Accelerating Barzilai-Borwein gradient method by imposing two-dimensional quadratic termination property

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Abstract The Barzilai-Borwein (BB) gradient method, computing the step size by imposing certain quasi-Newton property, is more efficient than the classic steepest descent (SD) method though it generally produces nonmonotone sequences. It is observed that the SD method adopts the Yuan stepsize is very competitive with the BB gradient method since the Yuan stepsize yields finite termination for two-dimensional strictly convex quadratic functions. In this paper, we investigate to accelerate the BB gradient method by imposing the above two-dimensional quadratic termination property. We introduce a novel equation and show that in the two-dimensional quadratic case it is equivalent to impose the gradient aligns with some eigendirection of the Hessian at next iteration, which will yield finite termination. Moreover, the Yuan stepsize can be recovered as a special solution of the equation. Based on the proposed equation, we derive a new stepsize for the BB gradient method. In addition to the aforementioned two-dimensional quadratic termination property, a remarkable feature of the new stepsize is that its computation only depends on the long and short BB stepsizes in two consecutive iterations, without the need for exact line search and Hessian. It thus has a great advantage of being easily extended.

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to solve a large class of constrained optimization problems. By adaptively taking long BB steps and some short steps associated with the new stepsizes, we develop an efficient gradient method for minimizing quadratic functions. The proposed method is further extended to solve general box-constrained and singly linearly box-constrained (SLB) optimization problems by incorporating nonmonotone line searches and gradient projection techniques. Numerical results on quadratic, box-constrained and SLB problems show that our proposed method outperforms the most successful gradient methods in the recent literature.

**Keywords** gradient methods · Barzilai-Borwein method · quadratic termination property · quadratic optimization · singly linearly and box-constrained optimization

**Mathematics Subject Classification (2000)** 90C25 · 90C30

1 Introduction

In 1988, Barzilai and Borwein [1] proposed a new efficient gradient method, referred to as the BB gradient method (also known as spectral gradient method), that has a surprisingly $R$-superlinear convergence rate when minimizing a two-dimensional strictly convex quadratic function. For a continuously differentiable function $f(x)$, the BB gradient method updates iterates as

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

where $g_k = \nabla f(x_k)$ and employs either of the following two stepsizes

$$\alpha_{k}^{BB1} = \arg\min_{\alpha > 0} \|\alpha^{-1} s_{k-1} - y_{k-1}\| = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T y_{k-1}},$$

and

$$\alpha_{k}^{BB2} = \arg\min_{\alpha > 0} \|s_{k-1} - \alpha y_{k-1}\| = \frac{s_{k-1}^T y_{k-1}}{s_{k-1}^T y_{k-1}},$$

where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$. Though it generally generates nonmonotone sequences, the BB gradient method performs much better than the classic steepest descent (SD) method in practice, see [19, 36, 44] for example. The above two stepsizes make the BB gradient method easy to extend to solve general constrained optimization problems [2, 31]. Successful applications of the BB gradient method and its variants have been found in sparse reconstruction [39, 41], nonnegative matrix factorization [32], optimization on manifolds [22, 33, 34, 40], machine learning [11, 38, 42], etc. Since optimization problems arising in different areas are often in large scale, BB-like methods have attracted increasingly attention in recent years due to their simplicity, numerical efficiency and low per-iteration cost, see [9, 12, 13, 17, 18, 21, 23, 36, 44, 49, 47] and references therein.
Recently, Yuan [13, 14] studied the gradient method for a quadratic objective, i.e.,
$$f(x) = \frac{1}{2}x^T Ax - b^T x,$$
where $b \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite. He derived a new stepsize, say $\alpha^Y_k$, by imposing finite termination in the two-dimensional case. In particular, the stepsize is such that $x_4$ is the minimizer when applying the following gradient method
$$x_2 = x_1 - \alpha^SD_1 g_1, \ x_3 = x_2 - \alpha^V_2 g_2, \ x_4 = x_3 - \alpha^SD_3 g_3,$$
where $\alpha^SD_k$ is the stepsize of the SD method [3] given by
$$\alpha^SD_k = \arg \min_{\alpha>0} f(x_k - \alpha g_k) = \frac{\sqrt{g_k^T g_k}}{f_k A g_k}.$$  
Yuan’s stepsize was modified by Dai and Yuan [14] as
$$\alpha^Y_k = \frac{2}{\frac{1}{\alpha_{k-1}} + \frac{1}{\alpha_k} + \sqrt{\left(\frac{1}{\alpha_{k-1}} - \frac{1}{\alpha_k}\right)^2 + \frac{4\|g_k\|^2}{(\alpha_k^2 + \|g_k\|)}}}.$$  
They suggested the so-called Dai-Yuan (DY) gradient method which uses $\alpha^Y_k$ and $\alpha^SD_k$ alternately as follows
$$\alpha^{DY}_k = \begin{cases} \alpha^SD_k, & \text{if } \text{mod}(k,4)<2; \\ \alpha^Y_k, & \text{otherwise}. \end{cases}$$
Since $\alpha^Y_k \leq \alpha^SD_k$, the DY gradient method [14] is monotone, which is observed to be very competitive with the nonmonotone BB gradient method [14]. Motivated by the success of the Yuan stepsize, Huang et al. [27] considered the following family of gradient methods
$$\alpha_k = \frac{g_k^T \psi(A) g_k}{g_k^T \psi(A) A g_k},$$
where $\psi$ is a real analytic function on $[\lambda_1, \lambda_n]$ and can be expressed by Laurent series $\psi(z) = \sum_{k=-\infty}^{\infty} c_k z^k$, $c_k \in \mathbb{R}$, such that $0 < \sum_{k=-\infty}^{\infty} c_k z^k < +\infty$ for all $z \in [\lambda_1, \lambda_n]$. Here, $\lambda_1$ and $\lambda_n$ are the minimum and maximum eigenvalues of $A$, respectively. Clearly, $\alpha^SD_k$ simply corresponds to the case $\psi(A) = I$. Huang et al. [27] suggested the following stepsize for the family [3]:
$$\alpha^H_k = \frac{2}{H_k^{(11)} + H_k^{(22)} + \sqrt{(H_k^{(11)} - H_k^{(22)})^2 + 4(H_k^{(12)})^2}},$$
where $H_k^{(ij)}$ is the component of $H_k$:
$$H_k = \begin{pmatrix} \frac{g_k^T \psi^2(A) A g_k}{\|\psi^2(A) g_k\|^2} & \frac{g_k^T \psi(A) g_k}{\alpha_{k-1} \|\psi(A) g_k\|^2} \\ \frac{g_k^T \psi(A) g_k}{\alpha_{k-1} \|\psi^2(A) g_k\|^2} & \frac{\alpha_{k-1} \|\psi^2(A) g_k\|^2}{\|\psi^2(A) g_k\|^2} \end{pmatrix}.$$
with $r \in \mathbb{R}$. Apparently, when $\psi(A) = I$, $\alpha_k^H$ reduces to $\alpha_k^{YY}$. It is shown that the stepsize $\alpha_k^H$ yields finite termination of the family (3) for two-dimensional strictly convex quadratic functions (or simply says, the stepsize $\alpha_k^H$ has the two-dimensional quadratic termination property).

One main contribution of this paper is to derive a new stepsize for the nonmonotone BB gradient method, which has the two-dimensional quadratic termination property, by the following equation

$$g_k^T v_1(k) \psi_1(A)(I - \alpha_k A)g_k \cdot g_k^T v_2(k) \psi_2(A)(I - \alpha_k A)g_k = g_k^T v_3(k) \psi_3(A)(I - \alpha_k A)g_k \cdot g_k^T v_4(k) \psi_4(A)(I - \alpha_k A)g_k,$$

where $v_1(k), v_2(k) \in \{1, \ldots, k\}$, $\psi_1, \psi_2, \psi_3, \psi_4$ are real analytic functions on $[\lambda_1, \lambda_n]$ as $\psi$ and satisfy $\psi_1(z)\psi_2(z) = \psi_3(z)\psi_4(z)$, $z \in \mathbb{R}$. It is proved that, for a two-dimensional strictly convex quadratic function, the equation (10) is equivalent to impose the new gradient $g_{k+1}$ aligns with some eigendirection of the Hessian, and hence any stepsize obtained by (10) enjoys the two-dimensional quadratic termination property. Based on the equation (10), we get the new stepsize

$$\alpha_k^{new} = \frac{2}{\phi_3 + \sqrt{\left(\frac{\phi_2}{\phi_3}\right)^2 - 4\frac{\phi_1}{\phi_3}}}.$$  

where

$$\phi_1 = \frac{\alpha_{BB1}^2 - \alpha_{BB2}}{\alpha_{BB1} - \alpha_{BB1}^2} \quad \text{and} \quad \phi_2 = \frac{\alpha_{BB2}^2 - \alpha_{BB1}^2}{\alpha_{BB1}^2 - \alpha_{BB1}^2}.$$ 

One distinguished feature of this stepsize is that it is computed by BB stepsizes in two consecutive iterations without using the exact line search and Hessian. So, it can easily be extended to solve a wide class of unconstrained and constrained optimization problems.

By adaptively using the new stepsize $\alpha_k^{new}$ and the two BB stepsizes, we propose an efficient gradient method to minimize quadratic functions. Then, with two modified BB stepsizes and gradient projection strategy and the Grippo-Lampariello-Lucidi (GLL) nonmonotone line search, we extend it to solve general box-constrained and singly linearly box-constrained (SLB) optimization problems. Numerical experiments on minimizing quadratic functions (4) show that our method performs much better than the most successful gradient methods developed in recent literature including BB1 [1], Dai-Yuan (DY) [14], ABB [36], ABBmin1 [20], ABBmin2 [20] and SDC [16]. In addition, numerical comparisons of our method with the spectral projected gradient (SPG) method [23] on box-constrained problems from the CUTEst collection [24] and with the Dai-Fletcher [11] and EQ-VABBmin methods [7] on random SLB problems and SLB problems arising in support vector machine (SVM) [6] highly suggest the potential benefits of our new proposed method for solving general box-constrained and SLB optimization problems.
The paper is organized as follows. In Section 2, we analyze properties of the equation (10) and derive our new stepsize for the BB gradient method. In Section 3, based on the new stepsize, we present a gradient method for minimizing quadratic functions. Section 4 generalizes the method in Section 3 to solve box-constrained and SLB optimization problems. In Section 5, we conduct extensive numerical experiments on quadratic functions, box-constrained and SLB optimization problems. Finally, some conclusion remarks are drawn in Section 6.

2 A new stepsize

This section aims at analyzing properties of the equation (10) and deriving our new stepsize.

The motivation of using equation (10) is as follows. For quadratics, \( \alpha_{SD}^{k} \) can be viewed as an approximate solution to \( Ag_k = 1/\alpha g_k \) while \( \alpha_{BB}^{1} \) is a least squares solution to \( Ag_k - 1 = 1/\alpha g_k - 1 \) with \( \alpha > 0 \) being the variable.

If we can compute a stepsize such that the next gradient is parallel to some eigendirection, i.e.,

\[
Ag_{k+1} = \alpha g_{k+1},
\]

we would have \( \alpha_{BB}^{k+2} = \alpha_{BB}^{k+2} = 1/\alpha \), which further implies that \( g_{k+3} = 0 \) and hence yields finite termination. Unfortunately, (13) does not hold in general. However, by (13), we get

\[
g_{v(k)}^T \psi(A)g_{k+1} = \psi(\alpha)g_{v(k)}^T g_{k+1},
\]

where \( v(k) \) is defined in (15). It follows from (14) that

\[
g_{v1(k)}^T \psi_1(A)g_{k+1} \cdot g_{v2(k)}^T \psi_2(A)g_{k+1} = g_{v1(k)}^T \psi_3(A)g_{k+1} \cdot g_{v2(k)}^T \psi_4(A)g_{k+1},
\]

which together with the update rule (1) gives the equation (10). We can get the formula of \( \alpha_k \) from (10) since it is a quadratic equation in \( \alpha_k \).

Next theorem shows that (10) is equivalent to (13) in the two-dimensional case, which implies that any stepsize deduced by (10) has the two-dimensional quadratic termination property.

**Theorem 1** When \( n = 2 \), any solution of (10) is such that (13) holds and hence has the two-dimensional quadratic termination property.

**Proof** Since the gradient method is invariant under translations and rotations when applying to minimize quadratics, without loss of generality, we assume that \( A = \text{diag}\{1, \lambda\} \) with \( \lambda > 1 \). By rearranging terms, the equation (10) can be written as

\[
\phi_1 \alpha_k^2 - \phi_2 \alpha_k + \phi_3 = 0,
\]

whose solutions are

\[
\alpha_k = \frac{\phi_2 \pm \sqrt{\phi_2^2 - 4\phi_1\phi_3}}{2\phi_1} = \frac{2}{\phi_2 \pm \sqrt{\left(\frac{\phi_2}{\phi_3}\right)^2 - 4\frac{\phi_2}{\phi_3}}},
\]

where

\[
\phi_1 = \frac{g_{v1(k)}^T}{g_{v2(k)}^T} \psi_1, \quad \phi_2 = \frac{g_{v1(k)}^T \psi_3}{g_{v2(k)}^T \psi_4}.
\]
Theorem 2 Suppose that $\alpha_{k-1} = \alpha_{k-1}^{SD}$ and $I - \alpha_{k-1}A$ is invertible. When $v_1(k) = k - 1$, $v_2(k) = k$, we have

(i) the stepsize $\alpha_k^{VV}$ is a solution of (10) with

$$\psi_1(A) = \psi_4(A) = (I - \alpha_{k-1}A)^{-1}, \quad \psi_2(A) = \psi_3(A) = I;$$

(ii) the stepsize $\alpha_k^H$ is a solution of (10) with

$$\psi_1(A) = (I - \alpha_{k-1}A)^{-1}\psi^{2r}(A), \quad \psi_2(A) = \psi^{2(1-r)}(A),$$

and

$$\psi_3(A) = \psi(A), \quad \psi_4(A) = (I - \alpha_{k-1}A)^{-1}\psi(A).$$
Proof (i) From (19) and the choices of \( v_1(k), v_2(k), \psi_1, \psi_2, \psi_3, \text{ and } \psi_4, \) we have that
\[
g_k^T(I-\alpha_k A)g_{k-1} \cdot g_k^T(g_k - \alpha_k A g_k) = g_k^T(I-\alpha_k A)g_{k-1},
\]
i.e.,
\[
(\zeta_{k-1} - \alpha_k \zeta_{k-1,1})(\zeta_{k,0} - \alpha_k \zeta_{k,1}) = (g_k^T g_k - g_k^T A g_k)^2,
\]
where \( \zeta_{k,j} = g_k^T A^j g_k \) for \( j = 0, 1 \). Since \( \alpha_{k-1} = \alpha_{SD}^{2D} \), we obtain \( g_k^T g_k = 0 \) and
\[
g_k^T A g_k = \frac{1}{\alpha_{SD}^{2D}}(g_k - g_k)^T g_k = -\frac{1}{\alpha_{SD}^{2D}} \zeta_{k,0},
\]
which together with (18) gives the equation (16) with
\[
\phi_1 = \zeta_{k-1,1} \zeta_{k,1} = \frac{1}{(\alpha_{SD}^{2D})^2} \zeta_{k,0}^2, \quad \phi_2 = \zeta_{k,0} \zeta_{k-1,1} + \zeta_{k-1,0} \zeta_{k,1}, \quad \phi_3 = \zeta_{k-1,0} \zeta_{k,0}.
\]

We further obtain
\[
\frac{\phi_1}{\phi_3} = \frac{\zeta_{k-1,1} \zeta_{k,1} - \frac{1}{(\alpha_{SD}^{2D})^2} \zeta_{k,0}^2}{\zeta_{k-1,0} \zeta_{k,0}} = \frac{1}{\alpha_{SD}^{2D} \alpha_{SD}^{2D}} \frac{||g_k||^2}{(\alpha_{SD}^{2D} ||g_k||)^2} \quad (19)
\]
and
\[
\frac{\phi_2}{\phi_3} = \frac{\zeta_{k,0} \zeta_{k-1,1} + \zeta_{k-1,0} \zeta_{k,1}}{\zeta_{k-1,0} \zeta_{k,0}} = \frac{1}{\alpha_{SD}^{2D}} + \frac{1}{\alpha_{SD}^{2D}}, \quad (20)
\]
where the last equality in (20) is due to the definition of \( \zeta_{k,0} \). From (17) we conclude that the stepsize \( \alpha_{SD}^{2D} \) is the smaller root of (10).

(ii) By using the same arguments as (i), we can prove the desired result. \( \square \)

Remark 2 Although the stepsize \( \alpha_{SD}^{2D} \) is a special solution of (10), it only has the two-dimensional quadratic termination property for the SD method because it uses \( g_k^T A g_k = 0 \) to eliminate some terms of the equation. Similarly, the stepsize \( \alpha_{SD}^{2D} \) only has the two-dimensional quadratic termination property for the family \( \{ \} \).

Remark 3 It is worth mentioning that, similar as \( \alpha_{SD}^{2D} \), the stepsize \( \alpha_{SD}^{2D} \) is also the smaller root of (10). As shown in Theorem 1 for a two-dimensional strictly convex quadratic function, the two roots of (10) are reciprocals of the largest and smallest eigenvalues of the Hessian. This is also true for the stepsize \( \alpha_{SD}^{2D} \) and the corresponding larger solution when \( n > 2 \), see [27]. The reason for preferring the smaller stepsize is that the larger one is generally not a good approximation of the reciprocal of the largest eigenvalue and may significantly increase the objective value, see [27] for details.
Thus, the equation (21) can be written in the form (16) where, by Theorem 3.

In order to get the formula of our new stepsize, we assume for the moment that the equation (21) has a solution, which will be specified by the proof of Theorem 5.

**Theorem 3** For the BB1 method, suppose that \( \alpha_k^{BB1} \neq \alpha_k^{BB1} \). Then the stepsize \( \alpha_k^{new} \) is a solution of (21).

**Proof** Let \( \zeta_{k,j} = g_k^T A^T g_k \). By the update rule (11), we have

\[
g_k^T (I - \alpha_k A)^{-1} (I - \alpha_k A) g_k = g_k^T (I - \alpha_k A) g_k = \zeta_{k-1,1} (\alpha_k - \alpha_k^{BB1} - \alpha_k),
\]

and

\[
g_k^T (I - \alpha_k A) g_k = \zeta_{k-1,1} (\alpha_k - \alpha_k^{BB1} - \alpha_k),
\]

Thus, the equation (21) can be written in the form (16) where, by \( \alpha_{k-1} = \alpha_k^{BB1} \),

\[
\phi_1 = \zeta_{k-2,1} (\alpha_k^{BB2} - \alpha_k^{BB1}) - \zeta_{k-1,1} \alpha_k^{BB1} - \zeta_{k-1,2} (\alpha_k^{BB2} - \alpha_k^{BB1})
\]

\[
= \zeta_{k-2,1} [\alpha_k^{BB2} (\alpha_k^{BB2} - \alpha_k^{BB1}) - \alpha_k^{BB1} (\alpha_k^{BB2} - \alpha_k^{BB1})]
\]

\[
= \zeta_{k-2,1} \alpha_k^{BB1} (\alpha_k^{BB2} - \alpha_k^{BB1}).
\]
\[ \phi_2 = \zeta_{k-2,2}\zeta_{k-1,1}\alpha_k^{BB_1}(\alpha_k^{BB_2} - \alpha_k^{BB_1}) - \zeta_{k-2,1}\zeta_{k-1,2}\alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1}) \]

\[ = \zeta_{k-2,2}\zeta_{k-1,1}\alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1}) \]

\[ = \zeta_{k-2,2}\zeta_{k-1,2}\alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1}) \]

and

\[ \phi_3 = -\zeta_{k-2,1}\zeta_{k-1,1}\alpha_k^{BB_1} \left( \alpha_k^{BB_1} - \alpha_k^{BB_1} \right), \]

which yield that

\[ \phi_1 = \frac{\zeta_{k-2,2}\zeta_{k-1,2}\alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1})}{\alpha_k^{BB_2} \left( \alpha_k^{BB_1} - \alpha_k^{BB_1} \right)} \]

\[ = \frac{\alpha_k^{BB_2} \alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1})}{\alpha_k^{BB_2} \left( \alpha_k^{BB_1} - \alpha_k^{BB_1} \right)} \]

and

\[ \phi_2 = \frac{\zeta_{k-2,2}\zeta_{k-1,2}\alpha_k^{BB_1} \left( \alpha_k^{BB_2} - \alpha_k^{BB_1} \right) - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1})}{\alpha_k^{BB_2} \left( \alpha_k^{BB_1} - \alpha_k^{BB_1} \right)} \]

\[ = \frac{\alpha_k^{BB_1} \alpha_k^{BB_2} - \zeta_{k-2,1}\zeta_{k-1,1}(\alpha_k^{BB_1} - \alpha_k^{BB_1})}{\alpha_k^{BB_2} \left( \alpha_k^{BB_1} - \alpha_k^{BB_1} \right)}. \]

This completes the proof by noting that \( \alpha_k^{\text{new}} \) is the smaller solution of (16). \( \Box \)

Remark 4 Although the derivation of \( \alpha_k^{\text{new}} \) is based on a quadratic objective function, \( \alpha_k^{\text{new}} \) is ready for general functions because it is only related to BB stepsizes in two consecutive iterations, which is quite different from the one in [29] who requires the Hessian.

Interestingly, the stepsize \( \alpha_k^{\text{new}} \) also satisfies the equation (21) for the BB2 method.

Theorem 4 Under the conditions of Theorem 3 for the BB2 method, \( \alpha_k^{\text{new}} \) is a solution of (21).

Proof For the BB2 method, the stepsize \( \alpha_k^{\text{new}} \) can be derived in the same way as Theorem 3 by noting

\[ \phi_1 = \zeta_{k-2,1}\zeta_{k-1,2}(\alpha_k^{BB_2} - \alpha_k^{BB_1}), \]

\[ \phi_2 = \zeta_{k-2,1}\zeta_{k-1,2}(\alpha_k^{BB_1} \alpha_k^{BB_2} - \alpha_k^{BB_1} \alpha_k^{BB_2}). \]
and

\[ \phi_3 = -\zeta_{k-2,1} \zeta_{k-1,1} \alpha_k^{BB_2} (\alpha_k^{BB_1} - \alpha_{k-1}^{BB_1}), \]

which give the same results of \( \phi_1/\phi_3 \) and \( \phi_2/\phi_3 \) as \((12)\). This completes the proof. \qed

Since the equation \((21)\) is a special case of \((10)\), by Theorems 1, 3 and 4, the stepsize \( \alpha_k^{\text{new}} \) has the desired two-dimensional quadratic termination property for both the BB1 and BB2 methods. To numerically verify this property, we applied the BB1 and BB2 methods with \( \alpha_k^{\text{new}} \) to minimize a quadratic function \((4)\) with

\[ A = \text{diag}\{1, \lambda\} \quad \text{and} \quad b = 0. \]  

(22)

The algorithm was run for five iterations using ten random starting points. Table 1 presents averaged values of \( \|g_6\| \) and \( f(x_6) \). It can be observed that for different \( \lambda \), the values of \( \|g_6\| \) and \( f(x_6) \) obtained by the BB1 and BB2 methods with \( \alpha_k^{\text{new}} \) are numerically very close to zero, whereas those values obtained by the unmodified BB1 method are far away from zero.

| \( \lambda \) | BB1 | BB1 with \( \alpha_k^{\text{new}} \) | BB2 with \( \alpha_k^{\text{new}} \) |
|---|---|---|---|
| | \( \|g_6\| \) | \( f(x_6) \) | \( \|g_6\| \) | \( f(x_6) \) | \( \|g_6\| \) | \( f(x_6) \) |
| 10 | 6.9873e-01 | 7.5641e-02 | 9.3863e-18 | 1.7612e-32 | 7.5042e-20 | 5.1740e-33 |
| 100 | 6.3834e+00 | 1.8293e+00 | 1.3555e-17 | 1.1388e-31 | 8.6044e-17 | 3.2604e-31 |
| 1000 | 1.5874e+00 | 6.6377e-03 | 8.8296e-16 | 3.2198e-30 | 3.7438e-28 | 9.5183e-31 |
| 10000 | 2.9710e+01 | 2.1038e-01 | 8.3267e-17 | 3.2828e-30 | 2.0988e-31 | 8.0889e-30 |

Next theorem shows that the equation \((21)\) always has a solution. It also provides upper and lower bounds for \( \alpha_k^{\text{new}} \), and a simple way to compute \( \phi_2/\phi_3 \).

**Theorem 5** The stepsize \( \alpha_k^{\text{new}} \) in Theorem 3 is well defined. Moreover, when \( \phi_1/\phi_3 \geq 0 \) and \( \phi_2 \neq 0 \), we have

\[ \frac{\phi_3}{\phi_2} \leq \alpha_k^{\text{new}} \leq \min\{\alpha_k^{BB_2}, \alpha_{k-1}^{BB_2}\}. \]  

(23)

**Proof** Clearly, \( \alpha_k^{\text{new}} \) is well defined when \( \phi_1/\phi_3 < 0 \). Now we consider the case \( \phi_1/\phi_3 \geq 0 \). Notice that \( \phi_2/\phi_3 \) can be rewritten as

\[ \frac{\phi_2}{\phi_3} = \frac{\alpha_{k-1}^{BB_2}(\alpha_k^{BB_1} - \alpha_{k-1}^{BB_1}) + \alpha_k^{BB_1}(\alpha_{k-1}^{BB_2} - \alpha_{k-1}^{BB_2})}{\alpha_k^{BB_2} \alpha_k^{BB_1} (\alpha_k^{BB_1} - \alpha_{k-1}^{BB_1})} = \frac{1}{\alpha_k^{BB_2}} + \frac{\phi_1}{\phi_3} \alpha_k^{BB_1}. \]  

(24)
By (24) and (12), we obtain
\[
\left( \frac{\phi_2}{\phi_3} \right)^2 \geq \left( \frac{\phi_2}{\phi_3} \right)^2 - 4 \frac{\phi_1}{\phi_3} \\
= \frac{1}{(\alpha_{BB2}^k)^2} + \frac{\phi_1}{\phi_3} \left( \alpha_{BB1}^k \right)^2 + 2 \frac{\phi_1}{\phi_3} \frac{\alpha_{BB1}^k}{\phi_3} \alpha_{BB2}^k - 4 \frac{\phi_1}{\phi_3} \\
= \frac{1}{(\alpha_{BB2}^k)^2} - \phi_3 (\alpha_{BB2}^k)^2 \\
\]
which indicates that \( \alpha_{new}^k \) is well defined and
\[
\frac{\phi_3}{\phi_2} \leq \alpha_{new}^k \leq \min \left\{ \alpha_{BB2}^k, \frac{\phi_3}{\alpha_{BB1}^k} \right\} \leq \alpha_{BB2}^k. \tag{25}
\]
Similarly as (24), we get
\[
\frac{\phi_2}{\phi_3} = \frac{1}{\alpha_{BB2}^k} + \frac{\phi_1}{\phi_3} \alpha_{BB1}^k \tag{26}
\]
Hence, we have
\[
\frac{\phi_3}{\phi_2} \leq \alpha_{new}^k \leq \min \left\{ \alpha_{BB2}^{k-1}, \frac{\phi_3}{\alpha_{BB1}^{k-1}} \right\} \leq \alpha_{BB2}^{k-1}. \tag{27}
\]
Combining (25) and (27), we get the desired inequalities (23). This completes the proof. \( \square \)

3 A new method for quadratics

With the aim of developing more efficient BB-like methods, different stepsize rules have been proposed. For example, Dai and Fletcher [10] suggested to alternately take \( \alpha_{BB1}^k \) for odd \( k \) and \( \alpha_{BB2}^k \) for even \( k \). Zhou et al. [46] designed the adaptive scheme, where \( \alpha_{BB2}^k \) is selected when \( \alpha_{BB2}^k / \alpha_{BB1}^k < \tau \) for some \( \tau \in (0, 1) \) and otherwise \( \alpha_{BB1}^k \) is selected. Recall that, under the condition \( s_{k-1}^T y_{k-1} > 0 \), \( \alpha_{BB1}^k \) is a long stepsize whereas \( \alpha_{BB2}^k \) is a short one since \( \alpha_{BB1}^k \geq \alpha_{BB2}^k \) follows by the Cauchy–Schwarz inequality. Both the above two schemes adopt short and long stepsizes, and perform better than using only one type of stepsize. Variants and other stepsize rules can be found in [4,7,9,20,21,29,37]. It has been observed that replacing \( \alpha_{BB2}^k \) with a short stepsize will further improve the performance of the adaptive scheme [3,20,29].

Notice that \( \alpha_{new}^k \) is a short stepsize under the condition of Theorem 5. Based on the above analysis, we consider to combine \( \alpha_{new}^k \) and the long
BB stepsize $\alpha_k^{BB1}$. However, using the same arguments as Theorem 5 when $\phi_1/\phi_3 < 0$ and $\phi_2 \neq 0$, we have
\[
\max\{\alpha_k^{BB2}, \alpha_{k-1}^{BB}\} \leq \alpha_k^{new} \leq \frac{\phi_3}{\phi_2},
\] (28)
which implies that $\alpha_k^{new}$ may be a long stepsize. To get a short stepsize in this case, we simply replace $\alpha_k^{new}$ by the upper bound in the case of Theorem 5, i.e., $\min\{\alpha_k^{BB2}, \alpha_{k-1}^{BB}\}$. More precisely, we compute a short stepsize by
\[
\begin{cases}
\alpha_k^{new}, & \text{if } \phi_1/\phi_3 \geq 0; \\
\min\{\alpha_k^{BB2}, \alpha_{k-1}^{BB}\}, & \text{if } \phi_1/\phi_3 < 0.
\end{cases}
\] (29)
Then, by (28) and Theorem 5 we write (29) in a compact form and get our alternate scheme
\[
\alpha_k = \begin{cases}
\min\{\alpha_k^{BB2}, \alpha_{k-1}^{BB}, \alpha_k^{new}\}, & \text{if } \text{mod}(k, m) = 0; \\
\alpha_k^{BB1}, & \text{otherwise},
\end{cases}
\] (30)
where $m$ is a positive integer. As for the adaptive scheme, the authors of [4, 7] suggested to update $\tau$ by
\[
\tau_{k+1} = \begin{cases}
\frac{\tau_k}{\gamma}, & \text{if } \alpha_k^{BB2}/\alpha_k^{BB1} < \tau_k; \\
\tau_k \gamma, & \text{otherwise},
\end{cases}
\] (31)
for some $\gamma \geq 1$. Such a dynamic strategy has the advantage of less dependent on the value of $\tau$ while keeping the efficiency of the stepsize [4, 7]. Based on the rule (31), we suggest the following adaptive scheme
\[
\alpha_k = \begin{cases}
\min\{\alpha_k^{BB2}, \alpha_{k-1}^{BB}, \alpha_k^{new}\}, & \text{if } \alpha_k^{BB2}/\alpha_k^{BB1} < \tau_k; \\
\alpha_k^{BB1}, & \text{otherwise}.
\end{cases}
\] (32)
In what follows, we will compare the alternate scheme (30) and the adaptive scheme (32) with fixed $\tau$, i.e., $\gamma = 1$, and with $\tau$ dynamically updated by (31) for some $\gamma > 1$.

We tested the two methods (30) and (32) on some randomly generated quadratic problems [43], whose objectives are given by
\[
f(x) = (x - x^*)^T \text{diag}(v_1, \ldots, v_n)(x - x^*),
\] (33)
where $x^*$ was randomly generated with components in $[-10, 10]$, $v_1 = 1$ and $v_j, j = 2, \ldots, n - 1$, were generated by the rand function in Matlab. The null vector was employed as the starting point. We stopped the iteration if the number of iteration exceeds 20000 or $\|g_k\| \leq \epsilon\|g_1\|$, where $\epsilon$ is a given tolerance. For each problem, we tested three different values of tolerances $\epsilon = 10^{-6}, 10^{-9}, 10^{-12}$ and condition numbers $\kappa = 10^4, 10^5, 10^6$. We randomly generated 10 instances of the problem for each value of $\kappa$ or $\epsilon$.

Table 2 compares the alternate method (30) with the adaptive method (32) using fixed $\tau$, where $m$ was set to $3, 5, 8, 10, 20, 30, 50$ and $\tau$ was set to $0.2, 0.5$, respectively. We can see that the value of $m$ has a significant impact on
Accelerating BB gradient method by imposing quadratic termination

performance of the alternate scheme while the choice of \( \tau \) does not affect performance of the adaptive scheme very much. In addition, the adaptive scheme performs much better than the alternate scheme. For example, the averaged number of iterations of the method (32) with \( \tau = 0.2 \) is less than 1/3 of that of the method (30) with \( m = 10 \) when \( \epsilon = 10^{-12} \).

Table 2: The numbers of averaged iterations of the method (30) with different \( m \) and the method (32) with different \( \tau \) on solving quadratic problem (33)

| \( n \)   | \( \epsilon \) \( 1e-06 \) | Method (30) | Method (32) |
|----------|-------------------------------|-------------|-------------|
|          | 3                            | 5           | 8           | 10          | 20          | 30          | 50          |
| 1e-06    | 911.9                        | 238.2       | 241.6       | 262.6       | 253.9       | 270.4       | 247.2       |
| 1e-09    | 6905.1                       | 2039.5      | 2580.0      | 1627.5      | 2164.5      | 2284.4      | 2299.4      |
| 1e-12    | 9784.9                       | 4852.6      | 5998.7      | 3503.2      | 3875.1      | 4601.4      | 4132.9      |
| 1000     | 1e-06                        | 263.1       | 259.2       | 290.4       | 285.5       | 276.6       | 261.2       |
| 1e-09    | 6136.7                       | 2304.9      | 2461.5      | 2461.5      | 2284.1      | 1857.8      | 1837.3      |
| 1e-12    | 9665.7                       | 5228.0      | 6239.0      | 4603.7      | 4469.7      | 4959.8      | 4350.3      |

To further investigate fixed and dynamic schemes of \( \tau \), we compared the method (32) with fixed \( \tau \) selected from \( \{0.1, 0.2, 0.3, 0.5, 0.7, 0.9\} \), and with \( \tau_1 \) also selected from the set but updated by (31). We employed the same settings as above to generate quadratic problems in the form (33) and set \( \gamma = 1.01 \) for the dynamic scheme. Table 3 presents averaged number of iterations of the two schemes on 1000- and 10000-dimensional problems. Clearly, when \( n = 1000 \), the dynamic scheme outperforms the fixed one for most values of \( \tau_1 \). When \( n = 10000 \), performance of the dynamic scheme is less dependent on the value of \( \tau_1 \) than the fixed scheme. Hence, in what follows, we will concentrate on the dynamic scheme.

Table 3: The numbers of averaged iterations of the method (32) with fixed \( \tau \) and dynamic scheme (31) on solving quadratic problem (33)

| \( n \)   | \( \epsilon \) \( 1e-06 \) | Fixed (\( \tau \)) | Dynamic (\( \tau_1 \)) |
|----------|-------------------------------|-------------------|---------------------|
|          | 0.1                           | 0.2               | 0.3                 | 0.7               | 0.9           | 0.1            | 0.2            | 0.3           | 0.5           | 0.7           | 0.9           |
| 1e-06    | 195.9                         | 199.1             | 188.4               | 189.9             | 192.9         | 202.6          | 191.7          | 192.1         | 190.7         | 181.9         |
| 1e-09    | 729.2                         | 757.8             | 895.5               | 1164.2            | 1351.9        | 734.0           | 637.7          | 670.2         | 623.6         | 660.4         |
| 1e-12    | 1020.5                        | 1078.9            | 1172.8              | 1330.0            | 1597.1        | 1046.7          | 919.5          | 970.6         | 880.8         | 901.5         |
| 1000     | 1e-06                         | 261.0             | 252.2               | 243.2             | 238.3         | 234.9           | 247.1          | 242.3         | 247.2         | 242.9         | 237.5         |
| 1e-09    | 1210.4                        | 1158.0            | 1243.4              | 1856.0            | 1725.6        | 1139.1          | 1162.8         | 1095.4        | 1140.4        | 1140.3        |
| 1e-12    | 1770.6                        | 1625.6            | 1686.8              | 2367.0            | 3223.0        | 1758.7          | 1865.7         | 1784.2        | 1888.5        | 1800.4        |

For the quadratic problem (4), the \( R \)-linear global convergence of the method (32) can easily be established by using the property in [9]. See the proof of Theorem 3 in [13] for example.
4 Extensions to box-constrained and SLB optimization

In this section, we extend the method presented in the former section to solve general box-constrained and SLB optimization problems.

To present a uniform algorithm framework for both box-constrained and SLB optimization, we consider the following general constrained optimization

$$\min_{x \in \Omega} f(x),$$

where $\Omega \subseteq \mathbb{R}^n$ is a closed convex set and $f$ is Lipschitz continuously differentiable on $\Omega$.

The overall algorithm for solving problem (34) is given in Algorithm 1, which updates the iterates as

$$x_{k+1} = x_k + \lambda_k d_k,$$

where $\lambda_k$ is a step length determined by some line search and $d_k$ is the search direction given by

$$d_k = P_{\Omega}(x_k - \alpha_k g_k) - x_k,$$

with $P_{\Omega}(\cdot)$ being the Euclidean projection onto $\Omega$ and $\alpha_k$ being a variant of (32) with safeguards.

As we know, for general objectives, BB-like methods are often more efficient with nonmonotone line searches than their monotone counterparts. Popular nonmonotone line search strategies including GLL [25], Dai-Zhang [15], Zhang-Hager [45] and Dai-Fletcher [10]. Here, we would like to adopt the GLL nonmonotone line search, which accepts the step length $\lambda_k$ when it satisfies the following inequality

$$f(x_k + \lambda_k d_k) \leq f_{\text{max}} + \sigma \lambda_k g_k^T d_k,$$

where $f_{\text{max}}$ is the maximal function value in recent $M$ iterations, i.e.,

$$f_{\text{max}} = \max_{0 \leq i \leq \min\{k, M-1\}} f(x_{k-i}).$$

Under standard assumptions, global convergence of Algorithm 1 can be established and the rate is $R$-linear for strongly convex objective functions, see [30] for example.

Although our method has a similar framework as that of the SPG algorithm in [2], the stepsize $\bar{\alpha}_k$ used here is quite different, which is given by

$$\bar{\alpha}_k = \begin{cases} \min\{\tilde{\alpha}_k, \bar{\alpha}_k, \tilde{\alpha}_k\}, & \text{if } \tilde{\alpha}_k < \tau_k; \\
\tilde{\alpha}_k, & \text{otherwise}, \end{cases}$$

where $\tau_k$ is updated by the rule (31), $\tilde{\alpha}_k^B_k$ and $\tilde{\alpha}_k^B$ are two modified BB stepsizes specified below. The stepsize $\tilde{\alpha}_k^B_k$ is defined by replacing $\alpha_k^B$ and $\alpha_k^B$ in $\alpha_k^B$ with $\alpha_k^B$ and $\alpha_k^B$, respectively.
where $l$ better performance than the original BB stepsizes, see for example [28,29].

Let us consider box-constrained problems, i.e., $\mathcal{O} = \{x \in \mathbb{R}^n \mid l \leq x \leq u\}$, where $l \leq x \leq u$ means componentwise $l_i \leq x_i \leq u_i$ for all $i = 1, \ldots, n$. We calculate the modified BB stepsizes from the Lagrangian function

$$\mathcal{L}(x, \delta, \zeta) = f(x) - \delta^T(x - l) - \zeta^T(u - x).$$

More precisely, denote

$$\bar{y}_{k-1} = \nabla_x \mathcal{L}(x_k, \delta_k, \zeta_k) - \nabla_x \mathcal{L}(x_{k-1}, \delta_{k-1}, \zeta_{k-1})$$

$$= y_{k-1} - (\delta_k - \delta_{k-1}) + (\zeta_k - \zeta_{k-1}). \quad (38)$$

We get

$$\bar{\alpha}_{BB1} = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T \bar{y}_{k-1}} \quad \text{and} \quad \bar{\alpha}_{BB2} = \frac{s_{k-1}^T \bar{y}_{k-1}}{\bar{y}_{k-1}^T \bar{y}_{k-1}}. \quad (39)$$

As pointed out by [28,29] a gradient projection method often eventually solves an unconstrained problem in the subspace corresponding to free variables. So, we only need to consider the free variables. To this end, using $\mathcal{I}_k$ and $\mathcal{J}_k = \mathcal{N} - \mathcal{I}_k$ to approximate the active and inactive sets, respectively, where $\mathcal{N} = \{1, 2, \ldots, n\}$. Since by first-order conditions of problem [34] (under standard assumption such as linear independence constraint qualification) the Lagrange multipliers for free variables are zeros at the solution, it is useful to set $\delta_{k-1}^{(i)} - \delta_{k-1}^{(i)} = 0$ and $\zeta_{k-1}^{(i)} - \zeta_{k-1}^{(i)} = 0$ for $i \in \mathcal{J}_k$. As for $i \in \mathcal{I}_k$, we simply set $\hat{y}_{k-1}^{(i)} = 0$. Hence, $\hat{y}_{k-1}$ can be written as

$$\hat{y}_{k-1}^{(i)} = \begin{cases} 0, & \text{if } i \in \mathcal{I}_k; \\ g_k^{(i)} - g_{k-1}^{(i)}, & \text{otherwise.} \end{cases} \quad (40)$$

In our test, we set $\mathcal{I}_k = \{i \in \mathcal{N} \mid s_{k-1}^{(i)} = 0\}$, which is suitable for box-constrained optimization. The above two modified BB stepsizes often yield better performance than the original BB stepsizes, see for example [28,29].
Now we investigate SLB problems, i.e.,
\[
\Omega = \{ x \in \mathbb{R}^n | l \leq x \leq u, a^T x = b \},
\]
where \( l \leq x \leq u, a \in \mathbb{R}^n \) and \( b \in \mathbb{R} \). As (38), we denote
\[
y_{k-1} = \nabla_x L(x_k, \delta_k, \zeta_k, t_k) - \nabla_x L(x_{k-1}, \delta_{k-1}, \zeta_{k-1}, t_{k-1})
= y_{k-1} - (\delta_k - \delta_{k-1}) + (\zeta_k - \zeta_{k-1}) - (t_k - t_{k-1})a,
\]
where
\[
L(x, \delta, \zeta, t) = f(x) - \delta^T(x - l) - \zeta^T(u - x) - t(a^T x - b).
\]
We also set \( y_{k-1}^{(i)} = 0 \) for \( i \in I_k \), and \( \delta_k^{(i)} - \delta_{k-1}^{(i)} = 0 \) and \( \zeta_k^{(i)} - \zeta_{k-1}^{(i)} = 0 \) for \( i \in J_k \). Again by first-order conditions of problem (34), \( \nabla_x L \) is zero at the solution. It is expected that
\[
y_{k-1}^{(J_k)} = y_{k-1}^{(J_k)} - (t_k - t_{k-1})a^{(J_k)} = 0.
\]
To compute \( y_{k-1}^{(J_k)} \), we need to estimate the Lagrange multipliers \( t_k \) and \( t_{k-1} \). A practical way is to estimate \( t_k - t_{k-1} \) by
\[
t_k - t_{k-1} = \frac{(a^{(J_k)})^T y_{k-1}^{(J_k)}}{(a^{(J_k)})^T a^{(J_k)}}.
\]
Thus, we have
\[
y_k^{(i)} = \begin{cases} 0, & \text{if } i \in I_k; \\ y_k^{(i)} - \frac{(a^{(J_k)})^T y_{k-1}^{(J_k)}}{(a^{(J_k)})^T a^{(J_k)}}a^{(J_k)}, & \text{otherwise}. \end{cases}
\]
Then we obtain the modified BB stepsizes for SLB problems by (39). For the case
\[
I_k = \{ i \in \mathcal{N} | x_k^{(i)} = x_{k-1}^{(i)} = l_i \text{ or } x_k^{(i)} = x_{k-1}^{(i)} = u_i \},
\]
see [7], where the stepsizes in (39) are derived from a different way.

5 Numerical results

In this section, we present numerical results of our method (32) on quadratic functions and Algorithm 1 on box-constrained and SLB optimization problems. Some recent very successful gradient descent methods are run for a comparison purpose. All the codes were written in Matlab (v.9.0-R2016a) and conducted on a laptop with an Intel Core i7, 2.9 GHz processor and 8 GB of RAM running Windows 10 system.
5.1 Quadratic problems

To show the efficiency of our method (32) on quadratic problems, we compared it with the following methods:

(i) BB1 [1]: the original BB method using long BB stepsize $\alpha_k^{BB1}$;
(ii) DY [14]: the monotone Dai-Yuan gradient method (7);
(iii) ABB [46]: the adaptive BB method;
(iv) ABBmin1 [20]: a gradient method adaptively uses $\alpha_k^{BB1}$ and $\min\{\alpha_j^{BB2} : j = \max\{1,k-m\},\ldots,k\}$;
(v) ABBmin2 [20]: a gradient method adaptively uses $\alpha_k^{BB1}$ and a short stepsize in [20];
(vi) SDC [16]: a gradient method takes $h$ SD iterates followed by $s$ steps with the same $\alpha_j^V$.

Firstly, we tested the methods on problem (33). We employed the same settings for initial points, condition numbers and tolerances as in Section 3. Five different distribution sets of the diagonal elements $v_j$, $j = 2,\ldots,n-1$ listed in Table 4 were generated. The problem dimension was set to $n = 10000$ in this test.

For the SDC method, the parameter pair $(h,s)$ was set to $(8,6)$ which is more efficient than other choices. As suggested in [20], $\tau = 0.15, 0.8, 0.9$ were used for the ABB, ABBmin1, ABBmin2 methods, respectively, whereas $m = 9$ was employed for the ABBmin1 method.

Figure 1 presents performance profiles [18] obtained by our method with $\tau_1 = 0.2$, $\gamma = 1.01$ and other compared methods on iteration metric, where the vertical axis shows the percentage of problems the method solves within the factor $\rho$ of the metric used by the most effective method in this comparison. It can be seen that our method (32) clearly outperforms other compared methods.

Table 4: Distributions of $v_j$

| Problem | Spectrum |
|---------|----------|
| 1       | $\{v_2,\ldots,v_{n-1}\} \subset (1,\kappa)$ |
| 2       | $\{v_2,\ldots,v_{n/5}\} \subset (1,100)$ $\{v_{n/5+1},\ldots,v_{n-1}\} \subset (\frac{\kappa}{2},\kappa)$ |
| 3       | $\{v_2,\ldots,v_{n/2}\} \subset (1,100)$ $\{v_{n/2+1},\ldots,v_{n-1}\} \subset (\frac{\kappa}{2},\kappa)$ |
| 4       | $\{v_2,\ldots,v_{4n/5}\} \subset (1,100)$ $\{v_{4n/5+1},\ldots,v_{n-1}\} \subset (\frac{\kappa}{2},\kappa)$ |
| 5       | $\{v_2,\ldots,v_{n/5}\} \subset (1,100)$ $\{v_{n/5+1},\ldots,v_{4n/5}\} \subset (100,\frac{\kappa}{2})$ $\{v_{4n/5+1},\ldots,v_{n-1}\} \subset (\frac{\kappa}{2},\kappa)$ |
Table 5 presents averaged iterations required by the compared methods to meet given tolerances. We see that, for the first problem set, our method is faster than the BB1, DY, SDC, ABB, and ABBmin1 methods, and is comparable to ABBmin2. For the second to fifth problem sets, our method (32) performs much better than the other compared methods. In addition, for each value of $\epsilon$, our method (32) always outperforms other compared methods in the sense of total number of iterations.

Secondly, we compared the methods on solving the non-random quadratic problem [16] with $A$ being a diagonal matrix given by

$$A_{jj} = 10^{\frac{\log_{10}(\kappa_n)}{n-j}(n-j)}, \quad j = 1, \ldots, n,$$

and $b = 0$. The problem dimension was also set as $n = 10000$. Parameter settings are the same as above except the pair $(h, s)$ used for the SDC method was set to $(30, 2)$ which performs better than other choices.

Averaged number of iterations over 10 different starting points with entries randomly generated in $[-10, 10]$ are presented in Table 6. Our method (32) again outperforms other compared methods for most of the problems.

5.2 Box-constrained problems

We compare Algorithm 1 with SPG [2,3] on solving box-constrained problems from the CUTEst collection [24] with dimension larger than 50. Three of the problems were deleted since none of these comparison algorithms can solve them which left 47 problems in our test.

\(^1\) codes available at https://www.ime.usp.br/~egbirgin/tango/codes.php
Table 5 The numbers of averaged iterations of our method [32], the BB1, DY, SDC, ABB, ABBmin1 and ABBmin2 methods on solving quadratic problem [33] with spectral distributions in Table 4

| set | $\epsilon$ | BB1 | DY | SDC | ABB | ABBmin1 | ABBmin2 | Method |
|-----|------------|-----|----|-----|-----|---------|---------|--------|
| 1   | 1e-06      | 274.3 | 239.2 | 241.6 | 256.1 | 264.5 | 296.3 | 244.9 |
|     | 1e-09      | 2352.9 | 2337.9 | 2012.6 | 1412.2 | 1754.8 | 1043.7 | 1202.1 |
|     | 1e-12      | 6173.9 | 6391.8 | 4363.0 | 2284.7 | 4059.7 | 1460.5 | 1916.8 |
| 2   | 1e-06      | 324.5 | 260.3 | 174.3 | 280.9 | 150.9 | 322.2 | 103.5 |
|     | 1e-09      | 1621.2 | 1332.5 | 726.6 | 1511.7 | 579.8 | 1361.3 | 397.4 |
|     | 1e-12      | 2910.0 | 2631.5 | 1359.3 | 2770.9 | 1023.7 | 2294.1 | 666.5 |
| 3   | 1e-06      | 437.6 | 316.5 | 213.3 | 357.4 | 179.8 | 382.4 | 134.5 |
|     | 1e-09      | 1782.3 | 1466.3 | 792.5 | 1627.2 | 634.6 | 1397.6 | 413.3 |
|     | 1e-12      | 2971.7 | 2899.0 | 1290.7 | 2814.8 | 1023.7 | 2294.1 | 666.9 |
| 4   | 1e-06      | 542.1 | 402.2 | 259.0 | 435.5 | 216.8 | 495.5 | 151.3 |
|     | 1e-09      | 1866.0 | 1654.0 | 818.6 | 1782.7 | 605.0 | 1605.6 | 444.5 |
|     | 1e-12      | 3316.7 | 2885.5 | 1391.6 | 2958.0 | 1081.6 | 2500.1 | 721.4 |
| 5   | 1e-06      | 863.4 | 645.1 | 689.0 | 706.5 | 688.8 | 896.7 | 667.6 |
|     | 1e-09      | 4002.4 | 3586.8 | 3551.0 | 3174.8 | 3062.7 | 3263.6 | 2623.7 |
|     | 1e-12      | 7218.5 | 6892.6 | 6071.4 | 5684.0 | 5432.1 | 4947.5 | 4452.8 |
| total | 1e-06      | 4761.2 | 4058.5 | 3890.7 | 4260.7 | 3943.7 | 4922.4 | 3538.6 |
|     | 1e-09      | 17404.6 | 15000.8 | 11379.0 | 10818.0 | 11538.1 | 11150.0 | 10048.7 |
|     | 1e-12      | 25040.0 | 24942.8 | 17720.1 | 17521.7 | 16957.5 | 15650.7 | 15650.7 |

Table 6 The numbers of iterations of the compared methods on problem [33] with $n = 10,000$

| $\kappa$ | $\epsilon$ | BB1 | DY | SDC | ABB | ABBmin1 | ABBmin2 | Method |
|----------|------------|-----|----|-----|-----|---------|---------|--------|
| $10^4$   | 1e-06      | 643.0 | 491.3 | 555.3 | 524.8 | 531.4 | 543.6 | 505.0 |
|          | 1e-09      | 1081.0 | 957.7 | 1045.1 | 950.9 | 990.7 | 897.5 | 924.5 |
|          | 1e-12      | 1488.6 | 1378.9 | 1479.7 | 1332.6 | 1427.7 | 1293.9 | 1318.0 |
| $10^5$   | 1e-06      | 1521.9 | 1334.3 | 1299.1 | 1203.9 | 1220.3 | 1329.6 | 1124.6 |
|          | 1e-09      | 3632.6 | 3117.9 | 2804.6 | 2720.1 | 2774.7 | 2689.3 | 2497.7 |
|          | 1e-12      | 5599.6 | 4764.8 | 4077.2 | 4065.0 | 4090.8 | 4030.3 | 3802.6 |
| $10^6$   | 1e-06      | 2596.3 | 2232.9 | 2036.3 | 2180.4 | 2229.6 | 3049.2 | 1909.0 |
|          | 1e-09      | 12691.0 | 10925.2 | 7529.3 | 7147.0 | 7772.7 | 7563.2 | 6626.5 |
|          | 1e-12      | 17951.8 | 18799.1 | 12163.2 | 12124.1 | 12110.8 | 11633.3 | 10530.1 |
| total    | 1e-06      | 4761.2 | 4058.5 | 3890.7 | 3909.1 | 3981.3 | 4024.4 | 3538.6 |
|          | 1e-09      | 17404.6 | 15000.8 | 11379.0 | 10818.0 | 11538.1 | 11150.0 | 10048.7 |
|          | 1e-12      | 25040.0 | 24942.8 | 17720.1 | 17521.7 | 16957.5 | 15650.7 | 15650.7 |
The parameters of the GLL nonmonotone line search were set as follows for Algorithm 1:

$$\alpha_{\min} = 10^{-30}, \quad \alpha_{\max} = 10^{30}, \quad M = 10, \quad \sigma = 10^{-4}. $$

And the initial stepsize was set to $\alpha_1 = 1/\|P_\Omega(x_1 - g_1) - x_1\|_\infty$. We updated the parameter $\tau_k$ for Algorithm 1 in the same way as the quadratic problems and adopted default parameters for SPG. The iteration was stopped when $\|P_\Omega(x_k - g_k) - x_k\|_\infty \leq 10^{-6}$, or the iteration number exceeds 200000.

Figure 2 presents the performance profiles of Algorithm 1 and SPG on iteration metric. We can see that Algorithm 1 performs significantly better than SPG.

5.3 SLB problems

In this subsection, we compare Algorithm 1 with the Dai-Fletcher [11] and EQ-VABBmin [7] methods, which were stopped once

$$\|x_k - x_{k-1}\|_2 \leq \epsilon,$$

or the iteration number exceeds 100000. We set $\tau_1 = 0.5$ and $\gamma = 1.3$ for Algorithm 1 and used default parameters for Dai-Fletcher and EQ-VABBmin.

To efficiently compute the projection onto the set $\Omega$, we adopted the secant-like algorithm developed in [11].

5.3.1 Random SLB problems

We employ the procedure in [11] to generate random SLB problems, which is based on the generation of random SPD box-constrained quadratic test problems in [35]. In particular, it uses five parameters $n$, $ncond$, $ndeg$, $na(x^*)$
and \(na(x_1)\) to determine the number of variables, condition number of the Hessian, amount of near-degeneracy, active variables at the solution \(x^*\) and active variables at the starting point \(x_1\), respectively. And it generates SLB problems in the following form

\[
\min \frac{1}{2} x^T A x - c^T x \\
\text{s.t. } l \leq x \leq u \\
a^T x = b,
\]

where \(A = PDP^T\) with

\[
P = (I - 2p_3p_3^T)(I - 2p_2p_2^T)(I - 2p_1p_1^T),
\]

where \(D\) is a diagonal matrix whose \(i\)-th component is defined by

\[
\log d_i = \frac{i - 1}{n - 1} ncond, \ i = 1, \ldots, n,
\]

and \(p_i, \ i = 1, 2, 3\) are random vectors whose elements are sampled from a uniform distribution in \((-1, 1)\). See [11] for more detail on generating the problems.

In our test, we set \(n = 10000\) and chose other parameters from

\[
ncond \in \{4, 5, 6\}, \ ndeg \in \{1, 3, 5, 7, 9\}, \ na(x^*) \in \{1000, 5000, 9000\}.
\]

For each case, we randomly generated one problem and got 45 problems in total. Four different starting points with \(na(x_1) \in \{0, 1000, 5000, 9000\}\) were generated for each problem. The tolerance parameter \(\epsilon\) was set to \(10^{-8}\) for this test. From Figure 3 we can see that Algorithm 1 performs much better than Dai-Fletcher and EQ-VABBmin.

![Fig. 3 Performance profiles of compared methods on random SLB problems, iteration metric](image-url)
5.3.2 Support vector machines

Support vector machines (SVMs) are popular models in machine learning, especially suitable for classification, which can be formulated as a SLB problem, see [6] for detail. Suppose that we are given a training set of labeled examples

\[ D = \{(z_i, w_i), \ i = 1, \ldots, n, \ z_i \in \mathbb{R}^m, \ w_i \in \{1, -1\}\}. \]

The SVM algorithm employs some kernel function, say \( K : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R} \), to classify new examples \( z \in \mathbb{R}^m \) by a decision function \( F : \mathbb{R}^m \rightarrow \{1, -1\} \) defined as

\[ F(z) = \text{sign}\left(\sum_{i=1}^{n} x^* w_i K(z_i, z_j) + b^*\right), \]

where \( x^* \) solves

\[
\begin{align*}
\min \ & \frac{1}{2} x^T G x - e^T x \\
\text{s.t.} \ & 0 \leq x \leq C e \\
& w^T x = 0.
\end{align*}
\]

Here, \( G \) has entries \( G_{ij} = w_i w_j K(z_i, z_j), \ i, j = 1, \ldots, n \), \( C \) is a parameter of the SVM algorithm, and \( e \) is the vector of all ones. The quantity \( b^* \in \mathbb{R} \) is easily derived after \( x^* \) is computed.

Using the Gaussian kernel

\[ K(z_i, z_j) = \exp\left(-\frac{\|z_i - z_j\|^2}{2\sigma^2}\right), \]

we have tested three real-world datasets for the binary classification: a9a, w8a, and ijcnn1 which can be downloaded from the LIBSVM website. For each dataset, we randomly selected 1000 examples to generate the test problem. The parameters \( C \) and \( \sigma \) were set to 1 and \( \sqrt{10} \) respectively in our test.

Three different tolerance values were tested: \( \epsilon = 10^{-3}, 10^{-6}, 10^{-9} \). The null vector was employed as the initial point for all the compared methods. Table 7 presents the number of iterations and CPU time in seconds costed by the compared methods for different tolerance requirements. It can be seen that Algorithm 1 often performs better than the other two methods.

6 Conclusion

We have introduced the equation (10) to derive the stepsize for gradient methods, and the solution of this equation is proved to have the two-dimensional quadratic termination property. Both \( \alpha_k^{YV} \) and \( \alpha_k^H \) are special solutions of the equation (10). A new stepsize \( \alpha_k^{new} \) which is calculated by the BB stepsizes in two consecutive iterations, for the BB gradient method is deduced based on the suggested equation. We developed a new method that adaptively uses
Table 7 Results of the compared methods on SVM problems with $n = 1000$

| methods      | $10^{-3}$ | $10^{-6}$ | $10^{-9}$ |
|--------------|-----------|-----------|-----------|
|              | iter      | CPU       | iter      | CPU       | iter      | CPU       |
| Dai-Fletcher | 253       | 0.79      | 537       | 1.64      | 687       | 2.22      |
| EQ-VABBmin   | 132       | 0.46      | 300       | 0.86      | 453       | 1.30      |
| Algorithm I  | 121       | 0.38      | 253       | 0.84      | 468       | 1.54      |
|              | w8a       |           |           |           |           |           |
| Dai-Fletcher | 202       | 0.55      | 782       | 2.21      | 1028      | 2.73      |
| EQ-VABBmin   | 107       | 0.32      | 454       | 1.33      | 679       | 1.92      |
| Algorithm I  | 78        | 0.24      | 284       | 0.81      | 550       | 1.59      |
|              | ijcnn1    |           |           |           |           |           |
| Dai-Fletcher | 293       | 0.81      | 41784     | 145.69    | 84698     | 290.48    |
| EQ-VABBmin   | 123       | 0.39      | 23928     | 82.99     | 29647     | 90.57     |
| Algorithm I  | 63        | 0.17      | 6487      | 20.44     | 21238     | 65.22     |

long BB stepsizes and short stepsizes associated with $\alpha_{k}^{new}$ for quadratic optimization. The method was further extended for solving box-constrained and SLB optimization problems by incorporating nonmonotone line searches and gradient projection techniques. Numerical comparisons with recent successful gradient methods on quadratic, general box-constrained and SLB optimization problems demonstrate the efficiency of our method.

A recent work of Huang et al. [29] generalizes the techniques in [27] to the following family of nonmonotone methods:

$$\alpha_k = \frac{q_{k-1}^T \psi(A) g_{k-1}}{g_{k-1}^T \psi(A) A g_{k-1}},$$

(45)

where $\psi$ is the same as the one in [27]. Clearly, the two BB stepsizes $\alpha_k^{BB1}$ and $\alpha_k^{BB2}$ simply corresponding to $\psi(A) = I$ and $\psi(A) = A$ in [27], respectively. They derived a stepsize, say $\tilde{\alpha}_k^H$, for the family [35] which also has the form (45) but with $H_k$ given by

$$H_k = \begin{pmatrix}
\frac{q_{k-1}^T \psi(A) g_{k-1}}{\|\psi(A) g_{k-1}\|^2} & \frac{q_{k-1}^T \psi(A) A g_k}{\|\psi(A) g_{k-1}\| \cdot \\|\psi^{(1-r)}(A) g_k\|} \\
\frac{q_{k-1}^T \psi(A) A g_k}{\|\psi(A) g_{k-1}\| \cdot \\|\psi^{(1-r)}(A) g_k\|} & \frac{\|\psi^{(1-r)}(A) g_k\|^2}{\|\psi(A) g_{k-1}\|^2}
\end{pmatrix},$$

where $q_k$ is a vector satisfying $(I - \alpha_{k-1} A) q_k = g_k$. This stepsize has the two-dimensional quadratic termination property, and can also be recovered by the equation (10) when $v_1(k) = k - 2$, $v_2(k) = k$.

$$\psi_1(A) = (I - \alpha_{k-2} A)^{-2}(I - \alpha_{k-1} A)^{-1} \psi^{2r}(A), \quad \psi_2(A) = \psi^{2(1-r)}(A),$$
and
\[ \psi_3(A) = (I - \alpha_{k-2} A)^{-1} \psi(A), \quad \psi_4(A) = (I - \alpha_{k-2} A)^{-1} (I - \alpha_{k-1} A)^{-1} \psi(A). \]
However, as we see from \( H_k \), the calculation of \( \tilde{\alpha}^H_k \) requires the Hessian which makes it not easy to extend to general problems.

To ensure global convergence, Algorithm 1 adopts the GLL nonmonotone line search. One may also employ other line searches mentioned before such as Dai-Zhang \[15\], Zhang-Hager \[45\] and Dai-Fletcher \[10\] strategies. Based on the analysis in \[10, 26, 30\], we can establish the convergence of Algorithm 1 under those line searches without difficulty. We shall conduct extensively numerical experiments for Algorithm 1 using the aforementioned line searches on various unconstrained and constrained optimization problems in our future work.

In \[27\], it is shown that, for general strictly convex quadratics, the stepsize \( \alpha^H_k \) converges to the reciprocal of the maximum eigenvalue of the Hessian when applying the family \( \{8\} \). An interesting question is whether our new stepsize \( \alpha^\text{new}_k \) enjoys similar spectral property as \( \alpha^H_k \) in the \( n \)-dimensional case. To answer this question, one needs to know the asymptotic behavior of the BB gradient method which is still an open issue. However, our results show that the gradient method incorporated with some stepsize that has the two-dimensional quadratic termination property can significantly improve its performance.

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