Numerical Optimization 08: Quasi-Newton methods

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Overview

1. Quasi-Newton's method
2. The DFP method
3. BFGS method
4. The Broyden Class
5. The L-BFGS method
6. Summary

Quasi-Newton's method

Just as the secant method approximates f" in the univariate case, quasi Newton approximate the inverse Hessian ($(\boldsymbol{H}^k)^{-1}$) which is needed for each step of update

$$\boldsymbol{x}^{k+1} \leftarrow \boldsymbol{x}^k - \alpha^k (\boldsymbol{H}^k)^{-1} \boldsymbol{g}^k$$

These methods typically set $(\boldsymbol{H}^k)^{-1}$ (let's call it $\boldsymbol{Q}$ from now on) to the identity matrix and then apply updates to reflect information learned with each iteration. To simplify the equations for various quasi-Newton methods, we define the following

$$\gamma^{k+1} = \boldsymbol{g}^{k+1} - \boldsymbol{g}^k$$
$$\delta^{k+1} = \boldsymbol{x}^{k+1} - \boldsymbol{x}^k$$

A new quadratic model

Instead of computing the exact $\boldsymbol{Q}$, we can update it in a simple manner to account for the curvature measured during the most recent step. Suppose, we have generated $\boldsymbol{x}^{k+1}$ and wish to construct a new quadratic model,

$$m^{k+1}(\boldsymbol{p}) = f(x^{k+1}) + \boldsymbol{g}^{k+1}p + \frac{1}{2}\boldsymbol{p}^T\boldsymbol{Q}^{k+1}\boldsymbol{p}$$

We let the gradient of m^{k+1} match the gradient of f for at least two steps $\boldsymbol{x}^{k+1}$ and $\boldsymbol{x}^k$.

$$\nabla m^{k+1}(-\alpha^k p^k) = \boldsymbol{g}^{k+1} - \alpha^k\boldsymbol{Q}^{k+1}\boldsymbol{p}^k = \boldsymbol{g}^k$$

Since $\nabla m^{k+1}(0) = g^{k+1}$, the second of these condition is satisfied automatically. Rearranging it, we obtain the so called secant condition.

$$\boldsymbol{Q}^{k+1}\alpha^k\boldsymbol{p}^k = \boldsymbol{g}^{k+1} - \boldsymbol{g}^k \quad \rightarrow \quad \boldsymbol{Q}^{k+1}\boldsymbol{\delta}^k = \boldsymbol{\gamma}^k \tag{1}$$

A new quadratic model

Given the displacements $\boldsymbol{\delta}^k$ and the change of gradients γ^k. It requires that the symmetric positive definite matrix $\boldsymbol{Q}^{k+1}$, it needs that

$$\boldsymbol{\delta}^k \gamma^k > 0$$

At this stage, there still exists an infinite number of solutions of $\boldsymbol{Q}^{k+1}$. To determine a unique solution, we impose another condition, which is that $\boldsymbol{Q}^{k+1}$ is close to the current $\boldsymbol{Q}^k$

$$\min_{\boldsymbol{Q}} ||\boldsymbol{Q} - \boldsymbol{Q}^k||$$
$$\text{s.t.} \qquad \boldsymbol{Q} = \boldsymbol{Q}^T, \qquad \boldsymbol{B}\delta^k = \gamma^k$$

Different matrix norms can be applied here to give different quasi-Newton methods.

The Davidon-Fletcher-Powell (DFP) method

Davidon proposed a relation to ensures that $\boldsymbol{Q}$ is symmetric.

$$\boldsymbol{Q}^{k+1} = \boldsymbol{Q}^k + auu^T + bvv^T$$

According to the secant condition

$$\boldsymbol{Q}^k \boldsymbol{\delta}^k + auu^T \boldsymbol{\delta}^k + bvv^T \boldsymbol{\delta}^k = \gamma^k$$

An obvious choice for u and v is

$$u = \boldsymbol{\gamma}^k, \qquad v = \boldsymbol{Q}^k \boldsymbol{\delta}^k \quad \rightarrow \quad au^T \boldsymbol{\delta}^k = 1, \quad bv^T \boldsymbol{\delta}^k = -1$$

where

$$a = 1/u^T \boldsymbol{\delta}^k = 1/u^T \boldsymbol{\delta}^k \quad b = -1/v^T \boldsymbol{\delta}^k = 1/u^T \boldsymbol{\delta}^k$$

$$\boldsymbol{Q}^{k+1} = \boldsymbol{Q}^k - \frac{\boldsymbol{Q}^k \gamma^k (\gamma^k)^T \boldsymbol{Q}^k}{(\gamma^k)^T \boldsymbol{Q}^k \gamma^k} + \frac{\boldsymbol{\delta}(\boldsymbol{\delta}^k)^T}{(\boldsymbol{\delta}^k)^T \boldsymbol{\gamma}^k}$$

W. C. Davidon, Variable Metric Method for Minimization
SIAM Journal on Optimization. 1. (1991), 1-17.

The Broyden-Fletcher-Goldfarb-Shanno (BFGS) method

In the BFGS algorithm, it does not approximate $\boldsymbol{Q}^k$, but handles $\boldsymbol{H}^k = (\boldsymbol{Q}^k)^{-1}$

$$\boldsymbol{H}^{k+1}\gamma^k = \boldsymbol{\delta}^k$$

The minimize condition is,

$$\begin{aligned} &\min_{\boldsymbol{H}} ||\boldsymbol{H} - \boldsymbol{H}^k|| \\ \text{s.t.} \qquad &\boldsymbol{H} = \boldsymbol{H}^T, \qquad \boldsymbol{H}\gamma^k = \boldsymbol{\delta}^k \end{aligned}$$

$$\boldsymbol{Q}^{k+1} = \boldsymbol{Q}^k - \frac{\boldsymbol{\delta}^k(\gamma^k)^T\boldsymbol{Q}^k + \boldsymbol{Q}^k\gamma^k(\boldsymbol{\delta}^{\boldsymbol{k}})^T}{(\boldsymbol{\delta}^k)^T\gamma^k} + \left(1 + \frac{(\gamma^k)^T\boldsymbol{Q}^k\gamma^k}{(\boldsymbol{\delta}^k)^T\boldsymbol{Q}^k}\right)\frac{\boldsymbol{\delta}^k(\boldsymbol{\delta}^k)^T}{(\boldsymbol{\delta}^k)^T\gamma^k}$$

BFGS does better than DFP with approximate line search.

The Broyden Class

Comparing the two solutions from DFP and BFGS,

$$\left\{\begin{aligned} \text{DFP:}\quad \boldsymbol{Q}^{k+1} &= \boldsymbol{Q}^k - \frac{\boldsymbol{Q}^k\gamma^k(\gamma^k)^T\boldsymbol{Q}^k}{(\gamma^k)^T\boldsymbol{Q}^k\gamma^k} + \frac{\boldsymbol{\delta}(\boldsymbol{\delta}^k)^T}{(\boldsymbol{\delta}^k)^T\gamma^k} \\ \text{BFGS:}\ \boldsymbol{Q}^{k+1} &= \boldsymbol{Q}^k - \frac{\boldsymbol{\delta}^k(\gamma^k)^T\boldsymbol{Q}^k + \boldsymbol{Q}^k\gamma^k(\boldsymbol{\delta}^{\boldsymbol{k}})^T}{(\boldsymbol{\delta}^k)^T\gamma^k} + \left(1 + \frac{(\gamma^k)^T\boldsymbol{Q}^k\gamma^k}{(\boldsymbol{\delta}^k)^T\boldsymbol{Q}^k}\right)\frac{\boldsymbol{\delta}^k(\boldsymbol{\delta}^k)^T}{(\boldsymbol{\delta}^k)^T\gamma^k} \\ &= \boldsymbol{Q}^k - \frac{\boldsymbol{Q}^k\gamma^k(\gamma^k)^T\boldsymbol{Q}^k}{(\gamma^k)^T\boldsymbol{Q}^k\gamma^k} + \frac{\boldsymbol{\delta}(\boldsymbol{\delta}^k)^T}{(\boldsymbol{\delta}^k)^T\gamma^k} + [(\boldsymbol{\delta}^k)^T\boldsymbol{Q}^k\boldsymbol{\delta}^k]\boldsymbol{v}^{\boldsymbol{k}}(\boldsymbol{v}^{\boldsymbol{k}})^T \end{aligned}\right.$$

where

$$\boldsymbol{v}^{\boldsymbol{k}} = \frac{\gamma^k}{(\gamma^k)^T\boldsymbol{\delta}^k} - \frac{\boldsymbol{Q}^k\boldsymbol{\delta}^k}{(\boldsymbol{\delta}^k)^T\boldsymbol{Q}^k\boldsymbol{\delta}^k}$$

In fact, there exists a family of solutions

$$\boldsymbol{Q}^k = (1-\lambda)\boldsymbol{Q}^k_{\text{BFGS}} + \lambda\boldsymbol{Q}^k_{\text{DFP}}$$

Changing λ from 0 to 1 is actually varying the u and v in

$$\boldsymbol{Q}^{k+1} = \boldsymbol{Q}^k + auu^T + bvv^T$$

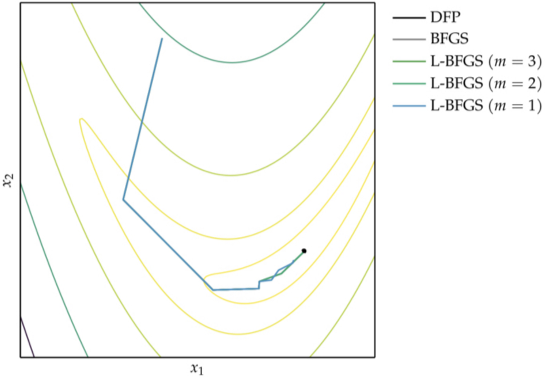
The Limited-memory BFGS

BFGS still uses an $n \times n$ dense matrix, which is a problem for storage of the hessian when dealing with very large scale problems. Inspecting the following update, can we do something smart?

$$\boldsymbol{Q}^{k+1} = \boldsymbol{Q}^{k} + auu^{T} + bvv^{T}$$

In L-BFGS, it stores the last m values for $\boldsymbol{\delta}$ and γ rather than the entire inverse of H.

Comparison of various quasi-Newton algorithms



Summary

- Quasi-Newton method attempted to approximate the Hessian from function and gradient evaluations.
- The first step approximation of hessian in the quasi-newton methods is usually an identity matrix
- BFGS performs better than DFP, but it still relies on the storage of big Hessian matrix
- L-BFGS is a more scalable approach for large scale problems.
- All quasi-Newton methods can work with the approximate line search.