



A gradient method exploiting the two dimensional quadratic termination property

Xinrui Li¹ · Yakui Huang²

Received: 10 January 2022 / Accepted: 13 September 2022 / Published online: 22 September 2022
© The Author(s), under exclusive licence to Springer-Verlag GmbH Germany, part of Springer Nature 2022

Abstract

The quadratic termination property is important to the efficiency of gradient methods. We consider equipping a family of gradient methods, where the stepsize is given by the ratio of two norms, with two dimensional quadratic termination. Such a desired property is achieved by cooperating with a new stepsize which is derived by maximizing the stepsize of the considered family in the next iteration. It is proved that each method in the family will asymptotically alternate in a two dimensional subspace spanned by the eigenvectors corresponding to the largest and smallest eigenvalues. Based on this asymptotic behavior, we show that the new stepsize converges to the reciprocal of the largest eigenvalue of the Hessian. Furthermore, by adaptively taking the long Barzilai–Borwein stepsize and reusing the new stepsize with retard, we propose an efficient gradient method for unconstrained quadratic optimization. We prove that the new method is R -linearly convergent with a rate of $1 - 1/\kappa$, where κ is the condition number of Hessian. Numerical experiments show the efficiency of our proposed method.

Keywords Gradient methods · Quadratic termination · Asymptotic convergence · R -linear convergence

1 Introduction

The gradient method is well-known for minimizing a smooth function $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}$, which updates the iterates by

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

✉ Yakui Huang
huangyakui2006@gmail.com

¹ School of Sciences, Hebei University of Technology, Tianjin 300401, China

² Institute of Mathematics, Hebei University of Technology, Tianjin 300401, China

where $g_k = \nabla f(x_k)$ and the stepsize $\alpha_k > 0$ depends on the method under consideration. The classic steepest descent (SD) [1] and minimal gradient (MG) [2] methods determine α_k by minimizing $f(x_k - \alpha g_k)$ and $\|g(x_k - \alpha g_k)\|_2$, respectively. Theoretically, the SD and MG methods will asymptotically perform zigzags between two directions, which often yield poor performance in many problems [3–7].

In 1988, Barzilai and Borwein [8] proposed the following two novel stepsizes from the view of quasi-Newton methods,

$$\alpha_k^{BB1} = \arg \min_{\alpha \in \mathbb{R}} \left\| \alpha^{-1} s_{k-1} - y_{k-1} \right\|_2 = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T y_{k-1}} \tag{2}$$

and

$$\alpha_k^{BB2} = \arg \min_{\alpha \in \mathbb{R}} \left\| s_{k-1} - \alpha y_{k-1} \right\|_2 = \frac{s_{k-1}^T y_{k-1}}{y_{k-1}^T y_{k-1}}, \tag{3}$$

where $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$. Apparently, $\alpha_k^{BB1} \geq \alpha_k^{BB2}$ follows from the Cauchy–Schwartz inequality if $s_{k-1}^T y_{k-1} > 0$. When $f(x)$ is a quadratic function

$$f(x) = \frac{1}{2} x^T A x - b^T x, \tag{4}$$

where $A \in \mathbb{R}^{n \times n}$ is a real symmetric positive definite matrix and $b \in \mathbb{R}^n$, α_k^{BB1} and α_k^{BB2} can be regarded as the SD and MG stepsizes with retard, respectively, i.e.

$$\alpha_k^{BB1} = \frac{g_{k-1}^T g_{k-1}}{g_{k-1}^T A g_{k-1}} = \alpha_{k-1}^{SD} \quad \text{and} \quad \alpha_k^{BB2} = \frac{g_{k-1}^T A g_{k-1}}{g_{k-1}^T A^2 g_{k-1}} = \alpha_{k-1}^{MG}.$$

Barzilai and Borwein [8] proved that the BB method is R -superlinearly convergent for the two dimensional strictly convex quadratic function. It has been shown that the BB method is globally convergent [9] with R -linear rate [10] for any dimensional cases. Although the BB method is nonmonotone, extensive numerical experimental results indicate that it performs much better than the SD method [11–13]. See [14, 15, 16, 17, 18, 19, 20 and 21] for more BB-like methods.

In [22], Yuan derived a new stepsize, which together with the SD method produces the minimizer of a two dimensional strictly convex quadratic function in three iterations. In what follows, if a method can give the exact minimizer of a two dimensional convex quadratic function within finite iterations, we call it has the property of two dimensional quadratic termination. Based on the following variant of the Yuan stepsize,

$$\alpha_k^{DY} = \frac{2}{\sqrt{\left(\frac{1}{\alpha_{k-1}^{SD}} - \frac{1}{\alpha_k^{SD}}\right)^2 + \frac{4\|g_k\|_2^2}{(\alpha_{k-1}^{SD})^2 \|g_{k-1}\|_2^2} + \frac{1}{\alpha_{k-1}^{SD}} + \frac{1}{\alpha_k^{SD}}}}, \tag{5}$$

Dai and Yuan [23] suggested the so-called Dai–Yuan (DY) gradient method with

$$\alpha_k = \begin{cases} \alpha_k^{SD}, & \text{if } \text{mod}(k, 4) < 2; \\ \alpha_k^{DY}, & \text{otherwise.} \end{cases} \tag{6}$$

Clearly, $\alpha_k^{DY} \leq \min\{\alpha_k^{SD}, \alpha_{k-1}^{SD}\}$, which implies that the DY method is monotone. Interestingly, the DY method can even outperform the nonmonotone BB method. Recently, Huang et al. [5] derived a new stepsize, say α_k^H , such that the gradient method

$$\alpha_k = \frac{g_k^T \psi(A) g_k}{g_k^T \psi(A) A g_k}$$

together with α_k^H achieves the two dimensional quadratic termination, where ψ is a real analytic function on $[\lambda_1, \lambda_n]$ and can be expressed by Laurent series

$$\psi(z) = \sum_{k=-\infty}^{\infty} d_k z^k, \quad d_k \in \mathbb{R}, \tag{7}$$

such that $0 < \sum_{k=-\infty}^{\infty} d_k z^k < +\infty$ for all $z \in [\lambda_1, \lambda_n]$. Here, λ_1 and λ_n are the smallest and largest eigenvalues of A , respectively. Furthermore, α_k^H reduces to α_k^{DY} when $\psi(A) = I$. The property of two dimensional quadratic termination has shown great potential in improving performances of gradient methods, see [24, 5, 25] for example.

To our knowledge, there is still lack of theoretical analysis for the two dimensional quadratic termination of the Dai–Yang method [26] whose stepsize is given by

$$\alpha_k^P = \frac{\|g_k\|_2}{\|A g_k\|_2}. \tag{8}$$

A remarkable property of the Dai–Yang method is that α_k^P converges to the optimal stepsize $\frac{2}{\lambda_1 + \lambda_n}$ (in the sense that it minimizes the modulus $\|I - \alpha A\|_2$, see [26, 27]). Moreover, the Dai–Yang method is able to find the eigenvectors corresponding to λ_1 and λ_n .

In this paper, for a uniform analysis, we consider equipping the family

$$\alpha_k = \frac{\|\psi(A) g_k\|_2}{\|\psi(A) A g_k\|_2} \tag{9}$$

with the two dimensional quadratic termination property, which will be achieved by cooperating with

$$\tilde{\alpha}_k = \arg \max_{\alpha_k \in \mathbb{R}} \alpha_{k+1} = \arg \max_{\alpha_k \in \mathbb{R}} \frac{\|\psi(A)(I - \alpha_k A) g_k\|_2}{\|\psi(A) A (I - \alpha_k A) g_k\|_2}. \tag{10}$$

The above strategy of maximizing the stepsize value in the next iteration has been employed in [28] for the SD method. However, the analysis in [28] can not be directly applied to the family (9). Clearly, α_k^P corresponds to the case $\psi(A) = I$ in (9). We prove that each method in the family (9) will asymptotically alternate in a two dimensional subspace associated with the two eigenvectors corresponding to λ_1 and λ_n . In addition, for any given ψ , the stepsize (9) tends to the above optimal stepsize as $k \rightarrow \infty$, and the eigenvectors corresponding to λ_1 and λ_n can be obtained. Then, we show that $\lim_{k \rightarrow \infty} \tilde{\alpha}_k = 1/\lambda_n$ for n dimensional strictly convex quadratics. By adaptively taking α_k^{BB1} and reusing $\tilde{\alpha}_{k-1}$ for some iterations, we propose a new method for quadratic minimization problems. It is proved that the proposed method is R -linearly convergent with the rate of $1 - 1/\kappa$, where $\kappa = \lambda_n/\lambda_1$ is the condition number of A . Our numerical comparisons with the BB1 [8], DY [23], SL (Alg.1 in [25]), ABBmin2 [28], SDC [29], and MGC [7] methods for solving unconstrained random and non-random quadratic optimization demonstrate that the proposed method is very efficient. Further, numerical experiments on quadratic problems whose Hessians are chosen from the SuiteSparse Matrix Collection [30] suggest that the proposed method is very competitive with the above methods.

The paper is organized as follows. In Sect. 2, we derive the new stepsize $\tilde{\alpha}_k$ and analyze its properties. The asymptotic behavior of the family (9) is also analyzed. Our new algorithm for quadratic minimization problems as well as its R -linear convergence are presented in Sect. 3. Section 4 presents some numerical comparisons of the proposed method and other successful gradient methods on solving quadratic problems. Finally, in Sect. 5 we give some concluding remarks.

2 A new stepsize and its properties

In this section, we derive the formula of $\tilde{\alpha}_k$ and analyze its properties.

To obtain $\tilde{\alpha}_k$, we consider

$$F(\alpha_k) := \alpha_{k+1}^2 = \frac{\|\psi(A)(I - \alpha_k A)g_k\|_2^2}{\|\psi(A)A(I - \alpha_k A)g_k\|_2^2}. \tag{11}$$

The maximum value of $F(\alpha_k)$ is achieved when $F'(\alpha_k) = 0$, which holds for any α_k satisfying

$$\phi_1 \alpha_k^2 - \phi_2 \alpha_k + \phi_3 = 0, \tag{12}$$

where $\phi_1 = c_1 c_4 - c_2 c_3$, $\phi_2 = c_0 c_4 - c_2^2$ and $\phi_3 = c_0 c_3 - c_1 c_2$ with

$$c_j = g_k^T A^j \psi^2(A) g_k, \quad j = 0, 1, 2, 3, 4. \tag{13}$$

The following lemma guarantees that (12) has two roots.

Lemma 1 Assume $g_k \neq 0$ and g_k is not parallel to Ag_k . Then, $\phi_1, \phi_2, \phi_3 > 0$ and $\phi_2^2 - 4\phi_1\phi_3 > 0$.

Proof It follows from the Cauchy-Schwartz inequality and (13) that

$$\begin{aligned} \left\| \psi(A)A^{\frac{j}{2}}g_k \right\|_2^2 \left\| \psi(A)A^{\frac{j+2}{2}}g_k \right\|_2^2 &> \left(\left(\psi(A)A^{\frac{j}{2}}g_k \right)^T \left(\psi(A)A^{\frac{j+2}{2}}g_k \right) \right)^2 \\ &= \left(g_k^T \psi^2(A)A^{j+1}g_k \right)^2 \end{aligned}$$

for $j \geq 0$. That is, $c_j/c_{j+1} > c_{j+1}/c_{j+2}$, which implies $\phi_1, \phi_2, \phi_3 > 0$.

By direct calculation, we obtain $c_1\phi_2 = c_0\phi_1 + c_2\phi_3$, which implies that

$$c_1^2\phi_2^2 = (c_0\phi_1 + c_2\phi_3)^2 \geq 4c_0c_2\phi_1\phi_3.$$

Combining with $c_0c_2 > c_1^2$, we have $\phi_2^2 - 4\phi_1\phi_3 > 0$. This completes the proof. \square

Using the square root law, we get the two roots of (12) as

$$\tilde{\alpha}_k = \frac{\phi_2 - \sqrt{\phi_2^2 - 4\phi_1\phi_3}}{2\phi_1} = \frac{2}{\frac{\phi_2}{\phi_3} + \sqrt{\left(\frac{\phi_2}{\phi_3}\right)^2 - 4\frac{\phi_1}{\phi_3}}} \tag{14}$$

and

$$\hat{\alpha}_k = \frac{\phi_2 + \sqrt{\phi_2^2 - 4\phi_1\phi_3}}{2\phi_1} = \frac{2}{\frac{\phi_2}{\phi_3} - \sqrt{\left(\frac{\phi_2}{\phi_3}\right)^2 - 4\frac{\phi_1}{\phi_3}}} \tag{15}$$

It is easy to see that $\tilde{\alpha}_k = \arg \max_{\alpha_k \in \mathbb{R}} \alpha_{k+1}$ and $\hat{\alpha}_k = \arg \min_{\alpha_k \in \mathbb{R}} \alpha_{k+1}$.

Next theorem presents the two dimensional quadratic termination of the gradient method using α_k in (9) and $\tilde{\alpha}_k$.

Theorem 1 (Two dimensional quadratic termination) Consider the gradient method (1) for minimizing the two dimensional quadratic function (4). If the stepsize α_k is given by (9) for all $k \neq k_0$ and $\alpha_{k_0} = \tilde{\alpha}_{k_0}$ at the k_0 -th iteration where $k_0 \geq 1$, it holds that $g_{k_0+i} = 0$ for some $1 \leq i \leq 3$.

Proof Without loss of generality, we assume that $A = \text{diag}\{1, \lambda\}$ with $\lambda > 0$. Let $g_k^{(1)}$ and $g_k^{(2)}$ be the first and second components of g_k , respectively. Notice that

$$c_j = g_k^T \psi^2(A)A^j g_k = \left(g_k^{(1)} \right)^2 \psi^2(1) + \lambda^j \left(g_k^{(2)} \right)^2 \psi^2(\lambda).$$

After direct calculation and simplification, we get

$$\begin{aligned} \phi_1 &= \left(g_k^{(1)}\right)^2 \left(g_k^{(2)}\right)^2 \psi^2(1) \psi^2(\lambda) (\lambda - 1)^2 (\lambda + 1) \lambda, \\ \phi_2 &= \left(g_k^{(1)}\right)^2 \left(g_k^{(2)}\right)^2 \psi^2(1) \psi^2(\lambda) (\lambda - 1)^2 (\lambda + 1)^2, \\ \phi_3 &= \left(g_k^{(1)}\right)^2 \left(g_k^{(2)}\right)^2 \psi^2(1) \psi^2(\lambda) (\lambda - 1)^2 (\lambda + 1). \end{aligned}$$

Therefore, we obtain

$$\frac{\phi_1}{\phi_3} = \lambda \quad \text{and} \quad \frac{\phi_2}{\phi_3} = \lambda + 1.$$

Thus, from (14) we know that $\tilde{\alpha}_k = 1/\lambda$ for all $k \geq 1$. The conclusion follows immediately from $\alpha_{k_0} = \tilde{\alpha}_{k_0}$ and $g_{k+1} = (I - \alpha_k A)g_k$. We complete the proof. \square

In what follows, we shall prove that $\tilde{\alpha}_k$ converges to $1/\lambda_n$ under each method in the family (9). To this aim, we have to analyze the asymptotic behavior of the family (9) first.

For convenience, we assume without loss of generality that the matrix A is diagonal with distinct eigenvalues, i.e.

$$A = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_n\}, \quad 0 < \lambda_1 < \lambda_2 < \dots < \lambda_n. \tag{16}$$

Let $\{\xi_1, \xi_2, \dots, \xi_n\}$ be the set of orthogonal eigenvectors associated with the eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$. Denoting by $\mu_k^{(i)}, i = 1, \dots, n$, the components of g_k along ξ_i , i.e.

$$g_k = \sum_{i=1}^n \mu_k^{(i)} \xi_i. \tag{17}$$

It follows from (1) and (17) that

$$g_{k+1} = (I - \alpha_k A)g_k = \prod_{j=0}^k (I - \alpha_j A)g_0 = \sum_{i=1}^n \mu_{k+1}^{(i)} \xi_i, \tag{18}$$

where

$$\mu_{k+1}^{(i)} = (1 - \alpha_k \lambda_i) \mu_k^{(i)} = \mu_0^{(i)} \prod_{j=0}^k (1 - \alpha_j \lambda_i). \tag{19}$$

The following lemma is useful in our analysis.

Lemma 2 [26] *Let p be a vector in \mathbb{R}^n such that (i) $p^{(1)} > 0$ and $p^{(n)} > 0$ (ii) $p^{(1)} + p^{(n)} = 1$. Further assume that $0 < \lambda_1 < \dots < \lambda_n$. Consider a transformation T such that*

$$(Tp)^{(i)} = \frac{(\lambda_i - \gamma(p))^2 p^{(i)}}{\sum_i (\lambda_i - \gamma(p))^2 p^{(i)}}, \quad \text{where} \quad \gamma(p) = \sqrt{\sum_i \lambda_i^2 p^{(i)}}.$$

Then

$$\lim_{k \rightarrow \infty} T^k p = \begin{cases} h_1, & \text{if } i = 1, \\ 0, & \text{if } i = 2, \dots, n - 1, \\ h_2, & \text{if } i = n, \end{cases}$$

where

$$h_1 = \frac{\lambda_1 + 3\lambda_n}{4(\lambda_1 + \lambda_n)} \quad \text{and} \quad h_2 = \frac{3\lambda_1 + \lambda_n}{4(\lambda_1 + \lambda_n)}. \tag{20}$$

Based on Lemma 2, we are able to show that each method in the family (9) will zigzag in a two dimensional subspace which generalizes the results in [26], where the case $\psi(A) = I$ (i.e. the Dai–Yang method) is considered.

Theorem 2 Assume that the starting point x_0 is such that

$$g_0^T \xi_1 \neq 0 \quad \text{and} \quad g_0^T \xi_n \neq 0.$$

Let $\{x_k\}$ be the sequence generated by applying a method in the family (9). Then

$$\lim_{k \rightarrow \infty} \frac{\psi(\lambda_i) \mu_{2k}^{(i)}}{\sqrt{\sum_{j=1}^n (\psi(\lambda_j) \mu_{2k}^{(j)})^2}} = \begin{cases} \text{sign}(\psi(\lambda_1) \mu_{2k}^{(1)}) \sqrt{h_1}, & \text{if } i = 1, \\ 0, & \text{if } i = 2, \dots, n - 1, \\ \text{sign}(\psi(\lambda_n) \mu_{2k}^{(n)}) \sqrt{h_2}, & \text{if } i = n, \end{cases} \tag{21}$$

and

$$\lim_{k \rightarrow \infty} \frac{\psi(\lambda_i) \mu_{2k+1}^{(i)}}{\sqrt{\sum_{j=1}^n (\psi(\lambda_j) \mu_{2k+1}^{(j)})^2}} = \begin{cases} \text{sign}(\psi(\lambda_1) \mu_{2k+1}^{(1)}) \sqrt{h_1}, & \text{if } i = 1, \\ 0, & \text{if } i = 2, \dots, n - 1, \\ -\text{sign}(\psi(\lambda_n) \mu_{2k+1}^{(n)}) \sqrt{h_2}, & \text{if } i = n, \end{cases} \tag{22}$$

where h_1 and h_2 are defined in (20). Further, the vectors

$$\frac{\psi(A)g_k}{\|\psi(A)g_k\|_2} + \frac{\psi(A)g_{k+1}}{\|\psi(A)g_{k+1}\|_2} \quad \text{and} \quad \frac{\psi(A)g_k}{\|\psi(A)g_k\|_2} - \frac{\psi(A)g_{k+1}}{\|\psi(A)g_{k+1}\|_2}$$

tend to be the eigenvectors corresponding to λ_1 and λ_n of A , respectively.

Proof By (17), we get

$$\psi(A)g_k = \sum_{i=1}^n \eta_k^{(i)} \xi_i, \tag{23}$$

where $\eta_k^{(i)} = \psi(\lambda_i)\mu_k^{(i)}$, which together with (19) yields

$$\eta_{k+1}^{(i)} = (1 - \alpha_k \lambda_i) \eta_k^{(i)}. \tag{24}$$

Defining the vector $p_k = (p_k^{(i)})$ with

$$p_k^{(i)} = \frac{(\eta_k^{(i)})^2}{\|\eta_k\|_2^2} \tag{25}$$

and

$$\gamma_k = \alpha_k^{-1} = \frac{\|\psi(A)Ag_k\|_2}{\|\psi(A)g_k\|_2} = \sqrt{\sum_i \lambda_i^2 p_k^{(i)}}. \tag{26}$$

We have from (24), (25) and (26) that

$$p_{k+1}^{(i)} = \frac{(\lambda_i - \gamma_k)^2 p_k^{(i)}}{\sum_i (\lambda_i - \gamma_k)^2 p_k^{(i)}}.$$

Clearly, according to the definition of p_k , we get that $p_k^{(i)} \geq 0$ for all i and

$$\sum_i p_k^{(i)} = 1, \quad \text{for all } k.$$

Let $p = p_1 \in \mathbb{R}^n$, based on the above analysis and Lemma 2, we know that $\lim_{k \rightarrow \infty} p_k = (h_1, 0, \dots, 0, h_2)^T$, where h_1 and h_2 are given in (20). It follows from (24) and $\lambda_n^{-1} < \alpha_k < \lambda_1^{-1}$ that

$$\text{sign}(\psi(\lambda_1)\mu_{k+1}^{(1)}) = \text{sign}(\psi(\lambda_1)\mu_k^{(1)}) \tag{27}$$

and

$$\text{sign}(\psi(\lambda_n)\mu_{k+1}^{(n)}) = -\text{sign}(\psi(\lambda_n)\mu_k^{(n)}). \tag{28}$$

Thus, by Lemma 2, (27) and (28), we know that (21) and (22) hold.

Furthermore, combining (23), (27) and (28), we find that

$$\lim_{k \rightarrow \infty} \frac{\psi(A)g_k}{\|\psi(A)g_k\|_2} + \frac{\psi(A)g_{k+1}}{\|\psi(A)g_{k+1}\|_2} = 2\text{sign}(\psi(\lambda_1)\mu_{2k}^{(1)})\sqrt{h_1}\xi_1$$

and

$$\lim_{k \rightarrow \infty} \frac{\psi(A)g_k}{\|\psi(A)g_k\|_2} - \frac{\psi(A)g_{k+1}}{\|\psi(A)g_{k+1}\|_2} = \pm 2\sqrt{h_2}\xi_n.$$

This completes our proof. □

From Theorem 2, we have the following asymptotic result of the stepsize (9).

Corollary 1 *Under the conditions of Theorem 2, for α_k in (9) it holds that*

$$\lim_{k \rightarrow \infty} \alpha_k = \frac{2}{\lambda_1 + \lambda_n}.$$

Next theorem shows that $\tilde{\alpha}_k$ converges to $1/\lambda_n$ under each method in the family (9).

Theorem 3 *Under the conditions of Theorem 2, let $\{g_k\}$ be the sequence generated by applying a method in the family (9) to minimize the n -dimensional quadratic function (4). Then $\lim_{k \rightarrow \infty} \tilde{\alpha}_k = 1/\lambda_n$.*

Proof From (18) and (13), we obtain

$$c_j = g_k^T A^j \psi^2(A)g_k = \sum_{i=1}^n \lambda_i^j \left(\psi(\lambda_i)\mu_k^{(i)} \right)^2. \tag{29}$$

When k is odd, by the definition of ϕ_1 , (22) and (29), we get

$$\begin{aligned} \lim_{k \rightarrow \infty} \frac{\phi_1}{c_0^2} &= \lim_{k \rightarrow \infty} \left(\frac{c_1 c_4}{c_0 c_0} - \frac{c_2 c_3}{c_0 c_0} \right) \\ &= \lim_{k \rightarrow \infty} \left[\sum_{i=1}^n \lambda_i \frac{\left(\psi(\lambda_i)\mu_k^{(i)} \right)^2}{\sum_{s=1}^n \left(\psi(\lambda_s)\mu_k^{(s)} \right)^2} \cdot \sum_{i=1}^n \lambda_i^4 \frac{\left(\psi(\lambda_i)\mu_k^{(i)} \right)^2}{\sum_{s=1}^n \left(\psi(\lambda_s)\mu_k^{(s)} \right)^2} \right] \\ &\quad - \lim_{k \rightarrow \infty} \left[\sum_{i=1}^n \lambda_i^2 \frac{\left(\psi(\lambda_i)\mu_k^{(i)} \right)^2}{\sum_{s=1}^n \left(\psi(\lambda_s)\mu_k^{(s)} \right)^2} \cdot \sum_{i=1}^n \lambda_i^3 \frac{\left(\psi(\lambda_i)\mu_k^{(i)} \right)^2}{\sum_{s=1}^n \left(\psi(\lambda_s)\mu_k^{(s)} \right)^2} \right] \tag{30} \\ &= (h_1 \lambda_1 + h_2 \lambda_n)(h_1 \lambda_1^4 + h_2 \lambda_n^4) - (h_1 \lambda_1^2 + h_2 \lambda_n^2)(h_1 \lambda_1^3 + h_2 \lambda_n^3) \\ &= h_1 h_2 \lambda_1 \lambda_n (\lambda_n - \lambda_1)^2 (\lambda_1 + \lambda_n). \end{aligned}$$

Similarly, we have

$$\lim_{k \rightarrow \infty} \frac{\phi_2}{c_0^2} = h_1 h_2 (\lambda_n - \lambda_1)^2 (\lambda_1 + \lambda_n)^2 \tag{31}$$

and

$$\lim_{k \rightarrow \infty} \frac{\phi_3}{c_0^2} = h_1 h_2 (\lambda_n - \lambda_1)^2 (\lambda_1 + \lambda_n). \tag{32}$$

Combining (30), (31) and (32), we obtain

$$\lim_{k \rightarrow \infty} \frac{\phi_1}{\phi_3} = \lambda_1 \lambda_n \quad \text{and} \quad \lim_{k \rightarrow \infty} \frac{\phi_2}{\phi_3} = \lambda_1 + \lambda_n. \tag{33}$$

It follows from (33) and (14) that $\lim_{k \rightarrow \infty} \tilde{\alpha}_k = 1/\lambda_n$. When k is even, we get the desired result in the same manner as above. This completes our proof. \square

From (33), we see that ϕ_1/ϕ_3 and ϕ_2/ϕ_3 are independent of $\psi(A)$. The following example shows that $\tilde{\alpha}_k$ converges to $1/\lambda_n$ under both the MG and Dai–Yang methods. In particular, we applied the MG and Dai–Yang methods to the quadratic function (4) with

$$A = \text{diag}\{a_1, a_2, \dots, a_n\} \quad \text{and} \quad b = 0, \tag{34}$$

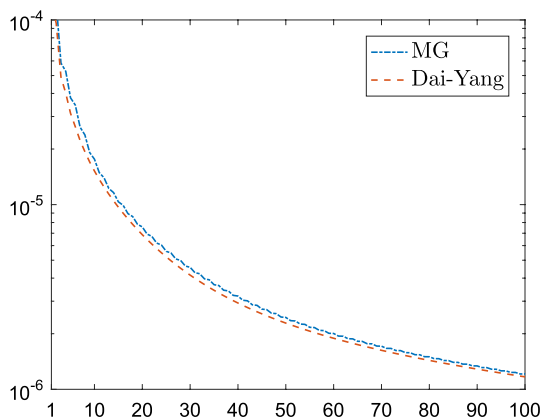
where $a_1 = 1$, $a_n = n$ and a_i was randomly generated in $(1, n)$, $i = 2, \dots, n - 1$. The starting point was set to the vector of all ones. From Fig. 1, we see that $\tilde{\alpha}_k$ approximates $1/\lambda_n$ with satisfactory accuracy after a small number of iterations under both the MG and Dai–Yang methods.

3 A new gradient method

In this section, we propose a new algorithm for unconstrained quadratic optimization and present its R -linear convergence result.

Extensive studies point out that adaptively choosing a short stepsize or α_k^{BB1} at each iteration is numerically better than the original BB method, see for example [31, 32, 33, 28, 34, 35]. Now we show that the new stepsize $\tilde{\alpha}_k$ is a short one.

Fig. 1 Problem (34) with $n = 1000$: convergence history of the sequence $\{|\tilde{\alpha}_k - 1/\lambda_n|\}$ for the first 100 iterations of the MG and Dai–Yang methods



Theorem 4 Under the conditions of Lemma 1, it holds that $\tilde{\alpha}_k < c_2/c_3$.

Proof According to (13) and (14), we get

$$\frac{c_2}{c_3} - \tilde{\alpha}_k = \frac{c_2\sqrt{\phi_2^2 - 4\phi_1\phi_3} + c_2\phi_2 - 2c_3\phi_3}{c_3\left(\phi_2 + \sqrt{\phi_2^2 - 4\phi_1\phi_3}\right)}. \tag{35}$$

If $c_2\phi_2 - 2c_3\phi_3 > 0$, we have $c_2/c_3 - \tilde{\alpha}_k > 0$; otherwise, it follows from (35) that

$$\begin{aligned} \frac{c_2}{c_3} - \tilde{\alpha}_k &= \frac{4(c_2c_3\phi_2\phi_3 - (c_3\phi_3)^2 - c_2^2\phi_1\phi_3)}{c_3\Delta\left(\phi_2 + \sqrt{\phi_2^2 - 4\phi_1\phi_3}\right)} \\ &= \frac{4\phi_3^2(c_2c_4 - c_3^2)}{c_3\Delta\left(\phi_2 + \sqrt{\phi_2^2 - 4\phi_1\phi_3}\right)}, \end{aligned}$$

where the last equality is due to $c_3\phi_2 = c_2\phi_1 + c_4\phi_3$ and $\Delta = c_2\sqrt{\phi_2^2 - 4\phi_1\phi_3} - (c_2\phi_2 - 2c_3\phi_3) > 0$. From $\phi_1, \phi_3 > 0$ and $c_2c_4 - c_3^2 > 0$, we know that $\tilde{\alpha}_k < c_2/c_3$ holds. This completes our proof. \square

Based on the above analysis, we can develop gradient method using $\tilde{\alpha}_k$ and α_k^{BB1} in an adaptive way. Notice that reusing the retard short stepsize for some iterations could reduce the computational cost and yield better performance, see [29, 36, 25, 13, 7]. So, we suggest to combine the adaptive and cyclic schemes with α_k^{BB1} and $\tilde{\alpha}_{k-1}$. In particular, our method reuses $\tilde{\alpha}_{k-1}$ for r iterations when $\alpha_k^{BB2}/\alpha_k^{BB1} < \tau$ for some $\tau \in (0, 1)$; otherwise, we set $\alpha_k = \alpha_k^{BB1}$. We use t as the index to keep track of the number of short stepsizes chosen during the iterative process. The stepsize for our algorithm is summarized as

$$\alpha_k = \begin{cases} \tilde{\alpha}_{k-1}, & \text{if } \text{mod}(t, r) = 0 \text{ and } \alpha_k^{BB2}/\alpha_k^{BB1} < \tau; \\ \alpha_k^{BB1}, & \text{if } \text{mod}(t, r) = 0 \text{ and } \alpha_k^{BB2}/\alpha_k^{BB1} \geq \tau; \\ \alpha_{k-1}, & \text{otherwise.} \end{cases} \tag{36}$$

We mention that the parameter τ can be chosen dynamically as [24]. However, in our test the dynamic scheme does not show much evidence over the above fixed one. Our method is formally presented in Algorithm 1.

Algorithm 1: A gradient method for unconstrained quadratic optimization

```

Choose  $x_0 \in \mathbb{R}^n$ ,  $\epsilon, \tau \in (0, 1)$ ,  $r \in \mathbb{N}$ . Set  $\alpha_0 = \alpha_0^{SD}$ ,  $k := 0$ ,  $t := 0$ .
while  $\|g_k\| > \epsilon$  do
   $x_{k+1} = x_k - \alpha_k g_k$ 
  if  $\text{mod}(t, r) = 0$  then
    if  $\alpha_{k+1}^{BB2} / \alpha_{k+1}^{BB1} < \tau$  then
      compute  $\tilde{\alpha}_k$ 
       $\alpha_{k+1} = \tilde{\alpha}_k$ 
       $t := t + 1$ 
    else
       $\alpha_{k+1} = \alpha_{k+1}^{BB1}$ 
    end
  else
     $\alpha_{k+1} = \alpha_k$ 
     $t := t + 1$ 
  end
   $k := k + 1$ 
end

```

To establish R -linear convergence of Algorithm 1, we first show the boundedness of $\tilde{\alpha}_k$.

Let us denote

$$f_1(\alpha) = \frac{g_k^T (I - \alpha A)^T \psi^2(A) (I - \alpha A) g_k}{g_k^T (I - \alpha A)^T \psi^2(A) A (I - \alpha A) g_k} \tag{37}$$

and

$$f_2(\alpha) = \frac{g_k^T (I - \alpha A)^T \psi^2(A) A (I - \alpha A) g_k}{g_k^T (I - \alpha A)^T \psi^2(A) A^2 (I - \alpha A) g_k}. \tag{38}$$

Using the same arguments as (12) and Lemma 1, we know that both $f_1'(\alpha) = 0$ and $f_2'(\alpha) = 0$ have two roots. In addition, the roots of $f_1'(\alpha) = 0$, say $\tilde{\beta}_k$ and $\hat{\beta}_k$ with $\tilde{\beta}_k \leq \hat{\beta}_k$, are the solutions of

$$\phi_4 \beta^2 - \phi_3 \beta + \phi_5 = 0, \tag{39}$$

and the roots of $f_2'(\alpha) = 0$, say $\tilde{\gamma}_k$ and $\hat{\gamma}_k$ with $\tilde{\gamma}_k \leq \hat{\gamma}_k$, satisfy

$$\phi_6 \gamma^2 - \phi_1 \gamma + \phi_4 = 0, \tag{40}$$

where ϕ_1, ϕ_3 are defined in the former section, and $\phi_4 = c_1 c_3 - c_2^2$, $\phi_5 = c_0 c_2 - c_1^2$ and $\phi_6 = c_2 c_4 - c_3^2$. Recall that $F(\alpha) = f_1(\alpha) f_2(\alpha)$. Since $f_1(\alpha) > 0$ and $f_2(\alpha) > 0$, any root of $F'(\alpha) = f_1'(\alpha) f_2(\alpha) + f_1(\alpha) f_2'(\alpha) = 0$ yields

$$f_1'(\alpha) = f_2'(\alpha) = 0 \quad \text{or} \quad f_1'(\alpha) f_2'(\alpha) < 0.$$

If the root is such that $f'_1(\alpha) \leq 0$ and $f'_2(\alpha) \geq 0$, we must have

$$\alpha \in [\tilde{\beta}_k, \hat{\beta}_k] \quad \text{and} \quad \alpha \in (-\infty, \tilde{\gamma}_k] \cup [\hat{\gamma}_k, +\infty). \tag{41}$$

Similarly, for the case $f'_1(\alpha) \geq 0$ and $f'_2(\alpha) \leq 0$, we get

$$\alpha \in [\tilde{\gamma}_k, \hat{\gamma}_k] \quad \text{and} \quad \alpha \in (-\infty, \tilde{\beta}_k] \cup [\hat{\beta}_k, +\infty). \tag{42}$$

Now we are ready to prove that $\tilde{\alpha}_k$ is bounded between $1/\lambda_n$ and $1/\lambda_1$.

Theorem 5 *Under the conditions of Lemma 1, it holds that $1/\lambda_n \leq \tilde{\alpha}_k \leq 1/\lambda_1$.*

Proof Since $F'(\tilde{\alpha}_k) = 0$, when $f'_1(\tilde{\alpha}_k) \leq 0$, it follows from (41) that

$$\tilde{\beta}_k \leq \tilde{\alpha}_k \leq \min\{\tilde{\gamma}_k, \hat{\beta}_k\} \quad \text{or} \quad \max\{\hat{\gamma}_k, \tilde{\beta}_k\} \leq \tilde{\alpha}_k \leq \hat{\beta}_k.$$

For the case $f'_1(\tilde{\alpha}_k) \geq 0$, by (42), we get

$$\tilde{\gamma}_k \leq \tilde{\alpha}_k \leq \min\{\tilde{\beta}_k, \hat{\gamma}_k\} \quad \text{or} \quad \max\{\hat{\beta}_k, \tilde{\gamma}_k\} \leq \tilde{\alpha}_k \leq \hat{\gamma}_k.$$

Thus, we only need to prove that $1/\lambda_n \leq \hat{\beta}_k, \tilde{\beta}_k, \hat{\gamma}_k, \tilde{\gamma}_k \leq 1/\lambda_1$.

To proceed, we first show that

$$\hat{\beta}_k = f_1(\tilde{\beta}_k). \tag{43}$$

Since $f'_1(\tilde{\beta}_k) = 0$, we have

$$(c_1 - 2c_2\tilde{\beta}_k + c_3\tilde{\beta}_k^2)(-c_1 + c_2\tilde{\beta}_k) - (c_0 - 2c_1\tilde{\beta}_k + c_2\tilde{\beta}_k^2)(-c_2 + c_3\tilde{\beta}_k) = 0,$$

which implies that

$$\begin{aligned} f_1(\tilde{\beta}_k) &= \frac{c_0 - 2c_1\tilde{\beta}_k + c_2\tilde{\beta}_k^2}{c_1 - 2c_2\tilde{\beta}_k + c_3\tilde{\beta}_k^2} = \frac{c_2\tilde{\beta}_k - c_1}{c_3\tilde{\beta}_k - c_2} \\ &= \hat{\beta}_k \frac{c_2\tilde{\beta}_k - c_1}{c_3\hat{\beta}_k\tilde{\beta}_k - c_2\hat{\beta}_k} = \hat{\beta}_k \frac{c_2\tilde{\beta}_k - c_1}{c_3 \frac{\phi_5}{\phi_4} - c_2\hat{\beta}_k}, \end{aligned}$$

where the last equality comes from the fact that $\tilde{\beta}_k\hat{\beta}_k = \phi_5/\phi_4$.

In order to prove (43), we are suffice to show that

$$c_2\tilde{\beta}_k - c_1 = c_3 \frac{\phi_5}{\phi_4} - c_2\hat{\beta}_k,$$

that is,

$$c_2\phi_4(\tilde{\beta}_k + \hat{\beta}_k) = c_1\phi_4 + c_3\phi_5,$$

which holds due to $\tilde{\beta}_k + \hat{\beta}_k = \phi_3/\phi_4$ and the definitions of $c_1, c_2, c_3, \phi_3, \phi_4, \phi_5$.

Thus, (43) is true. It follows from the definition of f_1 and the Rayleigh's quotient property that $1/\lambda_n \leq \hat{\beta}_k = f_1(\tilde{\beta}_k) \leq 1/\lambda_1$.

Using the same arguments as above, we get $1/\lambda_n \leq \tilde{\beta}_k, \tilde{\gamma}_k, \hat{\gamma}_k \leq 1/\lambda_1$. This completes the proof. \square

In [37], the authors prove that any gradient method with stepsizes satisfying the following Property B has R -linear convergence rate $1 - \lambda_1/M_1$ which implies a $1 - 1/\kappa$ rate when $M_1 \leq \lambda_n$. Similar results for gradient methods satisfying the Property A in [38] can be found in [39]. However, a stepsize satisfies Property B may not meet the conditions of Property A.

Property B: We say that the stepsize α_k has Property B if there exist an integer m and positive constant $M_1 \geq \lambda_1$ such that

- (i) $\lambda_1 \leq \alpha_k^{-1} \leq M_1$;
- (ii) for some real analytic function ψ defined as (7) and $v(k) \in \{k, k - 1, \dots, \max\{k - m + 1, 0\}\}$,

$$\alpha_k \leq \frac{g_{v(k)}^T \psi^2(A) g_{v(k)}}{g_{v(k)}^T A \psi^2(A) g_{v(k)}}. \tag{44}$$

Clearly, α_k^{BB1} satisfies Property B with $M_1 = \lambda_n, m = 2$ and $\psi^2(A) = I$, and the new stepsize $\tilde{\alpha}_k$ satisfies Property B with $M_1 = \lambda_n$. So, we are able to show R -linear convergence of Algorithm 1 with $1 - 1/\kappa$ rate as Theorem 2 in [37]. For completeness, we include the proof here.

Theorem 6 *Suppose that the sequence $\{g_k\}$ is generated by Algorithm 1. Then either $g_k = 0$ for some finite k or the sequence $\{\|g_k\|_2\}$ converges to zero R -linearly in the sense that*

$$|g_k^{(i)}| \leq C_i \theta^k, \quad i = 1, 2, \dots, n, \tag{45}$$

where $\theta = 1 - 1/\kappa$ and

$$\left\{ \begin{array}{l} C_1 = |g_0^{(1)}|; \\ C_i = \max \left\{ |g_0^{(i)}|, \frac{|g_1^{(i)}|}{\theta}, \dots, \frac{|g_{r-1}^{(i)}|}{\theta^{r-1}}, \frac{\max\{\sigma_i, \sigma_i^r\}}{\theta^r \psi(\lambda_i)} \sqrt{\sum_{j=1}^{i-1} \psi^2(\lambda_j) C_j^2} \right\}, \\ i = 2, 3, \dots, n, \end{array} \right.$$

with $\sigma_i = \max \left\{ \frac{\lambda_i}{\lambda_1} - 1, 1 - \frac{\lambda_i}{\lambda_n} \right\}$.

Proof It follows from $g_{k+1}^{(i)} = (1 - \alpha_k \lambda_i) g_k^{(i)}$ and (i) of Property B that

$$|g_{k+1}^{(i)}| \leq \sigma_i |g_k^{(i)}|, \quad i = 1, 2, \dots, n. \tag{46}$$

Clearly, (45) holds for $i = 1$.

In what follows, we prove (45) by induction on i . Assume that (45) holds for all $1 \leq i \leq L - 1$ with $L \in \{2, \dots, n\}$. When $i = L$, it follows from the definition of C_L that (45) holds for $k = 0, 1, \dots, r - 1$. Assume by contradiction that (45) does not hold for $k \geq r$ when $i = L$. Let $\hat{k} \geq r$ be the minimal index such that $|g_{\hat{k}}^{(L)}| > C_L \theta^{\hat{k}}$. Then, if $\alpha_{\hat{k}-1} \lambda_L \leq 1$, we get

$$|g_{\hat{k}}^{(L)}| = (1 - \alpha_{\hat{k}-1} \lambda_L) |g_{\hat{k}-1}^{(L)}| \leq \theta |g_{\hat{k}-1}^{(L)}| \leq C_L \theta^{\hat{k}},$$

which contradicts our assumption. Thus we must have $\alpha_{\hat{k}-1} \lambda_L > 1$, which combines with (46) and $\theta < 1$ gives that

$$\begin{aligned} \psi(\lambda_L) |g_{\hat{k}-j}^{(L)}| &\geq \frac{\psi(\lambda_L) |g_{\hat{k}}^{(L)}|}{\sigma_L^j} > \frac{\psi(\lambda_L) C_L \theta^{\hat{k}}}{\sigma_L^j} \geq \frac{\psi(\lambda_L) C_L \theta^{\hat{k}}}{\max\{\sigma_L, \sigma_L^r\}} \\ &\geq \theta^{\hat{k}-r} \sqrt{\sum_{i=1}^{L-1} \psi^2(\lambda_i) C_i^2} \geq \theta^{\hat{k}-r} \sqrt{\sum_{i=1}^{L-1} (\psi(\lambda_i) g_{\hat{k}-j}^{(i)})^2 \theta^{2(j-\hat{k})}} \\ &= \theta^{j-r} \sqrt{G(\hat{k}-j, L-1)} \geq \sqrt{G(\hat{k}-j, L-1)}, \quad j \in [1, r], \end{aligned}$$

where $G(k, l) = \sum_{i=1}^l (\psi(\lambda_i) g_k^{(i)})^2$. This together with Theorem 4 yields that

$$\begin{aligned} |1 - \tilde{\alpha}_{\hat{k}-1} \lambda_L| &= \tilde{\alpha}_{\hat{k}-1} \lambda_L - 1 \leq \frac{(\psi(A)g_{\hat{k}-1})^T A^2 (\psi(A)g_{\hat{k}-1})}{(\psi(A)g_{\hat{k}-1})^T A^3 (\psi(A)g_{\hat{k}-1})} \lambda_L - 1 \\ &= \frac{\sum_{i=1}^n (\lambda_L - \lambda_i) \lambda_i^2 (\psi(\lambda_i) g_{\hat{k}-1}^{(i)})^2}{\sum_{i=1}^n \lambda_i^3 (\psi(\lambda_i) g_{\hat{k}-1}^{(i)})^2} \\ &\leq \frac{(\lambda_L - \lambda_1) \lambda_1^2 G(\hat{k}-1, L-1)}{\lambda_1^3 G(\hat{k}-1, L-1) + \lambda_L^3 (\psi(\lambda_L) g_{\hat{k}-1}^{(L)})^2} \\ &\leq \frac{\lambda_L - \lambda_1}{\lambda_L + \lambda_1} < \theta. \end{aligned}$$

Using similar arguments, we can show $|1 - \alpha_{\hat{k}}^{BB1} \lambda_L| \leq \theta$. Thus, $|g_{\hat{k}}^{(L)}| \leq \theta |g_{\hat{k}-1}^{(L)}| \leq C_L \theta^{\hat{k}}$ which contradicts our assumption. Hence (45) holds for all i . We complete the proof. □

4 Numerical experiments

In this section, we provide numerical experiments of Algorithm 1 on solving quadratic problems. All our codes are written in MATLAB R2016b and carried out on a PC with an AMD Ryzen 5 PRO 2500U, 2.00 GHz processor and 8 GB of RAM running Windows 10 system.

For Algorithm 1, we use $\tilde{\alpha}_k$ with $\psi(A) = I$. Then, if we compute the vector $z = Ag_k$ at each iteration, and keep into memory $w = Ag_{k-1}$, $\tilde{\alpha}_{k-1}$ can be expressed as

$$c_0 = g_{k-1}^T g_{k-1}, \quad c_1 = g_{k-1}^T w, \quad c_2 = w^T w,$$

$$c_3 = \frac{g_k^T z - c_1 + 2\alpha_{k-1}c_2}{\alpha_{k-1}^2}, \quad c_4 = \frac{z^T z - c_2 + 2\alpha_k c_3}{\alpha_k^2}.$$

Hence only one matrix-vector product is required in per iteration for Algorithm 1.

Firstly, we compare Algorithm 1 with the BB1 [8], DY [13], ABBmin2 [28], SDC [29] and MGC [7] methods and the Alg.1 method in [25] (we note this method as SL) on solving the following quadratic problem [22]:

$$f(x) = (x - x^*)^T V(x - x^*), \tag{47}$$

where $V = \text{diag}\{v_1, \dots, v_n\}$ is a diagonal matrix and x^* is randomly generated with components in $[-10, 10]$. Five different distributions of the diagonal elements $v_j, j = 1, 2, \dots, n$, are generated, see Table 1.

The parameter m in SL uses the value $m = 5$ for the second problem set and $m = 6$ for other sets to get good performance. For ABBmin2, τ is set to 0.9 as suggested in [28]. For SDC and MGC, the parameter pairs (h, s) and (d_1, d_2) are all set to (8, 6), which are more efficient than other choices for this test. The parameters in Algorithm 1 are set to $\tau = 0.3$ and $r = 5$.

For all comparison methods, the stopping condition is $\|g_k\|_2 \leq \epsilon \|g_0\|_2$, where $\epsilon > 0$ is a given tolerance. The problem dimension is set to $n = 1000$. For each problem set, three different tolerance parameters $\epsilon = 10^{-6}, 10^{-9}, 10^{-12}$ and condition

Table 1 Distributions of v_j

Problem	Spectrum
1	$v_1 = 1, v_n = \kappa, \{v_2, \dots, v_{n-1}\} \subset (1, \kappa)$
2	$v_1 = 1, v_n = \kappa, \{v_2, \dots, v_{n/5}\} \subset (1, 100),$ $\{v_{n/5+1}, \dots, v_{n-1}\} \subset (\frac{\kappa}{2}, \kappa)$
3	$v_1 = 1, v_n = \kappa, \{v_2, \dots, v_{n/5}\} \subset (1, 100),$ $\{v_{n/5+1}, \dots, v_{4n/5}\} \subset (100, \frac{\kappa}{2}), \{v_{4n/5+1}, \dots, v_{n-1}\} \subset (\frac{\kappa}{2}, \kappa)$
4	$v_j = \kappa^{\frac{n-j}{n-1}}, \quad j = 1, \dots, n$
5	$v_j = \frac{\kappa}{2} \left(\cos \frac{n-j}{n-1} \pi + 1 \right), \quad j = 1, \dots, n$

Table 2 The average number of iterations required by Algorithm 1, the BB1, DY, SL, SDC, MGC and ABBmin2 methods on quadratic problem (47) with spectral distributions in Table 1

κ	ϵ	BB1	DY	SL	MGC	SDC	ABBmin2	Algorithm 1
<i>Problem set 1</i>								
10^4	10^{-6}	323.9	308.1	249.3	269.4	262.2	219.8	234.9
	10^{-9}	894.8	848.7	660.3	733.5	754.1	366.1	445.8
	10^{-12}	1359.1	1328.6	1029.3	1142.7	1176.0	528.6	649.2
10^5	10^{-6}	231.5	238.2	199.7	204.1	200.3	203.7	199.3
	10^{-9}	2265.1	2415.5	1586.9	1733.5	1806.7	525.6	600.3
	10^{-12}	4073.0	4335.5	2786.5	3130.5	3268.0	687.5	814.6
10^6	10^{-6}	221.0	222.1	185.3	196.6	184.3	173.8	182.9
	10^{-9}	5221.4	6446.6	3166.5	3891.2	3800.8	798.0	869.8
	10^{-12}	11834.4	15815.0	7378.4	8560.6	8276.9	1025.8	1151.6
<i>Problem set 2</i>								
10^4	10^{-6}	286.2	362.4	199.9	264.3	260.9	264.7	170.0
	10^{-9}	653.1	849.7	430.5	555.9	556.0	529.0	350.2
	10^{-12}	978.1	1301.3	651.2	840.2	810.0	786.7	523.9
10^5	10^{-6}	432.5	494.0	182.7	244.6	261.7	453.5	141.1
	10^{-9}	1444.2	1985.0	616.1	944.2	900.9	1141.2	402.9
	10^{-12}	2327.8	3534.1	1003.9	1427.1	1401.9	1809.0	635.7
10^6	10^{-6}	514.2	459.1	104.8	130.5	126.5	465.4	76.0
	10^{-9}	3256.7	3427.3	733.6	925.7	946.0	2556.5	410.9
	10^{-12}	5820.9	6938.1	1327.8	1790.8	1801.3	4322.4	742.3
<i>Problem set 3</i>								
10^4	10^{-6}	461.2	452.9	375.9	404.3	396.5	401.3	391.6
	10^{-9}	1021.5	1029.5	821.8	926.3	904.4	786.1	790.8
	10^{-12}	1550.0	1550.7	1237.5	1371.1	1370.5	1142.1	1165.4
10^5	10^{-6}	809.7	804.1	657.4	750.6	710.9	938.3	677.2
	10^{-9}	3089.1	3058.8	2285.1	2700.0	2555.1	2145.4	2052.6
	10^{-12}	5128.4	5104.9	3661.4	4092.1	4014.5	3300.3	3209.4
10^6	10^{-6}	1155.6	1119.2	856.7	1025.7	982.8	1266.0	694.5
	10^{-9}	8562.1	9690.6	6101.3	6876.4	6722.9	5968.5	4084.4
	10^{-12}	16239.6	19489.3	10609.8	12340.0	12342.7	9598.3	6956.4
<i>Problem set4</i>								
10^4	10^{-6}	628.7	602.1	497.5	541.3	531.1	514.3	509.9
	10^{-9}	1164.8	1159.7	946.6	1055.1	1021.8	913.9	910.3
	10^{-12}	1688.5	1670.4	1355.5	1507.8	1479.2	1296.5	1291.3
10^5	10^{-6}	1480.7	1442.2	1118.1	1304.5	1297.6	1330.6	1177.2
	10^{-9}	3440.9	3702.2	2705.9	3056.5	3038.8	2664.7	2469.3
	10^{-12}	5437.8	5795.1	4240.0	4665.7	4582.6	3891.6	3718.5
10^6	10^{-6}	2533.3	2667.0	1941.2	2422.4	2202.7	3119.5	1996.0
	10^{-9}	10849.6	12898.5	7542.4	9075.5	8508.5	7713.0	6570.9
	10^{-12}	18028.8	23430.2	12681.4	14396.4	13549.1	11838.3	10539.5

Table 2 (continued)

κ	ϵ	BB1	DY	SL	MGC	SDC	ABBmin2	Algorithm 1
<i>Problem set 5</i>								
10^4	10^{-6}	527.0	535.3	454.3	487.0	487.7	599.6	484.5
	10^{-9}	4455.5	5480.7	4115.5	4098.2	3805.4	2879.0	2993.8
	10^{-12}	9098.2	10185.5	7358.3	7815.6	7473.1	4312.4	4806.7
10^5	10^{-6}	552.7	573.5	467.7	525.8	497.4	635.6	489.5
	10^{-9}	4633.8	5142.8	3812.0	4047.6	3888.3	2837.5	2879.0
	10^{-12}	9007.1	10727.7	7141.0	7150.1	6967.7	4209.8	4767.2
10^6	10^{-6}	527.5	558.6	476.9	503.0	477.0	669.9	489.9
	10^{-9}	4859.5	5423.8	4121.7	4127.7	4363.2	2846.0	3060.0
	10^{-12}	9410.7	10661.0	7703.8	7299.8	7528.9	4379.8	5083.6

Bold values indicated by denote the best one among the compared methods

numbers $\kappa = 10^4, 10^5, 10^6$ are tested. For each value of κ and ϵ , 10 starting points are randomly generated in $[-10, 10]$ and the average results are presented in Table 2.

We see that Algorithm 1 clearly outperforms the BB1, DY, SDC and MGC methods. As compared with the SL method, Algorithm 1 is usually faster than it when a high accuracy is required. Moreover, Algorithm 1 often performs better than ABBmin2 for the second to fourth problem sets and is very competitive with ABBmin2 for the first and last problem sets.

Next, we compare the above methods on problem (4), where $b = Ax^*$ and x^* is a random vector as before. We test 14 sparse matrices from the SuiteSparse Matrix Collection [30] listed in Table 3. The iteration stops when $\|g_k\|_2 \leq 10^{-6}\|g_0\|_2$. In

Table 3 Test problems from Suitesparse Matrix Collection

Matrices	Size	Nonzeros	Condition number
bcsstk14	1806	63454	1.192324×10^{10}
bcsstk15	3948	117816	6.538185×10^9
bcsstk17	10974	428650	1.296064×10^{10}
bcsstk18	11948	149090	3.459995×10^{11}
msc01440	1440	44998	3.305875×10^6
msc04515	4515	97707	2.272772×10^6
ex15	6867	98671	8.612330×10^{12}
cbuckle	13681	676515	3.299134×10^7
gyro_k	17361	1021159	1.095832×10^9
s3dkq4m2	90449	4427725	1.896133×10^{11}
s3dkt3m2	90449	3686223	3.625322×10^{11}
s3rmq4m1	5489	262943	1.765559×10^{10}
s3rmt3m1	5489	217669	2.481977×10^{10}
s3rmt3m3	5357	207123	2.400640×10^{10}

Table 4 The average number of iterations required by Algorithm 1, the BB1, DY, SL, SDC, MGC and ABBmin2 methods on problem (4) with A given by Table 3

Matrices	BB1	DY	SL	MGC	SDC	ABBmin2	Algorithm 1
bcsstk14	2425.8	1948.7	1791.0	1705.9	1820.6	1667.4	1677.3
bcsstk15	2510.4	2219.6	1966.0	1778.3	2000.3	1788.1	1774.2
bcsstk17	4411.5	4335.5	3721.6	3428.0	3589.0	3035.4	3005.4
bcsstk18	4118.8	4194.9	3498.3	3655.1	4055.5	3334.6	3206.7
msc01440	1423.8	1623.9	1329.4	1233.0	1241.5	1151.9	1139.0
msc04515	1008.8	986.2	903.7	810.7	851.6	821.4	829.7
ex15	913.0	1002.5	802.6	806.7	778.9	716.9	775.4
cbuckle	2335.5	2092.8	2015.9	1884.0	1984.6	1665.4	1730.0
gyro_k	1672.8	1564.6	1461.1	1390.7	1366.9	1321	1329.2
s3dkq4m2	1611.8	1800.6	1600.3	1362.8	1493.4	1205.1	1178
s3dkt3m2	2048.6	2081.8	1802.5	1455.3	1644.5	1158.6	1236.5
s3rmq4m1	1153.7	1191.6	967.1	880.6	911.9	835.7	811.5
s3rmt3m1	1038.7	1099.9	929.4	871.6	906.4	879.8	904.1
s3rmt3m3	1606.7	1612.2	1457.9	1276.6	1286.6	1229.6	1206.6

Bold values indicated by denote the best one among the compared methods

Table 5 The CPU time required by Algorithm 1, the BB1, DY, SL, SDC, MGC and ABBmin2 methods on problem (4) with A given by Table 3

Matrices	BB1	DY	SL	MGC	SDC	ABBmin2	Algorithm 1
bcsstk14	0.40	0.17	0.16	0.31	0.16	0.30	0.15
bcsstk15	0.57	0.28	0.25	0.41	0.24	0.43	0.22
bcsstk17	6.44	3.51	2.99	5.04	2.81	4.49	2.41
bcsstk18	3.27	2.04	1.69	3.02	1.79	2.80	1.54
msc01440	0.13	0.09	0.07	0.12	0.06	0.11	0.06
msc04515	0.21	0.12	0.11	0.19	0.10	0.18	0.10
ex15	0.20	0.13	0.10	0.19	0.10	0.17	0.10
cbuckle	6.12	2.98	2.87	5.00	2.67	4.32	2.29
gyro_k	5.26	2.65	2.49	4.44	2.27	4.23	2.27
s3dkq4m2	26.91	16.35	14.33	23.59	12.91	20.97	10.60
s3dkt3m2	25.26	13.87	12.39	19.27	10.85	15.20	8.62
s3rmq4m1	0.60	0.32	0.26	0.51	0.25	0.51	0.22
s3rmt3m1	0.48	0.27	0.28	0.43	0.22	0.42	0.22
s3rmt3m3	0.79	0.44	0.39	0.67	0.33	0.62	0.32

Bold values indicated by denote the best one among the compared methods

our test, we choose the parameters so that each method achieves the best performance. Specifically, we set $m = 4$ for SL, $(h, s) = (3, 4)$ for SDC, $(d_1, d_2) = (4, 4)$ for MGC, $\tau = 0.3$ for ABBmin2 and $\tau = 0.1$ and $r = 5$ for Algorithm 1 .

For each matrix, ten initial points between -10 and 10 are randomly generated. The average number of iterations of compared methods are listed in Table 4. We see that for most matrices Algorithm 1 has better performance than BB1, DY, SL, MGC, SDC and is competitive with ABBmin2 in the sense of number of iterations. Table 5 lists the average CPU time in seconds for those methods. We observe that Algorithm 1 takes less CPU time than BB1, DY, MGC, ABBmin2, and is as fast as SL and SDC. One important reason for this phenomenon is that our method reuses the stepsize $\tilde{\alpha}_{k-1}$ for r iterations which can reduce computational cost.

5 Conclusions and discussions

For a uniform analysis, we considered a family of gradient methods whose stepsize is provided by α_k in (9), which includes the Dai–Yang method (5) as a special case. It is proved the family zigzags between two directions in a subspace spanned by the two eigenvectors corresponding to the smallest and largest eigenvalues of the Hessian. In order to achieve the two dimensional quadratic termination of the family, we derived a short stepsize $\tilde{\alpha}_k$ (14) that converges to $1/\lambda_n$. By using the long BB stepsize and $\tilde{\alpha}_{k-1}$ in a new adaptive cyclic manner, we designed Algorithm 1 for unconstrained quadratic optimization. We proved that Algorithm 1 converges R -linearly at a rate of $1 - 1/\kappa$. Our numerical results on minimizing quadratic functions indicate the efficiency of Algorithm 1 over other recent successful gradient methods.

By using the same arguments as those in the proof of Theorem 1, we find stepsizes $\tilde{\beta}_k$ and $\tilde{\gamma}_k$ are such that (37) and (38) achieve the two dimensional quadratic termination, respectively. For the n dimensional quadratic problem, by Theorem 1 in [5], we obtain

$$\lim_{k \rightarrow \infty} \tilde{\beta}_k = \frac{1}{\lambda_n}, \quad \lim_{k \rightarrow \infty} \tilde{\gamma}_k = \frac{1}{\lambda_n}$$

and

$$\lim_{k \rightarrow \infty} \hat{\beta}_k = \frac{1}{\lambda_1}, \quad \lim_{k \rightarrow \infty} \hat{\gamma}_k = \frac{1}{\lambda_1}.$$

In addition, we have $\lim_{k \rightarrow \infty} \hat{\alpha}_k = 1/\lambda_1$. However, $\hat{\alpha}_k$, $\hat{\beta}_k$ and $\hat{\gamma}_k$ would not be good approximations of $1/\lambda_1$, for more details see [36]. It is worth noting that the stepsize proposed in [28] is a special case of $\tilde{\beta}_k$ with $\psi(A) = I$. Moreover, it is not difficult to prove that $\tilde{\beta}_k$ and $\tilde{\gamma}_k$ are short stepsizes in the sense $\tilde{\beta}_k < c_2/c_3$ and $\tilde{\gamma}_k < c_1/c_2$. Hence, we can replace $\tilde{\alpha}_{k-1}$ in Algorithm 1 by $\tilde{\beta}_{k-1}$ and $\tilde{\gamma}_{k-1}$, which leads to two variants of Algorithm 1. Preliminary experimental results show that the two variants are competitive with Algorithm 1. Furthermore, we can obtain the same convergence results as Theorem 6.

The results of this paper show that the two dimensional quadratic termination property is useful for designing efficient gradient methods. It would be interesting to develop new algorithms for solving general unconstrained optimization problems based on such a property. We leave this as our future work.

6 Declarations

All data generated or analyzed during this study are included in this published article and are also available from the corresponding author on reasonable request.

Acknowledgements This work was supported by the National Natural Science Foundation of China (Grant No. 11701137) and Natural Science Foundation of Hebei Province (Grant No. A2021202010).

References

1. Cauchy, A.: Méthode générale pour la résolution des systèmes d'équations simultanées. *Comp. Rend. Sci. Paris* **25**, 536–538 (1847)
2. Dai, Y.H., Yuan, Y.X.: Alternate minimization gradient method. *IMA J. Numer. Anal.* **23**(3), 377–393 (2003)
3. Akaike, H.: On a successive transformation of probability distribution and its application to the analysis of the optimum gradient method. *Ann. Inst. Stat. Math.* **11**(1), 1–16 (1959)
4. Forsythe, G.E.: On the asymptotic directions of the s -dimensional optimum gradient method. *Numer. Math.* **11**(1), 57–76 (1968)
5. Huang, Y.K., Dai, Y.H., Liu, X.W., Zhang, H.: On the asymptotic convergence and acceleration of gradient methods. *J. Sci. Comput.* **90**, 7 (2022)
6. Nocedal, J., Sartenaer, A., Zhu, C.: On the behavior of the gradient norm in the steepest descent method. *Comput. Optim. Appl.* **22**(1), 5–35 (2002)
7. Zou, Q., Magoulès, F.: Fast gradient methods with alignment for symmetric linear systems without using Cauchy step. *J. Comput. Math.* **381**, 113033 (2021)
8. Barzilai, J., Borwein, J.M.: Two-point step size gradient methods. *IMA J. Numer. Anal.* **8**(1), 141–148 (1988)
9. Raydan, M.: On the Barzilai-Borwein choice of steplength for the gradient method. *IMA J. Numer. Anal.* **13**(3), 321–326 (1993)
10. Dai, Y.H., Liao, L.Z.: R -linear convergence of the Barzilai-Borwein gradient method. *IMA J. Numer. Anal.* **22**(1), 1–10 (2002)
11. Fletcher, R.: On the Barzilai-Borwein method. In: *Optimization and control with applications*, pp. 235–256. Springer, New York (2005)
12. Raydan, M.: The Barzilai-Borwein gradient method for the large scale unconstrained minimization problem. *SIAM J. Optim.* **7**(1), 26–33 (1997)
13. Yuan, Y.X.: Step-sizes for the gradient method. *AMS/IP Stud. Adv. Math.* **42**(2), 785–796 (2008)
14. Birgin, E.G., Martínez, J.M., Raydan, M.: Nonmonotone spectral projected gradient methods on convex sets. *SIAM J. Optim.* **10**(4), 1196–1211 (2000)
15. Birgin, E.G., Martínez, J.M., Raydan, M., et al.: Spectral projected gradient methods: review and perspectives. *J. Stat. Softw.* **60**(3), 539–559 (2014)
16. Dai, Y.H., Huang, Y.K., Liu, X.W.: A family of spectral gradient methods for optimization. *Comput. Optim. Appl.* **74**(1), 43–65 (2019)
17. Di Serafino, D., Ruggiero, V., Toraldo, G., Zanni, L.: On the steplength selection in gradient methods for unconstrained optimization. *Appl. Math. Comput.* **318**, 176–195 (2018)
18. Grippo, L., Lampariello, F., Lucidi, S.: A nonmonotone line search technique for Newton's method. *SIAM J. Numer. Anal.* **23**(4), 707–716 (1986)
19. Huang, Y.K., Liu, H.: Smoothing projected Barzilai-Borwein method for constrained non-lipschitz optimization. *Comput. Optim. Appl.* **65**(3), 671–698 (2016)
20. Huang, Y.K., Liu, H., Zhou, S.: Quadratic regularization projected Barzilai-Borwein method for nonnegative matrix factorization. *Data Min. Knowl. Discov.* **29**(6), 1665–1684 (2015)
21. Jiang, B., Dai, Y.H.: Feasible Barzilai-Borwein-like methods for extreme symmetric eigenvalue problems. *Optim. Method Softw.* **28**(4), 756–784 (2013)
22. Yuan, Y.X.: A new stepsize for the steepest descent method. *J. Comput. Math.* **24**(2), 149–156 (2006)

23. Dai, Y.H., Yuan, Y.X.: Analysis of monotone gradient methods. *J. Ind. Mang. Optim.* **1**(2), 181 (2005)
24. Huang, Y.K., Dai, Y.H., Liu, X.W.: Equipping the Barzilai-Borwein method with the two dimensional quadratic termination property. *SIAM J. Optim.* **31**(4), 3068–3096 (2021)
25. Sun, C., Liu, J.P.: New stepsizes for the gradient method. *Optim. Lett.* **14**(7), 1943–1955 (2020)
26. Dai, Y.H., Yang, X.: A new gradient method with an optimal stepsize property. *Comput. Optim. Appl.* **33**(1), 73–88 (2006)
27. Elman, H.C., Golub, G.H.: Inexact and preconditioned Uzawa algorithms for saddle point problems. *SIAM J. Numer. Anal.* **31**(6), 1645–1661 (1994)
28. Frassoldati, G., Zanni, L., Zanghirati, G.: New adaptive stepsize selections in gradient methods. *J. Ind. Mang. Optim.* **4**(2), 299–312 (2008)
29. De Asmundis, R., Di Serafino, D., Hager, W.W., Toraldo, G., Zhang, H.: An efficient gradient method using the Yuan steplength. *Comput. Optim. Appl.* **59**(3), 541–563 (2014)
30. Davis, T.A., Hu, Y.: The university of Florida sparse matrix collection. *ACM Trans. Math. Softw.* **38**(1), 1–25 (2011)
31. Crisci, S., Porta, F., Ruggiero, V., Zanni, L.: Spectral properties of Barzilai-Borwein rules in solving singly linearly constrained optimization problems subject to lower and upper bounds. *SIAM J. Optim.* **30**(2), 1300–1326 (2020)
32. Dai, Y.H., Fletcher, R.: Projected Barzilai-Borwein methods for large-scale box-constrained quadratic programming. *Numer. Math.* **100**(1), 21–47 (2005)
33. Dai, Y.H., Hager, W.W., Schittkowski, K., Zhang, H.: The cyclic Barzilai-Borwein method for unconstrained optimization. *IMA J. Numer. Anal.* **26**(3), 604–627 (2006)
34. Huang, Y.K., Dai, Y.H., Liu, X.W., Zhang, H.: On the acceleration of the Barzilai-Borwein method. *Comput. Optim. Appl.* **81**(3), 717–740 (2022)
35. Zhou, B., Gao, L., Dai, Y.H.: Gradient methods with adaptive step-sizes. *Comput. Optim. Appl.* **35**(1), 69–86 (2006)
36. Huang, Y.K., Dai, Y.H., Liu, X.W., Zhang, H.: Gradient methods exploiting spectral properties. *Optim. Method Softw.* **35**(4), 681–705 (2020)
37. Li, X., Huang, Y.K.: A note on the R -linear convergence of nonmonotone gradient methods. arXiv preprint, [arXiv:2207.05912](https://arxiv.org/abs/2207.05912) (2022)
38. Dai, Y.H.: Alternate step gradient method. *Optimization* **52**(4–5), 395–415 (2003)
39. Huang, N.: On R -linear convergence analysis for a class of gradient methods. *Comput. Optim. Appl.* **81**(1), 161–177 (2022)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.