

Optimization methods

Lecture 6: Conjugate gradient method, heavy-ball method and accelerated gradient method

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Brief reminder of the previous lecture

- ▶ Introduction to numerical optimization methods
- ▶ Convergence speed
- ▶ Gradient descent
- ▶ Convergence and condition number

Conjugate gradient method

- Consider the problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}),$$

where $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{b}^\top \mathbf{x}$ and $\mathbf{A} \in \mathbb{S}_{++}^n$

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- ▶ Denote $f'(\mathbf{x}_k) = \mathbf{A}\mathbf{x}_k - \mathbf{b} = \mathbf{r}_k$
- ▶ We reduce optimization problem to the problem of solving linear system

Motivation

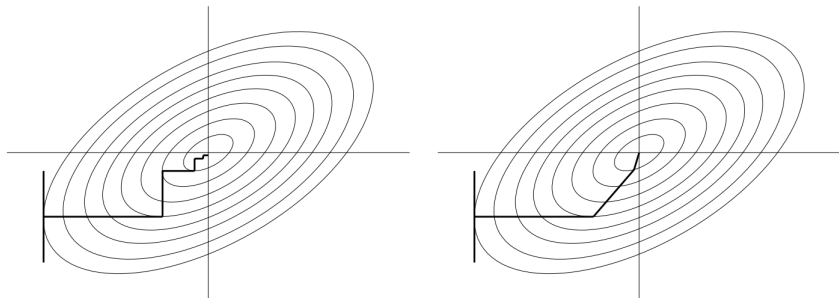
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- ▶ How to develop the method that converges at most after n iterations independently on the condition number?

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Plot is from [this page](#)

Conjugate directions

Definition

Non-zero vectors $\{\mathbf{p}_0, \dots, \mathbf{p}_l\}$ are called conjugate with respect to matrix $\mathbf{A} \in \mathbb{S}_{++}^n$, if

$$\mathbf{p}_i^\top \mathbf{A} \mathbf{p}_j = 0, \quad i \neq j$$

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- ▶ conjugate directions + the steepest descent step size selection = method that converges after n iterations

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Q: how to derive conjugate directions from the set of linear independent vectors?

Convergence

Theorem

Assume \mathbf{x}_k is generated by conjugate direction method. Then

1. $\langle \mathbf{r}_k, \mathbf{p}_i \rangle = 0, i = 1, \dots, k - 1$
2. $\mathbf{x}_k = \arg \min_{\mathbf{x} \in P} f(\mathbf{x}),$ where $P = \mathbf{x}_0 + \text{span}(\mathbf{p}_0, \dots, \mathbf{p}_{k-1})$

Conjugate gradients

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- ▶ $\mathbf{p}_0 = -\mathbf{r}_0$
- ▶ $\mathbf{p}_{k+1} = -\mathbf{r}_{k+1} + \beta_{k+1}\mathbf{p}_k$, where β_{k+1} guarantees that \mathbf{p}_k and \mathbf{p}_{k+1} are conjugate:

$$\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_{k+1} = \mathbf{p}_k^\top \mathbf{A} (-\mathbf{r}_{k+1} + \beta_{k+1} \mathbf{p}_k) = 0$$

$$\beta_{k+1} = \frac{\mathbf{p}_k^\top \mathbf{A} \mathbf{r}_{k+1}}{\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_k}$$

Pseudocode: basic version

```
def ConjugateGradientQuadratic(x0, A, b, eps):  
    r = A.dot(x0) - b  
    p = -r  
    while np.linalg.norm(r) > eps:  
        alpha = -r.dot(p) / p.dot(A.dot(p))  
        x = x + alpha * p  
        r = A.dot(x) - b  
        beta = r.dot(A.dot(p)) / p.dot(A.dot(p))  
        p = -r + beta * p  
    return x
```

Modifications of basic version

- How to compute α_k :

$$\alpha_k = -\frac{\mathbf{r}_k^\top \mathbf{p}_k}{\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_k} = -\frac{\mathbf{r}_k^\top (-\mathbf{r}_k + \beta_k \mathbf{p}_{k-1})}{\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_k} = \frac{\|\mathbf{r}_k\|_2^2}{\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_k}$$

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- How to compute β_k :

$$\beta_{k+1} = \frac{\mathbf{r}_{k+1}^\top \mathbf{A} \mathbf{p}_k}{\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_k} = \frac{\mathbf{r}_{k+1}^\top (\mathbf{r}_{k+1} - \mathbf{r}_k)}{(-\mathbf{r}_k + \beta_k \mathbf{p}_{k-1})^\top (\mathbf{r}_{k+1} - \mathbf{r}_k)} = \frac{\|\mathbf{r}_{k+1}\|_2^2}{\|\mathbf{r}_k\|_2^2}$$

Pseudocode: faster version

```
def ConjugateGradientQuadratic(x0, A, b, eps)
    r = A.dot(x0) - b
    p = -r
    while np.linalg.norm(r) > eps:
        alpha = r.dot(r) / p.dot(A.dot(p))
        x = x + alpha * p
        r_next = r + alpha * A.dot(p)
        beta = r_next.dot(r_next) / r.dot(r)
        p = -r_next + beta * p
        r = r_next
    return x
```

Why conjugate gradients are conjugate?

Theorem

Assume that after k iterations $\mathbf{x}_k \neq \mathbf{x}^*$. Then

1. $\langle \mathbf{r}_k, \mathbf{r}_i \rangle = 0, i = 1, \dots, k-1$
2. $\text{span}(\mathbf{r}_0, \dots, \mathbf{r}_k) = \text{span}(\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^k \mathbf{r}_0)$
3. $\text{span}(\mathbf{p}_0, \dots, \mathbf{p}_k) = \text{span}(\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^k \mathbf{r}_0)$
4. $\mathbf{p}_k^\top \mathbf{A} \mathbf{p}_i = 0, i = 1, \dots, k-1$

Krylov subspace

Definition

A subspace $\mathcal{K}_k(\mathbf{A}) = \text{span}(\mathbf{b}, \mathbf{A}\mathbf{b}, \dots, \mathbf{A}^{k-1}\mathbf{b})$ is called Krylov subspace.

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The main property

$$\mathbf{A}^{-1}\mathbf{b} \in \mathcal{K}_n(\mathbf{A})$$

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- ▶ $\mathbf{A}^{-1}\mathbf{b} = -\frac{1}{a_n}(\mathbf{A}^{n-1}\mathbf{b} + a_1\mathbf{A}^{n-2}\mathbf{b} + \dots + a_{n-1}\mathbf{b})$

Interpretation

- Search of the best approximation in the k -th Krylov subspace

$$\mathbf{x}_k = \arg \min_{\mathbf{x} \in \mathcal{K}_k} f(\mathbf{x})$$

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Brief description of the method

Search of the solution in the orthonormal Krylov basis

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- ▶ Convergence by objective:

$$\begin{aligned} f(\mathbf{x}) - f^* &= \frac{1}{2}\mathbf{x}^\top \mathbf{A} \mathbf{x} - \mathbf{b}^\top \mathbf{x} + \frac{1}{2}\|\mathbf{x}^*\|_{\mathbf{A}}^2 \\ &= \frac{1}{2}\|\mathbf{x}\|_{\mathbf{A}}^2 - \mathbf{x}^\top \mathbf{A} \mathbf{x}^* + \frac{1}{2}\|\mathbf{x}^*\|_{\mathbf{A}}^2 \\ &= \frac{1}{2}\|\mathbf{x} - \mathbf{x}^*\|_{\mathbf{A}}^2 \end{aligned}$$

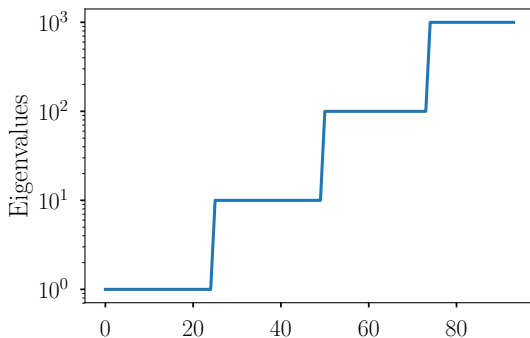
Convergence

Theorem

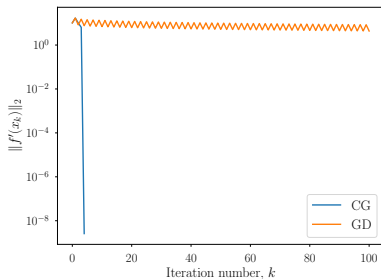
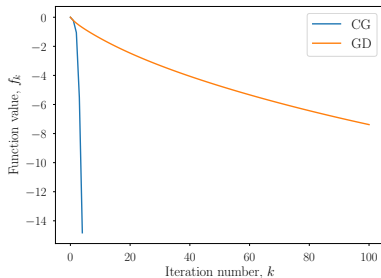
If matrix \mathbf{A} has only m different eigenvalues, then conjugate gradient method converges in m iterations.

Example

- ▶ $n = 100$
- ▶ Spectrum of \mathbf{A} : $\{1, 10, 100, 1000\}$
- ▶ $\kappa = 1000$



Convergence plot



Other estimates

- If no information about spectrum, then

$$f_k - f^* \leq C \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k$$

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- Fletcher-Reeves method

$$\beta_k = \frac{\|f'(\mathbf{x}_{k-1})\|_2^2}{\|f'(\mathbf{x}_{k-2})\|_2^2}$$

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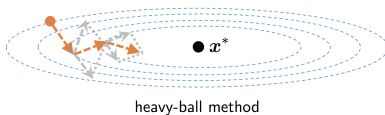
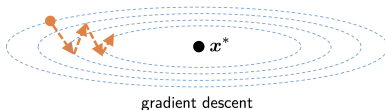
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- ▶ Hestenes-Stiefel method

$$\beta_k = \frac{\langle f'(\mathbf{x}_{k-1}), f'(\mathbf{x}_{k-1}) - f'(\mathbf{x}_{k-2}) \rangle}{\langle \mathbf{p}_{k-1}, f'(\mathbf{x}_{k-1}) - f'(\mathbf{x}_{k-2}) \rangle}$$

Heavy-ball method (B.T. Polyak, 1964)

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



This plot is from [this slides](#)

- ▶ Two-step non-monotone method
- ▶ CG is a particular case

Convergence

Theorem

If f is L -smooth strongly convex function, then

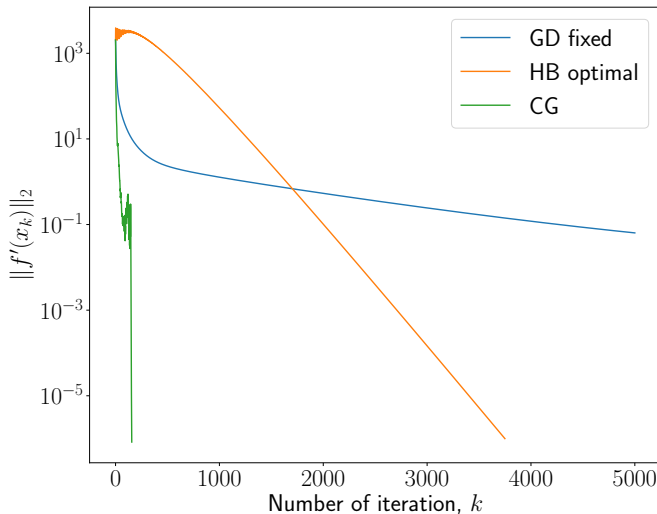
$\alpha_k = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}$ and $\beta_k = \max(|1 - \sqrt{\alpha_k L}|, |1 - \sqrt{\alpha_k \mu}|)^2$ gives

$$\left\| \begin{bmatrix} \mathbf{x}_{k+1} - \mathbf{x}^* \\ \mathbf{x}_k - \mathbf{x}^* \end{bmatrix} \right\|_2 \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \left\| \begin{bmatrix} \mathbf{x}_1 - \mathbf{x}^* \\ \mathbf{x}_0 - \mathbf{x}^* \end{bmatrix} \right\|_2$$

- ▶ Parameters depend on L and μ
- ▶ Faster than gradient descent
- ▶ Analogue of CG for non-quadratic but strongly convex function

Example

- ▶ $n = 100$
- ▶ Random strongly convex quadratic problem



Accelerated gradient method (Nesterov, 1983)

One of the form

$$\mathbf{y}_0 = \mathbf{x}_0$$

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

$$\mathbf{y}_{k+1} = \mathbf{x}_{k+1} + \frac{k}{k+3}(\mathbf{x}_{k+1} - \mathbf{x}_k)$$

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- Comparison with heavy-ball method

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- ▶ Comparison with heavy-ball method
- ▶ Non-monotone

Convergence

Theorem

If f is convex and L -smooth and step size $\alpha_k = \frac{1}{L}$, then accelerated gradient method converges as

$$f(\mathbf{x}_k) - f^* \leq \frac{2L\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2}{(k+1)^2} = \mathcal{O}(1/k^2)$$

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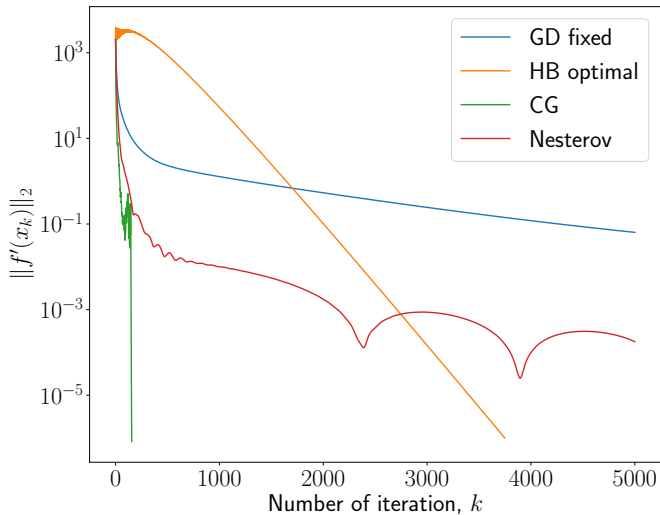
$$f(\mathbf{x}_k) - f^* \leq \frac{2L\|\mathbf{x}_0 - \mathbf{x}^*\|_2^2}{(k+1)^2} = \mathcal{O}(1/k^2)$$

Theorem

Accelerated gradient method used for minimizing strongly convex functions with step size $\alpha_k = \frac{1}{L}$ converges as

$$f(\mathbf{x}_k) - f^* \leq L\|\mathbf{x}_k - \mathbf{x}_0\|_2^2 \left(1 - \frac{1}{\sqrt{\kappa}}\right)^k$$

Example



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- ▶ How to process inexact gradients?
- ▶ How to select step sizes since in all methods they depend on unknown constants?
- ▶ How convergence speed is changed?

Summary

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