Conjugate gradients method

Optimization methods in machine learning

Aleksandr Beznosikov

Innopolis University

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Back to Cauchy again.

- Again we solve the system of linear equations:

$$Ax = b.$$

Try to find $x \in \mathbb{R}^d$

- $A \in \mathbb{R}^{d \times d}$ positive definite and $b \in \mathbb{R}^d$.

Conjugate directions

Definition of conjugate directions

A set of non-zero vectors $\{p_i\}_{i=0}^{n-1}$ is called conjugate with respect to a positive definite matrix A if for any $i \neq j \in \{0, \dots n-1\}$ follows

$$p_i^T A p_j = 0.$$

Conjugate directions: linear independence

Linear independence of conjugate directions

The conjugate vectors $\{p_i\}_{i=0}^{n-1}$ are linearly independent.

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- **Question:** what did we get? $\lambda_m = 0$.
- **Question:** what does that mean? We can run through all of them $m \neq i$ and get $\lambda_m = 0$, and then $p_i = 0$. Contradiction.

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- Take into account that $Ax^* = b$, then $p_j^T b = \lambda_j p_j^T A p_j$.
- Hence,

$$\lambda_j = \frac{p_j^T b}{p_j^T A p_j}.$$

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- **Question:** and can you see any problems? Everything is good except that we ourselves invented conjugate directions, we ourselves said that they exist, but how to get them in reality is still unclear.
- Let us start turning the reasoning into some iterative method:

$$\boxed{x^{k+1} = x^k + \alpha_k p_k.}$$

  That is, we are supposed to look for a new p_k at each iteration and find α_k for it.

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It turns out that $\alpha_i = \lambda_i$ if $x^0 = 0$. We need a formula to find α, since starting from 0 is good, but we may have a closer candidate as a starting point.

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- Then the following statement is true:

$$x^0 + \sum_{i=0}^{d-1} \alpha_i p_i = \sum_{i=0}^{d-1} \left(\frac{p_i^T A x^0}{p_i^T A p_i} + \alpha_i \right) p_i = \sum_{i=0}^{d-1} \lambda_i p_i = \sum_{i=0}^{d-1} \frac{p_i^T b}{p_i^T A p_i} p_i.$$

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- We get

$$\alpha_k = \frac{p_k^T (b - A x^0)}{p_k^T A p_k}.$$

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- The result is already normal, a little more can be done:

$$p_k^T A(x^k - x^0) = 0.$$

Question: why? $(x^k - x^0) = \sum_{i=0}^{k-1} \alpha_i p_i$, a p_i и p_k conjugate with respect to A.

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- Then we can do like this:

$$\alpha_k = \frac{p_k^T(b - Ax^k)}{p_k^T A p_k} = -\frac{p_k^T r_k}{p_k^T A p_k}.$$

Here we add notation: $r_k = Ax^k - b$.

Conjugate gradients method: physical meaning α

- Consider the step of the method $x^{k+1} = x^k + \alpha_k p_k$, as well as the function

$$f(x) = \frac{1}{2}x^T Ax - bx.$$

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- Consider:
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Where this function has a minimum on α^*? $\alpha^* = \frac{p_k^T(b - Ax^k)}{p_k^T A p_k} = \alpha_k$. That's physics — minimizing along p_k.

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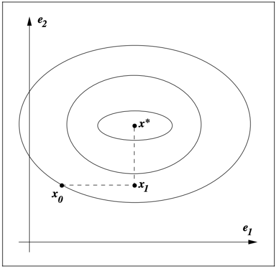

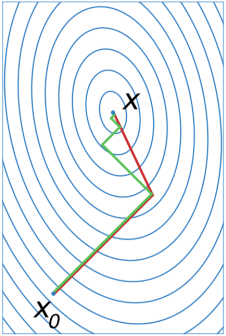

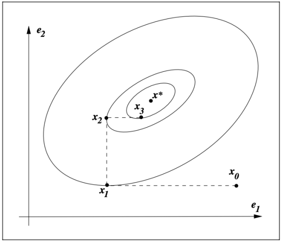

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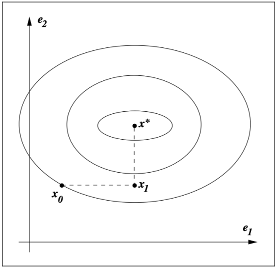

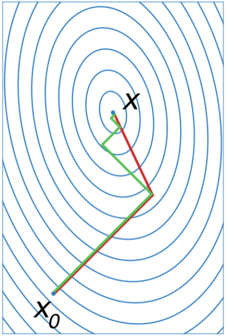

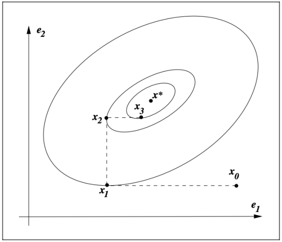

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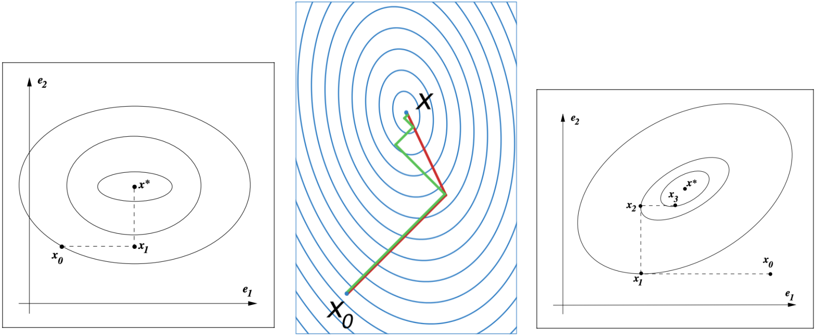

- The second picture shows that the conjugate directions are not orthogonal (in the usual sense of the word).
- The third picture shows that the directions are not conjugate with respect to A, which causes problems.

Conjugate gradients method: physical meaning p

Physical meaning of p

If $\{p_i\}_{i=0}^k$ conjugate directions, then for any $k \geq 0$ and $i \leq k$ it holds:

$$r_{k+1}^T p_i = 0 \text{ same as } \langle \nabla f(x^{k+1}), p_i \rangle.$$

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Whence, by virtue of choice α_k
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For $i < k$:
$$p_i^T r_{k+1} = p_i^T r_k + \alpha_k p_i^T Ap_k = 0.$$

Question: why?

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Question: why? By virtue of induction and conjugation.

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$$p_k = -r_k + \beta_k p_{k-1},$$

where β_k is some coefficient. To find p_k you only need to know p_{k-1} and r_k, and you can already forget the old r_i and p_i (they are accounted for in x^k).

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- **Question:** how to find β_k? The conjugacy of p_k and p_{k-1}:

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  from where

$$\beta_k = \frac{p_{k-1}^T A r_k}{p_{k-1}^T A p_{k-1}}.$$

Conjugate gradients method

Алгоритм 1 Conjugate gradients method

Input: starting point $x^0 \in \mathbb{R}^d$, $r_0 = Ax_0 - b$, $p_0 = -r_0$ number of iterations K

for $k = 0, 1, \ldots, K-1$ **do**

$\quad \alpha_k = -\frac{r_k^T p_k}{p_k^T A p_k}$

$\quad x^{k+1} = x^k + \alpha_k p_k$

$\quad r_{k+1} = Ax^{k+1} - b$

$\quad \beta_{k+1} = \frac{r_{k+1}^T A p_k}{p_k^T A p_k}$

$\quad p_{k+1} = -r_{k+1} + \beta_{k+1} p_k$

end for

Output: x^K

Conjugate gradients method

Алгоритм 2 Conjugate gradients method

Input: starting point $x^0 \in \mathbb{R}^d$, $r_0 = Ax_0 - b$, $p_0 = -r_0$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**

2: $\alpha_k = -\frac{r_k^T p_k}{p_k^T A p_k}$

3: $x^{k+1} = x^k + \alpha_k p_k$

4: $r_{k+1} = Ax^{k+1} - b$

5: $\beta_{k+1} = \frac{r_{k+1}^T A p_k}{p_k^T A p_k}$

6: $p_{k+1} = -r_{k+1} + \beta_{k+1} p_k$

7: **end for**

Output: x^K

Question: why the gradients?

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for $k = 0, 1, \ldots, K-1$ **do**

$\quad \alpha_k = -\frac{r_k^T p_k}{p_k^T A p_k}$

$\quad x^{k+1} = x^k + \alpha_k p_k$

$\quad r_{k+1} = Ax^{k+1} - b$

$\quad \beta_{k+1} = \frac{r_{k+1}^T A p_k}{p_k^T A p_k}$

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end for

Output: x^K

Question: why the gradients? $r_k = Ax^k - b = \nabla f(x^k)$. That's worth remembering.

Conjugate gradients method: proof

- **Question:** maybe we've already proved the convergence estimate?

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- **Question:** maybe we've already proved the convergence estimate? Close to this, we know that if all $\{p_i\}$ are conjugate directions, then we have enough d steps to recover the coefficients for x^* in the basis from $\{p_i\}$.

Conjugate gradients method: proof

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- **Question:** Do we know that all $\{p_i\}$ are conjugate?

Conjugate gradients method: proof

- **Question:** maybe we've already proved the convergence estimate? Close to this, we know that if all $\{p_i\}$ are conjugate directions, then we have enough d steps to recover the coefficients for x^* in the basis from $\{p_i\}$.
- **Question:** Do we know that all $\{p_i\}$ are conjugate? No, we only know that p_k and p_{k-1} are conjugate by virtue of the selection of β_k. We need to show a broader statement:

$$\text{For all } k \geq 1 \text{ for all } i < k \text{ it holds } p_k^T A p_i = 0.$$

Conjugate gradients method: proof

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- **Step:** Let us prove for $k+1$. p_{k+1} и p_k are conjugate by virtue of the selection of β_{k+1}. Consider $i < k$:

$$p_{k+1}^T A p_i = -r_{k+1}^T A p_i + \beta_{k+1} p_k^T A p_i = -r_{k+1}^T A p_i.$$

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Question: why is the second transition valid?

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Question: why is the second transition valid? Because of the induction assumption and the fact that $i < k$.

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  Question: why is the second transition valid? Because of the induction assumption and the fact that $i < k$.
- It remains to show that $r_{k+1}^T A p_i = 0$. Let us remember that.

Conjugate gradients method: proof

- We prove that for $k \geq 0$ the following holds $\text{span}\{r_0, \ldots r_k\} = \text{span}\{r_0, \ldots A^k r_0\}$ и $\text{span}\{p_0, \ldots p_k\} = \text{span}\{r_0, \ldots A^k r_0\}$.

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  Note that from the second assumption:
  $A^{k+1} r_0 = A(A^k r_0) \in \text{span}\{Ap_0, \ldots Ap_k\}$.

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  The inclusion of both sides is proven.

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- According to what has just been proven:

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- From what's just been proven.
$$Ap_i \in \mathrm{span}\{Ar_0, \ldots, A^{i+1} r_0\} \subseteq \mathrm{span}\{p_0, \ldots, p_{i+1}\}.$$
- But all p_j for j from 0 to i are orthogonal to r^{k+1} by virtue of the fact that $\{p_j\}$ are conjugate by virtue of the induction assumption. So we have what we need.

Conjugate gradients method: convergence

Theorem on convergence of conjugate gradients method

The conjugate gradient method for solving a system of linear equations with a square positive definite matrix of size d finds an exact solution in at most d iterations.

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Equivalent to minimizing a strong convex quadratic problem.

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Conjugate gradients method: convergence

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- The key word in the previous paragraph is «*exact*». The method of conjugate gradients can be stopped earlier, it is iterative. And this is already more interesting.

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- The key word in the previous paragraph is «*exact*». The method of conjugate gradients can be stopped earlier, it is iterative. And this is already more interesting.
- There are convergence features that make the method even faster.

Conjugate gradients method: convergence

Theorem on convergence of conjugate gradients method

The conjugate gradient method for solving a system of linear equations with a square positive definite matrix of size d finds an exact solution in at most r iterations, where r is the number of unique eigenvalues of the matrix.

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Theorem on convergence of conjugate gradients method

The method of conjugate gradients for solving a system of linear equations with a square positive definite matrix of size d has the following convergence estimate:

$$\|x^k - x^*\|_A^2 \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k \|x^0 - x^*\|_A^*.$$

Here $\|x\|_A^2 = x^T A x$ and $\kappa(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$.

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Question: and for which method is a similar estimate valid?

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Here $\|x\|_A^2 = x^T Ax$ and $\kappa(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$.

Question: and for which method is a similar estimate valid? Accelerated

Conjugate gradients method

Алгоритм 4 Conjugate gradients method (classical version)

Input: starting point $x^0 \in \mathbb{R}^d$, $r_0 = Ax_0 - b$, $p_0 = -r_0$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**

2: $\alpha_k = \frac{r_k^T r_k}{p_k^T A p_k}$

3: $x^{k+1} = x^k + \alpha_k p_k$

4: $r_{k+1} = r_k + \alpha_k A p_k$

5: $\beta_{k+1} = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$

6: $p_{k+1} = -r_{k+1} + \beta_{k+1} p_k$

7: **end for**

Output: x^K

Conjugate gradients method

Алгоритм 5 Conjugate gradients method (classical version)

Input: starting point $x^0 \in \mathbb{R}^d$, $r_0 = Ax_0 - b$, $p_0 = -r_0$ number of iterations K

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6: $p_{k+1} = -r_{k+1} + \beta_{k+1} p_k$

7: **end for**

Output: x^K

Recall that the gradient is $r_k = Ax^k - b = \nabla f(x^k)$.

Conjugate gradients method for general problems

Алгоритм 6 Conjugate gradients method (Fletcher - Reeves)

Input: staring point $x^0 \in \mathbb{R}^d$, $p_0 = -\nabla f(x_0)$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**
2: $\alpha_k = ?$
3: $x^{k+1} = x^k + \alpha_k p_k$
4: $\beta_{k+1} = \frac{\langle \nabla f(x^{k+1}), \nabla f(x^{k+1}) \rangle}{\langle \nabla f(x^k), \nabla f(x^k) \rangle}$
5: $p_{k+1} = -\nabla f(x^{k+1}) + \beta_{k+1} p_k$
6: **end for**

Output: x^K

Conjugate gradients method for general problems

Алгоритм 7 Conjugate gradients method (Fletcher - Reeves)

Input: staring point $x^0 \in \mathbb{R}^d$, $p_0 = -\nabla f(x_0)$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**
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3: $x^{k+1} = x^k + \alpha_k p_k$
4: $\beta_{k+1} = \frac{\langle \nabla f(x^{k+1}), \nabla f(x^{k+1}) \rangle}{\langle \nabla f(x^k), \nabla f(x^k) \rangle}$
5: $p_{k+1} = -\nabla f(x^{k+1}) + \beta_{k+1} p_k$
6: **end for**

Output: x^K

Question: how to find the step α_k?

Conjugate gradients method for general problems

Алгоритм 8 Conjugate gradients method (Fletcher - Reeves)

Input: staring point $x^0 \in \mathbb{R}^d$, $p_0 = -\nabla f(x_0)$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**

2: $\quad \alpha_k = ?$

3: $\quad x^{k+1} = x^k + \alpha_k p_k$

4: $\quad \beta_{k+1} = \frac{\langle \nabla f(x^{k+1}), \nabla f(x^{k+1}) \rangle}{\langle \nabla f(x^k), \nabla f(x^k) \rangle}$

5: $\quad p_{k+1} = -\nabla f(x^{k+1}) + \beta_{k+1} p_k$

6: **end for**

Output: x^K

Question: how to find the step α_k? We want to minimize along the direction p_k, we get a one-dimensional function depending on α. Let's remember about dichotomy and the golden ratio.

Conjugate gradients method for general problems

Алгоритм 9 Conjugate gradients method (Polak - Ribiere)

Input: starting point $x^0 \in \mathbb{R}^d$, $p_0 = -\nabla f(x_0)$ number of iterations K

1: **for** $k = 0, 1, \ldots, K-1$ **do**

2: $\alpha_k =$ Linesearch

3: $x^{k+1} = x^k + \alpha_k p_k$

4: $\beta_{k+1} = \frac{\langle \nabla f(x^{k+1}), \nabla f(x^{k+1}) - \nabla f(x^k) \rangle}{\langle \nabla f(x^k), \nabla f(x^k) \rangle}$

5: $p_{k+1} = -\nabla f(x^{k+1}) + \beta_{k+1} p_k$

6: **end for**

Output: x^K

Conjugate gradients method for general problems

- Generalizations work well, but the guarantees in theory are far from optimistic.

Conjugate gradients method for general problems

- Generalizations work well, but the guarantees in theory are far from optimistic.
- It is better to do «restarts» sometimes. In this case, «restarts» involve sometimes taking $\beta_k = 0$, forgetting history. **Question:** which method iterates then?

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- Generalizations work well, but the guarantees in theory are far from optimistic.
- It is better to do «restarts» sometimes. In this case, «restarts» involve sometimes taking $\beta_k = 0$, forgetting history. **Question:** which method iterates then? Gradient descent.

Conjugate gradients method for general problems

- Generalizations work well, but the guarantees in theory are far from optimistic.
- It is better to do «restarts» sometimes. In this case, «restarts» involve sometimes taking $\beta_k = 0$, forgetting history. **Question:** which method iterates then? Gradient descent.
- Suitable as a «starter» method, by which from an initial unknown point, we can get close, but not exactly to the solution.