Math 164: Optimization
Barzilai-Borwein Method

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online discussions on piazza.com

Main features of the Barzilai-Borwein (BB) method

- The BB method was published in a 8-page paper[1] in 1988
- It is a gradient method with modified step sizes, which are motivated by Newton's method but not involves any Hessian
- At nearly no extra cost, the method often significantly improves the performance of a standard gradient method
- The method is used along with non-monotone line search as a safeguard

[1] J. Barzilai and J. Borwein. Two-point step size gradient method. IMA J. Numerical Analysis 8, 141–148, 1988.

Motivation of the BB method

Let $\boldsymbol{g}^{(k)} = \nabla f(\boldsymbol{x}^{(k)})$ and $\boldsymbol{F}^{(k)} = \nabla^2 f(\boldsymbol{x}^{(k)})$.

- **gradient method**: $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \alpha_k \boldsymbol{g}^{(k)}$
  - choice of α_k: fixed, exact line search, or fixed initial + line search
  - **pros**: simple
  - **cons**: no use of 2nd order information, sometimes zig-zag
- **Newton's method**: $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - (\boldsymbol{F}^{(k)})^{-1} \boldsymbol{g}^{(k)}$
  - **pros**: 2nd-order information, 1-step for quadratic function, fast convergence near solution
  - **cons**: forming and computing $(\boldsymbol{F}^{(k)})^{-1}$ is expensive, need modifications if $\boldsymbol{F}^{(k)} \not\succ 0$

The BB method chooses α_k so that $\alpha_k \boldsymbol{g}^{(k)}$ approximates $(\boldsymbol{F}^{(k)})^{-1} \boldsymbol{g}^{(k)}$ without computing $\boldsymbol{F}^{(k)}$

Derive the BB method

- Consider

$$\underset{\boldsymbol{x}}{\text{minimize}}\ f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x},$$

  where $\boldsymbol{A} \succ 0$ is symmetric. Gradient is $\boldsymbol{g}^{(k)} = \boldsymbol{A}\boldsymbol{x}^{(k)} - \boldsymbol{b}$. Hessian is $\boldsymbol{A}$.

- Newton step: $\boldsymbol{d}^{(k)}_{\text{newton}} = -\boldsymbol{A}^{-1}\boldsymbol{g}^{(k)}$

- **Goal:** choose α_k so that $-\alpha_k\boldsymbol{g}^{(k)} = -(\alpha_k^{-1}I)^{-1}\boldsymbol{g}^{(k)}$ approximates $-\boldsymbol{A}^{-1}\boldsymbol{g}^{(k)}$

- Define: $\boldsymbol{s}^{(k-1)} := \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}$ and $\boldsymbol{y}^{(k-1)} := \boldsymbol{g}^{(k)} - \boldsymbol{g}^{(k-1)}$. Then $\boldsymbol{A}$ satisfies:

$$\boldsymbol{A}\boldsymbol{s}^{(k-1)} = \boldsymbol{y}^{(k-1)}.$$

- Therefore, given $\boldsymbol{s}^{(k-1)}$ and $\boldsymbol{y}^{(k-1)}$, how about choose α_k so that

$$(\alpha_k^{-1}I)\boldsymbol{s}^{(k-1)} \approx \boldsymbol{y}^{(k-1)}$$

- **Goal:**

$$(\alpha_k^{-1} I)\boldsymbol{s}^{(k-1)} \approx \boldsymbol{y}^{(k-1)}.$$

- **BB method:**
  - Least-squares problem: (let $\beta = \alpha^{-1}$)

$$\alpha_k^{-1} = \arg\min_{\beta} \frac{1}{2}\|\boldsymbol{s}^{(k-1)}\beta - \boldsymbol{y}^{(k-1)}\|^2 \implies \alpha_k^1 = \frac{\left(\boldsymbol{s}^{(k-1)}\right)^T \boldsymbol{s}^{(k-1)}}{\left(\boldsymbol{s}^{(k-1)}\right)^T \boldsymbol{y}^{(k-1)}}$$

  - Alternative Least-squares problem:

$$\alpha_k = \arg\min_{\alpha} \frac{1}{2}\|\boldsymbol{s}^{(k-1)} - \boldsymbol{y}^{(k-1)}\alpha\|^2 \implies \alpha_k^2 = \frac{\left(\boldsymbol{s}^{(k-1)}\right)^T \boldsymbol{y}^{(k-1)}}{\left(\boldsymbol{y}^{(k-1)}\right)^T \boldsymbol{y}^{(k-1)}}$$

- α_k^1 and α_k^2 are called the BB step sizes.

Apply the BB method

- Since $\boldsymbol{x}^{(k-1)}$ and $\boldsymbol{g}^{(k-1)}$ and thus $\boldsymbol{s}^{(k-1)}$ and $\boldsymbol{y}^{(k-1)}$ are unavailable at $k = 0$, we apply the standard gradient descent at $k = 0$ and start BB at $k = 1$
- We can use either α_k^1 or α_k^2 or alternate between them
- We can fix $\alpha_k = \alpha_k^1$ or $\alpha_k = \alpha_k^2$ for a few consecutive steps
- It performs very well on minimizing quadratic and many other functions
- However, f_k and $\|\nabla f_k\|$ are **not** monotonic!

Steepest descent versus BB on quadratic programming

- **Model:**

$$\underset{\boldsymbol{x}}{\text{minimize}}\ f(\boldsymbol{x}) := \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} - \mathbf{b}^T\boldsymbol{x}.$$

- Gradient iteration

$$\boldsymbol{x}^{k+1} \leftarrow \boldsymbol{x}^{(k)} - \alpha_k(\boldsymbol{A}\boldsymbol{x}^{(k)} - \mathbf{b}).$$

- **Steepest descent** selects α_k as $\arg\min_\alpha f(\boldsymbol{x}^{(k)} - \alpha_k(\boldsymbol{A}\boldsymbol{x}^{(k)} - \mathbf{b}))$

$$\alpha_k = \frac{(\boldsymbol{r}^k)^T\boldsymbol{r}^{(k)}}{(\boldsymbol{r}^k)^T\boldsymbol{A}\boldsymbol{r}^{(k)}}$$

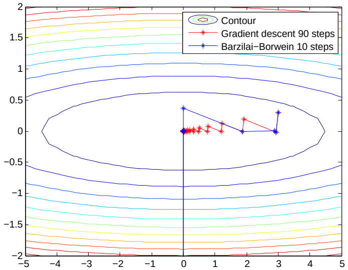
  where $\boldsymbol{r}^{(k)} := \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^{(k)}$.

- **BB** selects α_k as

$$\alpha_k^1 = \frac{(\boldsymbol{s}^{(k-1)})^T\boldsymbol{s}^{(k-1)}}{(\boldsymbol{s}^{(k-1)})^T\boldsymbol{y}^{(k-1)}}$$

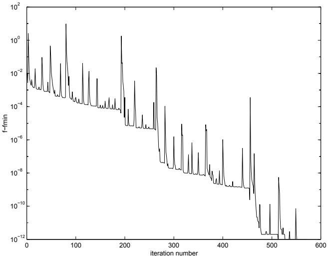
Numerical example

- Set symmetric matrix $\boldsymbol{A}$ to have the condition number $\frac{\lambda_{\max}(\boldsymbol{A})}{\lambda_{\min}(\boldsymbol{A})} = 50$.
- Stopping criterion:
$$\|\boldsymbol{r}^{(k)}\| < 10^{-8}$$
- **Steepest descent** stops in 90 iterations
- **BB** stops in 10 iterations



Properties of Barzilai-Borwein

- For quadratic functions, it has R-linear convergence[2]
- For 2D quadratic function, it has Q-superlinear convergence[3]
- No convergence guarantee for smooth convex problems. On these problems, we pair up BB with non-monotone line search.



BB on *Laplace2*: $\min \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x} + \frac{h^2}{4}\sum_{ijk} u_{ijk}^4.$

[2] Dai and Liao [2002]

[3] Barzilai and Borwein [1988], Dai [2013]

Nonmonotone line search

- Some growth in the function value is permitted
- Sometimes improve the likelihood of finding a global optimum
- Improve convergence speed when a monotone scheme is forced to creep along the bottom of a narrow curved valley
- Early nonmonotone line search method[4] developed for Newton's methods

$$f(\boldsymbol{x}^{(k)} + \alpha \boldsymbol{d}^{(k)}) \le \max_{0 \le j \le m_k} f(\boldsymbol{x}^{k-j}) + c_1 \alpha \nabla f_k^T \boldsymbol{d}^{(k)}$$

However, it may still kill R-linear convergence. **Example**: $x \in \mathbb{R}$,

$$\underset{x}{\text{minimize}}\, f(x) = \frac{1}{2}x^2, \quad x^0 \neq 0, \quad d^{(k)} = -x^{(k)}.$$

$$\alpha_k = \begin{cases} 1 - 2^{-k}, & k = i^2 \text{ for some integer } i, \\ 2, & \text{otherwise,} \end{cases}$$

converges R-linear but fails to satisfy the condition for k large.

[4] Grippo, Lampariello, and Lucidi [1986]

Zhang-Hager nonmonotone line search[5]

1. initialize $0 < c_1 < c_2 < 1,\ C_0 \leftarrow f(\boldsymbol{x}^0),\ Q_0 \leftarrow 1,\ \eta < 1,\ k \leftarrow 0$
2. while *not converged* do

3a. compute α_k satisfying the modified Wolfe conditions OR

3b. find α_k by backtracking, to satisfy the modified Armijo condition:

$$\text{sufficient decrease:} \quad f(\boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)}) \leq C_k + c_1 \alpha_k \nabla f_k^T \boldsymbol{d}^{(k)}$$

4. $\boldsymbol{x}^{k+1} \leftarrow \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)}$
5. $Q_{k+1} \leftarrow \eta Q_k + 1,\ C_{k+1} \leftarrow (\eta Q_k C_k + f(\boldsymbol{x}^{k+1}))/Q_{k+1}$.

Comments:

- If $\eta = 1$, then $C_k = \frac{1}{k+1} \sum_{j=0}^{k} f_j$.
- Since $\eta < 1$, C_k is a weighted sum of all past f_j, more weights on recent f_j.

[5] Zhang and Hager [2004]

Convergence (advanced topic)

The results below are left to the reader as an exercise.

If $f \in C^1$ and bounded below, $\nabla f_k^T \boldsymbol{d}^{(k)} < 0$, then

- $f_k \le C_k \le \frac{1}{k+1} \sum_{j=0}^{(k)} f_j$
- there exists α_k satisfying the modified Wolfe or Armijo conditions

In addition, if ∇f is Lipschitz with constant L, then

- $\alpha_k > C \frac{|\nabla f_k^T \boldsymbol{d}^{(k)}|}{\|\boldsymbol{d}^{(k)}\|}$ for some constant depending on c_1, c_2, L and the backing factor

Furthermore, if for all sufficiently large k, we have uniform bounds

$$\nabla f_k^T \boldsymbol{d}^{(k)} \le -c_3 \|\nabla f_k\|^2 \quad \text{and} \quad \|\boldsymbol{d}^{(k)}\| \le c_4 \|\nabla f_k\|$$

then

- $\lim_{k\to\infty} \nabla f_k = 0$

Once again, pairing with non-monotone linear search, Barzilai-Borwein gradient methods *work every well on general unconstrained differentiable problems*.

References:

Yu-Hong Dai and Li-Zhi Liao. R-linear convergence of the Barzilai and Borwein gradient method. *IMA Journal of Numerical Analysis*, 22(1):1–10, 2002.

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Luigi Grippo, Francesco Lampariello, and Stephano Lucidi. A nonmonotone line search technique for Newton's method. *SIAM Journal on Numerical Analysis*, 23(4): 707–716, 1986.

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