Regularized Barzilai-Borwein Method

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Abstract We develop a novel stepsize based on Barzilai-Borwein method for solving some challenging optimization problems efficiently, named regularized Barzilai-Borwein (RBB) stepsize. We indicate that the reciprocal of the RBB stepsize is the close solution to an $\ell_2$-regularized least squares problem. When the regularized item vanishes, the RBB stepsize reduces to the original Barzilai-Borwein stepsize. RBB stepsize includes a class of valid stepsizes, such as another version of Barzilai-Borwein stepsize. The global convergence of the corresponding RBB algorithm is proved in solving strictly convex quadratic optimization problems. One scheme for adaptively generating regularization parameters was proposed, named adaptive two-step parameter. An enhanced RBB stepsize is used for solving quadratic and general unconstrained optimization problems more efficiently. RBB stepsize could overcome the instability of BB stepsize in many ill-conditioned optimization problems. Moreover, RBB stepsize is more robust than BB stepsize in numerical experiments. Numerical examples show the advantage of using the proposed stepsize to solve some numerical optimization problems.

Keywords Barzilai-Borwein, regularization, least squares, stability, spectral

Mathematics Subject Classification (2000) 90C20 · 90C25 · 90C30
Introduction

In this paper, we consider the Barzilai and Borwein (BB) method \cite{BB1988} for the large scale unconstrained optimization problem

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

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a sufficiently smooth function. A minimizer is denoted by $x^*$. The BB method is defined by

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

where $x_k$ is the $k$th approximation to $x^*$, $g_k := \nabla f(x_k)$ is the gradient of $f$ at $x_k$. The scalar $\alpha_k$ is given by

$$\alpha_{BB1}^k := \alpha_k = \frac{s_{k-1}^T y_{k-1}}{s_{k-1}^T s_{k-1}},$$

where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$. $\frac{1}{\alpha_k}$ is called stepsize.

It is well known that the steepest descent (SD) method is the simplest gradient method in unconstrained optimization \cite{SD1946}. In this method, locally, $-g_k$ is the search direction in which the objective function value decreases the most, and the stepsize $\frac{1}{\alpha_k}$ is determined by exact line search

$$\frac{1}{\alpha_k} = \arg\min_{\alpha > 0} f(x_k + \frac{1}{\alpha} (-g_k)).$$

However, in practice, the SD method is not efficient and usually converges slowly due to zigzag behaviors \cite{Zigzag1991}. In the gradient method, if a new stepsize can break the zigzag behaviors, then the performance of SD method may be improved. Fortunately, BB method achieves this goal in a simple and effective way. Assuming $s_{k-1}^T y_{k-1} > 0$, the scalar $\alpha_{BB1}^k$ in \cite{BB1988} is the solution to the following least squares problem

$$\min_{\alpha \in \mathbb{R}} \|\alpha s_{k-1} - y_{k-1}\|_2^2.$$  \hspace{1cm} (3)

Here, another version of the BB scalar is to solve the least squares problem

$$\min_{\alpha \in \mathbb{R}} \|s_{k-1} - \frac{1}{\alpha} y_{k-1}\|_2^2,$$

the minimizer of which is

$$\alpha_{BB2}^k = \frac{y_{k-1}^T y_{k-1}}{s_{k-1}^T y_{k-1}}.$$  \hspace{1cm} (4)

By the Cauchy-Schwarz inequality \cite{CS1960}, we know that $\alpha_{BB1}^k \leq \alpha_{BB2}^k$ holds. For convenience, we use the abbreviation BB to indicate the BB1 in the next few sections.
From above, we know that the BB method approximates Hessian $\nabla^2 f(x_k)$ by the diagonal matrix $\alpha_k I$ at the $k$th iteration. Therefore, the BB method incorporates quasi-Newton approach to gradient method by the choice of step-size. Thus, the BB method obtains a faster convergence speed than that of the steepest descent method. In the seminal paper [9], the authors applied the BB method to solve the strictly convex quadratic optimization problem. Especially when $n = 2$, the authors proved that the BB method converges R-superlinearly to the global minimizer. In any dimension, it is still globally convergent [39] but the convergence is R-linear [13]. Raydan [40] adapted the method to unconstrained optimization by incorporating the non-monotone line search of Grippo et al. [38]. Since this work, the BB method has been successfully extended to many fields such as convex constrained optimization [16,15,22], nonlinear least squares [36], image processing [10,34], etc.

Despite impressive numerical performance of the BB method, one has to face the non-monotonic phenomenon of iterative residuals in numerical experiments [25,3,11]. As a matter of fact, this mysterious numerical phenomenon does not destroy the total downward tendency of iterative residual. But the unstable performance due to its non-monotonicity may lead to poor results in some ill-conditioned problems. In general, the non-monotonic phenomenon of the BB method stems form the fact that it frequently produces too long stepsizes [11]. An iteration point at a position with large curvature, and the long stepsize produced by the BB method will lead the function value to jump. In particular, when the problem is ill-conditioned, such a long stepsize may cause the iterate to oscillate violently, affecting the convergence speed.

Recently, the instability in the BB method has attracted some attention in the optimization community [11,24] and reference therein. From our point of view, the instability in the BB method could be regarded as an ill-posed inverse problem. It is well known that regularization is an effective technique to deal with such problems [4,28,44]. Therefore, we consider improving the stability of the BB method by adding a regularization term to (3). At the same time, we are interested in studying the instability index of the BB method as a regularization parameter to adaptively adjust the stepsize.

Assuming $\Phi_k$ is a symmetric positive definite matrix, we consider the following regularized least squares problem

$$\min_{\alpha \geq 0} \left\{ \| \alpha s_{k-1} - y_k - 1 \|_2^2 + \tau_k \| \alpha \Phi_k s_{k-1} - \Phi_k y_k - 1 \|_2^2 \right\}, \tag{5}$$

where $\tau_k \geq 0$ is regularization parameter, $\| \cdot \|_2$ is the usual Euclidean 2-norm. In the next section, we will show that the solution to above least squares problem as follows

$$\alpha_{RB} = \frac{s_{k-1}^T y_k - 1 + \tau_k s_{k-1}^T \Phi_k^T \Phi_k y_k - 1}{s_{k-1}^T s_{k-1} + \tau_k s_{k-1}^T \Phi_k^T \Phi_k s_{k-1}}. \tag{6}$$

If $\tau_k = 0$, (6) degenerates to the original BB scalar. After selecting a suitable matrix $\Phi_k$, we expect a more (less) regularization to lead to a shorter (longer)
stepsize. Through a skillful design of regularization parameters, the proposed stepsize can adaptively reduce the instability of the BB method without reducing the convergence speed.

In what follows, in Section 2, we propose regularized Barzilai-Borwein (RBB) method for solving strictly convex quadratic problems. In Section 3, we present global convergence properties, R-linear convergence rate of the RBB method. In Section 4, we propose a scheme for adaptively generating regularization parameters. In Section 5, we consider an enhanced RBB method for general unconstrained optimization problems, which has the advantages of low computing cost and fast convergence speed compared with the original RBB method. In Section 6, we present numerical results of the RBB and enhanced RBB methods for some ill-conditioned quadratics and general unconstrained optimization problems. We also demonstrate its numerical robustness. Finally, in Section 7, we present concluding remarks.

2 Regularized BB Method for Convex Quadratic Optimization

In this section, we consider the unconstrained quadratic optimization

$$
\min_{x \in \mathbb{R}^n} f(x) = \frac{1}{2} x^T A x - b^T x, \quad (7)
$$

where matrix $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite and $b \in \mathbb{R}^n$ is a given vector. We shall discuss some properties of RBB stepsize and the relationship between it and other stepsizes.

**Theorem 2.1** Let $\tau_k \geq 0$. Then the scalar $\alpha_{RBB}^k$ defined by (6) is the unique solution to (5).

**Proof** Because problem (5) is a strictly convex unconstrained optimization problem, the stationary point of the objective is none other than the unique solution to (5). Taking the first derivative of the objective in problem (5) with respect to $\alpha$ leads to the first-order optimality condition

$$
\alpha(s^T_{k-1}s_{k-1} + \tau_k s^T_{k-1}\Phi^T_{k}\Phi_{k}s_{k-1} - (s^T_{k-1}y_{k-1} + \tau_k s^T_{k-1}\Phi^T_{k}\Phi_{k}y_{k-1}) = 0. \quad (8)
$$

With the first-order optimality condition (8), we have

$$
\alpha = \frac{s^T_{k-1}y_{k-1} + \tau_k s^T_{k-1}\Phi^T_{k}\Phi_{k}y_{k-1}}{s^T_{k-1}s_{k-1} + \tau_k s^T_{k-1}\Phi^T_{k}\Phi_{k}s_{k-1}}. \quad (9)
$$

Since $\Phi^T_{k}\Phi_{k}$ is a symmetric positive definite matrix, the denominator of $\alpha$ in (9) is not equal to zero when $s_{k-1} \neq 0$. Consequently, the $\alpha$ in (9) is the $\alpha_{RBB}^k$ in (6), this completes the proof. □

For the convex optimization (7), we take $\Phi_k = A$ in (6), which implies

$$
\alpha_{RBB}^k = \frac{s^T_{k-1}(I + \tau_k A^2)y_{k-1}}{s^T_{k-1}(I + \tau_k A^2)s_{k-1}}. \quad (10)
$$
The above $\alpha_{RB}^{k}$ is the solution to
\[
\arg\min_{\alpha} \|\alpha s_{k-1} - y_{k-1}\|^{2}_{W},
\]
where $W = I + \tau_{k}A^{2}$ (cf. [24 Prop. 6]), $\|x\|_{W}^{2} = x^{T}Wx$. Let
\[
z_{\tau_{k}} = A_{\tau_{k}}s_{k-1},
\]
where $A_{\tau_{k}} = W^{\frac{1}{2}}$. For the $\alpha_{RB}^{k}$ in (10), we have
\[
\alpha_{RB}^{k} = \frac{z_{\tau_{k}}^{T}Az_{\tau_{k}}}{z_{\tau_{k}}^{T}z_{\tau_{k}}}. \tag{11}
\]
By the property of Rayleigh quotient [29], we have
\[
0 < \lambda_{1} \leq \alpha_{RB}^{k} \leq \lambda_{n}, \tag{12}
\]
where $\lambda_{1}$ and $\lambda_{n}$ denote the smallest and largest eigenvalues of $A$, respectively. This indicates that $\alpha_{RB}^{k}$ lies in the spectrum of $A$.

From the Cauchy-Schwarz inequality, we have a rather simple but interesting result as follows
\[
s_{k-1}^{T}y_{k-1}\frac{s_{k-1}}{s_{k-1}^{T}A^{2}s_{k-1}} \leq \frac{s_{k-1}^{T}A^{2}y_{k-1}}{s_{k-1}^{T}A^{2}s_{k-1}} \leq \frac{s_{k-1}^{T}A^{2}y_{k-1}}{s_{k-1}^{T}s_{k}}. \tag{13}
\]
Let $a = A^{\frac{1}{2}}s_{k-1}$, $\hat{a} = A^{\frac{1}{2}}y_{k-1}$. It follows $(a^{T}\hat{a})^{2} \leq (a^{T}a)(\hat{a}^{T}\hat{a})$ that the second inequality in (13) holds.

In the case of $\Phi_{k} = A$, the solution to the second term $\arg\min_{\alpha} \|\alpha \Phi_{k} s_{k-1} - \Phi_{k} y_{k-1}\|^{2}_{2}$ in the problem (5) is
\[
\beta_{k} = \frac{s_{k-1}^{T}A^{2}y_{k-1}}{s_{k-1}^{T}A^{2}s_{k-1}}.
\]
Inequalities (13) are equivalent to the following relationship
\[
\alpha_{RB1}^{k} \leq \alpha_{RB2}^{k} \leq \beta_{k}. \tag{14}
\]
Consequently, the regularization term in (5) is equivalent to a constraint imposed on the original least squares (3) to generate suitable small stepsize, improving the stability of BB method.

**Theorem 2.2** Assume that $s_{k-1}^{T}y_{k-1} > 0$ and $\tau_{k} \geq 0$. Then the $\alpha_{RB}^{k}$ lies in $[\alpha_{RB1}^{k}, \beta_{k}]$ and is monotonically increasing with respect to parameter $\tau_{k}$.

**Proof** Let $h_{\tau_{k}}(\alpha)$ be the derivative of the $\alpha_{RB}^{k}$ in (10) with respect to $\tau_{k}$. Then we have
\[
h_{\tau_{k}}(\alpha) = \frac{s_{k-1}^{T}A^{2}y_{k-1}s_{k-1}^{-1}s_{k-1}^{T} - s_{k-1}^{T}y_{k-1}s_{k-1}^{-1}A^{2}s_{k-1}}{(s_{k-1}^{T}(I + \tau_{k}A^{2})s_{k-1})^{2}}.
\]
According to (13), we have $s_{k-1}^T A^2 y_{k-1} = s_{k-1}^T s_{k-1} - s_{k-1}^T y_{k-1} A^2 s_{k-1} \geq 0$. And since $s_{k-1}^T y_{k-1} > 0$, we have $s_{k-1}^T (I + \tau_k A^2) s_{k-1} \neq 0$. Thus $h_\tau (\alpha) \geq 0$. This shows that $\alpha_k^{RBB}$ increases monotonically with respect to $\tau_k$. In the case of $\tau_k = 0$, we have $\alpha_k^{RBB} = \alpha_k^{BB}$. And by the result of (13), we have $\alpha_k^{RBB} \in [\alpha_k^{BB1}, \beta_k]$. The proof is completed.

We now consider the convex combination of $\alpha_k^{BB1}$ and $\alpha_k^{BB2}$ as follows

$$\alpha_k^{Con} = \gamma_k \alpha_k^{BB1} + (1 - \gamma_k) \alpha_k^{BB2},$$

where $\gamma_k \in [0, 1]$. Compared with the case in [17], the $\alpha_k^{Con}$ in this family is the solution to $\arg\min_{\alpha \in \mathbb{R}} \| \bar{\tau} (\alpha s_{k-1} - y_{k-1}) + (1 - \bar{\tau}) (s_{k-1} - \frac{1}{\gamma} y_{k-1}) \|^2_2$ for some $\bar{\tau} \in [0, 1]$.

**Proposition 2.1** Suppose $s_{k-1}^T y_{k-1} > 0$. For all $k$, each $\alpha_k^{Con} = \gamma_k \alpha_k^{BB1} + (1 - \gamma_k) \alpha_k^{BB2}$ can be regarded as a special case of the $\alpha_k^{RBB}$ (10) with

$$\tau_k = \frac{(1 - \gamma_k)(\alpha_k^{BB1} - \alpha_k^{BB2})}{\gamma_k \alpha_k^{BB1} + (1 - \gamma_k) \alpha_k^{BB2} - \beta_k},$$

where $0 \leq \gamma_k \leq 1$.

**Proof** From (13) and the results in (22), we know that $[\alpha_k^{BB1}, \alpha_k^{BB2}] \subset [\alpha_k^{BB1}, \beta_k]$ holds. For each $\gamma_k \in [0, 1]$, solving

$$\gamma_k \alpha_k^{BB1} + (1 - \gamma_k) \alpha_k^{BB2} = \frac{s_{k-1}^T (I + \tau_k A^2) y_{k-1}}{s_{k-1}^T (I + \tau_k A^2) s_{k-1}},$$

we obtain the resulting $\tau_k$. \hfill \square

In fact, the RBB method is a new spectral gradient method that produces a suitable quasi-Newton stepsize by adaptively adjusting the regularization parameter. In Section 4 an adaptive regularization parameter scheme is proposed. We now apply RBB method to construct Algorithm 1 for finding the optimal solution to the convex quadratic optimization problem (7).

**Algorithm 1** RBB: Regularized Barzilai-Borwein Algorithm for Solving (7)

**Require:** Stopping criterion: $\varepsilon > 0$, MaxIt $> 0$; Initialization: $A, b, x_0, g_0, k = 0$. Regularization parameter: $\tau_0 = 0$; initial stepsize $t_0$;

1: while $k < \text{MaxIt}$ and $\|g_k\|_2 > \varepsilon \|g_0\|_2$ do
2: $x_{k+1} = x_k - t_k g_k$.
3: $g_{k+1} = A x_{k+1} - b$.
4: $s = x_{k+1} - x_k, y = g_{k+1} - g_k$.
5: $t_k = \frac{s^T y}{s^T + t_k y}$, for some $t_k \geq 0$.
6: $k = k + 1$.
7: end while
3 Convergence Analysis of RBB Method

In this section, global convergence and R-linear convergence rate of Algorithm 1 will be proved. We state that the convergence analysis in this section is based on [39,35]. It is worth noting that the $\alpha_{k}^{RBB}$ in (10) can be seen as a special case of the family gradient stepsizes in [33] for $\rho_{k} = 0$, $v(k) = k - 1$ and a real analytic function $\Psi(A) = I + \tau_{k}A^{2}$, and [35] proves that they have global R-linear convergence rate. Therefore, for the proof of the global convergence rate of Algorithm 1, we directly adopt the results in [35]. However, for the sake of completeness, we give the proof of global convergence here. Throughout this paper, let $0 < \lambda_{1} \leq \lambda_{2} \leq \cdots \leq \lambda_{n}$ be the eigenvalues of $A$ and denote the Euclidean condition number of $A$ by

$$\kappa(A) := \|A\|_{2}\|A^{-1}\|_{2} = \frac{\lambda_{n}}{\lambda_{1}},$$

where $\lambda_{1}$ and $\lambda_{n}$ are the smallest and largest eigenvalues of $A$, respectively.

**Proposition 3.1** Let $f(x)$ be a strictly convex quadratic function. Let $\{x_{k}\}$ be the sequence of iterates generated by RBB method from a given vector $x_{0}$ and $x_{*}$ be the unique minimizer. Denote the residual vector by $e_{k} = x_{*} - x_{k}$. Then for all positive integer $k$, we have

1. $Ae_{k} = \alpha_{k}^{RBB}s_{k}$,
2. $e_{k+1} = \frac{1}{\alpha_{k}}(\alpha_{k}^{RBB}I - A)e_{k}$,
3. $s_{k+1} = \frac{1}{\alpha_{k}^{RBB}}(\alpha_{k}^{RBB}I - A)s_{k}$.

**Proof** Under the conditions in this theorem, we have $Ax_{*} - b = 0$. It follows from $s_{k-1} = x_{k} - x_{k-1}$ and $x_{k+1} = x_{k} - \frac{1}{\alpha_{k}}g_{k}$ that $Ae_{k} = A(x_{*} - x_{k}) = (Ax_{*} - b) - (Ax_{k} - b) = -g_{k} = \alpha_{k}^{RBB} s_{k}$ holds. It follows from $s_{k} = e_{k} - e_{k+1}$ and $Ae_{k} = \alpha_{k}^{RBB}s_{k}$ that $e_{k+1} = \frac{1}{\alpha_{k}^{RBB}}(\alpha_{k}^{RBB}I - A)e_{k}$. From $s_{k+1} = -\frac{1}{\alpha_{k+1}}g_{k+1}$, $s_{k} = -\frac{1}{\alpha_{k}^{RBB}}g_{k}$ and $g_{k+1} = (I - \frac{1}{\alpha_{k}^{RBB}}A)g_{k}$, the last equality follows directly. \(\Box\)

For any residual vector $e_{k}$ with $k \geq 0$, there are constants $e_{1}^{k}, e_{2}^{k}, \ldots, e_{n}^{k}$ such that

$$e_{k} = \sum_{i=1}^{n} e_{i}^{k} v_{i}, \quad (15)$$

where $v_{1}, v_{2}, \ldots, v_{n}$ are the orthonormal eigenvectors of $A$ associated with the eigenvalues $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$. From (15) and the iterative formula $e_{k+1} = \frac{1}{\alpha_{k}^{RBB}}(\alpha_{k}^{RBB}I - A)e_{k}$ in Proposition 3.1, we have

$$e_{k+1} = \frac{1}{\alpha_{k}}(\alpha_{k}^{RBB}I - A)\sum_{i=1}^{n} e_{i}^{k} v_{i} = \sum_{i=1}^{n} \frac{\alpha_{k}^{RBB} - \lambda_{i}}{\alpha_{k}} e_{i}^{k} v_{i}. \quad (16)$$
It follows from the orthonormality of the eigenvectors $v_1, v_2, \ldots, v_n$, there holds
\[
\|e_{k+1}\|^2 = \sum_{i=1}^{n} \left( \frac{\alpha_k^{BB} - \lambda_i}{\alpha_k^{BB}} \right)^2 (e_i^k)^2 \leq \max_{1 \leq i \leq n} \left| \frac{\alpha_k^{BB} - \lambda_i}{\alpha_k^{BB}} \right|^2 \|e_k\|^2. \tag{17}
\]
From (12), we have
\[
\max_{1 \leq i \leq n} \left| \frac{\alpha_k^{BB} - \lambda_i}{\alpha_k^{BB}} \right| < \lambda_n - \lambda_1. \tag{18}
\]
Combining (17) and (18), we know that if $1 < \kappa(A) < 2$, then $\{\|e_k\|\}$ is a monotonically decreasing sequence. Further, we know that the convergence properties of sequence $\{e_k\}$ depend on the behavior of each sequence $\{e_i^k\}$, $1 \leq i \leq n$. The following lemma shows that the sequence $\{e_1^k\}$ converges monotonically to zero Q-linearly [42].

**Lemma 3.1** Under the conditions in Proposition 3.1. Then the sequence $\{e_1^k\}$ converges to zero Q-linearly with convergence factor $\theta = 1 - \frac{\lambda_1}{\lambda_n}$.

**Proof** It follows from (16) that for all positive integer $k$, we have
\[
e_1^{k+1} = \left( \frac{\alpha_k^{BB} - \lambda_1}{\alpha_k^{BB}} \right) e_1^k.
\]
Since $\alpha_k^{BB}$ satisfies (12), we have $|e_1^{k+1}| = \left( \frac{\alpha_k^{BB} - \lambda_1}{\alpha_k^{BB}} \right) |e_1^k| \leq \theta |e_1^k|$, where
\[
\theta = 1 - \frac{\lambda_1}{\lambda_n} < 1.
\]
The proof is completed. \qed

It is observed that the coefficient $e_1^{k+1} = \frac{\alpha_k^{BB} - \lambda_1}{\alpha_k^{BB}} e_1^k$ of eigenvector $v_1$ in (16) asymptotically becomes zero whenever scalar $\alpha_k^{BB}$ approaches the eigenvalue $\lambda_1$ of $A$. As a member of the BB-like method, RBB method has the following convergence property.

**Lemma 3.2** (42, Lemma.2). Let $\{e_k\}$ be an infinite residual sequence generated by RBB method. Assume that sequences $\{e_1^k\}$, $\{e_2^k\}$, $\ldots$, $\{e_m^k\}$ all converge to zero for a fixed integer $m$, where $1 \leq m < n$. Then
\[
\liminf_{k \to \infty} |e_{m+1}^k| = 0.
\]

**Theorem 3.1** Let $f(x)$ be a strictly convex quadratic function. Let $\{x_k\}$ be an infinite sequence of iterates generated by RBB method, and let $x_*$ be the unique solution to the problem. Then $\lim_{k \to \infty} \|e_k\| = 0$, where $e_k = x_* - x_k$. 
Proof Combining (13) and the orthonormality of eigenvectors $v_1, v_2, \ldots, v_n$, we have
\[
\|e_k\|^2 = \sum_{i=1}^{n} (e^k_i)^2 \quad \forall \ k \geq 0.
\]
Hence, sequence $\{e_k\}$ converges to zero if and only if each one sequence $\{e^k_i\}$ for $i = 1, 2, \ldots, n$ converges monotonically to zero. From Lemma 3.1, sequence $\{e^k_i\}$ converges monotonically to zero. Therefore, it is sufficient to prove that $\{e^k_i\}$ converges to zero. Hence, sequence $\{e^k_i\}$ converges monotonically to zero. From Lemma 3.1, sequence $\{e^k_i\}$ converges monotonically to zero. Therefore, it is sufficient to prove that $\{e^k_i\}$ converges to zero. Then for any given $\varepsilon > 0$, there exists $\hat{k}$ sufficiently large such that
\[
\sum_{i=1}^{p-1} \lambda_i^2 (1 + \tau_k \lambda_i^2) (e^k_i)^2 < \frac{\varepsilon}{L} \quad \forall \ k \geq \hat{k} \text{ and } L \geq 2.
\] (19)

It follows from $z_k = A_{\tau_k} s_k = \frac{1}{\varepsilon} z_k = A_{\tau_k} A e_k$ and the orthonormality of eigenvectors $v_1, v_2, \ldots, v_n$ that the scalar $\alpha_{k+1}^{RBB}$ in (11) can be written as
\[
\alpha_{k+1}^{RBB} = \frac{z_k^T A_{\tau_k}}{z_k} = \frac{e^k_i A^T A_{\tau_k} A_{\tau_k} A e_k}{e^k_i A^T A_{\tau_k} A_{\tau_k} A e_k} = \sum_{i=1}^{n} \lambda_i^2 (1 + \tau_k \lambda_i^2) (e^k_i)^2
\] (20)
where $A_{\tau_k} = (I + \tau_k A^2) \hat{z}_k$. Combining (19) and (20), we have
\[
\sum_{i=p}^{n} \lambda_i^2 (1 + \tau_k \lambda_i^2) (e^k_i)^2 \leq \alpha_{k+1}^{RBB} \leq \lambda_n \quad \forall \ k \geq \hat{k} \text{ and } L \geq 2.
\] (21)

Further, it follows from Lemma 3.2 there exists $k_p > \hat{k}$ such that
\[
(\lambda_p)^2 (1 + \tau_k \lambda_p^2) (e_{k_p}^k)^2 < \varepsilon.
\]
Let $k_0 > k_p$ be any integer for which
\[
(\lambda_p)^2 (1 + \tau_k \lambda_p^2) (e_{k_0}^{k_0-1})^2 < \varepsilon,
\] (22)
and
\[
(\lambda_p)^2 (1 + \tau_k \lambda_p^2) (e_{k_0}^{k_0})^2 \geq \varepsilon.
\]
Clearly,
\[
\sum_{i=p}^{n} \lambda_i^2 (1 + \tau_k \lambda_i^2) (e^k_i)^2 \geq \lambda_p^2 (1 + \tau_k \lambda_p^2) (e_{k_0}^k)^2 \geq \varepsilon \quad \text{for } \ k_0 \leq k \leq r - 1,
\] (23)
where $r$ is the first integer greater than $k_0$ and such that
\[
\lambda_p^2 (1 + \tau_k \lambda_p^2) (e_{k_0}^r)^2 < \varepsilon.
\]
From (21) and (23), we have
\[
\frac{L}{L + 1} \lambda_p \leq \alpha_{k+1}^{RBB} \leq \lambda_n \quad \text{for } \ k_0 \leq k \leq r - 1 \text{ and } L \geq 2.
\]
It follows from the analysis in Lemma 3.2, there holds
\[ |e^{k+1}_p| = \frac{\alpha_{RBB}^{k+1} - \lambda_p}{\alpha_{RBB}^k} |e^k_p| \leq \hat{c} |e^k_p| \quad \text{for} \ k_0 + 1 \leq k \leq r, \]
(24)
where \( \hat{c} = \max\{\frac{1}{\hat{c}_2}, 1 - \frac{\lambda_1}{\lambda_n}\} < 1 \). From (17), we have
\[ (e^{k+1}_p)^2 \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_1}\right)^4 (e^{k_0}_p - 1)^2. \]
(25)
It follows from (22), (24) and (25) that there holds
\[ (e^{k+1}_p)^2 \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_1}\right)^4 (e^{k_0}_p - 1)^2 \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_1}\right)^4 \frac{\varepsilon}{\lambda_p^2(1 + \tau_k \lambda_p^2)}, \]
where \( k_0 \leq k \leq r \). Because \( \hat{k} \) is sufficiently large and \( \varepsilon > 0 \) can be chosen to be arbitrarily small and the conditions of \( k_p, k_0 \) and \( r \), we can deduce that \( \lim_{k \to \infty} |e^k_p| = 0 \) as required. The proof is completed. \( \square \)

4 Selecting Regularization Parameter \( \tau_k \)

In this section, we first propose an adaptive parameter scheme and then verify the effectiveness of this scheme through a typical numerical experiment.

4.1 A Two-Step Regularization Parameter Scheme

From the results in Theorem 2.2, we know that if the regularization parameter \( \tau_k \to 0 \), then \( \alpha_{RBB}^k \to \alpha_{BB}^k \), stability cannot be improved; conversely, if the regularization parameter \( \tau_k \to \infty \), then \( \alpha_{RBB}^k \to \beta_k \), convergence speed will be affected. An appropriate regularization parameter should balance the stability and convergence speed of RBB method in a suitable way.

The instability of BB method stems from its frequent occurrence of an extremely small \( \alpha_{BB}^k \) after a large \( \alpha_{BB}^l \) for \( l < k \) especially under ill-conditioning \( [25] \). Consequently, in order to improve the stability of the BB method, a natural idea is to generate a scalar \( \alpha_{RBB}^k \) larger than \( \alpha_{BB}^k \) after a large \( \alpha_{BB}^l \) by adjusting regularization parameter \( \tau_k \). In other words, we should control the magnitude of variation in the stepsizes over successive iterations by appropriate regularization parameter \( \tau_k \).

Based on this, we consider two successive scalars \( \alpha_{BB}^{k-1} \) and \( \alpha_{BB}^{k} \), and take
\[ \tau_k = \frac{\alpha_{BB}^{k+2}}{\alpha_{BB}^{k-1}}. \]
(26)
We call (26) a two-step regularization parameter. Let
\[ \theta_{k-2} = \angle(g_{k-2}, Ag_{k-2}), \quad \theta_{k-1} = \angle(g_{k-1}, Ag_{k-1}) \quad \text{for} \ k \geq 3, \]
be the angles between $g_{k-1}$ and $Ag_{k-1}$ for $i = 1, 2$, respectively. Then, we have

$$
\tau_k = \frac{\alpha_k^{BB2}}{\alpha_k^{BB1}} = \frac{\|y_{k-1}\|_2}{\|s_{k-1}\|_2} \frac{\cos(\theta_{k-2})}{\cos(\theta_{k-1})} = \frac{h_k \cos(\theta_{k-2})}{h_{k-1} \cos(\theta_{k-1})},
$$

where

$$
h_k = \frac{\|y_{k-1}\|_2}{\|s_{k-1}\|_2} = \sqrt{\frac{\alpha_k^{BB1} \alpha_k^{BB2}}{\alpha_k^{BB1}}}.
$$

is the geometric mean of $\alpha_k^{BB1}$ and $\alpha_k^{BB2}$, describing the current local mean curvature. We next analyze the principle of the regularization parameter (26).

We first analyze the ratio $\frac{\tau_k}{\tau_{k-1}}$ in (27). It is worth noting that, to minimize a general function, [43] tried to estimate the local Lipschitz constant of gradient by (28). In this way, $h_k$ would be sensitive to the local shape of the objective function. On the one hand, when the objective function is “steep”, i.e., (28) is large, we have to take a small value for the stepsize to guarantee convergence. On the other hand, when $f$ is “flat”, i.e., (28) is small, we have to take a large stepsize to accelerate convergence. BB method tends to produce a large stepsize, and the factor (28) reflects the local shape of $f$. Consequently, the factor $\frac{\tau_k}{\tau_{k-1}}$ in (27) serves as a correction for $\alpha_k^{BB1}$, and describes the variation in local mean curvature.

We now focus on analysis of $\frac{\cos(\theta_{k-2})}{\cos(\theta_{k-1})}$ in (27). To this end, we briefly recall the adaptive Barzilai-Borwein (ABB) method [46] as follows

$$
\alpha_k^{ABB} = \begin{cases} 
\alpha_k^{BB2}, & \text{if } \frac{\alpha_k^{BB1}}{\alpha_k^{BB2}} < \eta, \\
\alpha_k^{BB1}, & \text{otherwise},
\end{cases}
$$

where $\eta \in (0, 1)$. As in the previous section, we study the strictly convex quadratic case, so that $\alpha_k^{BB1} \leq \alpha_k^{BB2}$. The ABB scheme adaptively picks BB1 or BB2 step based on the value of $\frac{\alpha_k^{BB1}}{\alpha_k^{BB2}} = \cos^2 \theta_{k-1}$. The idea of the ABB scheme is to take a larger BB1 stepsize when $\cos^2 \theta_{k-1} \approx 1$, and a smaller stepsize when this is not the case, such as BB2 step. If $\cos^2 \theta_{k-1}$ is close to 1, this means that $-g_{k-1}$ is close to an eigenvector of $A$ corresponding to an eigenvalue $\lambda$. In this case, BB1 step performs better than BB2 step [24]. From the idea of ABB scheme (29), the term $\frac{\cos(\theta_{k-2})}{\cos(\theta_{k-1})}$ in (27) describes the local variation in search direction.

In summary, at current iteration, a large regularization parameter $\tau_k$ corresponds to a steep function (large $\frac{h_k}{h_{k-1}}$) and a search direction $-g_{k-1}$ away from an eigenvector of $A$ (large $\frac{\cos(\theta_{k-2})}{\cos(\theta_{k-1})}$), and leads to a short stepsize. A small regularization parameter $\tau_k$ corresponds to a flat function and a search direction $-g_{k-1}$ close to an eigenvector of $A$, and leads a long stepsize.

Here, naturally, one may ask, if the regularization parameter is set to

$$
\tau_k = \frac{\alpha_k^{BB1}}{\alpha_k^{BB1}},
$$
will it have the same effect as (26)? We claim this is not true. Below we provide an explanation. Since
\[ \tau_k = \frac{\alpha_k^{BB1}}{\alpha_k^{BB1-1}} = \frac{\|y_{k-1}\|_2/\|s_{k-1}\|_2 \cos(\theta_{k-1})}{\|y_{k-2}\|_2/\|s_{k-2}\|_2 \cos(\theta_{k-2})} = \frac{h_k \cos(\theta_{k-1})}{h_{k-1} \cos(\theta_{k-2})}, \]
the only difference between (27) and (30) is the term \( \frac{\cos(\theta_{k-1})}{\cos(\theta_{k-2})} \). Therefore, we get the opposite conclusion from (27) in the variation of search direction.

In order to tune the convergence speed and stability of the RBB method in various problems, we further expand the regularization parameters setting and consider
\[ \tau_k(r) = \left( \frac{\alpha_k^{BB2}}{\alpha_k^{BB1}} \right)^r, \]
for \( r \geq 0 \) is a real number. We will test various choice for \( r > 0 \) in Section 6.

Remark 4.1 It is worth noting that the regularization parameter scheme (26) implicitly adopts the idea of the trust region method and adaptively controls the fluctuation scale of the stepsize, making the RBB method very suitable for solving ill-conditioned optimization problems.

Remark 4.2 In fact, if \( \Phi_k = \sqrt{A} \), then the solution to \( \arg\min_{\alpha} \|\alpha \Phi_k s_{k-1} - \Phi_k y_{k-1}\|^2 \) is \( \hat{\beta}_k = \alpha_k^{BB2} \), in which case \( \alpha_k^{RBB} \in [\alpha_k^{BB1}, \alpha_k^{BB2}] \), and \( \alpha_k^{RBB} \) is monotonically increasing with respect to \( \tau_k \). In this case, \( \alpha_k^{ABB} \) can be seen as a discretized version of \( \alpha_k^{RBB} \), choosing \( \alpha_k^{BB1} \) or \( \alpha_k^{BB2} \) depending on the size of \( \frac{\alpha_k^{BB1}}{\alpha_k^{BB2}} \). The only difference is that we take \( \Phi_k = A \) in this article. But they have the same principle and belong to the same framework.

4.2 A Typical Numerical Experiment

To illustrate the performance of the RBB method with adaptive regularization parameter (26) in any dimensions. We apply it to the non-random quadratic minimization problem in [19], and consider function
\[ f(x) = \frac{1}{2}(x - x^*)^T A(x - x^*), \]
where \( A = \text{diag}(\lambda_1, \ldots, \lambda_n) \) with
\[ \lambda_i = 10^{\text{cond}(n-i)}, \quad i = 1, \ldots, n. \]
Here, \( \text{cond}(\kappa) = \log_{10}(\kappa) \) and \( \kappa > 0 \) is the condition number of \( A \). \( x^* \) is set as \( (1, \ldots, 1)^T \in \mathbb{R}^n \) and the initial guess is chosen as \( x_0 = 0 \in \mathbb{R}^n \). We set \( n = 50 \), \( \kappa = 10^8 \) and use the stopping condition \( \|g_k\|_2 \leq 10^{-8} \|g_0\|_2 \). Initial stepsize is \( t_0 = \frac{\gamma}{\|g_0\|^2 A g_0} \). For the RBB method, we set \( r = 1 \) in (31), and take \( \tau_0 = 0 \).

In the ABB scheme (29), after our testing, in such ill-conditioned problems, the parameter \( \eta = 0.7 \) performs better than that of the usual settings of
0.15 and 0.5. Therefore, we set $\eta = 0.7$ in (29). Since the ABBmin algorithm [26] usually has very good numerical performance, here we also consider the ABBmin algorithm, and set $m = 9$, $\nu_k = 0.8$, which is consistent with the parameter settings in Section 6.

Figure 1 reports the behave of gradient norms and inverse stepsizes $\alpha_k$ for the BB1, ABB, RBB and ABBmin methods at each iteration, respectively.

![Figure 1: On performances of BB1, ABB, RBB and ABBmin methods for a 50-dimensional ill-conditioned strictly convex quadratic problem](image)

Observing the results in Fig. 1, it can be seen from the four subgraphs in the first row that ABBmin performs best, RBB ranks second, and ABB’s performance is between RBB and BB1. The four subgraphs in the second row correspond to the $\alpha_k$ generated by these four different methods during the iteration progress, which explains why these methods show a large performance difference. As pointed out in the preceding, in the iterative progress, after a large $\alpha_{BB1}^l$ for $l < k$, BB method tends to generate an extremely small $\alpha_k^{BB1}$, causing the stepsizes to oscillate violently, so that the effects of several adjacent iterations almost cancel each other out and the components of the gradient cannot be quickly eliminated. The remaining three methods all have strategies for generating small stepsizes, which play a role in controlling local stability and speeding up convergence. Essentially, the so-called small step strategy is to control the fluctuation of stepsizes locally. Obviously, the inverse stepsizes $\alpha_k^{ABBmin}$ generated by ABBmin method have the best distribution and the smallest fluctuation among these methods. Compared with ABB and BB1 methods, the sequence $\alpha_k^{RBB}$ generated by RBB method is also well distributed.
5 Enhanced Regularized Barzilai-Borwein (ERBB) Method

In this section, we propose an enhanced RBB (ERBB) stepsize \( \alpha_k^{RBB} \) which utilizes a diagonal approximation of local Hessian, making it to be applied to both quadratic and general unconstrained optimization problems, and this operation substantially reduces the computational cost and improves the performance of RBB method. Meanwhile, an adaptive alternate stepsize strategy improves the convergence speed of RBB method. Therefore, based on the above two improvements, the overall performance of RBB method is enhanced.

5.1 ERBB Method for Convex Quadratic Optimization

In Section 2, for solving the strictly convex quadratic problems, we use the Hessian \( A \) of \( f(x) \) to generate \( \alpha_k^{RBB} \). By substituting \( \Phi_k = A \) into (6), we have

\[
\alpha_k^{RBB} = \frac{s_{k-1}^T y_{k-1} + \tau_k y_{k-1}^T A y_{k-1}}{s_{k-1}^T s_{k-1} + \tau_k y_{k-1}^T y_{k-1}}.
\]  

(33)

Observing (33), on the one hand, if \( f(x) \) is not quadratic, then calculating the local Hessian is a very expensive operation; on the other hand, even for the strictly convex quadratic function, this matrix-vector multiplication will increase the computational cost substantially as the size of problem becomes large.

To overcome these defects, combining the analysis in Section 2 and the \( \alpha_k^{RBB} \) in (33), we consider using a diagonal matrix \( \alpha_k^{BB2} I \) to approximate Hessian. As discussed in (cf. [38, P.178]), \( \alpha_k^{BB2} \) is a scaling factor that attempts to estimate the size of the true Hessian matrix along the most recent search direction and has been proved effective in practice. Meanwhile, in order to adjust the stepsize to various types of problems, we propose a new version of \( \alpha_k^{RBB} \) as follows

\[
\alpha_k^{RBB_{new}} = \frac{s_{k-1}^T y_{k-1} + \tau_k y_{k-1}^T \Phi_k y_{k-1}}{s_{k-1}^T s_{k-1} + \tau_k y_{k-1}^T y_{k-1}},
\]  

(34)

where the diagonal matrix

\[ \Phi_k = \phi_k I, \]  

(35)

where

\[ \phi_k = \max\{\alpha_j^{BB2} | j \in \{j_0, \ldots, k\}\} \]

with \( j_0 = \max\{1, k - \vartheta\} \), \( I \) is the identity matrix of order \( n \), \( \vartheta \geq 0 \) is an integer. From the fundamental property of the inequality, we have

\[ \alpha_k^{BB1} \leq \alpha_k^{RBB_{new}} \leq \phi_k \leq \lambda_n, \]

where \( \lambda_n \) is the largest eigenvalue of Hessian. The \( \alpha_k^{RBB_{new}} \) in (34) provides a family of spectral gradient stepsizes by choosing various \( \vartheta \). In general, it is
reasonable to choose a larger $\vartheta$ that contributes to produce a shorter stepsize. Conversely, a smaller $\vartheta$ leads to a longer stepsize.

The success of the ABBmin scheme in [26,10] inspires us to use the follow-
ing adaptively alternate stepsize scheme

$$\alpha_{ERBB}^k = \begin{cases} 
\max\{\alpha_{j}^{BBnew}|j \in \{j_0, \ldots, k\}\}, & \text{if } \alpha_k^{BB1}/\alpha_k^{BB2} < \nu_k, \\
\alpha_k^{BB1}, & \text{otherwise},
\end{cases} \quad (36)$$

where $j_0 = \max\{1, k - \varrho\}, \varrho \geq 0$ is an integer,

$$\nu_k = 1 - \frac{\alpha_k^{BB1}}{\alpha_k^{BBnew}} \in (0, 1). \quad (37)$$

In the following, we analyze the principle of the adaptive alternate stepsize scheme in (36). For simplicity, let

$$\bar{a} = \alpha_k^{BB1}/\alpha_k^{BB2} \in (0, 1), \quad \bar{b} = \alpha_k^{BB1}/\alpha_k^{BBnew} \in (0, 1).$$

It is worth noting that $\bar{b}$ describes the size of regularization parameter $\tau_k$, and the larger the parameter $\tau_k$, the smaller $\bar{b}$. We now discuss it in two cases.

Case I: $\alpha_k^{BB2} \geq \alpha_k^{BBnew}$, i.e., $\bar{a} \leq \bar{b}$. If $\bar{a} < 1 - \bar{b}$ holds, then we have $\bar{a} < 0.5$. In this case, we choose a short stepsize, which is consistent with ABBmin’s idea.

Case II: $\alpha_k^{BB2} < \alpha_k^{BBnew}$, i.e., $\bar{a} > \bar{b}$. If $\bar{a} < 1 - \bar{b}$ holds, then we have $\bar{a} < 0.5$. This implies that the current regularization parameter $\tau_k$ is large, which indicates that it is reasonable to take a small step. Specifically, for the case of $0.5 < \bar{a} < 1$ and $\bar{a} > 0.5$, we naturally choose a short stepsize based on the ABB scheme; for the case of $0.5 < \bar{a} < 1$ and $\bar{b} < 0.5$, this implies that the search direction close to an eigenvector of Hessian, but the local mean curvature may be large, it is advantageous to choose a short step.

Remark 5.1 In the threshold $\nu_k$ setting of the adaptively alternate stepsize scheme (36), we give priority to the search direction. If the search search direction is away from an eigenvector of Hessian (i.e., $\bar{a} < 0.5$), then we take a small step; if the search direction is already close to one of Hessian’s eigenvectors, we further need to consider the local mean curvature of function, which is represented by $\bar{b}$.

For the strictly convex quadratic problems (7), the $R$-linear convergence of the ERBB method (36) can be easily established using the results in [14, 35]. Therefore, we will not repeat it here. We call Algorithm 1 equipped with inverse stepsize (36) the ERBB algorithm.

Observing (34), ERBB method seems to require one more inner product per iteration than BB methods, but this extra computational work can be eliminated by using following formulas:

$$\begin{align*}
    s_{k-1}^T s_{k-1} &= t_{k-1}^2 g_{k-1}^T g_{k-1}, \\
    s_{k-1}^T y_{k-1} &= t_{k-1} (g_{k-1}^T g_{k-1} - g_k), \\
    y_{k-1}^T y_{k-1} &= g_k^T g_k - 2 g_k^T g_{k-1} + g_{k-1}^T g_{k-1},
\end{align*} \quad (38)$$
where $t_{k-1} = \frac{1}{g_{k-1}^T g_k}$. Notice that at every iteration, we only need to compute two inner products, i.e., $g_{k-1}^T g_k$ and $g_k^T g_k$. Our extensive numerical experiments show that these formulas are reliable in the quadratic case.

### 5.2 ERBB Method for General Unconstrained Optimization

To extend ERBB method for minimizing general objective functions \(^1\), we usually need to incorporate some line search to ensure global convergence. Among BB-like methods, nonmonotone line search is an effective strategy \(^40\).

Here we would like to adopt the Grippo-Lampariello-Lucidi (GLL) nonmonotone line search \(^30\), which accepts $\gamma_k$ when it satisfies

$$f(x_k + \gamma_k d_k) \leq \max_{1 \leq j \leq \min\{k, M - 1\}} \{f(x_{k-j})\} + \sigma \gamma_k g_k^T d_k,$$

(39)

where $\sigma \in (0, 1)$, $d_k$ is a descent direction.

The combination of the gradient method with the stepsize formula \(^36\) and the GLL nonmonotone line search strategy \(^39\) yields an algorithm, named Algorithm 2. Under some standard assumptions, global convergence of Algorithm 2 can similarly be established and the convergence rate is $R$-linear for strongly convex objective functions with Lipschitz continuous gradient \(^12\). Similarly, the equations in \(^38\) can be used in Algorithm 2 thus reducing the computational cost. For non-quadratic functions, the $\alpha_k^{ERBB}$ might be negative or zero, which could also happen while using the original BB method. In this case, we would use $\|s_{k-1}\|_2^2 / \|y_{k-1}\|_2^2$ as a stepsize.

#### Algorithm 2 ERBB: Enhanced Regularized Barzilai-Borwein Algorithm for Solving General Unconstrained Optimization

**Require**: stopping criterion: $\varepsilon > 0$, MaxIt $> 0$; Initialization: $x_0 \in \mathbb{R}^n$, $g_0 \in \mathbb{R}^n$, $t_{\text{max}} \geq t_{\text{min}} > 0$, initial stepsize $t_0 \in [t_{\text{min}}, t_{\text{max}}]$, $\sigma, \delta \in (0, 1)$, $M, \vartheta, \varkappa, k = 0$, regularization parameter: $\tau_0 = 0$.

1: while $k < \text{MaxIt}$ and $\|g_k\|_2 > \varepsilon \|g_0\|_2$ do
2:     $d_k = -t_k g_k$, $\gamma_k = 1$, $f_r = \max_{1 \leq j \leq \min\{k, M - 1\}} \{f(x_{k-j})\}$;
3: while the condition \(^39\) does not hold do
4:     $\gamma_k = \delta \gamma_k$;
5: end while
6:     $x_{k+1} = x_k + \gamma_k d_k$;
7: if $s_k^2 y_k > 0$ then
8:     compute $\tau_k$ by \(^26\), $t_k = \frac{1}{\alpha_k^{ERBB}}$ by \(^39\).
9: else
10:     $\bar{bb} = \frac{1}{\|s_k\|_2^2}$, $t_k = \min(\bar{bb}, \frac{1}{\|y_k\|_\infty})$.
11: end if
12: $k = \min\{t_{\text{min}}, \min\{t_k, t_{\text{max}}\}\}$.
13: $k = k + 1$.
14: end while
6 Numerical experiments

In this section, we present some numerical results to verify the analysis in the preceding sections. Since we are mainly concerned with the effect of regularization on original BB stepsize, it is only tested for numerical comparison with BB-like methods. Here, BB1 method refers to the method with BB1 stepsize, and BB2 method refers to the method with BB2 stepsize.

We report the number of iterations (Iter), CPU times in seconds (Time). All numerical experiments performed using Matlab R2019a under a Windows 11 operating system on a DELL G15 5200 personal computer with an Intel Core i7-12700H and 16 GB of RAM.

6.1 Convex Quadratic Optimization

We first test Algorithm 1 to examine the performance of regularization parameters $\tau_k(r)$ (31) with different $r$ for problem (32). We set $n = 100$, the initial point $x_0 = (x_1^0, \ldots, x_n^0)^T \in \mathbb{R}^n$ and $x^* = (x_1^*, \ldots, x_n^*)^T \in \mathbb{R}^n$, where $x_i^0 \in [-1,1]$ and $x_i^* \in [-1,1]$ are randomly generated, $i = 1,2,\ldots,n$, the termination condition is $\|g_k\|_2 \leq 10^{-10}\|g_0\|_2$. Initial stepsize is $t_0 = \frac{g_0^T g_0}{g_0^T A g_0}$.

Running independently 20 times, Table 1 reports the average number of iterations when the program meets the termination condition under different condition number $\kappa$ of $A$ and different $r$.

Table 1: Performance of regularization parameters with different $r$ for (32)

| $\kappa$ | $r$ | 0.5 | 1   | 1.5 | 2   | 2.5 | 3   | 3.5 | 4   |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1.0E+04  | 1.0E+04 | 1.199.2 | 1.110.3 | 979.5 | 990.9 | 1035.8 | 1038.9 | 1026.3 | 1088.8 |
| 1.0E+05  | 1.0E+05 | 1.949.7 | 1.948.8 | 1.999.3 | 2.018.3 | 2.124.2 | 2.277.8 | 2.351.9 | 2.552.3 |
| 1.0E+06  | 1.0E+06 | 2.190.4 | 2.201.3 | 2.238.3 | 2.568.2 | 3.094.1 | 3.641.6 | 4.776.3 | 4.118.7 |
| 1.0E+07  | 1.0E+07 | 2.709.6 | 2.860.4 | 2.790.4 | 2.896.4 | 3.467.4 | 4.944.6 | 4.347.4 | 5.456.9 |
| 1.0E+08  | 1.0E+08 | 2.962.6 | 3.450.3 | 3.166.8 | 3.440.9 | 4.950.3 | 4.944.3 | 5.400.7 | 5.948.3 |

Observing the results in Table 1, we see that the impact of $r$ on $\tau_k(r)$ in (31) is not significant when the condition number $\kappa = 10^4$. As the condition number increases, $r$ increases from 1.5 to 4, and the average number of iterations also increases. The average number of iterations is generally consistent when $r$ is taken as 0.5, 1 and 1.5. We take $r = 0.5$ in the later tests, but we can also see that $r = 1$ or 1.5 has advantages in some problems.

We test ERBB algorithm on some randomly generated quadratic problems. The objective function is given by

$$f(x) = \frac{1}{2}(x - x^*)^T A(x - x^*),$$

(40)

where $x^*$ was randomly generated with components in $[-10, 10]$, the matrix $A = \text{diag}(d_1, d_2, \ldots, d_n)$ is a diagonal matrix with nonzero elements $d_1 = 1,$
We further compare the performance of RBB, ERBB and other efficient gradient methods for solving the strictly convex quadratic problems with different spectral distributions. Table 2 lists four types of diagonal matrices with different spectral distributions, which derived from [17,31].

Table 2: Distributions of \( \{ d_i : i = 2, \ldots, n - 1 \} \)

| P | Spectrum | P | Spectrum |
|---|---|---|---|
| P1 | \( \{ d_2, \ldots, d_{n-1} \} \subset (1, \kappa) \) | P3 | \( \{ d_2, \ldots, d_{n/5} \} \subset (1, \zeta) \) |
| P2 | \( \{ d_{n/5+1}, \ldots, d_{n/5} \} \subset (\zeta, \kappa/2) \) \( \{ d_{4n/5+1}, \ldots, d_{n-1} \} \subset (\kappa/2, \kappa) \) | P4 | \( \{ d_2, \ldots, d_{4n/5} \} \subset (1, \zeta) \) \( \{ d_{4n/5+1}, \ldots, d_{n-1} \} \subset (\kappa/2, \kappa) \) |

We use the following stopping condition

\[
\| g_k \|_2 \leq \varepsilon \| g_0 \|_2,
\]

or the number of iterations exceeds MaxIt 20000. Initial stepsize is \( t_0 = \frac{g^T_0 g_0}{A g_0} \), we let \( \varepsilon = 10^{-9}, 10^{-12}, 10^{-15} \), and \( \kappa = 10^5, 10^6, 10^7, 10^8, 10^9, n = 100, 1000 \), respectively. In Table 2, we set \( \zeta = 999 \) for the test. For each value of \( \kappa \) and \( \varepsilon \), 10 different starting points with entries in \([-5, 5]\) were randomly generated.

To further illustrate the performance of RBB and ERBB algorithms for the strictly convex quadratic problems, they were compared with following BB-like methods:

1. BB1 [9]: the original BB method using \( \alpha_{BB1}^k \);
2. BB2 [9]: the original BB method using \( \alpha_{BB2}^k \);
3. ABB [46]: the adaptive BB method;
4. ABBmin [26]: a gradient method adaptively uses \( \alpha_{BB1}^k \) and \( \max \{ \alpha_j^{BB2} : j = \max \{1, k - m \}, \ldots, k \} \);
5. BBQ [32]: a BB method with two-dimensional quadratic termination property.

We use the same initial point, condition number and tolerance as before. As suggested in [20,32], \( \nu_k = 0.8 \) and \( m = 9 \) were used in ABBmin method, \( \nu_1 = 0.2, \gamma = 1.02 \) were employed in BBQ method. We set \( \eta = 0.7 \) in ABB method [29]. In ERBB algorithm [50], the parameters \( \vartheta \) and \( \varphi \) are taken as 6 and 7, respectively. And in the subsequent experiments, these two numbers are used as parameters in the ERBB algorithm. We present in Fig. 2 a log scaled view of the performance profiles [23] on the number of iterations for each tolerance \( \varepsilon \) obtained by the compared methods. For each method, the vertical axis \( \pi(\omega) \) of the figure shows the percentage of problems the method solves within the factor \( \omega \) of the minimum value of the metric.
Fig. 2: Performance profiles of RBB, ERBB, BB1, BB2, ABBmin, BBQ, ABB methods for ill-conditioned strictly convex quadratic problems with $n=100, 1000$, number of iterations.

As can be seen from the performance profiles, for the number of iterations, the ERBB method is significantly better than other compared methods under different tolerances.

Here, we consider the total variation metric $V_f = \sum_{j=0}^{n} |f(x_j) - f(x_{j+1})|$ of a function. We record the total variation indicators $V_{f1}$ and $V_{f2}$ of BB1 and RBB methods in Table 3, respectively. For the same tolerance, the total variation $V_f$ reflects the stability of the algorithm.

Table 3: The average total variation of the BB1 and RBB methods on problems in Table 2 with $n=100$

| Problem | P1 | P2 | P3 | P4 |
|---------|----|----|----|----|
| $\kappa$ | $\varepsilon$ | $V_{f1}$ | $V_{f2}$ | $V_{f1}$ | $V_{f2}$ | $V_{f1}$ | $V_{f2}$ | $V_{f1}$ | $V_{f2}$ |
| 10$^3$  | $10^{-9}$ | $4.0E+06$ | $4.5E+06$ | $4.3E+05$ | $4.3E+05$ | $7.8E+05$ | $1.2E+06$ | $4.5E+06$ | $1.2E+06$ |
| $10^{-12}$ | $4.0E+06$ | $4.5E+08$ | $4.4E+05$ | $5.4E+08$ | $8.5E+05$ | $1.1E+09$ | $5.0E+06$ | $9.6E+08$ |
| $10^{-15}$ | $4.5E+06$ | $3.6E+08$ | $3.8E+05$ | $5.4E+08$ | $7.5E+05$ | $1.3E+09$ | $4.7E+06$ | $2.2E+09$ |
| 10$^6$  | $10^{-9}$ | $5.2E+07$ | $2.6E+06$ | $2.9E+06$ | $7.6E+09$ | $3.7E+06$ | $5.8E+11$ | $5.1E+07$ | $1.5E+11$ |
| $10^{-12}$ | $5.1E+07$ | $7.6E+10$ | $3.2E+06$ | $1.3E+10$ | $4.5E+06$ | $6.1E+10$ | $5.2E+07$ | $7.4E+10$ |
| $10^{-15}$ | $5.0E+07$ | $2.9E+10$ | $3.1E+06$ | $5.3E+10$ | $1.4E+06$ | $1.0E+11$ | $5.0E+07$ | $3.7E+10$ |
| 10$^7$  | $10^{-9}$ | $5.2E+08$ | $2.7E+13$ | $2.6E+07$ | $1.4E+12$ | $2.7E+06$ | $1.9E+12$ | $5.9E+08$ | $2.6E+12$ |
| $10^{-12}$ | $4.8E+08$ | $6.5E+13$ | $2.6E+07$ | $1.3E+12$ | $6.7E+06$ | $2.8E+12$ | $4.8E+08$ | $3.0E+12$ |
| $10^{-15}$ | $4.9E+08$ | $5.3E+13$ | $3.1E+07$ | $1.3E+12$ | $7.1E+06$ | $1.5E+12$ | $4.3E+08$ | $5.4E+12$ |
| 10$^8$  | $10^{-9}$ | $4.8E+09$ | $1.6E+15$ | $2.3E+08$ | $2.9E+13$ | $1.3E+08$ | $8.0E+13$ | $4.8E+09$ | $9.4E+13$ |
| $10^{-12}$ | $4.3E+09$ | $3.8E+14$ | $2.1E+08$ | $4.0E+13$ | $1.2E+08$ | $9.0E+13$ | $4.8E+09$ | $6.6E+13$ |
| $10^{-15}$ | $4.4E+09$ | $2.9E+13$ | $2.3E+08$ | $2.1E+13$ | $1.1E+08$ | $9.0E+13$ | $5.0E+09$ | $1.3E+14$ |
| 10$^9$  | $10^{-9}$ | $5.2E+10$ | $6.8E+10$ | $2.9E+09$ | $6.4E+15$ | $7.5E+08$ | $5.4E+15$ | $4.1E+10$ | $8.6E+15$ |
| $10^{-12}$ | $5.8E+10$ | $7.9E+14$ | $2.3E+09$ | $1.0E+15$ | $8.9E+08$ | $1.5E+15$ | $4.3E+10$ | $2.4E+15$ |
| $10^{-15}$ | $5.4E+10$ | $9.1E+15$ | $2.8E+09$ | $2.3E+15$ | $6.8E+08$ | $3.6E+15$ | $3.7E+10$ | $4.1E+15$ |

From the results in Table 3, we can see that the stability of RBB is significantly better than that of BB1. It reflects that the RBB algorithm has strong robustness.
Furthermore, we again compare the above methods for the non-random strictly convex quadratic problem (32). The initial settings and termination conditions of this problem are the same as those in the previous test problems. Figure 4 illustrates the average numerical results of running these algorithms 10 times for dimension $n = 1000$. From Table 4, we can see that ERBB once again performs well among these compared methods.

Table 4: The average CPU time and number of iterations for the RBB, ERBB, BB1, BB2, ABBmin, BBQ and ABB methods on the non-random quadratic problems (32) with $n = 1000$

| Matrix | n | Nonzeros | Condition number |
|--------|---|-----------|-----------------|
| bundle1 | 10581 | 770,811 | 1.00E+03 |
| msc04 | 100 | 594 | 1.59E+00 |
| nasa2146 | 7,000 | 292,780 | 1.00E+03 |
| bodyc5 | 3,072 | 5,102 | 1.00E+03 |
| nos5 | 468 | 5,172 | 1.10E+04 |
| nos6 | 960 | 15,544 | 3.77E+04 |
| mhd4800b | 10,000 | 711,558 | – |
| msc00726 | 726 | 34,518 | 4.10E+05 |
| g6q | 685 | 3,249 | 4.23E+05 |
| lim0 | 147 | 2,449 | 2.80E+06 |
The results in Table 6 show that the performance of ERBB is comparable to that of BBQ, ABB, and ABBmin and significantly better than that of BB1 and BB2 methods.

### 6.2 General Unconstrained Optimization

In this section, we first test the performance of ERBB algorithm on a commonly used collection of unconstrained optimization test functions, and then conduct experiments on solving numerically spherical t-designs.

#### 6.2.1 Test on a Collection of Unconstrained Optimization Functions

For general objective functions, the performance of ERBB method was tested on a collection of unconstrained minimization problems from [5], which provides a standard starting point \( x_0 \) for each problem. We compare ERBB with the GBB [40], ABB [46], ABBmin [26, 21] and BBQ [32] methods. We delete the problem if either it can not be solved in 20000 iterations by any of the algorithms or the function evaluation exceeds one million and 57 problems are left. In the test, we uniformly set the dimension of these problems to \( n = 10000 \).

In the comparison experiment, we set \( t_0 = \|x_0\|_\infty/\|g_0\|_\infty \) if \( x_0^i > 0 \) for all \( i \geq 1 \) and otherwise \( t_0 = 1/\|g_0\|_\infty \), the range of stepsize and the parameters of nonmonotone line search as follows:

\[
\begin{align*}
t_{\min} &= 10^{-10}, & t_{\max} &= 10^{10}, & M &= 20, & \delta &= 0.5, & \gamma &= 10^{-4}.
\end{align*}
\]
In the ABB method, we set $\eta = 0.15$. Default parameter settings were used for the GBB, ABBmin and BBQ methods as before. The stopping condition $\|g_k\|_\infty \leq 10^{-6}(1 + |f_k|)$ was adopted for all the methods.

In this experiment, due to the existence of line search, we focus on CPU time consumption. To clearly compare the performance of these methods, the performance profiles on the CPU time metric plotted in Fig. 3. It can be seen from Fig. 3 that the performance of ERBB is better than that of the ABB, ABBmin and GBB methods, while the performance of BBQ is comparable to that of ERBB overall.

Fig. 3: Performance profiles of GBB, ABB, ABBmin, BBQ and ERBB methods for general unconstrained problems in [5], CPU time metric

6.2.2 Finding spherical $t$-designs

In this part, we consider a numerical computational problem of finding a set of points with “good” distribution on the unit sphere $S^2 := \{(x, y, z)^T \in \mathbb{R}^3 : x^2 + y^2 + z^2 = 1\}$.

A point set $X_N = \{x_1, \ldots, x_N\} \subset S^2$ is a spherical $t$-design if it satisfies

$$
\frac{1}{N} \sum_{j=1}^{N} p(x_j) = \frac{1}{4\pi} \int_{S^2} p(x) d\omega(x) \quad \forall \ p \in \mathbb{P}_t,
$$
where $d\omega(x)$ denotes area measure on the unit sphere, $\mathbb{P}_t := \mathbb{P}_t(S^2)$ is the space of spherical polynomials on $S^2$ with degree at most $t$. For more details on spherical designs, see [20,28]. In [41], the authors present a variational characterization of spherical $t$-design as follows

$$A_{N,t}(X_N) := \frac{4\pi}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{n=1}^{t} \frac{2n+1}{4\pi} P_n(\langle x_j, x_i \rangle),$$

(41)

where $P_n : [-1, 1] \to \mathbb{R}$ is the Legendre polynomial and $\langle x, y \rangle := x^T y$ is the inner product in $\mathbb{R}^3$. It is known that $X_N$ is a spherical $t$-design if and only if $A_{N,t}(X_N) = 0$ [41]. Therefore, the problem of finding a spherical $t$-design is expressed as solving a nonlinear optimization problem

$$\min_{X_N \subset S^2} A_{N,t}(X_N).$$

(42)

Given that the sphere has good geometric properties, problem (42) is actually an unconstrained optimization problem on a manifold. Therefore, for finding spherical $t$-designs, [3] numerically construct spherical $t$-designs by using BB method. Since the high-order Legendre polynomial has the property of highly oscillation and is locally unstable, we use ERBB method to solve spherical $t$-designs numerically. We perform comparison experiments of GBB, ABB, ABBmin, BBQ and ERBB methods. The termination condition of the algorithms is as follows

$$\|g_k\|_2 < \varepsilon_1 \text{ or } \|x_k - x_{k-1}\|_2 < \varepsilon_2,$$

where $\varepsilon_1 = 10^{-8}$, $\varepsilon_2 = 10^{-16}$. The maximum number of iterations and function evaluations are 10000 and one million, respectively. The parameter settings of these comparison methods are the same as those in the preceding experiments. The initial points in this experiment are consistent with those in [3].

Figure 4 presents the performance profiles of these methods on the CPU time metric. It can be seen from Fig. 4 that the performance of ERBB is significantly better than that of the other four compared algorithms, followed by BBQ, ABB, ABBmin algorithms and GBB performs the worst.

7 Conclusion

In this paper, we propose a regularized Barzilai-Borwein method for solving some ill-conditioned problems and analyze the convergence and stability of RBB algorithm. For general unconstrained optimization problems, we propose ERBB method. It improves the efficiency of original RBB method by a diagonal matrix that approximates the Hessian of objective function and an adaptive alternate stepsize strategy. We preliminarily discuss the selection of regularization parameters and obtain a scheme for adaptive generation of regularization parameters using adjacent old stepsizes. Some numerical experiments verify the performances of the RBB and ERBB methods with adaptive
Fig. 4: Performance profiles of the GBB, ABB, ABBmin, BBQ and ERBB methods for finding spherical t-designs, CPU time metric

regularization parameter. However, the selection of more appropriate regularization parameters and the relationship between the performance of RBB method and the spectral distribution of local Hessian still need to be further explored.

8 Declaration

8.1 Ethical Approval

Not Applicable.

8.2 Availability of supporting data

Data available on request from the authors.

8.3 Competing interests

The authors declare that there is no conflict of interest.
8.4 Funding

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8.5 Authors’ contribution

In this work, Congpei An was responsible for writing the abstract and introduction, and the rest was completed by Xin Xu.

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