

E(y) descent rate

How much closer does one step bring us to the solution $\mathbf{y}^* = \mathbf{0}$? In other words, how much smaller is $\mathbf{e}(\mathbf{y}_{k+1})$ relatively to $\mathbf{e}(\mathbf{y}_k)$? From the definition of $\mathbf{e}(\mathbf{y})$ and for \mathbf{y}_{k+1} , we obtain:

$$\begin{aligned} \frac{e(\mathbf{y}_k) - e(\mathbf{y}_{k+1})}{e(\mathbf{y}_k)} &= \frac{\mathbf{y}_k^T Q \mathbf{y}_k - \mathbf{y}_{k+1}^T Q \mathbf{y}_{k+1}}{\mathbf{y}_k^T Q \mathbf{y}_k} \\ &= \frac{\mathbf{y}_k^T Q \mathbf{y}_k - \left(\mathbf{y}_k - \frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_k^T Q \mathbf{g}_k} \mathbf{g}_k \right)^T Q \left(\mathbf{y}_k - \frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_k^T Q \mathbf{g}_k} \mathbf{g}_k \right)}{\mathbf{y}_k^T Q \mathbf{y}_k} \\ &= \frac{2 \frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_k^T Q \mathbf{g}_k} \mathbf{g}_k^T Q \mathbf{y}_k - \left(\frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_k^T Q \mathbf{g}_k} \right)^2 \mathbf{g}_k^T Q \mathbf{g}_k}{\mathbf{y}_k^T Q \mathbf{y}_k} \\ &= \frac{2 \mathbf{g}_k^T \mathbf{g}_k \mathbf{g}_k^T Q \mathbf{y}_k - (\mathbf{g}_k^T \mathbf{g}_k)^2}{\mathbf{y}_k^T Q \mathbf{y}_k \mathbf{g}_k^T Q \mathbf{g}_k}. \end{aligned} \tag{4}$$

Since Q is invertible, we have:

$$\mathbf{g}_k = Q\mathbf{y}_k \Rightarrow \mathbf{y}_k = Q^{-1}\mathbf{g}_k$$

And

$$\mathbf{y}_k^T Q\mathbf{y}_k = \mathbf{g}_k^T Q^{-1}\mathbf{g}_k$$

,what allows to rewrite (4) as:

$$\frac{e(\mathbf{y}_k) - e(\mathbf{y}_{k+1})}{e(\mathbf{y}_k)} = \frac{(\mathbf{g}_k^T \mathbf{g}_k)^2}{\mathbf{g}_k^T Q^{-1}\mathbf{g}_k \mathbf{g}_k^T Q\mathbf{g}_k}$$

or

$$e(\mathbf{y}_{k+1}) = \left(1 - \frac{(\mathbf{g}_k^T \mathbf{g}_k)^2}{\mathbf{g}_k^T Q^{-1}\mathbf{g}_k \mathbf{g}_k^T Q\mathbf{g}_k}\right) e(\mathbf{y}_k)$$

Kantorovich inequality.

Kantorovich inequality: Let Q be a positive definite, symmetric, $n \times n$ matrix.

Then, for any vector y there holds:

$$\frac{(\mathbf{y}^T \mathbf{y})^2}{\mathbf{y}^T Q^{-1} \mathbf{y} \mathbf{y}^T Q \mathbf{y}} \geq \frac{4\sigma_1 \sigma_n}{(\sigma_1 + \sigma_n)^2}$$

This inequality allows to prove the **Steepest Descent Rate** theorem.

Steepest Descent Rate Theorem

Steepest Descent Rate theorem:

Let

$$f(\mathbf{x}) = c + \mathbf{a}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T Q \mathbf{x}$$

be a quadratic function of \mathbf{x} , with Q symmetric and positive definite .

For any \mathbf{x}_0 , the method of steepest descent

,where

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{\mathbf{g}_k^T \mathbf{g}_k}{\mathbf{g}_k^T Q \mathbf{g}_k} \mathbf{g}_k$$

$$\mathbf{g}_k = \mathbf{g}(\mathbf{x}_k) = \left. \frac{\partial f}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} = \mathbf{a} + Q \mathbf{x}_k$$

Converges to the unique minimum point

$$\mathbf{x}^* = -Q^{-1}\mathbf{a}$$

The difference at every step satisfies

$$f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*) \leq \left(\frac{\sigma_1 - \sigma_n}{\sigma_1 + \sigma_n} \right)^2 (f(\mathbf{x}_k) - f(\mathbf{x}^*))$$

, where σ_1 and σ_n are the respectively the largest and the smallest singular values of Q

Proof

From the definitions

$$\mathbf{y} = \mathbf{x} - \mathbf{x}^* \quad \text{and} \quad e(\mathbf{y}) = \frac{1}{2} \mathbf{y}^T Q \mathbf{y}$$

we obtain

$$\begin{aligned} f(\mathbf{x}_{k+1}) - f(\mathbf{x}^*) &= e(\mathbf{y}_{k+1}) = \left(1 - \frac{(\mathbf{g}_k^T \mathbf{g}_k)^2}{\mathbf{g}_k^T Q^{-1} \mathbf{g}_k \mathbf{g}_k^T Q \mathbf{g}_k} \right) e(\mathbf{y}_k) \leq \\ &\leq \left(1 - \frac{4\sigma_1\sigma_n}{(\sigma_1 + \sigma_n)^2} \right) e(\mathbf{y}_k) = \left(\frac{\sigma_1 - \sigma_n}{\sigma_1 + \sigma_n} \right)^2 (f(\mathbf{x}_k) - f(\mathbf{x}^*)) \end{aligned}$$

Here, the Kantorovich inequality was used.

Analysis

The ratio

$$\kappa(\mathbf{Q}) = \sigma_1 / \sigma_n$$

Is called the *condition number* of \mathbf{Q} . The larger the condition number (ratio between the largest and the smallest singular values), the closer the ratio

$$(\sigma_1 - \sigma_n) / (\sigma_1 + \sigma_n)$$

to 1 and therefore the slower the convergence.

Illustration

Consider the two dimensional case, $x \in \mathbf{R}^2$. The figure shows a trajectory x_k , imposed in the contours of $f(x)$.

The greater the ratio between the singular values,

of Q (which is the aspect ratio of the

ellipses), the slower the

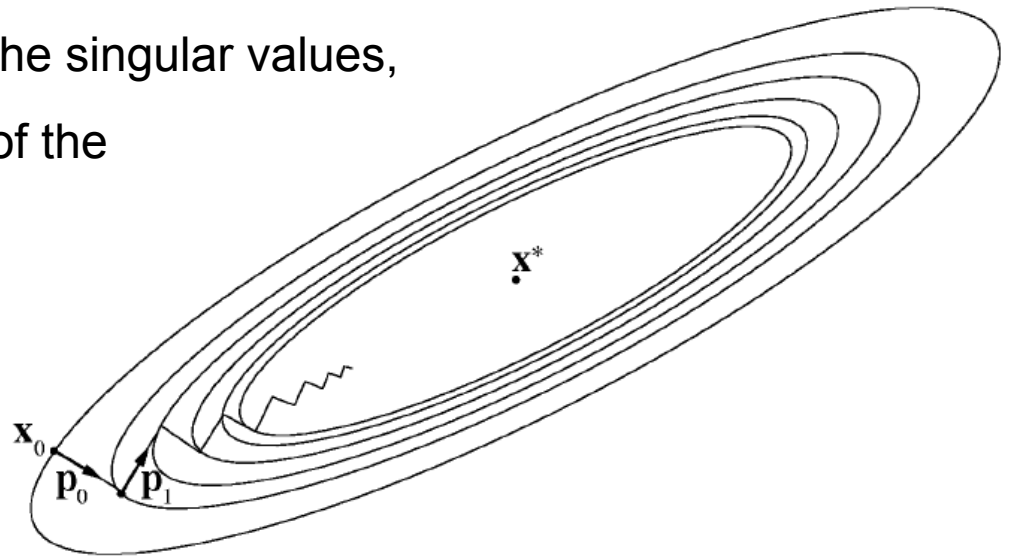
convergence rate. If

the isolines are

circular ($k(Q)=1$)

or the trajectory

started from the ellipses axis, a single step brings us to x^* .



Stopping criteria

We do not know the \mathbf{x}^* and therefore $\mathbf{f}(\mathbf{x}^*)$. Thus the stopping criteria is not trivial.

The criterion can be $|\mathbf{f}(\mathbf{x}_k) - \mathbf{f}(\mathbf{x}_{k-1})|$ or $|\mathbf{x}_k - \mathbf{x}_{k-1}|$. The second criterion is better, since it indicates proximity of \mathbf{x}^* .

Line search

The steepest descent can be applied to general cases of \mathbf{f} , not necessarily quadratic and not defined via

$$f(\mathbf{x}) = c + \mathbf{a}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x} \quad (1)$$

In these cases, \mathbf{Q} is the matrix of the second derivatives of \mathbf{f} with respect to \mathbf{x} , called a *Hessian* of \mathbf{f} . In this case, only n first derivatives are needed to calculate the direction \mathbf{p}_k . The step size requires calculation of Hessian of $f(\mathbf{x})$, which requires computing $\binom{n}{2}$ second derivatives, and therefore is very expensive.

Using the line search allows to reach the minimum of $f(\mathbf{x})$ in the direction \mathbf{p}_k without the Hessian calculation.