Greedy Quasi-Newton Method with Explicit Superlinear Convergence

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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 twice differentiable with Lipschitz and positive definite second derivative.

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

1. Set $x_{k+1} := x_k - H_k f'(x_k)$.
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2. Update H_k into H_{k+1}.

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? $O(c^{k^2})$, $O(c^{k^3})$, $O(k^{-k})$, $\ldots$?

Our goal:

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

Our goal:

$\boxed{\text{Present a new quasi-Newton method with an explicit superlinear rate.}}$

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 $f''(x)$.
- We want the distance between H and A^{-1} go to zero.

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Question: How to measure the distance between H and A^{-1}?

Norms

- Introduce a pair of conjugate norms induced by A:
$$\|x\|_A := \langle Ax, x\rangle^{\frac{1}{2}}, \qquad \|y\|_A^* := \langle y, A^{-1}y\rangle^{\frac{1}{2}}.$$

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- The corresponding operator norm in $\mathbb{S}^n$ is
$$\|W\|_A := \max_{\|y\|_A^*=1} \|Wy\|_A = \max_{\|x\|_A=1} \|WAx\|_A = \lambda_{\max}(WAWA)^{\frac{1}{2}}.$$

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Explanation: Consider a quadratic function
$$f(x) := \frac{1}{2}\langle Ax, x\rangle = \frac{1}{2}\|x\|_A^2.$$
Then the quasi-Newton step
$$x_{k+1} = x_k - H_k f'(x_k) = (A^{-1} - H_k)Ax_k$$
gives us
$$\|x_{k+1}\|_A = \|(H_k - A^{-1})Ax_k\|_A \leq \|H_k - A^{-1}\|_A \|x_k\|_A.$$
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Progress in matrix and greedy BFGS update

Lemma (Progress in matrix for the BFGS update)

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

$$\|H_+ - A^{-1}\|^2_{\mathrm{Fr}(A)} \leq \|H - A^{-1}\|^2_{\mathrm{Fr}(A)} - \frac{\|(H - A^{-1})As\|^2_A}{\|s\|^2_A}.$$

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

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- Makes the maximal progress keeping the update cost relatively small.

Main property of greedy BFGS update

Lemma (Linear convergence in matrix)

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

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

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

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$$r_k \le r_0 \prod_{i=0}^{k-1} ((1-\rho)^i \sigma_0) = \sigma_0^k (1-\rho)^{k^2} r_0.$$

Conclusion:

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Can we expect similar results when f is general nonlinear?

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

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

General nonlinear functions

Main assumption: (Lipschitz continuity of f'' relative to x^*)

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

Lemma (Progress of one step of GreedyBFGS)

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

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

$$\sigma_{k+1} \leq \left(1 - \frac{1-2r_{k+1}}{1+2r_{k+1}}\rho_k\right)\frac{1+2r_{k+1}}{1-2r_k}\sigma_k + \frac{2\sqrt{n}}{1-2r_k}(r_k + r_{k+1}).$$

Simplification:

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

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Convergence of GreedyBFGS

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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- It uses the classic BFGS rule with greedily selected direction.
- Explicit $O((1-\rho)^{k^2})$ superlinear convergence rate.

Thank you!

Bad initial matrix

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Idea: Successively improve H_k while not going to far away from x^*.

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GreedyBFGS–II

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

1. (Backtracking) Find smallest $j_k \geq 0$: $f(x_k - 2^{-j_k} H_k f'(x_k)) \leq f(x_k)$.
2. Set $x_{k+1} := x_k - 2^{-j_k} H_k f'(x_k)$.
3. Set $H_{k+1} :=$ GreedyBFGS$(H_k, f''(x_{k+1}))$.

Convergence of GreedyBFGS–II

Theorem (Local superlinear convergence of GreedyBFGS–II)

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

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

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

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

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and

$$\left.\begin{aligned} r_k &\leq \left(1 - \frac{\rho}{2}\right)^{\frac{k(k+1)}{2}} \bar{r}, \\ \sigma_k &\leq \left(1 - \frac{\rho}{2}\right)^k \frac{1}{2} \end{aligned}\right\} \quad k \geq T_0.$$

Computing the update

For doing the GreedyBFGS update, we need to compute

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

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\begin{aligned}
i_{\max}(H, A) &= \operatorname*{argmax}_{1 \le i \le n} \frac{\|(H - A^{-1})Ae_i\|_A^2}{\|e_i\|_A^2} \\
&= \operatorname*{argmax}_{1 \le i \le n} \frac{\langle A(H - A^{-1})A(H - A^{-1})Ae_i, e_i \rangle}{\langle Ae_i, e_i \rangle}
\end{aligned}
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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
$$f(x) := \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle,$$
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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

Now consider

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

where $\beta > 0$, Q is sparse with at most p non-zeros in each column.

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