Conjugate gradient method

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Optimization methods. MIPT

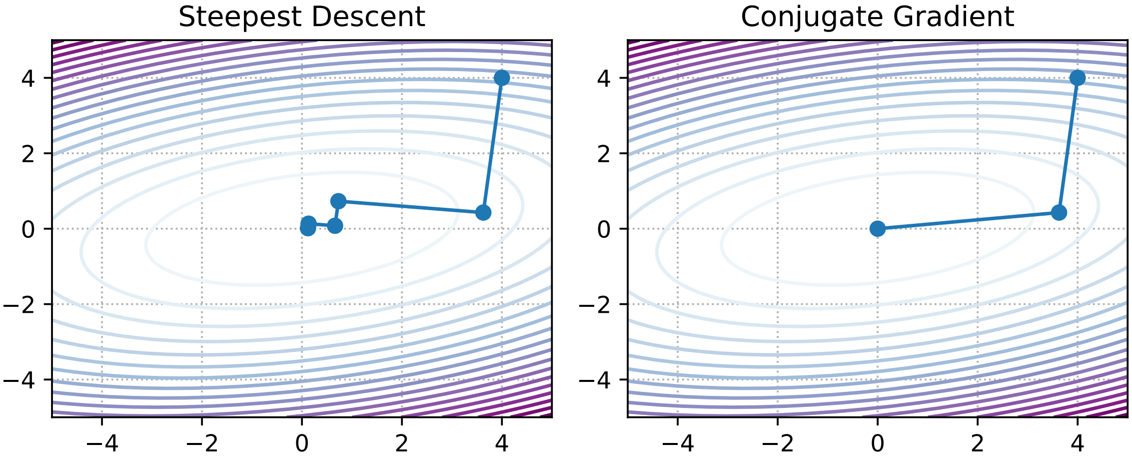
Strongly convex quadratics

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

$$Ax^* = b$$



Exact line search aka steepest descent

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

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot.
An interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

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Optimality conditions:

$$
\nabla f(x_k)^T \nabla f(x_{k+1}) = 0
$$

Optimal value for quadratics

$$
\nabla f(x_k)^\top A (x_k - \alpha \nabla f(x_k)) - \nabla f(x_k)^\top b = 0 \qquad \alpha_k = \frac{\nabla f(x_k)^T \nabla f(x_k)}{\nabla f(x_k)^T A \nabla f(x_k)}
$$

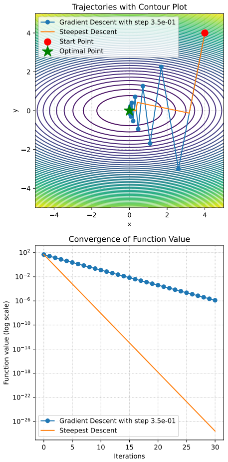
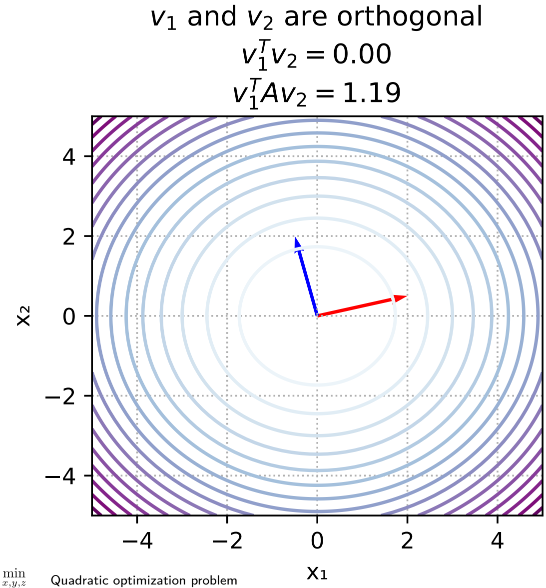
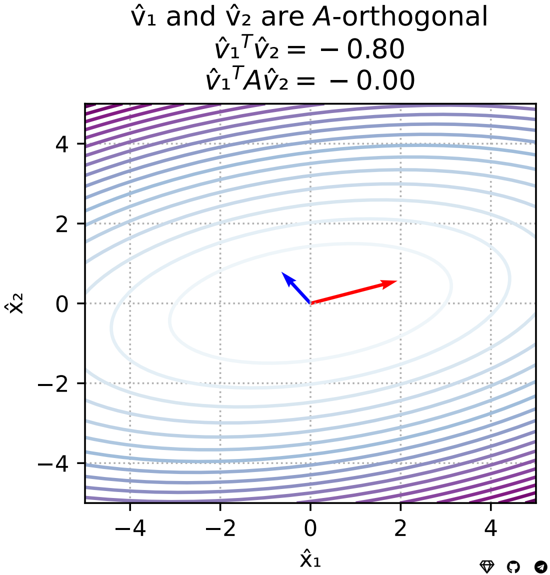


Figure 1: Steepest Descent

Open In Colab ♣

Conjugate directions. A-orthogonality.





Conjugate directions. A-orthogonality.

Suppose, we have two coordinate systems and some quadratic function $f(x) = \frac{1}{2}x^T I x$ looks just like on the left part of Figure 2, while in another coordinates it looks like $f(\hat{x}) = \frac{1}{2}\hat{x}^T A \hat{x}$, where $A \in \mathbb{S}^d_{++}$.

$$\frac{1}{2}x^T I x \qquad\qquad\qquad \frac{1}{2}\hat{x}^T A \hat{x}$$

Since $A = Q\Lambda Q^T$:

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A-orthogonal vectors

Vectors $x \in \mathbb{R}^d$ and $y \in \mathbb{R}^d$ are called A-orthogonal (or A-conjugate) if

$$x^T A y = 0 \qquad \Leftrightarrow \qquad x \perp_A y$$

When $A = I$, A-orthogonality becomes orthogonality.

Gram–Schmidt process

Idea of the method of conjugate directions

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4. update the direction: $d_{k+1} = -\nabla f(x_{k+1}) + \beta_k d_k$, where β_k is calculated by the formula:
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5. Repeat steps 2-4 until n directions are built, where n is the dimension of space (dimension of x).

Method of Conjugate Directions

If a set of vectors $d_1, \ldots, d_k$ - are A-conjugate (each pair of vectors is A-conjugate), these vectors are linearly independent. $A \in \mathbb{S}^n_{++}$.

Proof

We'll show, that if $\sum\limits_{i=1}^{k} \alpha_k d_k = 0$, than all coefficients should be equal to zero:

$$
\begin{aligned}
0 &= \sum_{i=1}^{n} \alpha_k d_k \\
&= d_j^\top A \left(\sum_{i=1}^{n} \alpha_k d_k \right) \\
&= \sum_{i=1}^{n} \alpha_k d_j^\top A d_k \\
&= \alpha_j d_j^\top A d_j + 0 + \ldots + 0
\end{aligned}
$$

Thus, $\alpha_j = 0$, for all other indices one have perform the same process

Conjugate Gradients

Conjugate Gradients

Conjugate Gradients

Conjugate gradient method

Conjugate Gradient = Conjugate Directions

+ Residuals as starting vectors for Gram–Schmidt

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

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

Convergence

Theorem 1. If matrix A has only r different eigenvalues, then the conjugate gradient method converges in r iterations.

Theorem 2. The following convergence bound holds

$$\|x_k - x^*\|_A \leq 2\left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}\right)^k \|x_0 - x^*\|_A,$$

where $\|x\|^2_A = x^\top Ax$ and $\kappa(A) = \frac{\lambda_1(A)}{\lambda_n(A)}$ is the conditioning number of matrix A, $\lambda_1(A) \geq ... \geq \lambda_n(A)$ are the eigenvalues of matrix A

Note: compare the coefficient of the geometric progression with its analog in gradient descent.

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.

Preconditioned conjugate gradient method