Greedy Quasi-Newton Method with Explicit Superlinear Convergence

Anton Rodomanov   Yurii Nesterov

Catholic University of Louvain, Belgium

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Quasi-Newton methods for minimizing functions

Problem: $\min_{x \in \mathbb{R}^n} f(x)$, where $f : \mathbb{R}^n \to \mathbb{R}$ is a smooth function.

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Initialize $x_0 \in \mathbb{R}^n$, $H_0 \in \mathbb{S}^n_{++}$ and iterate for $k \geq 0$:

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Denote $s_k := x_{k+1} - x_k$ and $y_k := f'(x_{k+1}) - f'(x_k)$.

- (SR1) $H_{k+1} := H_k + \frac{(s_k - H_k y_k)(s_k - H_k y_k)^T}{\langle y_k, s_k - H_k y_k \rangle}$.
- (DFP) $H_{k+1} := H_k - \frac{H_k y_k y_k^T H_k}{\langle y_k, H_k y_k \rangle} + \frac{s_k s_k^T}{\langle y_k, s_k \rangle}$.
- (BFGS) $H_{k+1} := \left(I - \frac{s_k y_k^T}{\langle y_k, s_k \rangle} \right) H_k \left(I - \frac{y_k s_k^T}{\langle y_k, s_k \rangle} \right) + \frac{s_k s_k^T}{\langle y_k, s_k \rangle}$.

Superlinear convergence of quasi-Newton methods

Theorem (Dennis-Moré 1974, 1977)

If (x_0, H_0) *is sufficiently close to* $(x^*, f''(x^*)^{-1})$*, then both DFP and BFGS are superlinearly convergent:* $\frac{\|x_{k+1}-x^*\|}{\|x_k-x^*\|} \to 0$.

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Main question: Rate of convergence? $O(c^{k^2})$, $O(c^{k^3})$, $O(k^{-k})$, ...?

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Our goal:

Present a new quasi-Newton method with an explicit superlinear rate.

BFGS update and norms

Definition (BFGS update)

For $A \in \mathbb{S}^n_{++}$, $H \in \mathbb{S}^n$ and $s \in \mathbb{R}^n$, define

$$\mathrm{BFGS}(H, A, s) := \left(I - \frac{ss^T A}{\langle As, s \rangle} \right) H \left(I - \frac{Ass^T}{\langle As, s \rangle} \right) + \frac{ss^T}{\langle As, s \rangle}.$$

- Here A plays the role of $f''(x)$ and $y := As$.

Our goal: Decrease the distance between H and A^{-1}.

Main property of BFGS update

- Introduce the Euclidean norm induced by A:
$$\|x\|_A := \langle Ax, x \rangle^{\frac{1}{2}}.$$

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For $H_+ := \mathrm{BFGS}(H, A, s)$, *we have*
$$\|H_+ - A^{-1}\|^2_{\mathrm{Fr}(A)} \leq \|H - A^{-1}\|^2_{\mathrm{Fr}(A)} - \frac{\|(HA - I)s\|_A^2}{\|s\|_A^2}.$$

Greedy BFGS update

Definition (Greedy BFGS update)

Let $e_1, \ldots, e_n$ be the standard orthonormal basis in $\mathbb{R}^n$. For

$$i_{\max}(H, A) := \operatorname*{argmax}_{1 \le i \le n} \frac{\|(HA - I)e_i\|_A^2}{\|e_i\|_A^2},$$

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$$\mathrm{GreedyBFGS}(H, A) := \mathrm{BFGS}(H, A, e_{i_{\max}(H,A)}).$$

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- Makes the maximal progress keeping the update cost relatively small.
- Computation of $i_{\max}(H, A)$ will be addressed later.

Main property of greedy BFGS update

Lemma (Linear convergence in matrix)

For $H_+ := \mathrm{GreedyBFGS}(H, A)$*, we have*

$$\|H_+ - A^{-1}\|_{\mathrm{Fr}(A)} \leq (1-\rho)\|H - A^{-1}\|_{\mathrm{Fr}(A)},$$

where $\rho := \rho(A)$ *is the coordinate condition number of* A*:*

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- Follows from lower bounding the maximum by the expectation for i chosen randomly with probability $\pi_i := \frac{\|a_i\|_A^2}{\mathrm{Tr}(A)}$.

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- The randomized version was first proposed in [Gower-Richtárik 2016].

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Can we expect similar results when f is general nonlinear?

GreedyBFGS method

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1. Set $x_{k+1} := x_k - H_k f'(x_k)$
2. Set $H_{k+1} := \mathrm{GreedyBFGS}(H_k, f''(x_{k+1}))$.

NB: $A := f''(x_{k+1})$ changes at every iteration.

General nonlinear functions

Lipschitz continuity of f'':

$$\|f''(x) - f''(x^*)\|_{f''(x^*)^{-1}} \leq L\|x - x^*\|_{f''(x^*)}.$$

Lemma (Progress of one step of GreedyBFGS)

For $r_k := \frac{L}{2}\|x_k - x^*\|_{f''(x^*)}$, $\sigma_k := \|H_k - f''(x_k)^{-1}\|_{\mathrm{Fr}(f''(x_k))}$ *and* $\rho := \rho(f''(x^*))$, *we have*

$$r_{k+1} \leq \frac{(1+r_k)^{\frac{3}{2}}}{(1-2r_k)\sqrt{1-r_k}}\sigma_k r_k + \frac{3\sqrt{1+r_k}}{(1-2r_k)\sqrt{1-r_k}} r_k^2$$

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Simplification: Assuming r_k is sufficiently small and $\sigma_0 \leq 1$, we get

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$$\begin{aligned} r_{k+1} &\leq \sigma_k r_k, \\ \sigma_{k+1} &\leq (1-\rho)\sigma_k \end{aligned} \quad \Rightarrow \quad \begin{aligned} r_k &\leq (1-\rho)^{k^2} r_0 \\ \sigma_k &\leq (1-\rho)^k. \end{aligned}$$

Theorem (Local superlinear convergence of GreedyBFGS)

If $r_0 \leq \bar{r}$ *and* $\sigma_0 \leq 0.5$*, where* $\bar{r} := \frac{2c\rho}{\sqrt{n}}$ *for* $c := 0.02$*, then*

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Reminder:

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Reminder: For quadratic f, we had

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Bad initial matrix

What to do if $\sigma_0 := \|H_0 - f''(x_0)^{-1}\|_{\mathrm{Fr}(f''(x_0))} > 0.5$? (Usually $H_0 := I$.)

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GreedyBFGS–II

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2. Set $H_{k+1} :=$ GreedyBFGS$(H_k, f''(x_{k+1}))$.

Convergence of GreedyBFGS–II

Theorem (Local superlinear convergence of GreedyBFGS–II)

Suppose $\frac{L}{2}\|x - x^*\|_{f''(x^*)} \le \bar{r}$ *for all* $L_f(x_0) := \{x : f(x) \le f(x_0)\}$, *and let*

$$T_0 := \begin{cases} 0 & \text{if } \sigma_0 \le 0.5 \\ 2\rho^{-1}\ln(5\sigma_0) & \text{otherwise.} \end{cases}$$

Then for $\delta := \frac{8c}{1-10c} = 0.2$ *and* $b := 1 - \frac{8c}{1-2c} = 0.8333\ldots$, *we have*

$$\left.\begin{aligned} r_k &\le \bar{r}, \\ \sigma_k &\le \delta + (1 - b\rho)^k(\sigma_0 - \delta) \end{aligned}\right. \qquad 0 \le k < T_0$$

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Computing the update

For doing the GreedyBFGS update, we need to compute

$$i_{\max}(H, A) = \underset{1 \le i \le n}{\operatorname{argmax}} \frac{\|(HA - I)e_i\|_A^2}{\|e_i\|_A^2}$$

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$$i_{\max}(H, A) = \operatorname*{argmax}_{1 \le i \le n} \frac{\|(HA - I)e_i\|_A^2}{\|e_i\|_A^2} = \operatorname*{argmax}_{1 \le i \le n} \frac{\langle (AH - I)A(HA - I)e_i, e_i \rangle}{\langle Ae_i, e_i \rangle}$$

- Need to compute the diagonal of A and
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(Note that $AHAHA = AHA(AH)^T$.)

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Complexity of each update: $O(n^2)$.

Example 1: Sparse quadratic

Let f be a strictly convex quadratic function

$$f(x) := \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle,$$

where $A \in \mathbb{S}^n_{++}$ has at most p non-zeros in each column.

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Fact: A^2 contains $\leq np^2$ non-zeros and can be computed in $O(np^2 + n^2)$.

Example 2: Sparse cubically regularized quadratic

A more complicated example:

$$f(x) := \frac{1}{2}\langle Qx, x\rangle + \langle b, x\rangle + \frac{\beta}{3}\|x\|^3,$$

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- Explicit $O((1-\rho)^{k^2})$ superlinear convergence rate.

Thank you!