

# Conjugate gradient method

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

## Strongly convex quadratics

Consider the following quadratic optimization problem:

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

Optimality conditions:

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

## Strongly convex quadratics

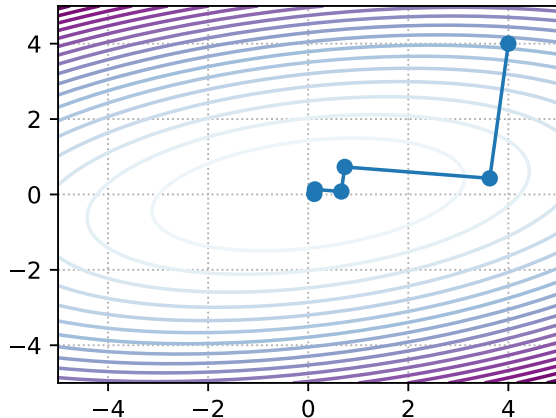
Consider the following quadratic optimization problem:

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

Optimality conditions:

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

### Steepest Descent



### Conjugate Gradient



# Overview of the CG method for the quadratic problem

1) **Initialization.**  $k = 0$  and  $x_k = x_0$ ,  $d_k = d_0 = -\nabla f(x_0)$ .

# Overview of the CG method for the quadratic problem

- 1) **Initialization.**  $k = 0$  and  $x_k = x_0$ ,  $d_k = d_0 = -\nabla f(x_0)$ .
- 2) **Optimal Step Length.** By the procedure of *line search* we find the optimal length of step. This involves calculate  $\alpha_k$  minimizing  $f(x_k + \alpha_k d_k)$ :

$$\alpha_k = -\frac{d_k^\top (Ax_k - b)}{d_k^\top A d_k}$$

# Overview of the CG method for the quadratic problem

- 1) **Initialization.**  $k = 0$  and  $x_k = x_0$ ,  $d_k = d_0 = -\nabla f(x_0)$ .
- 2) **Optimal Step Length.** By the procedure of *line search* we find the optimal length of step. This involves calculate  $\alpha_k$  minimizing  $f(x_k + \alpha_k d_k)$ :

$$\alpha_k = -\frac{d_k^\top (Ax_k - b)}{d_k^\top A d_k}$$

- 3) **Algorithm Iteration.** Update the position of  $x_k$  by moving in the direction  $d_k$ , with a step size  $\alpha_k$ :

$$x_{k+1} = x_k + \alpha_k d_k$$

# Overview of the CG method for the quadratic problem

- 1) **Initialization.**  $k = 0$  and  $x_k = x_0$ ,  $d_k = d_0 = -\nabla f(x_0)$ .
- 2) **Optimal Step Length.** By the procedure of *line search* we find the optimal length of step. This involves calculate  $\alpha_k$  minimizing  $f(x_k + \alpha_k d_k)$ :

$$\alpha_k = -\frac{d_k^\top (Ax_k - b)}{d_k^\top A d_k}$$

- 3) **Algorithm Iteration.** Update the position of  $x_k$  by moving in the direction  $d_k$ , with a step size  $\alpha_k$ :

$$x_{k+1} = x_k + \alpha_k d_k$$

- 4) **Direction Update.** Update the  $d_{k+1} = -\nabla f(x_{k+1}) + \beta_k d_k$ , where  $\beta_k$  is calculated by the formula:

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

# Overview of the CG method for the quadratic problem

- 1) **Initialization.**  $k = 0$  and  $x_k = x_0$ ,  $d_k = d_0 = -\nabla f(x_0)$ .
- 2) **Optimal Step Length.** By the procedure of *line search* we find the optimal length of step. This involves calculate  $\alpha_k$  minimizing  $f(x_k + \alpha_k d_k)$ :

$$\alpha_k = -\frac{d_k^\top (Ax_k - b)}{d_k^\top Ad_k}$$

- 3) **Algorithm Iteration.** Update the position of  $x_k$  by moving in the direction  $d_k$ , with a step size  $\alpha_k$ :

$$x_{k+1} = x_k + \alpha_k d_k$$

- 4) **Direction Update.** Update the  $d_{k+1} = -\nabla f(x_{k+1}) + \beta_k d_k$ , where  $\beta_k$  is calculated by the formula:

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

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



# Optimal Step Length

Exact line search:

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

# Optimal Step Length

Exact line search:

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

Let's find an analytical expression for the step  $\alpha_k$ :

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

# Optimal Step Length

Exact line search:

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

Let's find an analytical expression for the step  $\alpha_k$ :

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

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

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

## Direction Update

We update the direction in such a way that the next direction is  $A$  - orthogonal to the previous one:

$$d_{k+1} \perp_A d_k \iff d_{k+1}^\top A d_k = 0$$

## Direction Update

We update the direction in such a way that the next direction is  $A$  - orthogonal to the previous one:

$$d_{k+1} \perp_A d_k \iff d_{k+1}^\top A d_k = 0$$

Since  $d_{k+1} = -\nabla f(x_{k+1}) + \beta_k d_k$ , we choose  $\beta_k$  so that there is  $A$  - orthogonality:

$$d_{k+1}^\top A d_k = -\nabla f(x_{k+1})^\top A d_k + \beta_k d_k^\top A d_k = 0 \iff \beta_k = \frac{\nabla f(x_{k+1})^\top A d_k}{d_k^\top A d_k}$$

## Direction Update

We update the direction in such a way that the next direction is  $A$  - orthogonal to the previous one:

$$d_{k+1} \perp_A d_k \iff d_{k+1}^\top A d_k = 0$$

Since  $d_{k+1} = -\nabla f(x_{k+1}) + \beta_k d_k$ , we choose  $\beta_k$  so that there is  $A$  - orthogonality:

$$d_{k+1}^\top A d_k = -\nabla f(x_{k+1})^\top A d_k + \beta_k d_k^\top A d_k = 0 \iff \beta_k = \frac{\nabla f(x_{k+1})^\top A d_k}{d_k^\top A d_k}$$

### 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

$v_1$  and  $v_2$  are orthogonal

$$v_1^T v_2 = 0.00$$

$$v_1^T A v_2 = 1.19$$



$\hat{v}_1$  and  $\hat{v}_2$  are A-orthogonal

$$\hat{v}_1^T \hat{v}_2 = -0.80$$

$$\hat{v}_1^T A \hat{v}_2 = -0.00$$



# 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  $\alpha_i = -\frac{d_i^\top (Ax_i - b)}{d_i^\top Ad_i}$  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  $\alpha_k$  and the coefficient  $\beta_k$ :

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

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,  $r_i^\top r_k = 0, \forall i \neq k$  (**Lemma 5** from the lecture).

## CG method in practice

In practice, the following formulas are usually used for the step  $\alpha_k$  and the coefficient  $\beta_k$ :

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

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,  $r_i^\top r_k = 0, \forall i \neq k$  (**Lemma 5** from the lecture).

Let's get an expression for  $\beta_k$ :

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

## CG method in practice

In practice, the following formulas are usually used for the step  $\alpha_k$  and the coefficient  $\beta_k$ :

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

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,  $r_i^\top r_k = 0, \forall i \neq k$  (**Lemma 5** from the lecture).

Let's get an expression for  $\beta_k$ :

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

$$\text{Numerator: } r_{k+1}^\top A d_k = \frac{1}{\alpha_k} r_{k+1}^\top (r_k - r_{k+1}) = [r_{k+1}^\top r_k = 0] = -\frac{1}{\alpha_k} r_{k+1}^\top r_{k+1}$$

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

## CG method in practice

In practice, the following formulas are usually used for the step  $\alpha_k$  and the coefficient  $\beta_k$ :

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

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,  $r_i^\top r_k = 0, \forall i \neq k$  (**Lemma 5** from the lecture).

Let's get an expression for  $\beta_k$ :

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

$$\text{Numerator: } r_{k+1}^\top A d_k = \frac{1}{\alpha_k} r_{k+1}^\top (r_k - r_{k+1}) = [r_{k+1}^\top r_k = 0] = -\frac{1}{\alpha_k} r_{k+1}^\top r_{k+1}$$

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

### 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  $Ad_k = \frac{1}{c} (\nabla f(x_{k+1}) - \nabla f(x_k))$ , we get rid of the “knowledge” of the function in step definition  $\beta_k$ , 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 .