STABILIZED BARZILAI-BORWEIN METHOD*

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Abstract

The Barzilai-Borwein (BB) method is a popular and efficient tool for solving large-scale unconstrained optimization problems. Its search direction is the same as for the steepest descent (Cauchy) method, but its stepsize rule is different. Owing to this, it converges much faster than the Cauchy method. A feature of the BB method is that it may generate too long steps, which throw the iterates too far away from the solution. Moreover, it may not converge, even when the objective function is strongly convex. In this paper, a stabilization technique is introduced. It consists in bounding the distance between each pair of successive iterates, which often allows for decreasing the number of BB iterations. When the BB method does not converge, our simple modification of this method makes it convergent. For strongly convex functions with Lipschits gradients, we prove its global convergence, despite the fact that no line search is involved, and only gradient values are used. Since the number of stabilization steps is proved to be finite, the stabilized version inherits the fast local convergence of the BB method. The presented results of extensive numerical experiments show that our stabilization technique often allows the BB method to solve problems in a fewer iterations, or even to solve problems where the latter fails.

Mathematics subject classification: 65K05, 90C06, 90C30.

Key words: Unconstrained optimization, Spectral algorithms, Stabilization, Convergence analysis.

1. Introduction

In this paper, we consider spectral gradient methods for solving the unconstrained optimization problem

$$\min_{x \in R^n} f(x),\tag{1.1}$$

where $f: \mathbb{R}^n \to \mathbb{R}^1$ is a sufficiently smooth function. Its minimizer is denoted by x^* . Gradient-type iterative methods used for solving problem (1.1) have the form

$$x_{k+1} = x_k - \alpha_k g_k, \tag{1.2}$$

^{*} Received July 16, 2019 / Revised version received September 30, 2019 / Accepted November 11, 2019 / Published online November 21, 2019 /

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where $g_k = \nabla f(x_k)$ and $\alpha_k > 0$ is a stepsize. Methods of this type differ in the stepsize rules which they follow.

We focus here on the two choices of α_k proposed in 1988 by Barzilai and Borwein [1], usually referred to as the BB method. The rationale behind these choices is related to viewing the gradient-type methods as quasi-Newton methods, where α_k in (1.2) is replaced by the matrix $D_k = \alpha_k I$. This matrix is served as an approximation of the inverse Hessian matrix. Following the quasi-Newton approach, the stepsize is calculated by forcing either D_k^{-1} (BB1 method) or D_k (BB2 method) to satisfy the secant equation in the least squares sense. The corresponding two problems are formulated as

$$\min_{D=\alpha I} \|D^{-1}s_{k-1} - y_{k-1}\| \quad \text{and} \quad \min_{D=\alpha I} \|s_{k-1} - Dy_{k-1}\|, \tag{1.3}$$

where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$. The solutions to these problems are

$$\alpha_k^{BB1} = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T y_{k-1}} \quad \text{and} \quad \alpha_k^{BB2} = \frac{s_{k-1}^T y_{k-1}}{y_{k-1}^T y_{k-1}},$$
(1.4)

respectively. Here and in what follows, $\|\cdot\|$ denotes the Euclidean vector norm and the induced matrix norm. Other norms used in this paper will be denoted in a different way.

Barzilai and Borwein [1] proved that their method converges R-superlinearly for two-dimensional strictly convex quadratics. Dai and Fletcher [7] analyzed the asymptotic behavior of BB-like methods, and they obtained R-superlinear convergence of the BB method for the three-dimensional case. Global convergence of the BB method for the n-dimensional case was established by Raydan [20] and further refined by Dai and Liao [10] for obtaining the R-linear rate. For nonquadratic functions, local convergence proof of the BB method with R-linear rate was, first, sketched in some detail by Liu and Dai [19], and then it was later rigorously proved by Dai et al. [9]. Extensive numerical experiments show that the two BB stepsize rules significantly improve the performance of gradient methods (see, e.g., [14,21]), both in quadratic and nonquadratic cases.

A variety of modifications and extensions have been developed, such as gradient methods with retards [15], alternate BB method [8], cyclic BB method [9], limited memory gradient method [4] etc. Several approaches were proposed for dealing with nonconvex objective functions, in which case the BB stepsize (1.4) may become negative. In our numerical experiments, we use the one proposed in [6]. The BB method has been extended to solving symmetric and nonsymmetric linear equations [6,11]. Furthermore, by incorporating the nonmontone line search by Grippo et al. [17], Raydan [21] and Grippo et al. [18] developed the global BB method for general unconstrained optimization problems. Later, Birgin et al. [2] proposed the so-called spectral projected gradient method which extends Raydan's method to smooth convex constrained problems. For more works on BB-like methods, see [3,14,23] and references therein.

As it was observed by many authors, the BB method may generate too long steps, which throw the iterates too far away from the solution. In practice, it may not converge even for strongly convex functions (see, e.g., [14]). The purpose of this paper is to introduce a simple stabilization technique and to justify its efficiency both theoretically and practically. Our stabilization does not assume any objective function evaluations. It consists in uniformly bounding $||s_k||$, the distance between each pair of successive iterates. It should be emphasized that, if the BB method safely converges for a given function, then there is no necessity in stabilizing it. In such cases, the stabilization may increase the number of iterations. In other

cases, as it will be demonstrated by results of our numerical experiments, the stabilization may allow for decreasing the number of iterations or even to make the BB method convergent.

Although we focus here on stabilizing the conventional BB method, our approach can directly be combined with the existing modifications of the BB method, where a nonmonotone line search is used.

The paper is organized as follows. In the next section, we present an example of a strictly convex function and show that the BB method does not converge in this case. This contributes to a motivation for stabilizing this method. In the same section, its stabilized version is introduced. In Section 3, a global convergence of our stabilized BB algorithm as well as its R-linear rate of convergence are proved under suitable assumptions. Results of numerical experiments are reported and discussed in Section 4. Finally, some conclusions are included in the last section of the paper.

2. Stabilized Algorithm

Before formulating our stabilized algorithm, we wish to begin with a motivation based on presenting an example of a strongly convex function for which we theoretically prove that neither of the BB methods converge. To the best of our knowledge, no theoretical evidence of BB methods being divergent is available in the literature.

In the review paper by Fletcher [14], it is claimed that the BB method diverges in practice for certain initial points in the test problem referred to as Strictly Convex 2 by Raydan [21], in which

$$f(x) = \sum_{i=1}^{n} i(e^{x_i} - x_i)/10.$$
 (2.1)

This strongly convex function will be used in Section 4 for illustrating the efficiency of the stabilized algorithm. Our numerical experiments show that, in this specific case, the failure of the BB method is related to the underflow and overflow effects in the computer arithmetic. We are not acquainted with any theoretical justification of the divergence of the BB method for this or any other functions.

We will present now an instance of a function for which the BB method does not converge in the exact arithmetic. For this purpose, the notation

$$a = \sqrt{5} - 1$$
, $b = \sqrt{5} + 3$, $c_1 = \frac{3\sqrt{5} + 8}{4}$, $c_2 = -\frac{5\sqrt{5} + 11}{32}$, $f(a) = \frac{c_1 a^2}{2} + \frac{c_2 a^4}{4}$

will be used. Consider the univariate function

$$f(x) = \begin{cases} \frac{1}{4}(x+a)^2 - (\sqrt{5}+1)(x+a) + f(a), & x < -a, \\ \frac{c_1}{2}x^2 + \frac{c_2}{4}x^4, & -a \le x \le a, \\ \frac{1}{4}(x-a)^2 + (\sqrt{5}+1)(x-a) + f(a), & x > a. \end{cases}$$
 (2.2)

Its first derivative

$$g(x) = \begin{cases} \frac{1}{2}(x+a) - \sqrt{5} - 1, & x < -a, \\ c_1 x + c_2 x^3, & -a \le x \le a, \\ \frac{1}{2}(x-a) + \sqrt{5} + 1, & x > a \end{cases}$$

is continuously differentiable, and g(x) is an odd monotonically increasing function (see Fig. 2.1). It can be easily verified that the function f(x) is twice continuously differentiable with

$$1/2 \le f''(x) \le c_1, \quad \forall x \in R^1.$$

This means that this function is strongly convex, and its first derivative is Lipschitz-continuous.

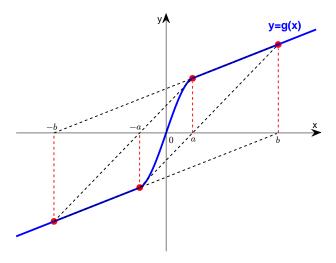


Fig. 2.1. Cyclic iterates generated by the BB method for function (2.2).

For any univariate objective function, there is no difference between BB1 and BB2 versions, and they are equivalent to the secant method applied to the first derivative. For function (2.2), if to initiate the BB method with $x_0 = -b$ and $x_1 = -a$, then the subsequent iterates are

$$\begin{aligned} x_2 &= x_1 - \frac{x_1 - x_0}{g(x_1) - g(x_0)} g(x_1) = b, \\ x_3 &= x_2 - \frac{x_2 - x_1}{g(x_2) - g(x_1)} g(x_2) = a, \\ x_4 &= x_3 - \frac{x_3 - x_2}{g(x_3) - g(x_2)} g(x_3) = -b = x_0, \\ x_5 &= x_4 - \frac{x_4 - x_3}{g(x_4) - g(x_3)} g(x_4) = -a = x_1. \end{aligned}$$

This clearly shows that the BB method cycles between four points (see Figure 2.1). The presented counter-example can be easily extended to n-dimensional case. As an example, one can consider a separable objective function equal to the sum of any number of functions of the form (2.2), where no variable appears in more than one of these functions.

After motivating the necessity of stabilizing the BB method, we can now proceed to presenting the basic idea of our stabilized BB algorithm, where $\Delta>0$ is a parameter. It consists in choosing the stepsize in (1.2) in the way that $\|x_{k+1}-x_k\|=\Delta$, whenever $\|\alpha_k^{BB}g_k\|>\Delta$, i.e. $\alpha_k^{BB}>\Delta/\|g_k\|$. In other cases, we choose $\alpha_k=\alpha_k^{BB}$, which results in $\|x_{k+1}-x_k\|\leq\Delta$. Thus, denoting

$$\alpha_k^{stab} = \frac{\Delta}{\|g_k\|},$$

we propose to choose

$$\alpha_k = \min\{\alpha_k^{BB}, \alpha_k^{stab}\}. \tag{2.3}$$

Here $\alpha_k^{BB} = \alpha_k^{BB1}$ or $\alpha_k^{BB} = \alpha_k^{BB2}$, depending on the specific BB method in (1.4). A formal description of our stabilized BB algorithm follows.

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Algorithm 2.1. BBstab.

Given: initial points x_0, x_1 \in \mathbb{R}^n such that x_0 \neq x_1, and scalar \Delta > 0.

Evaluate g_0 and g_1.

for k = 1, 2, \ldots do

if g_k = 0 then stop.

Set s_{k-1} \leftarrow x_k - x_{k-1} and y_{k-1} \leftarrow g_k - g_{k-1}.

Compute \alpha_k by formula (2.3).

Set x_{k+1} \leftarrow x_k - \alpha_k g_k and evaluate g_{k+1}.

end (for)
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This algorithm will be referred to as BB1stab or BB2stab depending on the corresponding choice of α_k^{BB} in (1.4). Note that, for $\Delta = +\infty$, it reduces to the underlying standard BB algorithm.

3. Convergence Analysis

In this section, global convergence of the BBstab algorithm will be proved. Whenever iterates $\{x_k\}$ are mentioned, they are assumed to be generated by BBstab, where it is required that $x_0 \neq x_1$.

Throughout this section, the objective function is assumed to comply with the following requirement.

A1. The function $f: \mathbb{R}^n \to \mathbb{R}^1$ is twice continuously differentiable, and there exist positive constants $\Lambda_1 \leq \Lambda_2$ such that

$$\Lambda_1 \|v\|^2 \le v^T \nabla^2 f(x) v \le \Lambda_2 \|v\|^2, \quad \forall x, v \in \mathbb{R}^n.$$
(3.1)

This assumption implies that

$$\Lambda_1 \|x - x^*\| \le \|g(x)\| \le \Lambda_2 \|x - x^*\|, \quad \forall x \in \mathbb{R}^n.$$
 (3.2)

Extra assumptions are introduced below in proper places.

We shall use the following notation:

$$\begin{split} &\Omega_{1} = \{x \in R^{n}: \ \|g(x)\| \leq \Lambda_{1}\Delta\}, \\ &\Omega_{2} = \{x \in R^{n}: \ \Lambda_{1}\Delta \ < \|g(x)\| \leq \Lambda_{2}\Delta\}, \\ &\Omega_{3} = \{x \in R^{n}: \ \Lambda_{2}\Delta \ < \|g(x)\|\}, \\ &\Omega_{3'} = \{x \in R^{n}: \ \Lambda_{2}\Delta \ < \|g(x)\| \leq \varkappa\Lambda_{2}\Delta\}, \end{split}$$

which will be motivated later. Here

$$arkappa = rac{\Lambda_2}{\Lambda_1}.$$

Obviously, $\Omega_{3'} \subset \Omega_3$, and $\Omega_{1,2,3} = \mathbb{R}^n$, where $\Omega_{1,2,3} = \Omega_1 \cup \Omega_2 \cup \Omega_3$. We shall use similar notation for other unions of sets Ω_i .

Inequalities (3.1) ensure that

$$\frac{1}{\Lambda_2} \le \alpha_k^{BB} \le \frac{1}{\Lambda_1}, \quad \forall k \ge 1, \tag{3.3}$$

which in turn means that

$$\alpha_k \le \min\left\{\frac{\Delta}{\|g_k\|}, \frac{1}{\Lambda_1}\right\}, \quad \forall k \ge 1,$$
(3.4)

$$\frac{1}{\varkappa \Lambda_2} \le \alpha_k \le \frac{1}{\Lambda_1}, \qquad \forall x_k \in \Omega_{1,2,3'}. \tag{3.5}$$

These bounds justify the implications

$$x_{k} \in \Omega_{1} \quad \Rightarrow \quad \alpha_{k} = \alpha_{k}^{BB},$$

$$x_{k} \in \Omega_{2} \quad \Rightarrow \quad \alpha_{k} = \min\{\alpha_{k}^{BB}, \alpha_{k}^{stab}\},$$

$$x_{k} \in \Omega_{3} \quad \Rightarrow \quad \alpha_{k} = \alpha_{k}^{stab}.$$

$$(3.6)$$

We can now prove the following result.

Lemma 3.1. Let $x_0, x_1 \in \mathbb{R}^n$ be arbitrary starting points. Then for any $\Delta > 0$, the iterates $\{x_k\}$ have the property that

$$||g_{k+1}|| \le \begin{cases} q_k ||g_k||, & \text{if } x_k \in \Omega_3, \\ \varkappa ||g_k||, & \text{otherwise,} \end{cases} \quad \forall k \ge 1, \tag{3.7}$$

where

$$q_k = 1 - \frac{\Lambda_1 \Delta}{\|g_k\|}.$$

Proof. Using Assumption A1, we get

$$g_{k+1} = g_k - \alpha_k H_k g_k,$$

where the matrix $H_k = \int_0^1 \nabla^2 f(x_k + ts_k) dt$ is symmetric, and it fulfills the relations

$$\Lambda_1 I \leq H_k \leq \Lambda_2 I$$
.

Clearly,

$$||g_{k+1}|| \le ||I - \alpha_k H_k|| ||g_k||. \tag{3.8}$$

Consider, first, the case when $x_k \in \Omega_3$. Using the inequality $\Lambda_2 \Delta < ||g(x)||$ and relations (3.6), we can derive for (3.8) the following upper bound

$$||I - \alpha_k^{stab} H_k|| = \max_{\|v\| = 1} |1 - \alpha_k^{stab} v^T H_k v| = 1 - \alpha_k^{stab} \min_{\|v\| = 1} v^T H_k v \le 1 - \frac{\Lambda_1 \Delta}{\|g_k\|}.$$

This proves the upper inequality in (3.7).

Suppose now that $x_k \in \Omega_{1,2}$, i.e., $||g_k|| \leq \Lambda_2 \Delta$. Then, using (3.4), we get the bounds $\Lambda_2^{-1} \leq \alpha_k \leq \Lambda_1^{-1}$, which together with the inequalities $\Lambda_1 \leq ||H_k|| \leq \Lambda_2$ yield

$$||I - \alpha_k H_k|| \le \max\{1 - \varkappa^{-1}, \varkappa - 1\} = \varkappa - 1 < \varkappa.$$

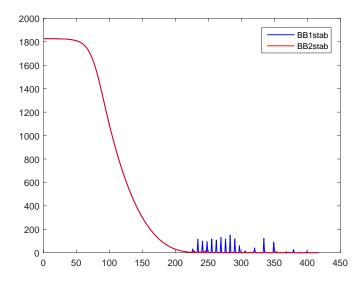


Fig. 3.1. Graphs of $||g_k||$ for BB1stab and BB2stab with $\Delta = 2$ for Raydan function (2.1).

By combining this estimate with (3.8), we finally prove the lower inequality in (3.7).

Lemma 3.1 implies that the stabilization steps have the following properties

$$q_k \in (0,1), \quad \forall x_k \in \Omega_3,$$
 (3.9)

$$q_{k+1} < q_k, \qquad \forall x_k, x_{k+1} \in \Omega_3. \tag{3.10}$$

Next, we prove that, after a finite number of iterations, all iterates belong to the bounded set $\Omega_{1,2,3'}$.

Lemma 3.2. For any $x_0, x_1 \in \mathbb{R}^n$ and $\Delta > 0$, there exists an integer $K \geq 1$ such that the inequality

$$||g_k|| \le \varkappa \Lambda_2 \Delta \tag{3.11}$$

holds, that is $x_k \in \Omega_{1,2,3'}$, for all $k \geq K$. Moreover, K is the iteration number corresponding to the first iterate x_K that belongs to $\Omega_{1,2,3'}$.

Proof. Notice that (3.11) is satisfied if and only if $x_k \in \Omega_{1,2,3'}$. We first show that if $x_k \in \Omega_{1,2,3'}$, then so does the next iterate. Indeed, in view of (3.7) and (3.9), if $x_k \in \Omega_{3'}$, then $x_{k+1} \in \Omega_{1,2,3'}$. On the other hand, if $x_k \in \Omega_{1,2}$, i.e. $||g_k|| \leq \Lambda_2 \Delta$, then, by Lemma 3.1, we have $||g_{k+1}|| \leq \varkappa \Lambda_2 \Delta$.

Suppose now that $x_1 \in \Omega_3 \setminus \Omega_{3'}$. Then it immediately follows from relations (3.9) and (3.10), that there exists K > 1 such that $x_K \in \Omega_{1,2,3'}$. As it was shown above, this means that $x_k \in \Omega_{1,2,3'}$ for all $k \geq K$.

It follows from (3.9) that, when iterates belong to the set Ω_3 , the value $||g_k||$ monotonically decreases as indicated by (3.7). Furthermore, the actual decrease may speed-up in accordance with (3.10). When the iterates reach $\Omega_{1,2}$, the decrease is naturally expected to slow down, and this is followed by a non-monotonic behavior of $||g_k||$, which is a typical feature of the BB steps. One can observe all these stages in the behavior of BBstab in Figure 3.1. It presents changes of $||g_k||$ with k in the process of minimizing Raydan function (2.1). Details of these

runs are discussed in Section 4. Note that both BB1 and BB2 fail to solve this problem starting from the same points. The figure illustrates the role of stabilization in providing convergence of BBstab. One can clearly recognize the first stage of the process when the stabilization steps ensure a monotonic decrease of $||g_k||$. For the BB1stab and BB2stab, the iteration when the standard BB step was used for the first time is 228 and 226, respectively. For them, the last stabilization step was used in iteration 379 and 353, respectively. Observe that the spikes of $||g_k||$ produced by BB1 is much larger than those for BB2.

Lemma 3.2 allows us to deduce an interesting property of the BB method, namely, that if it generates bounded steps, it cannot generate unbounded iterates because one can choose a sufficiently large Δ , which is not binding. The same lemma indicates that a proper choice of Δ allows for BBstab to reach any neighborhood of x^* . We use the notation

$$B_{\delta}(x^*) = \{x \in \mathbb{R}^n : ||x - x^*|| \le \delta\}.$$

in the following formulation of this useful feature of BBstab.

Lemma 3.3. Let $x_0, x_1 \in R^n$ be any starting points. Then for any $\delta > 0$ and positive $\Delta \leq \frac{\delta}{\varkappa^2}$, there exists $K(\Delta) \geq 1$ such that the iterates $\{x_k\}$ satisfy the condition

$$x_k \in B_\delta(x^*), \quad \forall k \ge K(\Delta).$$

Proof. Combining (3.2) and Lemma 3.2, we get the relations

$$||x_k - x^*|| \le \frac{||g_k||}{\Lambda_1} \le \varkappa^2 \Delta \le \delta,$$

which are satisfied for all sufficiently large k. This completes the proof.

We shall make use of Lemma 3.2 for proving global convergence result for BBstab. We show also that its local rate of convergence is R-linear, which means that there exist positive γ and $c \in (0,1)$ such that

$$||x_{k+1} - x^*|| \le \gamma c^k ||x_1 - x^*||. \tag{3.12}$$

These convergence results are based on our convergence analysis presented in the next subsection for convex quadratic functions.

3.1. Convergence in Quadratic Case

In this sub-section, we focus on minimizing convex quadratic functions of the form

$$f(x) = \frac{1}{2}x^{T}Ax - b^{T}x,$$
(3.13)

where the matrix $A \in \mathbb{R}^{n \times n}$ is positive definite, and $b \in \mathbb{R}^n$. For these functions, we derive the convergence with R-linear rate. To this end, we will make use of the following property which is the same as Property A in [5].

Definition 3.1. We say that the choice of the stepsize in (1.2) has property P if there exist an integer m and positive constants M_1 and M_2 such that, for all $k \geq 1$,

- (i) $\Lambda_1 \leq \alpha_k^{-1} \leq M_1$;
- (ii) for any integer $\ell \in [1, n-1]$ and real number $\epsilon > 0$, if $R(k-j, \ell) \le \epsilon$ and $(g_{k-j}^{(\ell+1)})^2 \ge M_2 \epsilon$ hold for $j \in [0, \min\{k, m\} 1]$, then $\alpha_k^{-1} \ge \frac{2}{3} \lambda_{\ell+1}$.

Theorem 3.1. Let $x_0, x_1 \in R^n$ be arbitrary starting points. Then for any $\Delta > 0$, the sequence $\{x_k\}$ converges to x^* with R-linear rate. Moreover, there exists a positive integer \bar{j} , such that, for any $\Delta > 0$, $x_0 \in R^n$ and $x_1 \in \Omega_{1,2,3'}$, the inequality

$$||g_{k+\bar{j}}|| \le \frac{1}{2} ||g_k||$$

holds for all $k \geq 1$.

Proof. It is well known that the BB method is invariant under orthogonal transformation of the variables and, as it can be easily seen, so does its stabilized version. Hence, we can assume without loss of generality that the matrix A is of the form

$$A = \operatorname{diag}(\lambda_1, \dots, \lambda_n), \tag{3.14}$$

where $0 < \Lambda_1 = \lambda_1 < \lambda_2 < \ldots < \lambda_n = \Lambda_2$. Here, like it is often done for the gradient methods (see, e.g., [20]), it is assumed without loss of generality that the matrix A has distinct eigenvalues. Then denoting the *i*-th component of g_k by $g_k^{(i)}$, we have

$$g_{k+1}^{(i)} = (1 - \alpha_k \lambda_i) g_k^{(i)}, \quad i = 1, \dots, n.$$
 (3.15)

We will also make use of the following notation:

$$R(k, \ell) = \sum_{i=1}^{\ell} (g_k^{(i)})^2.$$

Firstly, we prove that the step size α_k has property **P**. Lemma 3.2 ensures that $x_k \in \Omega_{1,2,3'}$ for all $k \geq 1$. Then the bounds (3.5) show that α_k has property **P**(i) with $M_1 = \varkappa \Lambda_2$.

Next, we will show, for any integer $\ell \in [1, n-1]$ and real number $\epsilon > 0$, that the inequality $\alpha_k^{-1} \geq \frac{2}{3}\lambda_{\ell+1}$ is satisfied, whenever $R(k-1,\ell) \leq \epsilon$ and $(g_{k-1}^{(\ell+1)})^2 \geq 2\epsilon$. This will be done separately for BB1- and BB2-based iterates.

For the BB1 case, we have

$$\alpha_k^{-1} \ge \frac{g_{k-1}^T A g_{k-1}}{\|g_{k-1}\|^2} = \frac{\sum_{i=1}^n \lambda_i (g_{k-1}^{(i)})^2}{R(k-1,n)} \ge \frac{\lambda_{\ell+1} \sum_{i=\ell+1}^n (g_{k-1}^{(i)})^2}{R(k-1,\ell) + \sum_{i=\ell+1}^n (g_{k-1}^{(i)})^2}$$
$$\ge \frac{\lambda_{\ell+1} \sum_{i=\ell+1}^n (g_{k-1}^{(i)})^2}{\epsilon + \sum_{i=\ell+1}^n (g_{k-1}^{(i)})^2} \ge \frac{2\lambda_{\ell+1}\epsilon}{\epsilon + 2\epsilon} = \frac{2}{3}\lambda_{\ell+1}.$$

For BB2, we obtain

$$(\alpha_k)^{-1} \ge \frac{g_{k-1}^T A^2 g_{k-1}}{g_{k-1}^T A g_{k-1}} \ge \frac{\lambda_{\ell+1} \sum_{i=\ell+1}^n \lambda_i (g_{k-1}^{(i)})^2}{\lambda_{\ell+1} R(k-1,\ell) + \sum_{i=\ell+1}^n \lambda_i (g_{k-1}^{(i)})^2}$$
$$\ge \frac{\lambda_{\ell+1}^2 (g_{k-1}^{(\ell+1)})^2}{\lambda_{\ell+1} R(k-1,\ell) + \lambda_{\ell+1} (g_{k-1}^{(\ell+1)})^2} \ge \frac{2\lambda_{\ell+1} \epsilon}{\epsilon + 2\epsilon} = \frac{2}{3} \lambda_{\ell+1}.$$

Thus, $\mathbf{P}(ii)$ holds for m=2 and $M_2=2$. This implies that BBstab stepsize α_k satisfies \mathbf{P} . Then we can skip the rest of the proof because it is similar to the proof of Theorem 4.1 in [5].

It should be emphasized that, in this lemma, the value of \bar{j} depends only on Λ_1 and Λ_2 .

3.2. Convergence in General Case

For nonquadratic functions, we shall first prove local R-linear convergence of BBstab. This result will then be used for showing that it converges from any starting point.

Throughout this sub-section, we need to additionally assume that the Hessian matrix $\nabla^2 f(x)$ is Lipschitz-continuous at x^* . In what follows, we use the notation $H = \nabla^2 f(x^*)$.

A2. There exist a radius $\rho > 0$ and a Lipschitz constant $L \geq 0$ such that

$$\|\nabla^2 f(x) - H\| \le L\|x - x^*\|, \quad \forall x \in B_\rho(x^*).$$

This assumption implies that

$$||g(x) - H(x - x^*)|| \le \frac{L}{2} ||x - x^*||^2, \quad \forall x \in B_{\rho}(x^*).$$
 (3.16)

The second-order Taylor approximation to f around x^* is given by the quadratic function

$$\hat{f}(x) = f(x^*) + \frac{1}{2}(x - x^*)^T H(x - x^*). \tag{3.17}$$

Define new iterates $\hat{x}_{k,j}$ associated with \hat{f} as follows:

$$\begin{cases} \hat{x}_{k,0} = x_k, \\ \hat{x}_{k,j+1} = \hat{x}_{k,j} - \hat{\alpha}_{k,j} \hat{g}_{k,j}, \quad j \ge 0, \end{cases}$$
 (3.18)

where

$$\hat{\alpha}_{k,j} = \left\{ \begin{array}{ll} \alpha_k, & \text{if } j = 0, \\ \min\{\hat{\alpha}_{k,j}^{BB}, \, \hat{\alpha}_{k,j}^{stab}\}, & \text{otherwise.} \end{array} \right.$$

Here $\hat{\alpha}_{k,j}^{BB}=\hat{\alpha}_{k,j}^{BB1}$ or $\hat{\alpha}_{k,j}^{BB}=\hat{\alpha}_{k,j}^{BB2}$ and $\hat{\alpha}_{k,j}^{stab}=\frac{\Delta}{\|\hat{g}_{k,j}\|}$ with

$$\hat{\alpha}_{k,j}^{BB1} = \frac{\hat{s}_{k+j-1}^T \hat{s}_{k+j-1}}{\hat{s}_{k+j-1}^T \hat{y}_{k+j-1}}, \qquad \hat{\alpha}_{k,j}^{BB2} = \frac{\hat{s}_{k+j-1}^T \hat{y}_{k+j-1}}{\hat{y}_{k+j-1}^T \hat{y}_{k+j-1}},$$

 $\hat{s}_{k+j-1} = \hat{x}_{k,j} - \hat{x}_{k,j-1}, \ \hat{g}_{k,j} = H(\hat{x}_{k,j} - x^*)$ and $\hat{y}_{k+j-1} = \hat{g}_{k,j} - \hat{g}_{k,j-1}$. In what follows, whenever we mention $\hat{x}_{k,j}$ and $\hat{\alpha}_{k,j}$, they are assumed to be generated as defined above.

The next result follows immediately from Theorem 3.1.

Lemma 3.4. Let $\Delta > 0$ be any scalar, such that $\Omega_{1,2,3'} \subseteq B_{\rho}(x^*)$. Then there exists a positive integer \bar{j} , dependent only on Λ_1 and Λ_2 , such that, for any $x_{k-1} \in R^n$ and $x_k \in \Omega_{1,2,3'}$, the inequality holds

$$\|\hat{g}_{k,\bar{j}}\| \le \frac{1}{2} \|\hat{g}_{k,0}\|.$$

It can be easily seen that if $x_k \in \Omega_{1,2,3'}$, then all corresponding $\hat{x}_{k,j} \in \Omega_{1,2,3'}$. In this case, BBstab stepsize α_k satisfies the bounds (3.5), and similarly for $\hat{\alpha}_{k,j}$, we have the bounds

$$\frac{1}{\varkappa \Lambda_2} \le \hat{\alpha}_{k,j} \le \frac{1}{\Lambda_1}, \quad \forall j \ge 0. \tag{3.19}$$

The following result will be used for proving local R-linear convergence.

Lemma 3.5. Let integer $\bar{j} \geq 1$ be arbitrary. Then there exist positive scalars $\bar{\Delta}$ and γ with the following property: for any $\Delta \in (0, \bar{\Delta}]$, $x_{k-1} \in R^n$, $x_k \in \Omega_{1,2,3'} \subset B_{\rho}(x^*)$ and $m \in [0, \bar{j}]$, for which

$$\|\hat{g}_{k,j}\| \ge \frac{1}{2} \|\hat{g}_{k,0}\|, \quad \forall j \in [0, \max\{0, m-1\}],$$
 (3.20)

we have the inequality

$$||x_{k+j} - \hat{x}_{k,j}|| \le \gamma ||x_k - x^*||^2 \tag{3.21}$$

satisfied for all $j \in [0, m]$.

Proof. Throughout the proof, let c denote a generic positive constant, which may depend on some of fixed constants, such as $\bar{\Delta}$, \bar{j} , Λ_1 , Λ_2 or L, but not on the choice of Δ or $x_k \in \Omega_{1,2,3'} \subset B_{\rho}(x^*)$. For brevity, we will use the same notation in all inequalities, even though every specific value of c depends on the one, where it is used. What is important is that the number of these inequalities is finite.

We first notice that, by Lemma 3.2, the relation $x_{k+j} \in \Omega_{1,2,3'} \subseteq B_{\rho}(x^*)$ holds for all $j \geq 0$. The process of proving (3.21) will be combined with showing that the inequalities

$$||g(x_{k+j}) - \hat{g}(\hat{x}_{k,j})|| \le c||x_k - x^*||^2, \tag{3.22}$$

$$||s_{k+i}|| \le c||x_k - x^*||, \tag{3.23}$$

$$|\alpha_{k+j} - \hat{\alpha}_{k,j}| \le c||x_k - x^*||,$$
 (3.24)

are satisfied for all $j \in [0, m]$.

The proof of (3.21)-(3.24) is by induction on m. For m=0, noticing that $\hat{x}_{k,0}=x_k$, $\hat{\alpha}_{k,0}=\alpha_k$ and $s_k=-\alpha_k g_k$, by (3.2), (3.5) and (3.16), we can immediately get (3.21)-(3.24) satisfied for j=0.

Suppose that there exist $M \in [1, \bar{j})$ and $\bar{\Delta} > 0$ with the property that if (3.20) holds for any $m \in [0, M-1]$, then (3.21)-(3.24) are satisfied for all $j \in [0, m]$. Next, we shall show that for a smaller choice of $\bar{\Delta} > 0$, we can replace M by M+1. Hence, we suppose that (3.20) holds for all $j \in [0, M]$. Since (3.20) holds for all $j \in [0, M-1]$, it follows from the induction hypothesis and (3.23) that

$$||x_{k+M+1} - x^*|| \le ||x_k - x^*|| + \sum_{i=0}^{M} ||s_{k+i}|| \le c||x_k - x^*||.$$
(3.25)

By analogy with the proof of Lemma 2.2 in [9], we derive from (3.2), (3.5), (3.16), (3.19), (3.25) and the induction hypothesis that (3.21)-(3.23) hold for j = M + 1. Then we just need to show that

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| \le c||x_k - x^*||. \tag{3.26}$$

It follows from (3.2) that

$$||x_k - x^*|| \le \frac{||g_k||}{\Lambda_1} \le \varkappa^2 \Delta \le \varkappa^2 \bar{\Delta}.$$

Then by choosing any $\bar{\Delta} < 1/(2\gamma \varkappa^3)$, using relations (3.1), (3.5), (3.19)-(3.21), (3.23) and the same reasoning as in the proof of Lemma 2.2 in [9], we obtain

$$|\alpha_{k+M+1}^{BB} - \hat{\alpha}_{k,M+1}^{BB}| \le c||x_k - x^*||. \tag{3.27}$$

In the following, the proof of (3.26) will be done by separately considering four different cases.

Case I: $\alpha_{k+M+1}^{BB} \leq \alpha_{k+M+1}^{stab}$ and $\hat{\alpha}_{k,M+1}^{BB} \leq \hat{\alpha}_{k,M+1}^{stab}$. Then (3.27) directly leads to

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| = |\alpha_{k+M+1}^{BB} - \hat{\alpha}_{k,M+1}^{BB}| \le c||x_k - x^*||.$$

Case II: $\alpha_{k+M+1}^{BB} \leq \alpha_{k+M+1}^{stab}$ and $\hat{\alpha}_{k,M+1}^{BB} > \hat{\alpha}_{k,M+1}^{stab}$. If $\hat{\alpha}_{k,M+1}^{stab} \geq \alpha_{k+M+1}^{BB}$, then (3.27) implies

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| = \hat{\alpha}_{k,M+1}^{stab} - \alpha_{k+M+1}^{BB} < \hat{\alpha}_{k,M+1}^{BB} - \alpha_{k+M+1}^{BB} \le c ||x_k - x^*||.$$

Suppose now that $\hat{\alpha}_{k,M+1}^{stab} < \alpha_{k+M+1}^{BB}$. Then we have

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| = \alpha_{k+M+1}^{BB} - \hat{\alpha}_{k,M+1}^{stab} \le \alpha_{k+M+1}^{stab} - \hat{\alpha}_{k,M+1}^{stab}. \tag{3.28}$$

It follows from (3.5) and (3.19) that

$$\|\hat{g}_{k,M+1}\| = \frac{\Delta}{\hat{\alpha}_{k,M+1}^{stab}} > \frac{\Delta}{\hat{\alpha}_{k,M+1}^{BB}} \ge \Delta\Lambda_1. \tag{3.29}$$

By (3.2) and (3.16), we get

$$||g_{k+M+1} - \hat{g}_{k,M+1}|| \le \frac{L}{2} ||x_{k+M+1} - x^*||^2 \le \frac{L}{2\Lambda_1^2} ||g_{k+M+1}||^2 \le \frac{1}{2} \varkappa^4 \Delta^2 L.$$

This along with (3.29) leads to

$$||g_{k+M+1}|| \ge ||\hat{g}_{k,M+1}|| - ||g_{k+M+1} - \hat{g}_{k,M+1}|| \ge \Delta \left(\Lambda_1 - \frac{1}{2}\varkappa^4 \Delta L\right) \ge \Delta C(\bar{\Delta}),$$

where $C(\bar{\Delta}) = \Lambda_1 - \varkappa^4 \bar{\Delta} L/2 > 0$ whenever $\bar{\Delta} < 2\Lambda_1/(\varkappa^4 L)$. Then we obtain

$$\begin{split} |\alpha_{k+M+1}^{stab} - \hat{\alpha}_{k,M+1}^{stab}| &= \left|\frac{\Delta}{\|g_{k+M+1}\|} - \frac{\Delta}{\|\hat{g}_{k,M+1}\|}\right| = \Delta \frac{|\|\hat{g}_{k,M+1}\| - \|g_{k+M+1}\|\|}{\|g_{k+M+1}\|\|\hat{g}_{k,M+1}\|} \\ &\leq \Delta \frac{\|\hat{g}_{k,M+1} - g_{k+M+1}\|}{\|g_{k+M+1}\|\|\hat{g}_{k,M+1}\|} \leq \frac{c\|x_k - x^*\|^2}{\Delta \Lambda_1 C(\bar{\Delta})} \leq \frac{c\|g_k\|\|x_k - x^*\|}{\Delta \Lambda_1^2 C(\bar{\Delta})} \\ &\leq \frac{c \varkappa \Lambda_2 \Delta \|x_k - x^*\|}{\Delta \Lambda_1^2 C(\bar{\Delta})} = \frac{c \varkappa^2}{\Lambda_1 C(\bar{\Delta})} \|x_k - x^*\|. \end{split}$$

This together with (3.28) shows that (3.26) holds.

Case III: $\alpha_{k+M+1}^{BB} > \alpha_{k+M+1}^{stab}$ and $\hat{\alpha}_{k,M+1}^{BB} \leq \hat{\alpha}_{k,M+1}^{stab}$. If $\alpha_{k+M+1}^{stab} \geq \hat{\alpha}_{k,M+1}^{BB}$, then by (3.27), we have

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| = \alpha_{k+M+1}^{stab} - \hat{\alpha}_{k,M+1}^{BB} \leq \alpha_{k+M+1}^{BB} - \hat{\alpha}_{k,M+1}^{BB} \leq c \|x_k - x^*\|.$$

Suppose now that $\alpha_{k+M+1}^{stab} < \hat{\alpha}_{k,M+1}^{BB}$. Then we get

$$|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| = \hat{\alpha}_{k,M+1}^{BB} - \alpha_{k+M+1}^{stab} \le \hat{\alpha}_{k,M+1}^{stab} - \alpha_{k+M+1}^{stab}.$$

To use the same reasoning as in Case II, we need to have lower bounds for $||g_{k+M+1}||$ and $||\hat{g}_{k,M+1}||$. To this end, applying (3.5) and (3.19), we obtain

$$||g_{k+M+1}|| = \frac{\Delta}{\alpha_{k+M+1}^{stab}} > \frac{\Delta}{\alpha_{k+M+1}^{BB}} \ge \Delta \Lambda_1.$$
(3.30)

Furthermore, (3.2), (3.16) and (3.30) yield

$$\|\hat{g}_{k,M+1}\| \ge \|g_{k+M+1}\| - \|g_{k+M+1} - \hat{g}_{k,M+1}\| \ge \Delta C(\bar{\Delta}).$$

This lower bound is positive whenever $\bar{\Delta} < 2\Lambda_1/(\varkappa^4 L)$. The two lower bounds allows us to conclude, by analogy with Case II, that (3.26) holds.

Case IV: $\alpha_{k+M+1}^{BB} > \alpha_{k+M+1}^{stab}$ and $\hat{\alpha}_{k,M+1}^{BB} > \hat{\alpha}_{k,M+1}^{stab}$. It follows from (3.2), (3.22), (3.29) and (3.30) that

$$\begin{split} &|\alpha_{k+M+1} - \hat{\alpha}_{k,M+1}| \\ &\leq & \Delta \frac{\|\hat{g}_{k,M+1} - g_{k+M+1}\|}{\|g_{k+M+1}\| \|\hat{g}_{k,M+1}\|} \leq \Delta \frac{c\|x_k - x^*\|^2}{\Delta^2 \Lambda_1^2} \leq \frac{c\|g_k\| \|x_k - x^*\|}{\Delta \Lambda_1^3} \\ &\leq & \frac{c\varkappa \Lambda_2 \Delta \|x_k - x^*\|}{\Delta \Lambda_1^3} \leq \frac{c\varkappa \Lambda_2}{\Lambda_1^3} \|x_k - x^*\|. \end{split}$$

Collecting the results in the considered four cases, one can see that (3.26) is satisfied for any

$$\Delta < \min \left\{ \frac{1}{2\gamma \varkappa^3}, \frac{2\Lambda_1}{\varkappa^4 L} \right\}.$$

This completes the induction and finally proves that inequalities (3.21)-(3.24) hold for all $j \in [0, m]$.

Next we will establish the local convergence property of BBstab for nonquadratic functions.

Theorem 3.2. There exists positive $\bar{\Delta}$ such that, for any positive $\Delta \leq \bar{\Delta}$ and any starting points $x_0, x_1 \in \Omega_{1,2,3'}$, the sequence $\{x_k\}$ converges to x^* with R-linear rate.

Lemma 3.5 allows us to skip the proof of this theorem because the reasoning is similar to the proof of Theorem 2.3 in [9].

We complete the analysis by presenting the following global convergence result.

Theorem 3.3. There exists positive $\bar{\Delta}$ such that, for any positive $\Delta \leq \bar{\Delta}$ and any starting points $x_0, x_1 \in \mathbb{R}^n$, the sequence $\{x_k\}$ converges to x^* with R-linear rate.

Proof. Let $\bar{\Delta} > 0$ be given by Theorem 3.2, which ensures local convergence to x^* . According to Lemma 3.2, after a finite number of BBstab iterations, all iterates will belong to $\Omega_{1,2,3'}$. This finally proves global convergence with R-linear rate.

4. Numerical Results

Our algorithms were implemented in MATLAB. The algorithms are terminated when either the number of iterations exceeds 10^5 , or

$$||g_k|| \le 10^{-6} \cdot ||g_0||.$$

In the next two subsections, results of numerical experiments are presented separately for quadratic and nonquadratic test functions.

A successful value of Δ is obviously problem dependent. In our implementation, we try to estimate its order of magnitude by setting $\Delta = +\infty$ for the first few iterations and making use of $||s_k||$ produced at these iterations by the standard BB algorithm. At the subsequent iterations, the constant value

$$\Delta = c \cdot \min\{\|s_1\|, \|s_2\|, \|s_3\|\},\tag{4.1}$$

is applied, where c>0 is a parameter. It turns out that this adaptive choice of Δ is less problem dependent.

Table 4.1: Numerical results for linear systems from the SuiteSparse Matrix Collection, Part I.

							,			
PROBLEM		BB1	BB1s	tab	PROB	LEM	BB1	BB1st	tab	
name	n	it	it	c	name	n	it	it	c	
1138_bus	1138	35202	21384	0.3	ex33	1733	1303	958	0.2	
2cubes_sphere	101492	5576	4662	0.3	$Flan_1565$	1564794	13781	16537	0.25	
af_0_k101	503625	4433	$\mathbf{2634}$	0.2	fv3	9801	449	449	0.2	
af_1_k101	503625	2473	2766	0.25	G2_circuit	150102	1139	1139	0.25	
af_2_k101	503625	4034	2499	0.25	G3_circuit	1585478	2177	2177	0.2	
af_3_k101	503625	3627	$\mathbf{2378}$	0.2	Geo_1438	1437960	32134	29095	0.3	
af_4_k101	503625	3047	5368	0.3	gyro	17361	10611	11925	0.3	
af_5_k101	503625	2397	2753	0.2	gyro_m	17361	3325	2225	0.25	
af_shell3	504855	1956	4565	0.3	hood	220542	4073	4308	0.25	
af_shell7	504855	2495	5515	0.3	Hook_1498	1498023	7839	7358	0.25	
apache1	80 800	18017	9143	0.2	$inline_1$	503712	20490	16833	0.3	
apache2	715176	17807	17807	0.2	jnlbrng1	40000	124	108	0.2	
audikw_1	943695	92730	65818	0.2	Kuu	7102	1733	949	0.3	
bcsstk08	1074	4627	5113	0.3	ldoor	952203	9133	9281	0.3	
bcsstk09	1083	747	713	0.3	LF10000	19998	48867	38250	0.2	
bcsstk10	1086	3416	$\mathbf{2383}$	0.25	LFAT5000	19994	22358	$\mathbf{22358}$	0.25	
bcsstk11	1473	2204	1699	0.2	m_t1	97578	1826	1826	0.2	
bcsstk13	2003	6848	8171	0.3	mhd3200b	3200	2065	$\mathbf{2065}$	0.2	
bcsstk14	1806	3577	$\mathbf{2682}$	0.25	mhd4800b	4800	2466	2466	0.2	
bcsstk15	3948	7006	4872	0.25	msc01050	1050	15187	11529	0.25	
bcsstk16	4884	401	401	0.25	msc01440	1440	807	807	0.2	
bcsstk17	10974	27014	14841	0.25	msc04515	4515	8066	6889	0.2	
bcsstk18	11948	5895	4332	0.3	msc10848	10848	3356	3356	0.2	
bcsstk21	3600	1455	1594	0.25	msc23052	23052	19088	7340	0.2	
bcsstk23	3134	8182	5619	0.2	msdoor	415863	8113	6655	0.25	
bcsstk24	3562	2383	1537	0.3	nasa1824	1824	9520	6515	0.3	
bcsstk25	15439	8369	8971	0.25	nasa2146	2146	355	355	0.2	
bcsstk26	1922	12624	8761	0.2	nasa2910	2910	19574	13683	0.3	
bcsstk27	1224	863	887	0.3	nasa4704	4704	43448	32961	0.2	
bcsstk36	23052	15466	12001	0.25	nasasrb	54870	10302	10223	0.3	
bcsstk38	8032	1584	1584	0.25	nd3k	9000	67509	86986	0.25	
bcsstm08	1074	4183	4183	0.2	nd6k	18000	92468	41133	0.2	
bcsstm11	1473	623	287	0.3	nd24k	72000	84165	73216	0.3	
bcsstm12	1473	2838	2375	0.3	offshore	259789	3826	3949	0.3	
bcsstm23	3134	2143	1857	0.25	oilpan	73752	4647	3899	0.3	
bcsstm24	3562	2102	1611	0.25	olafu	16146	69575	80804	0.3	

It is necessary to emphasize that the stabilization was designed not to speed-up the BB method when it safely converges. In such cases, it may increase the number of iterations, which is a negative outcome. The main purpose of the stabilization is to prevent the BB method from making too long steps. This serves for decreasing the number of BB iterations in case of its poor convergence or even making the method convergent when it fails, which is a positive outcome. Outcomes of all these aforementioned types were observed in our numerical experiments with stabilizing the BB method. One can easily recognize them in the tables presented below.

We focus here on demonstrating the potentials of improving convergence for the BB method. Therefore, our stabilized version is not checked here against another optimization algorithms. Since the computational cost of one iteration for the BB algorithms are practically the same as for their stabilized versions, only the number of iterations are compared. Notice that the

Table 4.2: Numerical results for linear systems from the SuiteSparse Matrix Collection, Part II.

PROBL	EM	BB1	BB1st	ab	PROBLE	M	BB1	BB1st	tab
name	n	it	it	c	name	n	it	it	c
bcsstm25	15 439	2 266	2 119	0.2	parabolic_fem	525825	5 451	2 989	0.2
bcsstm26	1922	1614	1239	0.2	plat1919	1919	3297	$\mathbf{2804}$	0.2
bcsstm39	46772	575	575	0.2	plbuckle	1282	5601	3726	0.3
BenElechi1	245874	3137	$\bf 3121$	0.3	Pres_Poisson	14822	17291	13461	0.25
bloweybq	10001	107	107	0.2	pwtk	217918	26060	$\mathbf{21798}$	0.25
$bmw7st_1$	141347	2463	$\mathbf{2463}$	0.2	s1rmq4m1	5489	9043	6890	0.2
bmwcra_1	148770	86966	123528	0.25	s1rmt3m1	5489	10092	11576	0.25
bodyy4	17546	154	154	0.25	s2rmq4m1	5489	5371	8958	0.2
bodyy5	18589	405	405	0.3	s2rmt3m1	5489	7850	6039	0.25
bodyy6	19366	809	853	0.3	s3dkq4m2	90449	16169	16169	0.2
bone010	986703	55659	$\mathbf{55659}$	0.25	s3dkt3m2	90449	18654	10739	0.2
boneS01	127224	7688	5669	0.2	s3rmq4m1	5489	8413	$\mathbf{7848}$	0.25
boneS10	914898	28584	24899	0.2	s3rmt3m1	5489	16901	19625	0.3
bundle1	10581	244	244	0.2	s3rmt3m3	5357	15586	6737	0.25
cant	62451	19609	22895	0.2	Serena	1391349	47765	23155	0.25
cbuckle	13681	6963	10770	0.25	ship_001	34920	17575	17499	0.2
cfd1	70656	4475	3555	0.2	ship_003	121728	64349	69948	0.3
cfd2	123440	5515	8145	0.25	shipsec1	140874	8730	6681	0.2
Chem97ZtZ	2541	125	114	0.25	shipsec5	179860	2565	3113	0.3
consph	83334	15034	11232	0.25	shipsec8	114919	3900	5827	0.3
crankseg_1	52804	4012	4012	0.2	smt	25710	38442	$\mathbf{24695}$	0.25
crankseg_2	63838	4914	3614	0.3	sts4098	4098	8262	12042	0.2
crystm01	4875	100	100	0.2	t2dah_e	11445	2557	1612	0.3
crystm02	13965	114	114	0.2	t2dal_e	4257	1585	1171	0.25
ct20stif	52329	6482	$\mathbf{6482}$	0.25	t3dl_e	20360	503	361	0.2
cvxbqp1	50000	383	383	0.2	thermal1	82654	5812	$\mathbf{5812}$	0.2
Dubcova1	16129	181	181	0.2	thermal2	1228045	22201	7170	0.25
Dubcova2	65025	372	348	0.3	tmt_sym	726713	40335	40335	0.25
Dubcova3	146689	520	429	0.2	Trefethen_2000	2000	258	258	0.2
ex3	1821	508	387	0.2	Trefethen_20000	20000	358	358	0.2
ex9	3363	1202	1202	0.3	Trefethen_20000b	19999	404	404	0.2
ex10	2410	3038	2023	0.25	vanbody	47072	19354	19133	0.2
ex10hs	2548	2412	1628	0.2	wathen100	30401	238	238	0.25
ex13	2568	2972	2972	0.2	wathen120	36441	308	308	0.2
ex15	6 867	3022	3298	0.3					

number of iterations is the same as the number of gradient evaluations.

In our numerical experiments, the BB1 algorithm was generating too long steps more frequently than the BB2 algorithm. This is often caused by relatively too small values of the scalar product $s_{k-1}^T y_{k-1}$ in the denominator of α_k^{BB1} . This explains why the stabilization is, in general, more important for the BB1 stepsize choice than for the BB2. Therefore, the numerical results presented here refer mainly to the BB1.

4.1. Quadratic test functions

A part of the numerical experiments was related to minimizing convex quadratic functions (3.13). This problem is equivalent to solving the system of linear equations

$$Ax = b$$
.

The matrices in our set of test problems come from the SuiteSparse Matrix Collection [12, 22]. For generating the vector b, we assumed that the solution $x^* = e$, i.e., b = Ae, where $e = (1, 1, ..., 1)^T$. The total number of problems in our test set is 141, where the problem size n varies from thousands to millions.

For the adaptive selection of Δ by formula (4.1), we tried just a few values of the parameter c, namely, 0.2, 0.25 and 0.3. In Tables 4.1 and 4.2, the number of iterations are reported for algorithms BB1 and BB1stab. For the latter, the best of the three results is presented along with the corresponding value of c. If the reported result is the same as for the BB1 algorithm, then it is obvious that the number of iterations remains the same for all values of c larger than the indicated one. The number of iterations, which is not worse than for the BB1 algorithm, are highlighted in this and other tables in this paper. One can see that, comparing with the BB1, its stabilized version is faster in solving 74 problems, while it is slower in 30 problems. Furthermore, the reduction in the number of iterations obtained by virtue of the stabilization was often substantial. We also tested the BB2 and BB2stab algorithms for these same 141 problems. We tried c = 0.1, 0.2, 0.25 and 0.3 in the adaptive selection of Δ by formula (4.1). Comparing with the BB2, BB2stab is faster in solving 58 problems, while for the given values of c, the stabilization is unable to decrease the number of BB2 iterations in 58 problems.

4.2. Nonquadratic test functions

For general functions, it is more difficult than for quadratic ones to avoid the cases, when x_1 is chosen too close to x_0 or too far away of it. In order to avoid such poor choices of these two points, our BBstab algorithms are initialized with only one point, namely, x_0 . The point x_1 is produced in the algorithms by checking if the inequality $f(x_0 + s_0) < f(x_0)$ is satisfied for $s_0 = -\alpha_0 g_0$, where $\alpha_0 = 1/||g_0||_{\infty}$. Otherwise, a number, typically few, of backtracking steps are performed by dividing the current vector s_0 by 4, while the required inequality is violated.

We begin here by comparing the performance of the BB algorithms and their stabilized versions on the strongly convex Raydan function (2.1) for n=1000. The point $x_0=-10 \cdot e$ was used for starting the algorithms. The standard BB1 algorithm failed to solve the problem. After two iterations, an overflow in computing $s_k^T y_k$ was reported. If to introduce the bounds $[10^{-30}, 10^{30}]$ for α^{BB1} , like it is often done in practice, then it also fails, although after a larger number of iterations. Namely, at iteration 123 and all subsequent iterations, an underflow was observed in calculating x_{k+1} for $||s_k|| < 10^{-26}$. In these two cases, the standard BB2 also failed. However, the same test problem for the same x_0 was successfully solved by BB1stab

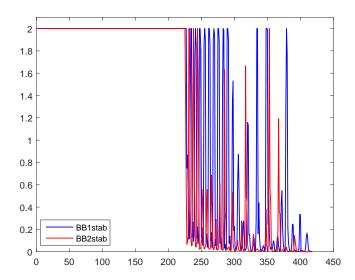


Fig. 4.1. Graphs of $||s_k||$ for BB1stab and BB2stab with $\Delta = 2$ for Raydan function (2.1).

and BB2stab with $\Delta=2$ in 418 and 416 iterations, respectively. No bounds, like $[10^{-30}, 10^{30}]$, are used in our implementation of the BB algorithms and their stabilized versions. Fig. 4.1 illustrates the stabilization effect. One can see that the BB1 was generating too long steps more frequently than the BB2. This observation is in general agreement with the other numerical experiments that we performed and also with the theory, which says that $\alpha_k^{BB1} \geq \alpha_k^{BB2}$.

The performance of our algorithms was compared also for unconstrained minimization problems from the CUTEst collection [16], which provides a standard starting point x_0 for each of them. We excluded from our comparison quadratic problems and those, in which the BB1/BB2 algorithm converged in less than 20 iterations. The results reported here concern only the

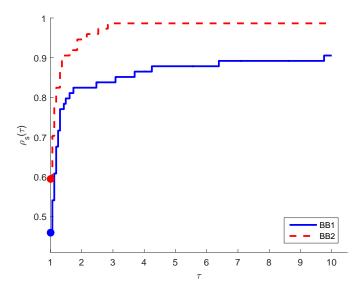


Fig. 4.2. Performance profiles of the BB1 and BB2 algorithms adapted to solving nonconvex unconstrained minimization problems (based on solving problems from the CUTEst collection).

problems, where at least one of the compared algorithms converged, and also those, where the both algorithms converged to the same point.

Table 4.3: Numerical results for unconstrained minimization problems from the CUTEst collection, adaptive selection of Δ .

PROBLE	M	BB1	BB1s	tab	PROBLE	M	BB1	BB1st	tab
name	n	it	it	c	name	n	it	it	c
ALLINITU	4	21	21	0.1	EXTROSNB	1 000	23	23	0.5
ARGTRIGLS	200	626	626	0.5	FLETCBV2	5000	30225	98735	1
BA-L1LS	57	34	33	1	FLETCHCR	1000	1892	1964	1
BA-L16LS	66462	64	66	0.5	FREUROTH	5000	52	52	0.5
BA-L21LS	34134	197	179	1	HEART8LS	8	44	44	0.5
BA-L49LS	23769	65	60	1	HYDC20LS	99	35	35	1
BA-L52LS	192627	280	277	0.1	LUKSAN11LS	100	31	32	1
BA-L73LS	33753	65	69	0.5	LUKSAN12LS	98	40	38	0.5
BDQRTIC	5000	41	41	0.5	LUKSAN17LS	100	230	187	0.1
BROWNBS	2	4110	961	0.1	LUKSAN21LS	100	6284	28255	1
BROYDN3DLS	5000	21	21	0.1	LUKSAN22LS	100	64	51	0.1
BROYDN7D	5000	29	29	0.1	MOREBV	5000	54926	$> 10^5$	1
BROYDNBDLS	5000	58	58	1	MSQRTALS	1024	71	56	0.5
CHAINWOO	4000	96	42	1	MSQRTBLS	1024	56	59	0.5
CHNROSNB	50	133	133	0.5	NCB20	5010	23	${\bf 22}$	0.1
CHNRSNBM	50	93	93	0.1	NONDQUAR	5000	40401	89179	1
CRAGGLVY	5000	56	50	1	NONMSQRT	4900	54	54	0.1
CUBE	2	$> 10^5$	61	1	OSCIGRAD	100000	81	81	1
CURLY10	10000	64	56	0.1	OSCIPATH	10	30	30	0.1
CURLY20	10000	56	56	0.5	PENALTY2	200	730	1909	1
CURLY30	10000	57	57	0.5	PENALTY3	200	21	21	0.5
DENSCHNF	2	122	31	0.5	POWELLSG	5000	65	47	1
DIXMAANE	3000	24	23	0.1	ROSENBR	2	$> 10^5$	$\bf 332$	1
DIXMAANF	3000	24	23	0.1	ROSENBRTU	2	$> 10^5$	85	1
DIXMAANI	3000	22	22	1	SCURLY30	10000	252	234	0.1
DIXMAANJ	3000	23	23	1	SPMSRTLS	4999	335	268	0.1
DIXMAANM	3000	773	515	1	SROSENBR	5000	$> 10^5$	55	0.5
DIXMAANN	3000	711	$\bf 502$	0.5	SSBRYBND	5000	4247	11005	1
DIXMAANO	3000	589	417	1	SSCOSINE	5000	3882	10414	1
DIXMAANP	3000	310	305	0.1	TOINTGOR	50	40	44	0.5
EDENSCH	2000	48	36	1	TOINTGSS	5000	5006	5004	1
EIGENALS	2550	41	41	0.1	VAREIGVL	50	415	323	0.5
EIGENCLS	2652	145	170	0.5	VESUVIALS	8	235	$> 10^{5}$	1
ERRINROS	50	2920	746	1	VESUVIOULS	8	256	$> 10^{5}$	1
ERRINRSM	50	25807	7 366	0.1	WATSON	12	120	217	0.1

Recall that the BB method was originally designed for solving convex problems in which case it is guaranteed that α_k^{BB} is nonnegative. Since the most of the unconstrained minimization test problems in the CUTEst collection are nonconvex, we had to adapt the BB method to solving this kind of problems. In our implementation of the BB method and its stabilized version, we follow paper [6] in setting

$$\alpha_k^{BB} \leftarrow \frac{\|s_k\|}{\|y_k\|},\tag{4.2}$$

whenever $\alpha_k^{BB} \leq 0$. This makes our algorithms much more robust. Fig. 4.2 presents results of solving 74 problems from the CUTEst collection. The BB1 and BB2 algorithms failed in 4 and 3 cases, respectively. The plots of the performance profiles introduced in [13] indicate that the BB2 algorithm is more robust than the BB1. Furthermore, the former algorithm required, on average, fewer iterations for solving problems. The main reason is that the BB1 algorithm generates too long steps more frequently. In what follows, we focus on presenting here results of stabilizing the BB1 algorithm, because it gains more from the stabilization than the BB2 algorithm.

Table 4.3 presents results of solving 70 nonquadratic test problems from the CUTEst collection. We tried only three values of the parameter c in the adaptive choice of Δ using (4.1), namely, 0.1, 0.5 and 1.0. The BB1 and BB1stab algorithms were not able to solve problems during 10^5 iterations in 4 and 3 cases, respectively. The BB1stab requires fewer number of iterations in 32 cases, while the BB1 performs better only in 17 cases. In 21 cases, the BB1stab with the indicated values of c requires the same number of iterations as the BB1.

We made experiments also with directly setting a certain value of Δ in the BB1stab. The trial values were 0.01, 0.1 and 1.0. For a few test problems, the results are better than for the aforementioned adaptive choice with $c=0.1,\,0.5$ and 1.0. For 22 of 71 problems, the number of iterations is smaller than in case of the BB1. These results are reported in Table 4.4. The preselected values of Δ allowed the BB1stab to solve five problems of those not solved by the BB1, including problems MOREBV and TQUARTIC, in which the adaptive choice of Δ failed. In case of TQUARTIC, the BB1 terminated because of producing NaN (Not a Number) in Matlab. The experiments with the preselected values of Δ indicate that there is plenty of room for improving the very simple adaptive strategy proposed in this paper.

Table 4.4: Numerical results for unconstrained minimization problems from the CUTEst collection, preselected Δ .

PROBLE	PROBLEM BB1		BB1st	ab	PROBLEM		BB1	BB1st	tab
name	n	it	it	Δ	name	n	it	it	Δ
BROWNBS	2	4110	80	1	LUKSAN11LS	100	31	23	1
CHNROSNB	50	133	50	1	LUKSAN17LS	100	230	166	1
CHNRSNBM	50	93	41	1	MOREBV	5000	54926	44712	0.01
CUBE	2	$> 10^5$	94	0.1	MSQRTALS	1024	71	66	0.1
DENSCHNF	2	122	31	1	NONMSQRT	4900	54	51	1
DIXMAANM	3000	773	715	1	OSCIPATH	10	30	27	1
DIXMAANO	3000	589	514	1	ROSENBR	2	$> 10^{5}$	129	0.1
ERRINROS	50	2920	923	1	ROSENBRTU	2	$> 10^{5}$	$\boldsymbol{664}$	0.1
ERRINRSM	50	25807	6165	0.1	SPMSRTLS	4999	335	294	1
FLETCBV2	5000	30225	25325	1	SROSENBR	5000	$> 10^{5}$	206	1
FLETCHCR	1000	1892	572	1	TQUARTIC	5000	\mathbf{F}	5325	0.1

For the BB2stab algorithm, we still tried the same three values of the parameter c in the adaptive choice of Δ using (4.1) as for BB1stab. In 77 test problems, the BB2stab performs better in 25 cases, while the BB2 performs better only in 15 cases. Table 4.5 presents results for all the cases when the BB2stab requires fewer number of iterations.

Table 4.5: Numerical results for unconstrained minimization problems from the CUTEst collection, adaptive selection of Δ .

PROBLE	PROBLEM		BB2s	stab	PROBLEM		BB2	BB2st	ab
name	n	it	it	c	name	n	it	it	c
BA-L21LS	34134	191	187	1	EIGENALS	2550	44	39	0.5
BA-L52LS	192627	358	316	1	EIGENCLS	2652	201	177	0.1
BDQRTIC	5000	41	37	0.1	INDEFM	100000	23	21	1
BROWNBS	2	4110	961	0.1	LUKSAN17LS	100	198	183	0.1
CHNRSNBM	50	54	45	0.1	MSQRTALS	1024	77	72	0.5
DENSCHNF	2	29	28	1	MSQRTBLS	1024	59	58	0.5
DIXMAANE	3000	21	20	0.1	NONDIA	5000	-	10599	0.5
DIXMAANF	3000	24	22	0.1	OSCIPATH	10	26	25	0.1
DIXMAANI	3000	25	20	0.1	PENALTY3	200	22	21	0.1
DIXMAANJ	3000	24	22	0.1	POWELLSG	5000	44	38	0.5
DIXMAANM	3000	610	425	0.1	VAREIGVL	50	490	407	0.1
DIXMAANN	3000	611	448	0.1	WATSON	12	340	170	0.5
DIXMAANO	3000	464	414	0.1					

5. Conclusions

In the present paper, it was proposed to stabilize the conventional BB method by virtue of bounding the distance between sequential iterates. The purpose was to improve its convergence, when it is affected by too long steps $\|\alpha_k^{BB}g_k\|$, and also to make the BB method convergent, when it fails to converge. Both a theoretical and numerical study of the stabilized version was conducted. We have proved that the stabilization provides the BB method with a global convergence without recourse to using any line search. The numerical results presented here are highly encouraging. The proposed very simple adaptive selection of Δ was able to successfully trap a value which is appropriate for each specific problem. However, we hope that this paper will stimulate development of more efficient algorithms for adaptive selection of Δ .

Acknowledgments. Part of this work was done during Oleg Burdakovs visit to the Chinese Academy of Sciences, which was supported by the Visiting Scientist award under the Chinese Academy of Sciences President's International Fellowship Initiative for 2017. The second author was supported by the Chinese Natural Science Foundation (No. 11631013) and the National 973 Program of China (No. 2015CB856002).

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