Numerical Optimization 05: 1st order methods

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June 25, 2020

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

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

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

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

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

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:

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

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

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

$$(-g^{k+1} + \beta^k d^{(k)})^T A d^{(k)} = 0$$

$$-g^{k+1} A d^{(k)} + \beta^k d^{(k)T} A d^{(k)} = 0$$

$$\beta^k = \frac{g^{(k+1)T} A d^{(k)}}{d^{(k)T} A d^{(k)}}$$

The conjugate method is exact for quadratic functions. But it can be applied to non quadractic 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.

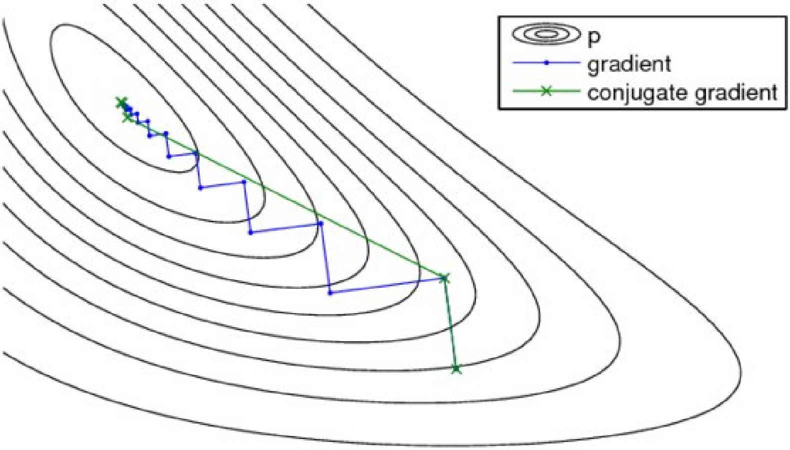
Fletcher-Reeves

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

Polak-Ribiere

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

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