Optimization methods
Lecture 8: Newton method. Quasi-Newton methods

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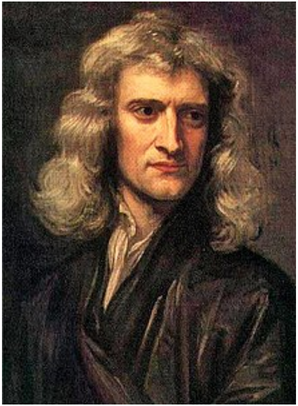
Brief reminder of the previous lecture

- Randomness in optimization problems
- Stochastic gradient descent
- Variance reduction technique

Newton method

$$\min_{\mathbf{x}} f(\mathbf{x})$$



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- Newton method $\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - f''(\mathbf{x}_k)^{-1} f'(\mathbf{x}_k)}$

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- Assume the function $f(\mathbf{x})$ in problem

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$$f'(\mathbf{x}^*) = G(\mathbf{x}) = 0$$

- Linear system to get direction $\mathbf{h}$

$$f'(\mathbf{x}) + f''(\mathbf{x})\mathbf{h} = 0$$

  is equivalent to the system in Newton method for problem (1)

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- converge
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Damped Newton method

$$\boxed{\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k f''(\mathbf{x}_k)^{-1} f'(\mathbf{x}_k)}$$

- Adaptive step size is similar to the gradient descent
- Adaptive step size expands convergence region

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- Local superlinear convergence $(\mathbf{x}_k \neq \mathbf{x}^*)$

$$\lim_{k\to\infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} = \lim_{k\to\infty} \frac{o(\|\mathbf{x}_k - \mathbf{x}^*\|)}{\|\mathbf{x}_k - \mathbf{x}^*\|} = 0$$

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Theorem

Let

- $f(\mathbf{x})$ *be local strongly convex with constant* μ*:*
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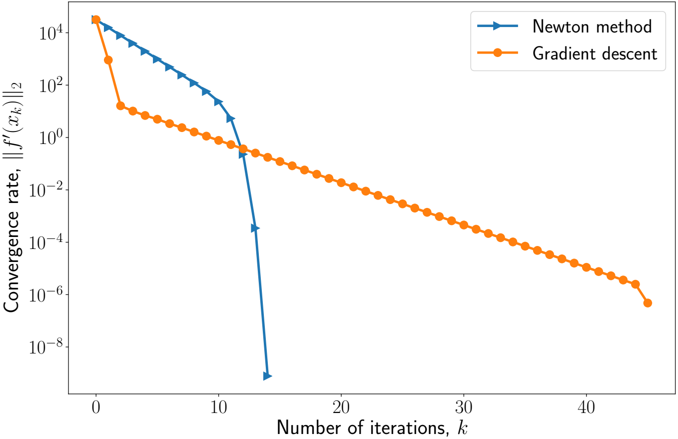
then Newton method converges ***quadratically***

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\| \leq \frac{M\|\mathbf{x}_k - \mathbf{x}^*\|^2}{2(\mu - M\|\mathbf{x}_k - \mathbf{x}^*\|)}$$

Example

$$
-\sum_{i=1}^{m} \log(1 - \mathbf{a}_i^\top \mathbf{x}) - \sum_{i=1}^{n} \log(1 - x_i^2) \to \min_{\mathbf{x} \in \mathbb{R}^n}
$$



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2. The well-known fact from calculus

$$\phi(b) - \phi(a) = \int_0^1 \phi'(a + t(b-a))(b-a)dt$$

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$$\mathbf{r}_{k+1} = \underbrace{\left(\mathbf{I} - f''(\mathbf{x}_k)^{-1} \int_0^1 [f''(\mathbf{x}^* + t\mathbf{r}_k)]dt\right)}_{\mathbf{G}_k} \mathbf{r}_k$$

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5. $\|\mathbf{r}_{k+1}\| \leq \|\mathbf{G}_k\| \|\mathbf{r}_k\|$

6. Hessian is Lipschitz, then

$$\mathbf{G}_k = f''(\mathbf{x}_k)^{-1} \int_0^1 [f''(\mathbf{x}_k) - f''(\mathbf{x}^* + t\mathbf{r}_k)]dt$$

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8. From the Lipschitz hessian and strong convexity of f at $\mathbf{x}^*$ follows that

$$f''(\mathbf{x}_k) \succeq f''(\mathbf{x}^*) - M\|\mathbf{r}_k\|\mathbf{I} \succeq (\mu - M\|\mathbf{r}_k\|)\mathbf{I}$$

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9. Estimate norm of the inverse hessian

$$\|f''(\mathbf{x}_k)^{-1}\| \leq \frac{1}{\mu - M\|\mathbf{r}_k\|}$$

Pro & Contra

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Pro

- Quadratic convergence
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Contra

- Storage of hessian: $O(n^2)$ memory cost
- Linear system is solved in every iteration: $O(n^3)$ operations in general case
- Hessian can be singular

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- Gradient descent

$$
\begin{aligned}
& f(\mathbf{x}+\mathbf{h}) \leq f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{h} \rangle + \frac{1}{2\alpha}\mathbf{h}^\top \mathbf{I}\mathbf{h} \equiv f_g(\mathbf{h}) \\
& \min_{\mathbf{h}} f_g(\mathbf{h}) \Rightarrow \mathbf{h}^* = -\alpha f'(\mathbf{x}) \\
& \mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k f'(\mathbf{x}_k)
\end{aligned}
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$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k f'(\mathbf{x}_k)$$

- Newton method

$$f(\mathbf{x}+\mathbf{h}) \approx f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{h}\rangle + \frac{1}{2}\mathbf{h}^\top f''(\mathbf{x})\mathbf{h} \equiv f_N(\mathbf{h})$$

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- Something better than $f_g(\mathbf{x})$, but faster than $f_N(\mathbf{x})$?

Quasi-Newton method

- Quadratic estimate $f(\mathbf{x}_{k+1})$

$$f_q(\mathbf{h}) = f(\mathbf{x}_k) + \langle f'(\mathbf{x}_k), \mathbf{h} \rangle + \frac{1}{2}\mathbf{h}^\top \mathbf{B}_k \mathbf{h}, \quad \mathbf{B}_k \succ 0$$

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- Fast update $\mathbf{B}_k \to \mathbf{B}_{k+1}$, **that uses only gradient**
- Fast search of $\mathbf{h}_k$

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- Fast update $\mathbf{B}_k \to \mathbf{B}_{k+1}$, **that uses only gradient**
- Fast search of $\mathbf{h}_k$
- Efficient storing $\mathbf{B}_k$

Quasi-Newton method

- Quadratic estimate $f(\mathbf{x}_{k+1})$

$$f_q(\mathbf{h}) = f(\mathbf{x}_k) + \langle f'(\mathbf{x}_k), \mathbf{h} \rangle + \frac{1}{2}\mathbf{h}^\top \mathbf{B}_k \mathbf{h}, \quad \mathbf{B}_k \succ 0$$

- Minimum of $f_q(\mathbf{h})$ is at point

$$\mathbf{h}_k = -\mathbf{B}_k^{-1} f'(\mathbf{x}_k)$$

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How update $\mathbf{B}_k$?

Two gradients rule

- $f'_q(-\alpha_k \mathbf{h}_k) = f'(\mathbf{x}_k) \Rightarrow f'(\mathbf{x}_{k+1}) - \alpha_k \mathbf{B}_{k+1} \mathbf{h}_k = f'(\mathbf{x}_k)$
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Examples of quasi-Newton methods

- Barzilai-Borwein
- BFGS

Barzilai-Borwein method

- Approximate hessian by diagonal matrix:

$$\alpha_k f'(\mathbf{x}_k) = \alpha_k \mathbf{I} f'(\mathbf{x}_k) = \left(\frac{1}{\alpha_k}\mathbf{I}\right)^{-1} f'(\mathbf{x}_k) \approx (f''(\mathbf{x}_k))^{-1} f'(\mathbf{x}_k)$$

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- It has stochastic modifications, paper from NIPS 2016

BFGS method

Broyden, Fletcher, Goldfarb, Shanno

BFGS method

- The problem

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\mathbf{H}_{k+1} = (\mathbf{I} - \rho_k \mathbf{s}_k \mathbf{y}_k^\top)\mathbf{H}_k(\mathbf{I} - \rho_k \mathbf{y}_k \mathbf{s}_k^\top) + \rho_k \mathbf{s}_k \mathbf{s}_k^\top,
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where $\rho_k = \dfrac{1}{\mathbf{y}_k^\top \mathbf{s}_k}$

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Almost theorem

If f is strongly convex and the hessian is Lipschitz. The BFGS converges superlinearly under some mild technical assumptions.

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- Unroll m steps of recursion

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&\mathbf{H}_{k+1} = \mathbf{V}_k^\top \mathbf{H}_k \mathbf{V}_k + \rho_k \mathbf{s}_k \mathbf{s}_k^\top \\
&= \mathbf{V}_k^\top \mathbf{V}_{k-1}^\top \mathbf{H}_{k-1} \mathbf{V}_{k-1} \mathbf{V}_k + \rho_{k-1} \mathbf{V}_k^\top \mathbf{V}_{k-1}^\top \mathbf{s}_{k-1} \mathbf{s}_{k-1}^\top \mathbf{V}_{k-1} \mathbf{V}_k \\
&+ \rho_k \mathbf{s}_k \mathbf{s}_k^\top = \mathbf{V}_k^\top \ldots \mathbf{V}_{k-m+1}^\top \mathbf{H}_{m,0} \mathbf{V}_{k-m+1} \ldots \mathbf{V}_k \\
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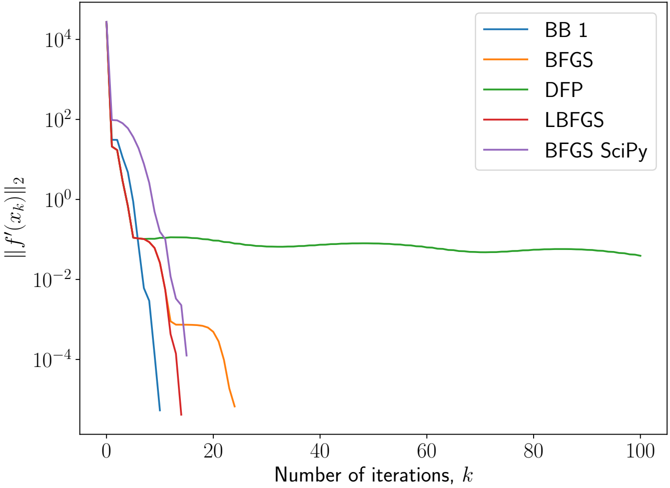
&+ \ldots + \rho_k \mathbf{s}_k \mathbf{s}_k^\top
\end{aligned}$$

- Efficient computing of $\mathbf{H}_k f'(\mathbf{x})$ without explicit forming of $\mathbf{H}_k$

Example

$$
-\sum_{i=1}^{m} \log(1 - \mathbf{a}_i^\top \mathbf{x}) - \sum_{i=1}^{n} \log(1 - x_i^2) \to \min_{\mathbf{x} \in \mathbb{R}^n}
$$



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- One iteration complexity is $O(n^2) + ...$ in contrast to the Newton method $O(n^3) + ...$
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Contra

- Stochastic generalization does not work
- Initialization of $\mathbf{B}_0$ or $\mathbf{H}_0$
- Convergence theory is still under development