

Numerical Optimization 05: 1st order methods

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Overview

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The choice of descent direction

In the previous chapter, we have talked about the general strategy for optimization is to decide a direction and then use the line search method to obtain a sufficient decrease. Repeating it for many time, we expect to arrive at the local minimum.

$$x^{k+1} = x^k + \alpha^k d^k$$

The search direction often has the form

$$d^k = -(B^k)^{-1} \nabla f(x^k) \quad (1)$$

where B^k is a symmetric and nonsingular matrix. In some method (e.g., steepest descent), B^k is the identify matrix, while in (quasi-) Newton's method, B^k is the approximate or exact Hessian.

In this lecture, we will cover the **first-order** methods which **purely rely on the gradient information**.

Gradient descent

An intuitive choice for the descent direction is the direction of steepest descent ($g^k = \nabla f(x^k)$).

$$d^k = -\frac{g^k}{\|g^k\|}$$

If we optimize the step size at each step, we have

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

Since

$$\nabla f(x^k + \alpha d^k)^T d^k = 0$$

$$d^{k+1} = -\frac{\nabla f(x^k + \alpha d^k)}{\|\nabla f(x^k + \alpha d^k)\|}$$

It is obvious that the two consecutive directions are **orthogonal**.

$$(d^{k+1})^T d^k = 0$$

Conjugate gradient

Gradient descent can perform poorly in narrow valleys. The conjugate gradient method overcomes this issue by doing a small transformation. When minimizing the quadratic functions:

$$\underset{\alpha}{\text{minimize}} : f(x) = \frac{1}{2}x^T Ax - b^T x$$

is equivalent to solving the linear equation

$$Ax = b$$

where A is $N \times N$ symmetric and positive definite, and thus f has a unique local minimum.

When solving $Ax = b$, a powerful method is to find a sequence of N **conjugate directions** satisfying

$$(d^i)^T A d^j = 0 \quad (i \neq j)$$

To find the successive conjugate directions

One can start with the direction of steepest descent

$$d^1 = -g^1$$

We then use line search to find the next design point. For quadratic functions $f = \frac{1}{2}x^T Ax - b^T x$, the step factor α can be computed as

$$\begin{aligned}\frac{\partial f(x + \alpha d)}{\partial \alpha} &= \frac{\partial}{\partial \alpha} \left[\frac{1}{2}(x + \alpha d)^T A(x + \alpha d) + b^T(x + \alpha d) + c \right] \\ &= d^T A(x + \alpha d) + d^T b \\ &= d^T (Ax + b) + \alpha d^T Ad\end{aligned}$$

Let the gradient be zero,

$$\alpha = -\frac{d^T (Ax + b)}{d^T Ad}$$

Then the update is

$$x^2 = x^1 + \alpha d^1$$

To find the successive conjugate directions (continued)

For the next step

$$d^{k+1} = -g^{k+1} + \beta^k d^k$$

where β^k is a series of scalar parameters. Larger values of β indicate that the previous descent direction contributes strongly.

We solve β , from the followings

$$\begin{aligned} d^{(k+1)T} A d^k &= 0 \\ (-g^{k+1} + \beta^k d^{(k)})^T A d^{(k)} &= 0 \\ -g^{k+1} A d^{(k)} + \beta^k d^{(k)T} A d^{(k)} &= 0 \\ \beta^k &= \frac{g^{(k+1)T} A d^{(k)}}{d^{(k)T} A d^{(k)}} \end{aligned}$$

The conjugate method is exact for quadratic functions. But it can be applied to non quadratic functions as well when the quadratic function is a good approximation.

To Approximate A and β

Unfortunately, we don't know the value of A that best approximate f around x^k . So we choose some way to compute β .

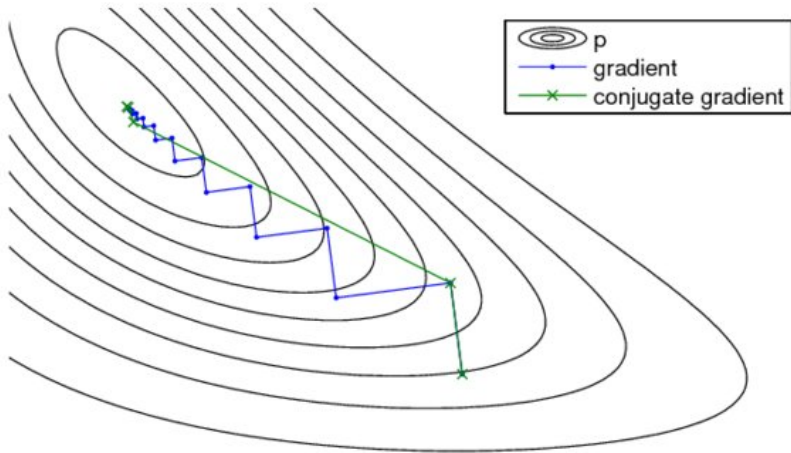
Fletcher-Reeves

$$\beta^k = \frac{g^{(k)T} g^{(k)}}{g^{(k-1)T} g^{(k-1)}}$$

Polak-Ribiere

$$\beta^k = \frac{g^{(k)T} (g^{(k)} - g^{(k-1)})}{g^{(k-1)T} g^{(k-1)}}$$

Comparison between Conjugate Gradient and Steepest Descent



Summary

- Gradient descent follows the direction of steepest descent
- Two consecutive search directions in gradient descent are orthogonal
- In conjugate gradient, the search directions are conjugate with respect to an approximate hessian.
- Both SD and CG work with the line search method