MATH 4211/6211 – Optimization

Conjugate Gradient Method

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Motivation: Design an improved gradient method without storing or inverting Hessian.

Definition. Let $\boldsymbol{Q} \succ \boldsymbol{0}$. The directions $\boldsymbol{d}^{(0)}, \boldsymbol{d}^{(1)}, \dots, \boldsymbol{d}^{(k)}$ are called (mutually) $\boldsymbol{Q}$-**conjugate** if ${\boldsymbol{d}^{(i)}}^\top \boldsymbol{Q} \boldsymbol{d}^{(j)} = 0$ for all $i \neq j$.

Remark: We can define $\boldsymbol{Q}$-inner product by $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{Q}} := \boldsymbol{x}^\top \boldsymbol{Q} \boldsymbol{y}$. Then $\boldsymbol{x}$ and $\boldsymbol{y}$ are $\boldsymbol{Q}$-conjugate if they are orthogonal, i.e., $\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{Q}} = 0$, in the sense of $\boldsymbol{Q}$-inner product. Also note that $\langle \boldsymbol{x}, \boldsymbol{x} \rangle_{\boldsymbol{Q}} = \|\boldsymbol{x}\|_{\boldsymbol{Q}}^2$.

Lemma. Let $\boldsymbol{Q} \succ \mathbf{0}$ be an n-by-n positive definite matrix. If $\boldsymbol{d}^{(0)}, \ldots, \boldsymbol{d}^{(k)}$ ($k \leq n-1$) are $\boldsymbol{Q}$-conjugate, then they are linearly independent.

Proof. Suppose $\alpha_0 \boldsymbol{d}^{(0)} + \alpha_1 \boldsymbol{d}^{(1)} + \cdots + \alpha_k \boldsymbol{d}^{(k)} = \mathbf{0}$. For each i, multiplying ${\boldsymbol{d}^{(i)}}^\top \boldsymbol{Q}$ yields $\alpha_i {\boldsymbol{d}^{(i)}}^\top \boldsymbol{Q} \boldsymbol{d}^{(i)} = 0$ due to the mutual $\boldsymbol{Q}$-conjugacy. Hence $\alpha_i = 0$.

Example. Find a set of $\boldsymbol{Q}$-conjugate directions $\boldsymbol{d}^{(0)}, \boldsymbol{d}^{(1)}, \boldsymbol{d}^{(2)} \in \mathbb{R}^3$ where

$$\boldsymbol{Q} = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 4 & 2 \\ 1 & 2 & 3 \end{bmatrix}$$

Solution. We first check that $\boldsymbol{Q} \succ \mathbf{0}$ by its leading principal minors:

$$3 > 0, \qquad \begin{vmatrix} 3 & 0 \\ 0 & 4 \end{vmatrix} = 12 > 0, \qquad \begin{vmatrix} 3 & 0 & 1 \\ 0 & 4 & 2 \\ 1 & 2 & 3 \end{vmatrix} = 22 > 0$$

We can set $\boldsymbol{d}^{(0)}$ to any nonzero vector. For instance, we can set with $\boldsymbol{d}^{(0)} = [1, 0, 0]^\top$.

Then we need to find $\boldsymbol{d}^{(1)} = [d_1^{(1)}, d_2^{(1)}, d_3^{(1)}]^\top$ such that

$$\boldsymbol{d}^{(1)\top}\boldsymbol{Q}\boldsymbol{d}^{(0)} = 3d_1^{(1)} + d_3^{(1)} = 0$$

For example, we can set $d_1^{(1)} = 1$, $d_2^{(1)} = 0$, and $d_3^{(1)} = -3$, and hence $\boldsymbol{d}^{(1)} = [1, 0, -3]^\top$.

Finally we need $\boldsymbol{d}^{(2)} = [d_1^{(2)}, d_2^{(2)}, d_3^{(2)}]^\top$ such that

$$\boldsymbol{d}^{(2)\top}\boldsymbol{Q}\boldsymbol{d}^{(0)} = 3d_1^{(2)} + d_3^{(2)} = 0$$
$$\boldsymbol{d}^{(2)\top}\boldsymbol{Q}\boldsymbol{d}^{(1)} = -6d_2^{(2)} - 8d_3^{(2)} = 0$$

from which we solve for $\boldsymbol{d}^{(2)}$ to get $\boldsymbol{d}^{(2)} = [1, 4, -3]^\top$.

In the end, we obtain $\boldsymbol{d}^{(0)} = [1, 0, 0]^\top, \boldsymbol{d}^{(1)} = [1, 0, -3]^\top, \boldsymbol{d}^{(2)} = [1, 4, -3]^\top$.

The idea of **Gram-Schmidt process** can be used to produce $\boldsymbol{Q}$-conjugate directions:

First select an arbitrary set of linearly independent directions $\boldsymbol{v}^{(0)}, \dots, \boldsymbol{v}^{(n-1)}$. Set $\boldsymbol{d}^{(0)} = \boldsymbol{v}^{(0)} / \|\boldsymbol{v}^{(0)}\|_{\boldsymbol{Q}}$.

Suppose we have got $\boldsymbol{d}^{(0)}, \dots, \boldsymbol{d}^{(k-1)}$, then compute $\boldsymbol{d}^{(k)}$ by

$$\boldsymbol{d}^{(k)} = \boldsymbol{v}^{(k)} - \sum_{i=0}^{k-1} (\boldsymbol{v}^{(k)\top} \boldsymbol{Q} \boldsymbol{d}^{(i)}) \boldsymbol{d}^{(i)}$$

and then normalize $\boldsymbol{d}^{(k)} \leftarrow \boldsymbol{d}^{(k)} / \|\boldsymbol{d}^{(k)}\|_{\boldsymbol{Q}}$.

It is easy to verify that $\boldsymbol{d}^{(k)\top} \boldsymbol{Q} \boldsymbol{d}^{(i)} = 0$ for $i = 0, \dots, k-1$.

Now we consider using conjugate directions $\boldsymbol{d}^{(0)}, \dots, \boldsymbol{d}^{(n-1)}$ (assume given) to solve

$$\underset{\boldsymbol{x}\in\mathbb{R}^n}{\text{minimize}}\; f(\boldsymbol{x}), \quad \text{where} \quad f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} - \boldsymbol{b}^\top \boldsymbol{x}$$

Basic conjugate direction algorithm: For $k = 0, 1, \dots, n-1$, do

$$\begin{aligned} \boldsymbol{g}^{(k)} &= \nabla f(\boldsymbol{x}^{(k)}) = \boldsymbol{Q}\boldsymbol{x}^{(k)} - \boldsymbol{b} \\ \alpha_k &= -\frac{\boldsymbol{g}^{(k)\top}\boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}} \\ \boldsymbol{x}^{(k+1)} &= \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)} \end{aligned}$$

Note that above $\alpha_k = \arg\min_{\alpha>0} f(\boldsymbol{x}^{(k)} + \alpha \boldsymbol{d}^{(k)})$ is the steepest step size.

Theorem. The basic conjugate direction algorithm converges in n steps.

Proof. First keep in mind that

$$\begin{aligned} \boldsymbol{x}^{(n)} &= \boldsymbol{x}^{(n-1)} + \alpha_{n-1}\boldsymbol{d}^{(n-1)} \\ &= \dots \\ &= \boldsymbol{x}^{(0)} + \alpha_0\boldsymbol{d}^{(0)} + \cdots + \alpha_{n-1}\boldsymbol{d}^{(n-1)} \end{aligned}$$

Now suppose $\boldsymbol{x}^* - \boldsymbol{x}^{(0)} = \beta_0\boldsymbol{d}^{(0)} + \cdots + \beta_{n-1}\boldsymbol{d}^{(n-1)}$ (this is possible since $\boldsymbol{d}^{(0)}, \dots, \boldsymbol{d}^{(n-1)}$ is a basis of $\mathbb{R}^n$.)

Now we will check that $\beta_k = \alpha_k$ for all $k = 0, \dots, n-1$: multiplying $\boldsymbol{x}^* - \boldsymbol{x}^{(0)}$ by ${\boldsymbol{d}^{(k)}}^\top \boldsymbol{Q}$, we obtain ${\boldsymbol{d}^{(k)}}^\top \boldsymbol{Q}(\boldsymbol{x}^* - \boldsymbol{x}^{(0)}) = \beta_k {\boldsymbol{d}^{(k)}}^\top \boldsymbol{Q}\boldsymbol{d}^{(k)}$.

We can solve for β_k:

$$\begin{aligned}\beta_k &= \frac{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}(\boldsymbol{x}^* - \boldsymbol{x}^{(0)})}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}} \\ &= \frac{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}[(\boldsymbol{x}^* - \boldsymbol{x}^{(k)}) + (\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(0)})]}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}} \\ &= -\frac{\boldsymbol{d}^{(k)\top}\boldsymbol{g}^{(k)}}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}} = \alpha_k\end{aligned}$$

where the 3rd equality above is due to $\boldsymbol{Q}(\boldsymbol{x}^* - \boldsymbol{x}^{(k)}) = -(\boldsymbol{Q}\boldsymbol{x}^{(k)} - \boldsymbol{b}) = -\boldsymbol{g}^{(k)}$ and that $\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(0)} = \sum_{j=0}^{k-1} \alpha_j \boldsymbol{d}^{(j)}$ which is a linear combination of $\left\{\boldsymbol{d}^{(j)} : 0 \le j \le k-1\right\}$ that are all $\boldsymbol{Q}$-conjugate with $\boldsymbol{d}^{(k)}$.

Therefore $\boldsymbol{x}^{(n)} - \boldsymbol{x}^{(0)} = \boldsymbol{x}^* - \boldsymbol{x}^{(0)}$, hence $\boldsymbol{x}^{(n)} = \boldsymbol{x}^*$.

Lemma. For any $k = 0, 1, \dots, n-1$, there are

$$\boldsymbol{g}^{(k+1)^\top} \boldsymbol{d}^{(j)} = 0, \quad \forall\, j \le k.$$

Proof. Multiplying both sides of $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)}$ by $\boldsymbol{Q}$:

$$\boldsymbol{Q}\boldsymbol{x}^{(k+1)} = \boldsymbol{Q}\boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{Q}\boldsymbol{d}^{(k)}$$

which yields $\boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \alpha_k \boldsymbol{Q}\boldsymbol{d}^{(k)}$ since $\boldsymbol{g}^{(k)} = \boldsymbol{Q}\boldsymbol{x}^{(k)} - \boldsymbol{b}$ for all k.

We will use this and induction to prove the claim.

Proof (cont). It is easy to show ${g^{(1)}}^\top d^{(0)} = 0$.

Suppose the claim holds for k, i.e.,

$$ {g^{(k)}}^\top d^{(i)} = 0, \quad \text{for } i = 0, 1, \ldots, k-1. $$

Then ${g^{(k+1)}}^\top d^{(i)} = {g^{(k)}}^\top d^{(i)} + \alpha_k {d^{(k)}}^\top Q d^{(i)}$.

If $i \le k-1$, then ${g^{(k+1)}}^\top d^{(i)} = 0$ due to induction hypothesis and Q-conjugacy. If $i = k$, then ${g^{(k+1)}}^\top d^{(k)} = {g^{(k)}}^\top d^{(k)} + \alpha_k {d^{(k)}}^\top Q d^{(k)} = 0$ due to the definition of α_k. Therefore the claim also holds for $k+1$.

Conjugate direction method can also be interpreted as an "expanding subspace" method:

Denote $\boldsymbol{D}^{(k)} := \text{span}\{\boldsymbol{d}^{(0)}, \boldsymbol{d}^{(1)}, \dots, \boldsymbol{d}^{(k-1)}\}$. Then $\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(0)} \in \boldsymbol{D}^{(k)}$, and $\boldsymbol{x}^{(k)}$ is selected such that

$$\boldsymbol{x}^{(k)} = \underset{\boldsymbol{x} \in \boldsymbol{x}^{(0)} + \boldsymbol{D}^{(k)}}{\arg\min} f(\boldsymbol{x})$$

Therefore $\boldsymbol{D}^{(0)} \subset \boldsymbol{D}^{(1)} \subset \cdots \subset \boldsymbol{D}^{(n)} = \mathbb{R}^n$, and $\boldsymbol{x}^{(n)}$ is the minimizer of $f(\boldsymbol{x})$ over $\boldsymbol{D}^{(n)} = \mathbb{R}^n$.

Now we have one more practical issue to solve: how to get $\boldsymbol{Q}$-conjugate directions?

Conjugate gradient method generates a new conjugate direction in every iteration.

More specifically, suppose we have got $\boldsymbol{x}^{(k)}$ and $\boldsymbol{d}^{(k)}$, then compute

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)}$$

where $\alpha_k = -\frac{\boldsymbol{g}^{(k)\top}\boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}}$.

The new conjugate direction is given by

$$\boldsymbol{d}^{(k+1)} = -\boldsymbol{g}^{(k+1)} + \beta_k \boldsymbol{d}^{(k)}$$

where $\beta_k = \frac{\boldsymbol{g}^{(k+1)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)\top}\boldsymbol{Q}\boldsymbol{d}^{(k)}}$.

Conjugate gradient method for quadratic function $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} - \boldsymbol{b}^\top \boldsymbol{x}$.

First give initial $\boldsymbol{x}^{(0)}$, compute $\boldsymbol{g}^{(0)} = \nabla f(\boldsymbol{x}^{(0)})$ and set $\boldsymbol{d}^{(0)} = -\boldsymbol{g}^{(0)}$.

For $k = 0, 1, 2, \dots, n-1$, iterate

$$
\begin{aligned}
\alpha_k &= -\frac{\boldsymbol{g}^{(k)\top} \boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)\top} \boldsymbol{Q} \boldsymbol{d}^{(k)}} \\
\boldsymbol{x}^{(k+1)} &= \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)} \\
\boldsymbol{g}^{(k+1)} &= \nabla f(\boldsymbol{x}^{(k)}) = \boldsymbol{Q}\boldsymbol{x}^{(k+1)} - \boldsymbol{b} \\
\beta_k &= \frac{\boldsymbol{g}^{(k+1)\top} \boldsymbol{Q} \boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)\top} \boldsymbol{Q} \boldsymbol{d}^{(k)}} \\
\boldsymbol{d}^{(k+1)} &= -\boldsymbol{g}^{(k+1)} + \beta_k \boldsymbol{d}^{(k)}
\end{aligned}
$$

Most expensive computation is $\boldsymbol{Qd}^{(k)}$, which requires n^2 multiplications and $n(n-1) = O(n^2)$ summations. This is done 1 time in every iteration.

We also need storing $\boldsymbol{Qx}^{(k)}$ which is updated for every k by $\boldsymbol{Qx}^{(k+1)} = \boldsymbol{Qx}^{(k)} + \alpha_k \boldsymbol{Qd}^{(k)}$.

Also, $\boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \alpha_k \boldsymbol{Qd}^{(k)}$ can be updated by vector summation.

But all these computations are of order $O(n)$.

Now we show CG converges in n steps for quadratic $f(\boldsymbol{x})$. To this end, we only need the following result.

Proposition. The directions $\boldsymbol{d}^{(0)}, \boldsymbol{d}^{(1)}, \dots, \boldsymbol{d}^{(n-1)}$ generated by CG algorithm are $\boldsymbol{Q}$-conjugate.

Proof. We prove this by induction.

First, ${\boldsymbol{d}^{(1)}}^\top \boldsymbol{Q}\boldsymbol{d}^{(0)} = (-\boldsymbol{g}^{(1)} + \beta_0 \boldsymbol{d}^{(0)})^\top \boldsymbol{Q}\boldsymbol{d}^{(0)} = 0$ due to defintion of β_0.

Now assume $\boldsymbol{d}^{(0)}, \dots, \boldsymbol{d}^{(k)}$ are $\boldsymbol{Q}$-conjugate. We need to show $\boldsymbol{d}^{(k+1)}$ is $\boldsymbol{Q}$-conjugate with all of them.

Proof (cont).

We need the following facts:

- $\boldsymbol{d}^{(k)} = -\boldsymbol{g}^{(k)} + \beta_{k-1}\boldsymbol{d}^{(k-1)}$, $\forall\, k$, by definition of $\boldsymbol{d}^{(k)}$ in CG.

- $\boldsymbol{g}^{(k+1)} = \boldsymbol{g}^{(k)} + \alpha_k \boldsymbol{Q}\boldsymbol{d}^{(k)}$, $\forall\, k$, by $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \alpha_k \boldsymbol{d}^{(k)}$ in CG.

- ${\boldsymbol{g}^{(k+1)}}^\top \boldsymbol{d}^{(j)} = 0$, $\forall\, j \le k$, by previous lemma.

- ${\boldsymbol{g}^{(k+1)}}^\top \boldsymbol{g}^{(j)} = 0$, $\forall\, j \le k$, since ${\boldsymbol{g}^{(k+1)}}^\top \boldsymbol{g}^{(j)} = {\boldsymbol{g}^{(k+1)}}^\top (\boldsymbol{d}^{(j)} - \beta_{j-1}\boldsymbol{d}^{(j)}) = 0$.

Proof (cont).

Now we come back to $LHS := \boldsymbol{d}^{(k+1)^\top} \boldsymbol{Q} \boldsymbol{d}^{(j)} = (-\boldsymbol{g}^{(k+1)} + \beta_k \boldsymbol{d}^{(k)})^\top \boldsymbol{Q} \boldsymbol{d}^{(j)}$.

If $j < k$, then $LHS = -\boldsymbol{g}^{(k+1)^\top} \boldsymbol{Q} \boldsymbol{d}^{(j)} = -\boldsymbol{g}^{(k+1)^\top} \frac{\boldsymbol{g}^{(j+1)} - \boldsymbol{g}^{(j)}}{\alpha_j} = 0$.

If $j = k$, then $LHS = \boldsymbol{d}^{(k+1)^\top} \boldsymbol{Q} \boldsymbol{d}^{(k)} = (-\boldsymbol{g}^{(k+1)} + \beta_k \boldsymbol{d}^{(k)})^\top \boldsymbol{Q} \boldsymbol{d}^{(k)} = 0$ due to definition of β_k.

Therefore $\boldsymbol{d}^{(k+1)^\top} \boldsymbol{Q} \boldsymbol{d}^{(j)}$ for all $j \leq k$.

We now consider **Conjugate Gradient** method for **non-quadratic** problems.

If we have $\boldsymbol{x}^{(k)}$ and $\boldsymbol{d}^{(k)}$, we can get step size α_k using line search such as

$$\alpha_k = \arg\min_{\alpha \geq 0} f(\boldsymbol{x}^{(k)} + \alpha \boldsymbol{d}^{(k)})$$

So we only need to find β_k for $\boldsymbol{d}^{(k+1)} = \boldsymbol{g}^{(k+1)} + \beta_k \boldsymbol{d}^{(k)}$, so $\boldsymbol{d}^{(0)}, \dots, \boldsymbol{d}^{(n)}$ are $\boldsymbol{Q}$-conjugate. In quadratic case

$$\beta_k = \frac{\boldsymbol{g}^{(k+1)^\top} \boldsymbol{Q} \boldsymbol{d}^{(k)}}{\boldsymbol{d}^{(k)^\top} \boldsymbol{Q} \boldsymbol{d}^{(k)}}$$

However, for non-quadratic f, the Hessian $\nabla^2 f(\boldsymbol{x})$ is not constant $\boldsymbol{Q}$.

There are several modifications to get β_k by eliminating the need of $\boldsymbol{Q}\boldsymbol{d}^{(k)}$.

- **Hestenes-Stiefel** formula:

$$\beta_k = \frac{\boldsymbol{g}^{(k+1)^\top}(\boldsymbol{g}^{(k+1)} - \boldsymbol{g}^{(k)})}{\boldsymbol{d}^{(k)^\top}(\boldsymbol{g}^{(k+1)} - \boldsymbol{g}^{(k)})}$$

- **Polak-Ribière** formula:

$$\beta_k = \frac{\boldsymbol{g}^{(k+1)^\top}(\boldsymbol{g}^{(k+1)} - \boldsymbol{g}^{(k)})}{\|\boldsymbol{g}^{(k)}\|^2}$$

- **Fletcher-Reeves** formula:

$$\beta_k = \frac{\|\boldsymbol{g}^{(k+1)}\|^2}{\|\boldsymbol{g}^{(k)}\|^2}$$

Remark.

- All three modifications are identical if f is quadratic;
- Need reinitialization $\boldsymbol{d}^{(k)} = -\boldsymbol{g}^{(k)}$ for $k = n, 2n, \dots$;
- Line search accuracy affects overall performance.

Some experience.

- Use Hestenes-Stiefel if line search is inaccurate.
- Use Polak-Ribière if $\boldsymbol{g}^{(k)}$ are bounded away from $\mathbf{0}$.
- Fletcher-Reeves has better global convergence property.