k) dk \| \geq \lambda.
\]
Here, we have used the fact that \( \langle F(x_k), F'(x_k) dk \rangle < 0 \).

The following lemma provides an estimate about \( \| E_k(\eta) \| \).

**Lemma 4.4.** If Assumption A3 holds, then there exists a \( \Gamma > 0 \) independent of \( k \) such that
\[
\| E_k(\eta) \| \leq \Gamma (1 - \eta) \| F(x_k) \|, \quad \eta \in [\tilde{\eta}_k, 1],
\] whenever \( x_k \in N_\delta(x^*) \).

**Proof.** From Lemma 4.3 we know that there exists a \( \lambda > 0 \) independent of \( k \) such that (25) holds for all \( x_k \in N_\delta(x^*) \). Therefore, for \( x_k \in N_\delta(x^*) \), by Lemma 7.2 in [14] we know that
\[
\| E_k(\eta) \| \leq \frac{2 \| F'(x_k)^{-1} \|}{\lambda} \cdot (1 - \eta) \| F(x_k) \|, \quad \text{for } \max \{ \tilde{\eta}_k, \sqrt{1 - \lambda^2} \} \leq \eta \leq 1.
\] (28)

Let \( \Gamma_1 = \frac{4\zeta}{\lambda}, \quad \Gamma_2 = \frac{4\zeta}{1 - \sqrt{1 - \lambda^2}} \).

Then, for \( \sqrt{1 - \lambda^2} \leq \tilde{\eta}_k \leq \eta \leq 1 \) or \( \tilde{\eta}_k < \sqrt{1 - \lambda^2} \leq \eta \leq 1 \), the estimate (28) shows that
\[
\| E_k(\eta) \| \leq \Gamma_1 (1 - \eta) \| F(x_k) \|.
\]

Therefore, (27) holds for our taking \( \Gamma := \Gamma_1 \). Suppose that \( \tilde{\eta}_k < \eta < \sqrt{1 - \lambda^2} \). Then it follows from (26) that
\[
\| E_k(\eta) \| \leq \| dk \|
\leq \| F'(x_k)^{-1} \| \left( \| F'(x_k) dk + F(x_k) \| + \| F(x_k) \| \right)
\leq 2\zeta \left( 1 + \sqrt{1 - \lambda^2} \right) \| F(x_k) \|
= 2\zeta \cdot \frac{1 + \sqrt{1 - \lambda^2}}{1 - \eta} \cdot (1 - \eta) \| F(x_k) \|
\leq 2\zeta \cdot \frac{1 + \sqrt{1 - \lambda^2}}{1 - \sqrt{1 - \lambda^2}} \cdot (1 - \eta) \| F(x_k) \|
\leq \frac{4\zeta}{1 - \sqrt{1 - \lambda^2}} \cdot (1 - \eta) \| F(x_k) \|
= \Gamma_2 (1 - \eta) \| F(x_k) \|.
\]

Therefore, (27) holds for our taking \( \Gamma := \Gamma_2 \), too. Consequently, we see that (27) holds for \( \Gamma = \max \{ \Gamma_1, \Gamma_2 \} \).

From the proof of Theorem 6.1 in [14], we have the following result.

**Lemma 4.5.** If Assumption A3 holds, then
\[
\| \sigma_k(\eta) \| \leq \Gamma (1 - \eta) \| F(x_k) \|
\]
whenever \( x_k \in N_\delta(x^*) \), where
\[
\Gamma = 2 \| F'(x^*)^{-1} \| \cdot \frac{1 + \eta_{\max}}{1 - \eta_{\max}},
\]
and \( \sigma_k(\eta) \) is defined by (24).
The following theorem demonstrates a relationship between the convergence of an NGQCGB iteration sequence and its subsequence.

**Theorem 4.1.** If Assumption A₃ holds, then \( x_k \to x^* \) (\( k \to +\infty \)).

**Proof.** Suppose that \( x_k \in N_\delta(x^*) \). Then Lemma 4.4 shows that there exists a \( \Gamma' > 0 \) independent of \( k \) such that
\[
\| \Delta_k \| = \| E_k(\eta_k) \| \leq \Gamma'(1 - \eta_k) \| F(x_k) \| ,
\]
when \( \Delta_k \) is computed by the QCGB strategy. In addition, from Lemma 4.5 we know that there exists a \( \Gamma'' > 0 \) independent of \( k \) such that
\[
\| \Delta_k \| \leq \Gamma''(1 - \eta_k) \| F(x_k) \| ,
\]
when \( \Delta_k \) is computed by the backtracking-loop strategy. Hence, if we define \( \Gamma = \max\{\Gamma', \Gamma''\} \), it holds that
\[
\| \Delta_k \| \leq \Gamma(1 - \eta_k) \| F(x_k) \| ,
\]
for \( x_k \in N_\delta(x^*) \). Because \( x^* \) is a limit point of the iteration sequence, by Lemma 4.2 we immediately know that \( x_k \to x^* \) (\( k \to +\infty \)). \( \Box \)

Now, we are ready to demonstrate the global convergence theorem for the NGQCGB method.

**Theorem 4.2.** If Assumption A₃ holds, then \( x_k \to x^* \) (\( k \to +\infty \)) and \( F(x^*) = 0 \). Moreover, \( x_{k+1} = x_k + \bar{s}_k \) for all sufficiently large \( k \).

**Proof.** By Theorem 4.1, it is obvious that \( x_k \to x^* \) (\( k \to +\infty \)). Now, we prove that \( F(x^*) = 0 \).

If there is a subsequence \( \{ x_{k_i} \} \subset \{ x_k \} \) that is generated by the backtracking-loop strategy, then it follows easily from Theorem 5.2 in [14] and its proof that \( F(x_{k_i}) \to 0 \) (\( k \to +\infty \)). Otherwise, there must be a subsequence \( \{ x_{k_i} \} \subset \{ x_k \} \) that is generated by the QCGB strategy, and we will prove that in this case \( F(x_{k_i}) \to 0 \) (\( k \to +\infty \)), too.

Let \( z_{k_i-1} = g_{k_i} - g_{k_i-1} \). Since \( x_{k_i} \) is generated by the QCGB strategy, from (14) and the monotonically decreasing property of \( \{ \| F(x_k) \| \} \) we get
\[
\sum_{i \geq 0} -s_{k_i-1}^T \Delta_{k_i-1} < +\infty \quad \text{and} \quad z_{k_i-1}^T \Delta_{k_i-1} \geq -(1 - \beta)g_{k_i-1}^T \Delta_{k_i-1}, \quad i \geq 0.
\]
These two inequalities show that
\[
\sum_{i \geq 0} \frac{(g_{k_i-1}^T \Delta_{k_i-1})^2}{z_{k_i-1}^T \Delta_{k_i-1}} < +\infty. \tag{29}
\]
From Assumption A₁ we know that
\[
z_{k_i-1}^T \Delta_{k_i-1} \leq \gamma \| \Delta_{k_i-1} \|^2, \quad i \geq 0. \tag{30}
\]
It then follows from (29) and (30) that
\[
\sum_{i \geq 0} \frac{(g_{k_i-1}^T d_{k_i-1})^2}{\| d_{k_i-1} \|^2} < +\infty,
\]
and consequently,
\[
\frac{-g_{k_i-1}^T d_{k_i-1}}{\| d_{k_i-1} \|} \to 0, \quad i \to +\infty. \tag{31}
\]
On the other hand, by Lemma 4.3 we know that there exists a \( \lambda > 0 \) independent of \( k \) such that
\[
\frac{\| F(x_k) \|}{\| F'(x_k) d_k \|} \geq \lambda.
\]
whenever \( x_k \in N_\delta(x^*) \). Because
\[
\| F(x_k)^T F'(x_k) \| \| d_k \| \leq \kappa \left( F'(x_k) \right) \| F(x_k) \| \| F'(x_k) d_k \|
\]
holds for \( x_k \in N_\delta(x^*) \), when \( x_{k-1} \in N_\delta(x^*) \) we have
\[
-\frac{\bar{g}_k}{d_k} \|d_k\| = \frac{| \langle F(x_{k-1}), F'(x_{k-1})d_{k-1} \rangle |}{\| F(x_{k-1})^T F'(x_{k-1}) \| \| d_{k-1} \|} \cdot \| F(x_{k-1})^T F'(x_{k-1}) \|
\geq \kappa \left( F'(x_{k-1}) \right)^{-1} \cdot \| F(x_{k-1})^T F'(x_{k-1}) \| \cdot \frac{| \langle F(x_{k-1}), F'(x_{k-1})d_{k-1} \rangle |}{\| F(x_{k-1}) \| \| F'(x_{k-1})d_{k-1} \|}
\geq \frac{\lambda}{2 \xi_1} \| F(x_{k-1})^T F'(x_{k-1}) \|
\geq \frac{\lambda}{4 \xi_1} \| F(x_{k-1}) \|.
\]
Therefore, by (31), we immediately get
\[
F(x_{k-1}) \rightarrow 0, \quad i \rightarrow +\infty.
\]
It then follows from the monotonically decreasing property of the sequence \( \| F(x_k) \| \) that \( F(x_k) \rightarrow 0 \) \( (k \rightarrow +\infty) \). Thus, in either case, we have \( F(x^*) = 0 \).

Since \( x_k \rightarrow x^* \) and \( F(x_k) \rightarrow 0 \), it follows easily from Lemma 5.1 in [14] that the backtracking loop along \( \tilde{s}_k \) will be successfully terminated with \( \eta_k = \tilde{\eta}_k \) for all \( k \) sufficiently large, which immediately results in \( x_{k+1} = x_k + \tilde{s}_k \) for all \( k \) sufficiently large. \( \square \)

Theorem 4.2 shows that if the NGQCGB iteration sequence \( \{x_k\} \subset \mathbb{R}^n \) converges to a solution \( x^* \) of the system of nonlinear equations \( (1) \), then the ultimate convergence speed of the \( \{x_k\} \) is determined by the choice of \( \tilde{\eta}_k \).

5. Restarting and preconditioning

In Section 3, we studied the NGQCGB method where neither restarting nor preconditioning is used for GMRES. However, since storage and work requirement increases very much when the number of iterations in GMRES becomes large, restarting technique is often needed; in addition, preconditioning is often required for Krylov subspace methods to accelerate their convergence rate. In this section, we outline how to combine the NGQCGB method with restarting and preconditioning strategies. The techniques adopted here is similar to those in [7].

In fact, with careful examination about the construction of the NGQCGB method in Section 3 and the proof of its convergence in Section 4, we find that if there is a subspace in which the inexact Newton step \( \tilde{s}_k \) lies, and the projection of the gradient on this subspace is computable, then the NGQCGB method can be applied and its convergence can be guaranteed. So, a proper subspace is the key for constructing the QCGB strategy. When neither restarting nor preconditioning is used, and \( s^0_k = 0 \), the Krylov subspace is the standard one. If either restarting or preconditioning is employed, then a different subspace must be constructed so that the NGQCGB method can still be applied.

5.1. Restarting

When GMRES is restarted every \( m_{\text{max}} \) iteration steps, the initial guess \( s^0_k \) at every restart is set to be the latest GMRES iterate. Then, after a restart, the new initial guess \( s^0_k \) is nonzero.

If \( s^0_k \neq 0 \), then, in general, \( K_m \neq \hat{s}^0_k + \hat{K}_m \). Noticing that \( \tilde{s}_k \in s^0_k + \hat{K}_m \), following the lines of [7] we can let \( \hat{g}_k \) be the projection of \( g_k \) onto the subspace \( \hat{K}_m \), where
\[
\hat{K}_m := \text{span} \{ V_m, s^0_k \}.
\]
For details about the computation of \( \hat{g}_k \) in this case, we refer to [7]. Here, we only point out that NGQCGB with restart admits matrix-free implementation, too.
5.2. Preconditioning

Since the left-preconditioning affects the residual of the corresponding linear system, we consider only the right-preconditioning for our method. That is to say, we will focus on the transformed Newton equation

\[(F'(x_k)P)(P^{-1}s) = -F(x_k),\]

or

\[(F'(x_k)P)z = -F(x_k), \quad \text{where } z = P^{-1}s.\]

For possible choices of the transforming/preconditioning matrix \(P\), we refer to [1,3,2] and references therein.

Without loss of generality, we assume that the initial guess of GMRES is \(z_0 = 0\) and no restarting is employed. In this case, the Krylov subspace generated by GMRES is

\[K_{m,P}(F'(x_k)P, r_k^0) := \text{span}\{r_k^0, (F'(x_k)P)r_k^0, \ldots, (F'(x_k)P)^{m-1}r_k^0\},\]

where \(r_k^0 = -F(x_k)\). Meanwhile, we note that (6) becomes \((F'(x_k)P)V_m = V_{m+1}H_m\), where \(v_1 = r_k^0/\beta_k\), with \(\beta_k = \|F(x_k)\|\). As the approximate solution for the Newton equation is \(\tilde{z}_k = P\tilde{z}_k\), where \(\tilde{z}_k \in K_{m,P}\), is such that

\[\|F(x_k) + (F'(x_k)P)\tilde{z}_k\| \leq \eta_k \|F(x_k)\|,\]

it follows that \(\tilde{z}_k \in PK_{m,P}\). Therefore, we can define \(\tilde{g}_k\) as the projection of \(g_k\) onto \(PK_{m,P}\). Since \(PV_m\) is a basis of \(PK_{m,P}\), it clearly holds that

\[\tilde{g}_k = (PV_m)(PV_m)^TF(x_k) = (PV_m)(PV_m)^TF'(x_k)\]

Then, the QCGB strategy with preconditioning can also be implemented without explicitly forming the Jacobian matrix.

6. Numerical tests

In this section, we use ten typical examples to examine the feasibility and effectiveness of the NGQCGB method, as well as to show that it outperforms both the NGB and the NGECB methods.

In all tests, we take \(\eta_{\max} = 0.9, \alpha = 10^{-4}, \beta = 0.4, \theta_l = 0.1\) and \(\theta_u = 0.5\). We use the “choice 2 safeguard” proposed in [15] to choose the forcing term \(\tilde{\eta}_k\); the GMRES method without restarting is employed, with the starting vector \(s_k = 0\) and the number of its maximal iteration steps \(m_{\max} = 40\). We stopped the inexact Newton method when the current iterate \(x_k\) satisfies

\[\max \left\{ \frac{1}{\sqrt{m}} \|F(x_k)\|, \frac{\|F(x_k)\|}{\|F(x_0)\|} \right\} \leq 10^{-6},\]

or when the number of iteration steps has exceeded 300. After \(m = m_{\max}\) GMRES iterations, if \(\|r_m\| > \tilde{\eta}_k \|F(x_k)\|\) we will adopt the proposal in [7], i.e., the inexact Newton step \(\tilde{s}_k\) is set to be \(\tilde{s}_k := s_k^m\) and \(\tilde{\eta}_k\) is set to be

\[\tilde{\eta}_k = \frac{\|F'(x_k)s_k^m + F(x_k)\|}{\|F(x_k)\|}.\]

Within each nonlinear iteration, the maximal numbers of the backtracking iterations are limited by 50. In addition, a failure is declared if one of the following three situations occurs during the iteration process:

**F1.** The number of nonlinear iterations is over \(k_{\max} = 300\);  
**F2.** Fifty backtracks are performed (along \(\tilde{s}_k\) for NGB, in ECB strategy for NGECB, and in QCGB strategy for NGQCGB) without producing a satisfactory step; and  
**F3.** \(\|F(x_{k-1})\| - \|F(x_k)\| \leq 10^{-6}\|F(x_k)\|\), which means that the method cannot manage to escape from a local minimizer of the merit function, see [16,18].
In our tests, most of the failures are due to $F_3$, and only a few result from $F_1$ and $F_2$.

Because the number of the backtracking steps $N_b$ affects the numerical behavior of the corresponding method, we implement NGQCGB and NGECB methods for different values of $N_b$. For clarity, we use NGQCGB($N_b$) and NGECB($N_b$) to denote the corresponding methods, respectively. In our computations, we let $N_b \leq 5$, which yields better numerical performance than the choice of $N_b > 5$; see [7]. We point out that in our tests the choice of $N_b$ is not critical for both NGQCGB and NGECB methods when $N_b \leq 5$.

Our test problems are typical systems of nonlinear equations in literature. They are listed in Table 1 along with their names and standard initial guesses, say $x_s$.

Besides the standard initial guess $x_s$, we used also the initial guesses $x_0 = \pm j x_s$, $\pm j e$, $j = 1, 2, \ldots, 5$, and $x_0 = 0$, where $e$ represents the vector with all entries being 1, and 0 denotes the zero vector. For some problems, some of the above initial guesses solve the problem or some of them are repeated. Therefore, we omit such initial guesses and obtain a total of 182 tests.

### 6.1. Performance profile

To assess the performance of the NGB, the NGECB and the NGQCGB methods, we use the “performance profile” proposed in [13] as evaluation tool. We briefly describe it here.

Assume that we have a solver set $\mathcal{S}$ with $n_s$ solvers and a problem set $\mathcal{P}$ with $n_p$ problems. Let $\mathcal{M}$ be a performance measure of the solvers, for example, the number of function evaluations or iterations, etc., and let $\mathcal{M}_{p,s}$ be the measure result for problem $p$ when the solver $s$ is used. For each problem $p$, let

$$\mathcal{M}_{p,\text{min}} = \min\{\mathcal{M}_{p,s} \mid s \in \mathcal{S}, \text{ and } p \text{ can be solved by } s\},$$

which is the best performance result for all solvers on problem $p$. Based on the performance measure $\mathcal{M}$, we define the **performance ratio** as

$$r_{p,s} = \begin{cases} \frac{\mathcal{M}_{p,s}}{\mathcal{M}_{p,\text{min}}}, & \text{if } p \text{ can be solved by } s, \\ r_{\infty}, & \text{if } p \text{ cannot be solved by } s, \end{cases}$$

where $r_{\infty} > e^\xi$ is a given sufficiently large number, and

$$\xi \equiv \max\{\ln r_{p,s} \mid s \in \mathcal{S}, \ p \in \mathcal{P}, \text{ and } p \text{ can be solved by } s\}.$$

Note that $r_{p,s}$ reflects the ratio of the performance of the solver $s$ to the best performance on problem $p$. Now, define the **performance profile** as

$$\rho_s(\tau) = \frac{1}{n_p} \left| \Omega_s^T \right|_F, \quad \tau \in [0, \ln r_{\infty}].$$

---

The definition here is slightly different from that in [13], but they are essentially the same.
where $\Omega_{\tau}^s = \{ p \in \mathcal{P} \mid \ln r_{p,s} \leq \tau \}$ and $|\Omega_{\tau}^s|$ represents the number of elements contained in $\Omega_{\tau}^s$. Note that $\rho_s(\tau)$ denotes the probability for the solver $s$ that a log-scale performance ratio is not greater than the factor $\tau$. Furthermore, it is easy to see that

(i) $\rho_s(0)$ represents the probability that the solver $s$ can solve a problem with the best performance;
(ii) $\rho_s(\xi)$ represents the probability that the solver $s$ can solve a problem successfully.

In our tests, the solver set contains the NGB, the NGECB and the NGQCGB methods, while the problem set is made up of the 182 tests. We use the number of nonlinear iterations and function evaluations as performance measure, since they reflect the main computational cost for each method.

6.2. Numerical results

First, we fixed $N_b = 4$ for the NGQCGB and the NGECB methods, and carried out the 182 tests for each of the three methods: NGQCGB(4), NGECB(4) and NGB. The performance profiles of these methods are plotted in Figs. 1–2.

Fig. 1 shows the performance profiles of the methods that are based on numbers of nonlinear iterations. From this figure, we see that the performance profile of NGQCGB(4) is always greater than that of NGECB(4) and NGB, so NGQCGB(4) is the winner in the tests. Observing the value of the performance profiles at the point 0, we see that the probability that NGQCGB(4) can give the best performance is nearly 0.8, while that of NGECB(4) is only a little more than 0.5, and that of NGB is about 0.51. We point out that in some tests, NGQCGB(4) and NGECB(4) are reduced to NGB. Thus, the sum of the probabilities that these methods perform best is larger than 1. By observing the highest parts of the three curves of the performance profiles, we can see that NGQCGB(4) succeeds in solving about 85% of the total tests, NGECB(4) can succeed in solving about 77%, and NGB can succeed in solving only about 64%. This shows that NGQCGB is more effective and robust than both NGECB and NGB methods.

Fig. 2 shows the performance profiles of the methods that are based on the numbers of function evaluations. We can see that the trends of the curves in Fig. 2 are almost the same as those in Fig. 1. Therefore, we can conclude from this figure again that NGQCGB is the optimal method among these three methods.

From the numerical results about Problems $P_1$ and $P_2$, we observed that by varying the parameter $N_b$ the chances of success of the NGQCGB and the NGECB methods are not improved much. However, different choices of $N_b$ will affect the efficiency of the methods. As an example, we list some results about NGQCGB for Problems $P_3$ and $P_4$ in Tables 2 and 3, where we use the following notations:
Fig. 2. Performance profile based on numbers of function evaluations ($\xi = 2.86$).

Table 2
Results of NGB and NGQCGB($N_b$) with $N_b = 1, 3, 5$ for Problem $P_3$

<table>
<thead>
<tr>
<th>$x_0$</th>
<th>NGB</th>
<th>NGQCGB(1)</th>
<th>NGQCGB(3)</th>
<th>NGQCGB(5)</th>
<th>NGB</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NI</td>
<td>FE</td>
<td>BT</td>
<td>SW</td>
<td>NI</td>
</tr>
<tr>
<td>$-x_s$</td>
<td>16</td>
<td>98</td>
<td>25</td>
<td>7</td>
<td>23</td>
</tr>
<tr>
<td>$-2x_s$</td>
<td>21</td>
<td>120</td>
<td>35</td>
<td>8</td>
<td>24</td>
</tr>
<tr>
<td>$-5x_s$</td>
<td>25</td>
<td>180</td>
<td>70</td>
<td>12</td>
<td>28</td>
</tr>
</tbody>
</table>

Table 3
Results of NGB and NGQCGB($N_b$) with $N_b = 0, 2, 4$ for Problem $P_4$

<table>
<thead>
<tr>
<th>$x_0$</th>
<th>NGB</th>
<th>NGQCGB(0)</th>
<th>NGQCGB(2)</th>
<th>NGQCGB(4)</th>
<th>NGB</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NI</td>
<td>FE</td>
<td>BT</td>
<td>SW</td>
<td>NI</td>
</tr>
<tr>
<td>$-x_s$</td>
<td>9</td>
<td>26</td>
<td>0</td>
<td>1</td>
<td>9</td>
</tr>
<tr>
<td>$-2x_s$</td>
<td>6</td>
<td>18</td>
<td>0</td>
<td>1</td>
<td>12</td>
</tr>
<tr>
<td>$-5x_s$</td>
<td>10</td>
<td>27</td>
<td>0</td>
<td>1</td>
<td>10</td>
</tr>
</tbody>
</table>

- NI: the number of nonlinear iterations;
- FE: the number of function evaluations;
- BT: the number of backtracking iterations;
- SW: the number of switches between the two backtracking strategies; and
- *: the case that a failure occurred in either of the situations $F_1$–$F_3$.

In Table 2, we list the numerical results of NGB and NGQCGB($N_b$) with $N_b = 1, 3$ and 5 for Problem $P_3$ when $x_0 = -x_s$, $-2x_s$ and $-5x_s$. From this table, we see that when $x_0 = -5x_s$, NGB failed but NGQCGB succeeded for all three choices of $N_b$. This shows that QCGB strategy is critical for the success of NGQCGB method in this case. By comparing the cases of $x_0 = -x_s$ and $-2x_s$, we see that the NGB method needs much more nonlinear iterations and function evaluations than the NGQCGB method. Thus, NGQCGB is more efficient than NGB in these two cases. Comparing the performance of the NGQCGB method for different values of $N_b$, we see that NGQCGB(5) is the most efficient one when $x_0 = -x_s$, while NGQCGB(1) is the winner for $x_0 = -2x_s$ and $-5x_s$. In addition, we see that, for $x_0 = -2x_s$ and $-5x_s$, the larger $N_b$ is, the more numbers of nonlinear iterations and function evaluations are needed.

When $x_0 = -x_s$, $-2x_s$ and $-5x_s$ for Problem $P_4$, we list the numerical results of NGB and NGQCGB($N_b$) with $N_b = 0, 2$ and 4 in Table 3. It can be seen from this table that the results of NGQCGB(4) exactly coincide with those of
NGB for all of the three initial guesses, as the QCGB strategy is never used in NGQCGB(4) in our implementations. By comparing the performance of NGQCGB for different values of $N_b$, we see that NGQCGB(0) shows the best performance. Furthermore, the larger $N_b$ is, the much more nonlinear iterations and function evaluations are needed for all the three cases.

7. Conclusions

We have presented a class of globally convergent inexact Newton methods, the Newton-GMRES with quasi-conjugate-gradient backtracking (NGQCGB) methods, for solving large sparse systems of nonlinear equations. These methods are a suitable combination of the Newton-GMRES iteration and some efficient backtracking strategies, and can be considered as an improvement of the known Newton-GMRES with backtracking (NGB) method. The convergence property of the NGQCGB method has been established similarly to that of the NECB method [7]. Numerical experiments have shown that the NGQCGB method is much more robust and effective than both NGB and NECB methods on the used test set of problems.

References