Conjugate gradient method

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

Strongly convex quadratics

Consider the following quadratic optimization problem:

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\min_{x \in \mathbb{R}^d} f(x) = \min_{x \in \mathbb{R}^d} \frac{1}{2} x^\top A x - b^\top x + c, \text{ where } A \in \mathbb{S}^d_{++}.
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Optimality conditions:

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\nabla f(x^*) = Ax^* - b = 0 \iff Ax^* = b
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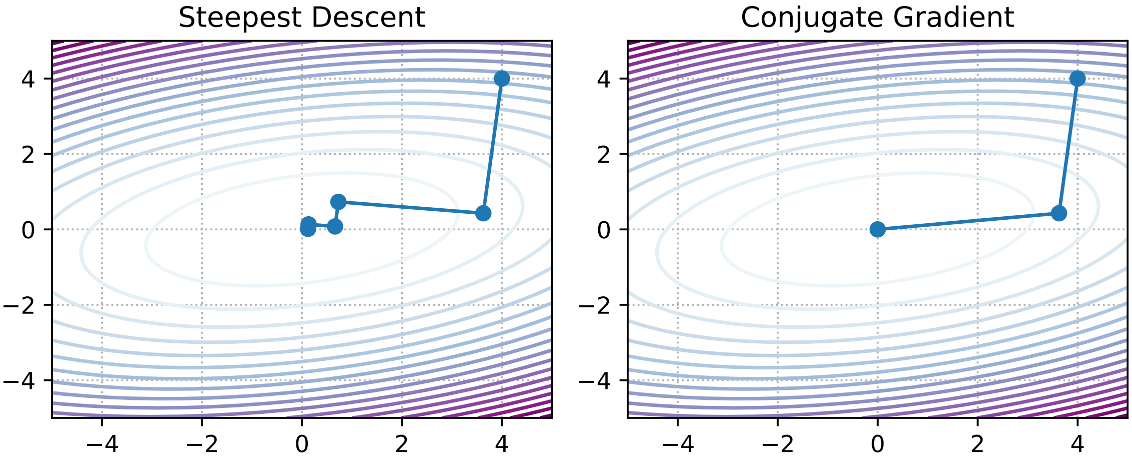

Overview of the CG method for the quadratic problem

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5) **Convergence Loop.** Repeat steps 2-4 until n directions are built, where n is the dimension of space (dimension of x).

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Exact line search:

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}^+} f(x_{k+1}) = \arg\min_{\alpha \in \mathbb{R}^+} f(x_k + \alpha d_k)$$

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$$f(x_k + \alpha d_k) = \frac{1}{2}(x_k + \alpha d_k)^\top A (x_k + \alpha d_k) - b^\top (x_k + \alpha d_k) + c$$
$$= \frac{1}{2}\alpha^2 d_k^\top A d_k + d_k^\top (A x_k - b)\alpha + \left(\frac{1}{2} x_k^\top A x_k + x_k^\top d_k + c\right)$$

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&= \frac{1}{2}\alpha^2 d_k^\top A d_k + d_k^\top (A x_k - b)\alpha + \left(\frac{1}{2} x_k^\top A x_k + x_k^\top d_k + c\right)
\end{aligned}$$

We consider $A \in \mathbb{S}^d_{++}$, so the point with zero derivative on this parabola is a minimum:

$$\left(d_k^\top A d_k\right)\alpha_k + d_k^\top (A x_k - b) = 0 \iff \alpha_k = -\frac{d_k^\top (A x_k - b)}{d_k^\top A d_k}$$

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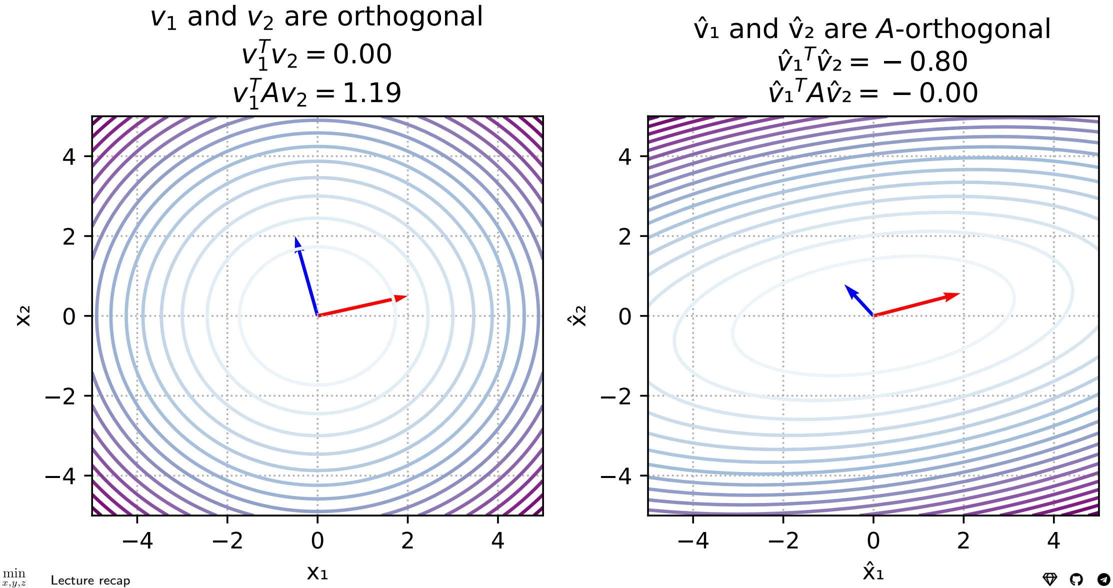
Lemma 1

All directions of construction using the procedure described above are orthogonal to each other:

$$d_i^\top A d_j = 0, \text{ if } i \neq j$$

$$d_i^\top A d_j > 0, \text{ if } i = j$$

A-orthogonality



Convergence of the CG method

Lemma 2

Suppose, we solve n-dimensional quadratic convex optimization problem. The conjugate directions method:

$$x_{k+1} = x_0 + \sum_{i=0}^{k} \alpha_i d_i,$$

where $\alpha_i = -\dfrac{d_i^\top (Ax_i - b)}{d_i^\top A d_i}$ taken from the line search, converges for at most n steps of the algorithm.

CG method in practice

In practice, the following formulas are usually used for the step α_k and the coefficient β_k:

$$\alpha_k = \frac{r_k^\top r_k}{d_k^\top A d_k} \qquad \beta_k = \frac{r_k^\top r_k}{r_{k-1}^\top r_{k-1}},$$

where $r_k = b - Ax_k$, since $x_{k+1} = x_k + \alpha_k d_k$ then $r_{k+1} = r_k - \alpha_k A d_k$. Also, $r_i^T r_k = 0, \forall i \neq k$ (**Lemma 5** from the lecture).

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Let's get an expression for β_k:

$$\beta_k = \frac{\nabla f\left(x_{k+1}\right)^\top A d_k}{d_k^\top A d_k} = -\frac{r_{k+1}^\top A d_k}{d_k^\top A d_k}$$

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Denominator: $d_k^\top A d_k = (r_k + \beta_{k-1} d_{k-1})^\top A d_k = \frac{1}{\alpha_k} r_k^\top (r_k - r_{k+1}) = \frac{1}{\alpha_k} r_k^\top r_k$

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Question

Why is this modification better than the standard version?

CG method in practice. Pseudocode

$\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$

if $\mathbf{r}_0$ is sufficiently small, then return $\mathbf{x}_0$ as the result

$\mathbf{d}_0 := \mathbf{r}_0$

$k := 0$

repeat

$$\alpha_k := \frac{\mathbf{r}_k^\top \mathbf{r}_k}{\mathbf{d}_k^\top \mathbf{A}\mathbf{d}_k}$$

$\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{d}_k$

$\mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k \mathbf{A}\mathbf{d}_k$

if $\mathbf{r}_{k+1}$ is sufficiently small, then exit loop

$$\beta_k := \frac{\mathbf{r}_{k+1}^\top \mathbf{r}_{k+1}}{\mathbf{r}_k^\top \mathbf{r}_k}$$

$\mathbf{d}_{k+1} := \mathbf{r}_{k+1} + \beta_k \mathbf{d}_k$

$k := k + 1$

end repeat

return $\mathbf{x}_{k+1}$ as the result

Non-linear conjugate gradient method

In case we do not have an analytic expression for a function or its gradient, we will most likely not be able to solve the one-dimensional minimization problem analytically. Therefore, step 2 of the algorithm is replaced by the usual line search procedure. But there is the following mathematical trick for the fourth point:

For two iterations, it is fair:

$$x_{k+1} - x_k = cd_k,$$

where c is some kind of constant. Then for the quadratic case, we have:

$$\nabla f(x_{k+1}) - \nabla f(x_k) = (Ax_{k+1} - b) - (Ax_k - b) = A(x_{k+1} - x_k) = cAd_k$$

Expressing from this equation the work $Ad_k = \dfrac{1}{c}\left(\nabla f(x_{k+1}) - \nabla f(x_k)\right)$, we get rid of the "knowledge" of the function in step definition β_k, then point 4 will be rewritten as:

$$\beta_k = \frac{\nabla f(x_{k+1})^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}{d_k^\top (\nabla f(x_{k+1}) - \nabla f(x_k))}.$$

This method is called the Polack - Ribier method.

Computational experiments

Run code in Colab. The code taken from .