A new Barzilai-Borwein steplength from the viewpoint of total least squares

Shiru Li · Yong Xia

Received: date / Accepted: date

Abstract Barzilai-Borwein (BB) steplength is a popular choice in gradient descent method. By observing that the two existing BB steplengths correspond to the ordinary and the data least squares, respectively, we employ the third kind of least squares, the total least squares, to create a new BB steplength, which is shown to lie between the two existing BB steplengths.

Keywords gradient descent · BB steplength · least squares · data least squares · total least squares

1 Introduction

The classical iterative formulation of the gradient descent method for unconstrained minimization reads as

\[ x_{k+1} = x_k - \alpha_k g_k, \quad k = 0, 1, \ldots, \]

where \( g_k \) is the gradient of the objective function at the \( k \)-th iteration point \( x_k \), and \( \alpha_k \) is a steplength with many choices. BB steplength, proposed by Barzilai

This research was supported by the Beijing Natural Science Foundation under grant Z180005, and the National Natural Science Foundation of China under grants 11822103, 11571029, and 11771056.

S. Li · Y. Xia
LMIB of the Ministry of Education, School of Mathematical Sciences, Beihang University, Beijing, 100191, P. R. China E-mail: lishiru@buaa.edu.cn (S. Li); yxia@buaa.edu.cn (Y. Xia, corresponding author)
and Borwein [2], is one of the popular choices of $\alpha_k$. The idea is to approximate the quasi-Newton matrix by $\alpha_k I$ (where $I$ is an identity matrix). It leads to the simplified quasi-Newton equations and their inverse version as $s_k \approx \alpha y_k$ and $\frac{1}{\alpha} s_k \approx y_k$, respectively, where $y_k = g_{k+1} - g_k$ and $s_k = x_{k+1} - x_k$. Due to the over-determination, the ordinary least squares is introduced to solve the simplified equations:

$$\alpha_{BB1}^{k+1} = \arg \min_{\alpha} \| s_k - \alpha y_k \|^2 = \frac{s_k^T y_k}{y_k^T y_k},$$  
(1)

$$\alpha_{BB2}^{k+1} = \arg \min_{\beta} \| \beta s_k - y_k \|^2 = \frac{s_k^T s_k}{s_k^T y_k},$$  
(2)

where $\| \cdot \|$ is the standard Euclidean norm.

BB gradient method achieved many successes in practice, for recent applications, we refer to [1,10,13]. Though in general BB method is not convergent [8], many studies focused on convergence analysis on strongly convex quadratic functions [2,3,4,5,12,15], and variant BB method [6,13].

In this note, we take a new look at BB steplengths from the viewpoint of different kinds of least squares. As we can observe that $\alpha_{BB1}$ and $\alpha_{BB2}$ correspond to the ordinary and the data least squares, respectively, as presented in Section 2, it implies from the total least squares a new BB steplength formula, which is located between $\alpha_{BB1}$ and $\alpha_{BB2}$. We use an example to show the good balance of the newly proposed BB steplength. Conclusions are made in Section 3.

2 Total least squares and the third BB steplength

The main contribution of this section is to derive a new BB steplength from the perspective of total least squares.

2.1 Least squares

We briefly review three kinds of least squares in this subsection. The goal is to solve an over-determined linear system $Ax \approx b$, where $A \in \mathbb{R}^{m \times n}$ is the data matrix, and $b \in \mathbb{R}^m$ is the observation vector.
If we assume that only \( b \) contains a noise \( r \), solving
\[
\min_{r,x} \{ \|r\|^2 : Ax = b + r \} = \min_{x} \|Ax - b\|^2,
\]
yields the well-known ordinary least squares problem.

The less popular data least squares problem \cite{7} corresponds the case where only \( A \) is noised by \( E \):\[
\min_{E,x} \{ \|E\|_F^2 : (A + E)x = b \} = \min_{x} \frac{\|Ax - b\|^2}{\|x\|^2},
\]
where \( \| \cdot \|_F \) is the Frobenius norm.

In case that both \( A \) and \( b \) are noised, the total least squares problem reads as follows:
\[
\min_{E,r,x} \{ \|E\|_F^2 + \|r\|^2 : (A + E)x = b + r \} = \min_{x} \frac{\|Ax - b\|^2}{\|x\|^2 + 1},
\]
which was firstly proposed in \cite{9}.

\subsection*{2.2 A new formula and its property}

First, by replacing the ordinary least squares in (1)-(2) with the data least squares, we obtain \( \alpha_{BB2} \) and \( \alpha_{BB1} \), respectively.

Now we apply the total least squares to solve the simplified quasi-Newton equations \( s_k \approx \alpha_{y_k} \):
\[
\min_{\alpha} q(\alpha) = \frac{\|\alpha y_k - s_k\|^2}{\alpha^2 + 1},
\]
which gives the solution
\[
\alpha_{BB3}^{k+1} = \frac{s_k^T s_k - y_k^T y_k + \sqrt{(y_k^T y_k - s_k^T s_k)^2 + 4(s_k^T y_k)^2}}{2s_k^T y_k}.
\]

Moreover, if we apply the total least squares to solve the inverse quasi-Newton equations \( \beta s_k \approx y_k \) with respect to \( \beta := 1/\alpha \), we can obtain the same formula (3).

We can reformulate \( \alpha_{BB3} \) as a function in terms of \( \alpha_{BB1} \) and \( \alpha_{BB2} \). It reveals how \( \alpha_{BB3} \) keeps a balance between \( \alpha_{BB1} \) and \( \alpha_{BB2} \). We list these observations in the following and omit the trivial proof.
Theorem 1 Suppose $\alpha_{BB1} > 0$, then we have

$$
\alpha_{BB3} = \frac{1}{\alpha_{BB1}} + \sqrt{\frac{1}{\alpha_{BB1}} - \alpha_{BB2}^2} + 4.
$$

Moreover, it holds that

$$
\alpha_{BB1} \leq \alpha_{BB3} \leq \alpha_{BB2},
$$

$$
\lim_{\alpha_{BB1} \to \infty} \frac{\alpha_{BB3}}{\alpha_{BB1}} = 1, \quad \lim_{\alpha_{BB2} \to 0} \frac{\alpha_{BB3}}{\alpha_{BB1}} = 1.
$$

Roughly speaking, BB method with $\alpha_{BB1}$ converges more robustly and hence less fast than that with $\alpha_{BB2}$. Theorem 1 suggests that $\alpha_{BB3}$ seems to be a balance between $\alpha_{BB1}$ and $\alpha_{BB2}$. If both $\alpha_{BB1}$ and $\alpha_{BB2}$ are small (or large) enough, $\alpha_{BB3}$ automatically approaches to the smaller (or larger) one.

We numerically show the benefit of the balance by a classical example. Consider the two-dimensional Rosenbrock function \[ f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2, \quad (x_0^0, x_0^1) = (-1.2, 1). \]

Starting from the same initial points $(x_1^0, x_2^0) = (x_0^0, x_0^1)$, we independently run the three BB methods with $\alpha_{BB1}$, $\alpha_{BB2}$, and $\alpha_{BB3}$, respectively. We set the stop criterion as $\| (x_k^1, x_k^2) - (x_1^*, x_2^*) \| \leq \epsilon$ together with a maximum iteration number 5000, where $(x_1^*, x_2^*) = (1, 1)$ is the minimizer of $f(x)$. We report in Table 1 the iteration numbers with different setting of $\epsilon$, where “–” stands for the situation that the maximum iteration number is reached.

Table 1 Comparison of iteration numbers in minimizing the planar Rosenbrock function.

| $\epsilon$ | BB1 | BB2 | BB3 |
|------------|-----|-----|-----|
| $10^{-2}$  | 154 | 32  |     |
| $10^{-4}$  | 160 | 38  |     |
| $10^{-4}$  | 166 | 44  |     |
| $10^{-8}$  | 172 | 46  |     |

3 Conclusions

From the perspective of least squares, we show the two existing BB steplengths correspond to the ordinary and data least squares, respectively. Then, based
on the third one, the total least squares, we propose a new BB steplength in this note. We prove that it lies (and hence keeps a balance) between the two existing BB steplengths. Future studies include more convergence analysis and variants of BB methods based on the new steplength.

References

1. A. B. Abubakar, P. Kumam, H. Mohammad, and A. M. Awwal. A barzilai-borwein gradient projection method for sparse signal and blurred image restoration. *Journal of the Franklin Institute*, 357(11):7266–7285, 2020.
2. J. Barzilai and J. M. Borwein. Two-point step size gradient methods. *IMA Journal of Numerical Analysis*, 8(1):141–148, 1988.
3. Y. H. Dai. A new analysis on the barzilai-borwein gradient method. *Journal of the Operations Research Society of China*, 1(2):187–198, 2013.
4. Y. H. Dai and L. Z. Liao. R-linear convergence of the barzilai and borwein gradient method. *IMA Journal of Numerical Analysis*, 22(1):1–10, 2002.
5. Yu Hong Dai and Roger Fletcher. On the asymptotic behaviour of some new gradient methods. *Mathematical Programming*, 103(3):541–559, 2005.
6. Yu Hong Dai, William W Hager, Klaus Schittkowski, and Hongchao Zhang. The cyclic barzilai—borwein method for unconstrained optimization. *IMA Journal of Numerical Analysis*, 26(3):604–627, 2006.
7. Ronald D DeGroat and Eric M Dowling. The data least squares problem and channel equalization. *IEEE Transactions on Signal Processing*, 41(1):407–411, 1993.
8. Roger Fletcher. On the barzilai-borwein method. In *Optimization and control with applications*, pages 235–256. Springer, 2005.
9. Gene H Golub and Charles F Van Loan. An analysis of the total least squares problem. *SIAM journal on numerical analysis*, 17(6):883–893, 1980.
10. J. Liang, Y. Xu, C. Bao, Y. Quan, and H. Ji. Barzilai–borwein-based adaptive learning rate for deep learning. *Pattern Recognition Letters*, 128:197–203, 2019.
11. J. J. Moré, B. S. Garbow, and K. E. Hillstrom. Testing unconstrained optimization software. *ACM Transactions on Mathematical Software*, 7(1):17–41, 1981.
12. M. Raydan. On the barzilai and borwein choice of steplength for the gradient method. *IMA Journal of Numerical Analysis*, 13(3):321–326, 1993.
13. M. Raydan. The barzilai and borwein gradient method for the large scale unconstrained minimization problem. *SIAM Journal on Optimization*, 7(1):26–33, 1997.
14. T. Yu, X. W. Liu, Y. H. Dai, and J. Sun. A minibatch proximal stochastic recursive gradient algorithm using a trust-region-like scheme and barzilai-borwein stepsizes. *IEEE Transactions on Neural Networks and Learning Systems*, 2020. doi [10.1109/tnnls.2020.3025383](https://doi.org/10.1109/tnnls.2020.3025383)
15. Y.-x. Yuan. *Numerical Methods for Nonlinear Programming*. Shanghai Scientific and Technical Publishers, 1993.