Quasi-Newton methods for minimization

Lectures for PHD course on
Non-linear equations and numerical optimization

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Outline

1. Quasi Newton Method
2. The symmetric rank one update
3. The Powell-symmetric-Broyden update
4. The Davidon Fletcher and Powell rank 2 update
5. The Broyden Fletcher Goldfarb and Shanno (BFGS) update
6. The Broyden class

Algorithm (General quasi-Newton algorithm)

$k \leftarrow 0$;
$\boldsymbol{x}_0$ *assigned;*
$\boldsymbol{g}_0 \leftarrow \nabla \mathsf{f}(\boldsymbol{x}_0)$;
$\boldsymbol{H}_0 \leftarrow \nabla^2 \mathsf{f}(\boldsymbol{x}_0)^{-1}$;
while $\|\boldsymbol{g}_k\| > \epsilon$ **do**
  — compute search direction
  $\boldsymbol{d}_k \leftarrow \boldsymbol{H}_k \boldsymbol{g}_k$;
  Approximate $\arg\min_{\lambda>0} \mathsf{f}(\boldsymbol{x}_k - \lambda \boldsymbol{d}_k)$ *by linsearch;*
  — perform step
  $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k - \lambda_k \boldsymbol{d}_k$;
  $\boldsymbol{g}_{k+1} \leftarrow \nabla \mathsf{f}(\boldsymbol{x}_{k+1})$;
  — update $\boldsymbol{H}_{k+1}$
  $\boldsymbol{H}_{k+1} \leftarrow$ *some_algorithm*$(\boldsymbol{H}_k, \boldsymbol{x}_k, \boldsymbol{x}_{k+1}, \boldsymbol{g}_k, \boldsymbol{g}_{k+1})$;
  $k \leftarrow k+1$;
end while

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- Let $\boldsymbol{B}_k$ and approximation of the Hessian of $f(\boldsymbol{x})$. Let $\boldsymbol{x}_k$, $\boldsymbol{x}_{k+1}$, $\boldsymbol{g}_k$ and $\boldsymbol{g}_{k+1}$ and if we use the Broyden update formula to force secant condition to $\boldsymbol{B}_{k+1}$ we obtain

$$\boldsymbol{B}_{k+1} \leftarrow \boldsymbol{B}_k + \frac{(\boldsymbol{y}_k - \boldsymbol{B}_k\boldsymbol{s}_k)\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{s}_k},$$

where $\boldsymbol{s}_k = \boldsymbol{x}_{k+1} - \boldsymbol{x}_k$ and $\boldsymbol{y}_k = \boldsymbol{g}_{k+1} - \boldsymbol{g}_k$. By using Sherman–Morrison formula and setting $\boldsymbol{H}_k = \boldsymbol{B}_k^{-1}$ we obtain the update:

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k - \frac{(\boldsymbol{H}_k\boldsymbol{y}_k - \boldsymbol{s}_k)\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{s}_k + \boldsymbol{s}_k^T\boldsymbol{H}_k\boldsymbol{g}_{k+1}}\boldsymbol{H}_k$$

- The previous update do not maintain symmetry. In fact if $\boldsymbol{H}_k$ is symmetric then $\boldsymbol{H}_{k+1}$ not necessarily is symmetric.

- To avoid loss of symmetry we can consider an update of the form:

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \boldsymbol{u}\boldsymbol{u}^T$$

- Imposing the secant condition (on the inverse)

$$\boldsymbol{H}_{k+1}\boldsymbol{y}_k = \boldsymbol{s}_k \qquad \Rightarrow \qquad \boldsymbol{H}_k\boldsymbol{y}_k + \boldsymbol{u}\boldsymbol{u}^T\boldsymbol{y}_k = \boldsymbol{s}_k$$

from previous equality

$$\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k + \boldsymbol{y}_k^T\boldsymbol{u}\boldsymbol{u}^T\boldsymbol{y}_k = \boldsymbol{y}_k^T\boldsymbol{s}_k \qquad \Rightarrow$$

$$\boldsymbol{y}_k^T\boldsymbol{u} = \left(\boldsymbol{y}_k^T\boldsymbol{s}_k - \boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k\right)^{1/2}$$

we obtain

$$\boldsymbol{u} = \frac{\boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k}{\boldsymbol{u}^T\boldsymbol{y}_k} = \frac{\boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k}{\left(\boldsymbol{y}_k^T\boldsymbol{s}_k - \boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k\right)^{1/2}}$$

- substituting the expression of $\boldsymbol{u}$

$$\boldsymbol{u} = \frac{\boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k}{\left(\boldsymbol{y}_k^T\boldsymbol{s}_k - \boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k\right)^{1/2}}$$

in the update formula, we obtain

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \frac{\boldsymbol{w}_k\boldsymbol{w}_k^T}{\boldsymbol{w}_k^T\boldsymbol{y}_k} \qquad \boldsymbol{w}_k = \boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k$$

- The previous update formula is the symmetric rank one formula (SR1).
- To be definite the previous formula needs $\boldsymbol{w}_k^T\boldsymbol{y}_k \neq 0$. Moreover if $\boldsymbol{w}_k^T\boldsymbol{y}_k < 0$ and $\boldsymbol{H}_k$ is positive definite then $\boldsymbol{H}_{k+1}$ not necessarily is positive definite.
- Have $\boldsymbol{H}_k$ symmetric and positive definite is important for global convergence

This lemma is used in the forward theorems

Lemma

Let be

$$q(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x} + c$$

with $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ symmetric and positive definite. Then

$$\begin{aligned} \boldsymbol{y}_k &= \boldsymbol{g}_{k+1} - \boldsymbol{g}_k \\ &= \boldsymbol{A}\boldsymbol{x}_{k+1} - \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_k + \boldsymbol{b} \\ &= \boldsymbol{A}\boldsymbol{s}_k \end{aligned}$$

where $\boldsymbol{g}_k = \nabla q(\boldsymbol{x}_k)^T$.

Theorem (property of SR1 update)

Let be

$$\mathsf{q}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x} + c$$

with $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ symmetric and positive definite. Let be $\boldsymbol{x}_0$ and $\boldsymbol{H}_0$ assigned. Let $\boldsymbol{x}_k$ and $\boldsymbol{H}_k$ produced by

1. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{s}_k$;
2. $\boldsymbol{H}_{k+1}$ *updated by the SR1 formula*

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \frac{\boldsymbol{w}_k\boldsymbol{w}_k^T}{\boldsymbol{w}_k^T\boldsymbol{y}_k} \qquad \boldsymbol{w}_k = \boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k$$

If $\boldsymbol{s}_0$, $\boldsymbol{s}_1$, ..., $\boldsymbol{s}_{n-1}$ are linearly independent then $\boldsymbol{H}_n = \boldsymbol{A}^{-1}$.

Proof. (1/2).

We prove by induction the hereditary property $\boldsymbol{H}_i\boldsymbol{y}_j = \boldsymbol{s}_j$.
BASE: For $i = 1$ is exactly the secant condition of the update.
INDUCTION: Suppose the relation is valid for $k > 0$ the we prove that it is valid for $k+1$. In fact, from the update formula

$$\boldsymbol{H}_{k+1}\boldsymbol{y}_j = \boldsymbol{H}_k\boldsymbol{y}_j + \frac{\boldsymbol{w}_k^T\boldsymbol{y}_j}{\boldsymbol{w}_k^T\boldsymbol{y}_k}\boldsymbol{w}_k \qquad \boldsymbol{w}_k = \boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k$$

by the induction hypothesis for $j < k$ and using lemma on slide 8 we have

$$\begin{aligned}\boldsymbol{w}_k^T\boldsymbol{y}_j &= \boldsymbol{s}_k^T\boldsymbol{y}_j - \boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_j = \boldsymbol{s}_k^T\boldsymbol{y}_j - \boldsymbol{y}_k^T\boldsymbol{s}_j \\ &= \boldsymbol{y}_k^T\boldsymbol{A}\boldsymbol{y}_j - \boldsymbol{y}_k^T\boldsymbol{A}\boldsymbol{y}_j = 0\end{aligned}$$

so that $\boldsymbol{H}_{k+1}\boldsymbol{y}_j = \boldsymbol{H}_k\boldsymbol{y}_j = \boldsymbol{s}_j$ for $j = 0, 1, \dots, k-1$. For $j = k$ we have $\boldsymbol{H}_{k+1}\boldsymbol{y}_k = \boldsymbol{s}_k$ trivially by construction of the SR1 formula.

Proof. (2/2).

To prove that $\boldsymbol{H}_n = \boldsymbol{A}^{-1}$ notice that

$$\boldsymbol{H}_n\boldsymbol{y}_j = \boldsymbol{s}_j, \qquad \boldsymbol{A}\boldsymbol{s}_j = \boldsymbol{y}_j, \qquad j = 0, 1, \dots, n-1$$

and combining the equality

$$\boldsymbol{H}_n\boldsymbol{A}\boldsymbol{s}_j = \boldsymbol{s}_j, \qquad j = 0, 1, \dots, n-1$$

due to the linear independence of $\boldsymbol{s}_i$ we have $\boldsymbol{H}_n\boldsymbol{A} = \boldsymbol{I}$ i.e. $\boldsymbol{H}_n = \boldsymbol{A}^{-1}$. □

Properties of SR1 update (1/2)

1. The SR1 update possesses the natural quadratic termination property (like CG).
2. SR1 satisfy the hereditary property $\boldsymbol{H}_k\boldsymbol{y}_j = \boldsymbol{s}_j$ for $j < k$.
3. SR1 does maintain the positive definitiveness of $\boldsymbol{H}_k$ if and only if $\boldsymbol{w}_k^T\boldsymbol{y}_k > 0$. However this condition is difficult to guarantee.
4. Sometimes $\boldsymbol{w}_k^T\boldsymbol{y}_k$ becomes very small or 0. This results in serious numerical difficulty (roundoff) or even the algorithm is broken. We can avoid this breakdown by the following strategy

Breakdown workaround for SR1 update

1. if $|\boldsymbol{w}_k^T\boldsymbol{y}_k| \geq \epsilon \|\boldsymbol{w}_k^T\| \|\boldsymbol{y}_k\|$ (i.e. the angle between $\boldsymbol{w}_k$ and $\boldsymbol{y}_k$ is far from 90 degree), then we update with the SR1 formula.
2. Otherwise we set $\boldsymbol{H}_{k+1} = \boldsymbol{H}_k$.

Properties of SR1 update (2/2)

Theorem (Convergence of nonlinear SR1 update)

Let $f(\boldsymbol{x})$ satisfying standard assumption. Let be $\{\boldsymbol{x}_k\}$ a sequence of iterates such that $\lim_{k\to\infty} \boldsymbol{x}_k = \boldsymbol{x}_\star$. Suppose we use the breakdown workaround for SR1 update and the steps $\{\boldsymbol{s}_k\}$ are uniformly linearly independent. Then we have

$$\lim_{k\to\infty} \left\| \boldsymbol{H}_k - \nabla^2 f(\boldsymbol{x}_\star)^{-1} \right\| = 0.$$

A.R.Conn, N.I.M.Gould and P.L.Toint
Convergence of quasi-Newton matrices generated by the symmetric rank one update.
Mathematic of Computation **50** 399–430, 1988.

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- The SR1 update, although symmetric do not have minimum property like the Broyden update for the non symmetric case.
- The Broyden update

$$\boldsymbol{A}_{k+1} = \boldsymbol{A}_k + \frac{(\boldsymbol{y}_k - \boldsymbol{A}_k\boldsymbol{s}_k)\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{s}_k}$$

solve the minimization problem

$$\|\boldsymbol{A}_{k+1} - \boldsymbol{A}_k\|_F \leq \|\boldsymbol{A} - \boldsymbol{A}_k\|_F \qquad \text{for all } \boldsymbol{A}\boldsymbol{s}_k = \boldsymbol{y}_k$$

- If we solve a similar problem in the class of symmetric matrix we obtain the Powell-symmetric-Broyden (PSB) update

Lemma (Powell-symmetric-Broyden update)

Let $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ symmetric and $\boldsymbol{s}, \boldsymbol{y} \in \mathbb{R}^n$ with $\boldsymbol{s} \neq \boldsymbol{0}$. Consider the set

$$\mathcal{B} = \left\{ \boldsymbol{B} \in \mathbb{R}^{n\times n} \,|\, \boldsymbol{B}\boldsymbol{s} = \boldsymbol{y},\, \boldsymbol{B} = \boldsymbol{B}^T \right\}$$

if $\boldsymbol{s}^T\boldsymbol{y} \neq 0$[a] then there exists a unique matrix $\boldsymbol{B} \in \mathcal{B}$ such that

$$\|\boldsymbol{A} - \boldsymbol{B}\|_F \leq \|\boldsymbol{A} - \boldsymbol{C}\|_F \qquad \text{for all } \boldsymbol{C} \in \mathcal{B}$$

moreover $\boldsymbol{B}$ has the following form

$$\boldsymbol{B} = \boldsymbol{A} + \frac{\boldsymbol{\omega}\boldsymbol{s}^T + \boldsymbol{s}\boldsymbol{\omega}^T}{\boldsymbol{s}^T\boldsymbol{s}} - (\boldsymbol{\omega}^T\boldsymbol{s})\frac{\boldsymbol{s}\boldsymbol{s}^T}{(\boldsymbol{s}^T\boldsymbol{s})^2} \qquad \boldsymbol{\omega} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{s}$$

then $\boldsymbol{B}$ is a rank two perturbation of the matrix $\boldsymbol{A}$.

[a] This is true if Wolfe line search is performed

Proof. (1/11).

First of all notice that $\mathcal{B}$ is not empty, in fact

$$\frac{1}{\boldsymbol{s}^T\boldsymbol{y}}\boldsymbol{y}\boldsymbol{y}^T \in \mathcal{B} \qquad \left[\frac{1}{\boldsymbol{s}^T\boldsymbol{y}}\boldsymbol{y}\boldsymbol{y}^T\right]\boldsymbol{s} = \boldsymbol{y}$$

So that the problem is not empty. Next we reformulate the problem as a constrained minimum problem:

$$\arg\min_{\boldsymbol{B}\in\mathbb{R}^{n\times n}} \frac{1}{2}\sum_{i,j=1}^{n}(A_{ij}-B_{ij})^2 \quad \text{subject to } \boldsymbol{B}\boldsymbol{s}=\boldsymbol{y} \text{ and } \boldsymbol{B}=\boldsymbol{B}^T$$

The solution is a stationary point of the Lagrangian:

$$g(\boldsymbol{B},\boldsymbol{\lambda},\boldsymbol{M}) = \frac{1}{2}\|\boldsymbol{A}-\boldsymbol{B}\|_F^2 + \boldsymbol{\lambda}^T(\boldsymbol{B}\boldsymbol{y}-\boldsymbol{s}) + \sum_{i<j}\mu_{ij}(B_{ij}-B_{ji})$$

Proof. (2/11).

taking the gradient we have

$$\frac{\partial}{\partial B_{ij}}g(\boldsymbol{B},\boldsymbol{\lambda},\boldsymbol{B}) = A_{ij} - B_{ij} + \lambda_i s_j + M_{ij} = 0$$

where

$$M_{ij} = \begin{cases} \mu_{ij} & \text{if } i<j; \\ -\mu_{ij} & \text{if } i>j; \\ 0 & \text{If } i=j. \end{cases}$$

The previous equality can be written in matrix form as

$$\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{\lambda}\boldsymbol{s}^T + \boldsymbol{M}.$$

Proof. (3/11).

Imposing symmetry for $\boldsymbol{B}$

$$\boldsymbol{A} + \boldsymbol{\lambda}\boldsymbol{s}^T + \boldsymbol{M} = \boldsymbol{A}^T + \boldsymbol{s}\boldsymbol{\lambda}^T + \boldsymbol{M}^T = \boldsymbol{A} + \boldsymbol{s}\boldsymbol{\lambda}^T - \boldsymbol{M}$$

solving for $\boldsymbol{M}$ we have

$$\boldsymbol{M} = \frac{\boldsymbol{s}\boldsymbol{\lambda}^T - \boldsymbol{\lambda}\boldsymbol{s}^T}{2}$$

substituting in $\boldsymbol{B}$ we have

$$\boldsymbol{B} = \boldsymbol{A} + \frac{\boldsymbol{s}\boldsymbol{\lambda}^T + \boldsymbol{\lambda}\boldsymbol{s}^T}{2}$$

Proof. (4/11).

Imposing $\boldsymbol{s}^T\boldsymbol{B}\boldsymbol{s} = \boldsymbol{s}^T\boldsymbol{y}$

$$\boldsymbol{s}^T\boldsymbol{A}\boldsymbol{s} + \frac{\boldsymbol{s}^T\boldsymbol{s}\boldsymbol{\lambda}^T\boldsymbol{s} + \boldsymbol{s}^T\boldsymbol{\lambda}\boldsymbol{s}^T\boldsymbol{s}}{2} = \boldsymbol{s}^T\boldsymbol{y} \qquad \Rightarrow$$

$$\boldsymbol{\lambda}^T\boldsymbol{s} = (\boldsymbol{s}^T\boldsymbol{\omega})/(\boldsymbol{s}^T\boldsymbol{s})$$

where $\boldsymbol{\omega} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{s}$. Imposing $\boldsymbol{B}\boldsymbol{s} = \boldsymbol{y}$

$$\boldsymbol{A}\boldsymbol{s} + \frac{\boldsymbol{s}\boldsymbol{\lambda}^T\boldsymbol{s} + \boldsymbol{\lambda}\boldsymbol{s}^T\boldsymbol{s}}{2} = \boldsymbol{y} \qquad \Rightarrow$$

$$\boldsymbol{\lambda} = \frac{2\boldsymbol{\omega}}{\boldsymbol{s}^T\boldsymbol{s}} - \frac{(\boldsymbol{s}^T\boldsymbol{\omega})\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

next we compute the explicit form of $\boldsymbol{B}$.

Proof. (5/11).

Substituting

$$\boldsymbol{\lambda} = \frac{2\boldsymbol{\omega}}{\boldsymbol{s}^T\boldsymbol{s}} - \frac{(\boldsymbol{s}^T\boldsymbol{\omega})\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^2} \qquad \text{in} \qquad \boldsymbol{B} = \boldsymbol{A} + \frac{\boldsymbol{s}\boldsymbol{\lambda}^T + \boldsymbol{\lambda}\boldsymbol{s}^T}{2}$$

we obtain

$$\boldsymbol{B} = \boldsymbol{A} + \frac{\boldsymbol{\omega}\boldsymbol{s}^T + \boldsymbol{s}\boldsymbol{\omega}^T}{\boldsymbol{s}^T\boldsymbol{s}} - (\boldsymbol{\omega}^T\boldsymbol{s})\frac{\boldsymbol{s}\boldsymbol{s}^T}{(\boldsymbol{s}^T\boldsymbol{s})^2} \qquad \boldsymbol{\omega} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{s}$$

next we prove that $\boldsymbol{B}$ is the unique minimum.

Proof. (6/11).

The matrix $\boldsymbol{B}$ is a minimum, in fact

$$\|\boldsymbol{B} - \boldsymbol{A}\|_F = \left\| \frac{\boldsymbol{\omega}\boldsymbol{s}^T + \boldsymbol{s}\boldsymbol{\omega}^T}{\boldsymbol{s}^T\boldsymbol{s}} - (\boldsymbol{\omega}^T\boldsymbol{s})\frac{\boldsymbol{s}\boldsymbol{s}^T}{(\boldsymbol{s}^T\boldsymbol{s})^2} \right\|_F$$

To bound this norm we need the following properties of Frobenius norm:

- $\|\boldsymbol{M} - \boldsymbol{N}\|_F^2 = \|\boldsymbol{M}\|_F^2 + \|\boldsymbol{N}\|_F^2 - 2\boldsymbol{M}\cdot\boldsymbol{N}$;

where $\boldsymbol{M}\cdot\boldsymbol{N} = \sum_{ij} M_{ij}N_{ij}$ setting

$$\boldsymbol{M} = \frac{\boldsymbol{\omega}\boldsymbol{s}^T + \boldsymbol{s}\boldsymbol{\omega}^T}{\boldsymbol{s}^T\boldsymbol{s}} \qquad \boldsymbol{N} = (\boldsymbol{\omega}^T\boldsymbol{s})\frac{\boldsymbol{s}\boldsymbol{s}^T}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

now we compute $\|\boldsymbol{M}\|_F$, $\|\boldsymbol{N}\|_F$ and $\boldsymbol{M}\cdot\boldsymbol{N}$.

Proof. (7/11).

$$\begin{aligned}
\boldsymbol{M}\cdot\boldsymbol{N} &= \frac{\boldsymbol{\omega}^T\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^3}\sum_{ij}(\omega_i s_j + \omega_j s_i)s_i s_j \\
&= \frac{\boldsymbol{\omega}^T\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^3}\sum_{ij}\left[(\omega_i s_i)s_j^2 + (\omega_j s_j)s_i^2\right] \\
&= \frac{\boldsymbol{\omega}^T\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^3}\left[\sum_i(\omega_i s_i)\sum_j s_j^2 + \sum_j(\omega_j s_j)\sum_i s_i^2\right] \\
&= \frac{\boldsymbol{\omega}^T\boldsymbol{s}}{(\boldsymbol{s}^T\boldsymbol{s})^3}\left[(\boldsymbol{\omega}^T\boldsymbol{s})(\boldsymbol{s}^T\boldsymbol{s}) + (\boldsymbol{\omega}^T\boldsymbol{s})(\boldsymbol{s}^T\boldsymbol{s})\right] \\
&= \frac{2(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2}
\end{aligned}$$

Proof. (8/11).

To bound $\|\boldsymbol{N}\|_F^2$ and $\|\boldsymbol{M}\|_F^2$ we need the following properties of Frobenius norm:

- $\left\|\boldsymbol{u}\boldsymbol{v}^T\right\|_F^2 = (\boldsymbol{u}^T\boldsymbol{u})(\boldsymbol{v}^T\boldsymbol{v})$;
- $\left\|\boldsymbol{u}\boldsymbol{v}^T + \boldsymbol{v}\boldsymbol{u}^T\right\|_F^2 = 2(\boldsymbol{u}^T\boldsymbol{u})(\boldsymbol{v}^T\boldsymbol{v}) + 2(\boldsymbol{u}^T\boldsymbol{v})^2$;

Then we have

$$\|\boldsymbol{N}\|_F^2 = \frac{(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^4}\left\|\boldsymbol{s}\boldsymbol{s}^T\right\|_F^2 = \frac{(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^4}(\boldsymbol{s}^T\boldsymbol{s})^2 = \frac{(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

$$\|\boldsymbol{M}\|_F^2 = \frac{\boldsymbol{\omega}\boldsymbol{s}^T + \boldsymbol{s}\boldsymbol{\omega}^T}{\boldsymbol{s}^T\boldsymbol{s}} = \frac{2(\boldsymbol{\omega}^T\boldsymbol{\omega})(\boldsymbol{s}^T\boldsymbol{s}) + 2(\boldsymbol{s}^T\boldsymbol{\omega})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

Proof. (9/11).

Putting all together and using Cauchy-Schwartz inequality ($\boldsymbol{a}^T\boldsymbol{b} \leq \|\boldsymbol{a}\|\,\|\boldsymbol{b}\|$):

$$\|\boldsymbol{M}-\boldsymbol{N}\|_F^2 = \frac{(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2} + \frac{2(\boldsymbol{\omega}^T\boldsymbol{\omega})(\boldsymbol{s}^T\boldsymbol{s}) + 2(\boldsymbol{s}^T\boldsymbol{\omega})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2} - \frac{4(\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

$$= \frac{2(\boldsymbol{\omega}^T\boldsymbol{\omega})(\boldsymbol{s}^T\boldsymbol{s}) - (\boldsymbol{\omega}^T\boldsymbol{s})^2}{(\boldsymbol{s}^T\boldsymbol{s})^2}$$

$$\leq \frac{\boldsymbol{\omega}^T\boldsymbol{\omega}}{\boldsymbol{s}^T\boldsymbol{s}} = \frac{\|\boldsymbol{\omega}\|^2}{\|\boldsymbol{s}\|^2} \qquad \text{[used Cauchy-Schwartz]}$$

Using $\boldsymbol{\omega} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{s}$ and noticing that $\boldsymbol{y} = \boldsymbol{C}\boldsymbol{s}$ for all $\boldsymbol{C} \in \mathcal{B}$. so that

$$\|\boldsymbol{\omega}\| = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{s}\| = \|\boldsymbol{C}\boldsymbol{s} - \boldsymbol{A}\boldsymbol{s}\| = \|(\boldsymbol{C}-\boldsymbol{A})\boldsymbol{s}\|$$

Proof. (10/11).

To bound $\|(\boldsymbol{C}-\boldsymbol{A})\boldsymbol{s}\|$ we need the following property of Frobenius norm:

- $\|\boldsymbol{M}\boldsymbol{x}\| \leq \|\boldsymbol{M}\|_F\,\|\boldsymbol{x}\|$;

in fact

$$\|\boldsymbol{M}\boldsymbol{x}\|^2 = \sum_i\Big(\sum_j M_{ij}s_j\Big)^2 \leq \sum_i\Big(\sum_j M_{ij}^2\Big)\Big(\sum_k s_k^2\Big)$$

$$= \|\boldsymbol{M}\|_F^2\,\|\boldsymbol{s}\|^2$$

using this inequality

$$\|\boldsymbol{M}-\boldsymbol{N}\|_F \leq \frac{\|\boldsymbol{\omega}\|}{\|\boldsymbol{s}\|} = \frac{\|(\boldsymbol{C}-\boldsymbol{A})\boldsymbol{s}\|}{\|\boldsymbol{s}\|} \leq \frac{\|\boldsymbol{C}-\boldsymbol{A}\|_F\,\|\boldsymbol{s}\|}{\|\boldsymbol{s}\|}$$

i.e. we have $\|\boldsymbol{A}-\boldsymbol{B}\|_F \leq \|\boldsymbol{C}-\boldsymbol{A}\|_F$ for all $\boldsymbol{C} \in \mathcal{B}$.

Proof. (11/11).

Let $\boldsymbol{B}'$ and $\boldsymbol{B}''$ two different minimum. Then $\frac{1}{2}(\boldsymbol{B}'+\boldsymbol{B}'') \in \mathcal{B}$ moreover

$$\left\|\boldsymbol{A} - \frac{1}{2}(\boldsymbol{B}'+\boldsymbol{B}'')\right\|_F \leq \frac{1}{2}\|\boldsymbol{A}-\boldsymbol{B}'\|_F + \frac{1}{2}\|\boldsymbol{A}-\boldsymbol{B}''\|_F$$

If the inequality is strict we have a contradiction. From the Cauchy–Schwartz inequality we have an equality only when $\boldsymbol{A}-\boldsymbol{B}' = \lambda(\boldsymbol{A}-\boldsymbol{B}'')$ so that

$$\boldsymbol{B}' - \lambda\boldsymbol{B}'' = (1-\lambda)\boldsymbol{A}$$

and

$$\boldsymbol{B}'\boldsymbol{s} - \lambda\boldsymbol{B}''\boldsymbol{s} = (1-\lambda)\boldsymbol{A}\boldsymbol{s} \quad \Rightarrow \quad (1-\lambda)\boldsymbol{y} = (1-\lambda)\boldsymbol{A}\boldsymbol{s}$$

but this is true only when $\lambda = 1$, i.e. $\boldsymbol{B}' = \boldsymbol{B}''$. □

Algorithm (PSB quasi-Newton algorithm)

$k \leftarrow 0$;
$\boldsymbol{x}$ *assigned*; $\boldsymbol{g} \leftarrow \nabla \mathsf{f}(\boldsymbol{x})$; $\boldsymbol{B} \leftarrow \nabla^2\mathsf{f}(\boldsymbol{x})$;
while $\|\boldsymbol{g}\| > \epsilon$ **do**
  — *compute search direction*
  $\boldsymbol{d} \leftarrow \boldsymbol{B}^{-1}\boldsymbol{g}$;   *[solve linear system* $\boldsymbol{B}\boldsymbol{d} = \boldsymbol{g}$*]*
  Approximate $\arg\min_{\alpha>0} \mathsf{f}(\boldsymbol{x} - \alpha\boldsymbol{d})$ *by linsearch;*
  — *perform step*
  $\boldsymbol{x} \leftarrow \boldsymbol{x} - \alpha\boldsymbol{d}$;
  — *update* $\boldsymbol{B}_{k+1}$
  $\boldsymbol{\omega} \leftarrow \nabla\mathsf{f}(\boldsymbol{x}) + (\alpha-1)\boldsymbol{g}$; $\boldsymbol{g} \leftarrow \nabla\mathsf{f}(\boldsymbol{x})$;
  $\beta \leftarrow (\alpha\boldsymbol{d}^T\boldsymbol{d})^{-1}$; $\gamma \leftarrow \beta^2\alpha\boldsymbol{d}^T\boldsymbol{\omega}$;
  $\boldsymbol{B} \leftarrow \boldsymbol{B} - \beta\big(\boldsymbol{d}\boldsymbol{\omega}^T + \boldsymbol{\omega}\boldsymbol{d}^T\big) + \gamma\boldsymbol{d}\boldsymbol{d}^T$;
  $k \leftarrow k+1$;
end while

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- The SR1 and PSB update maintains the symmetry but do not maintains the positive definitiveness of the matrix $\boldsymbol{H}_{k+1}$. To recover this further property we can try the update of the form:

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \alpha \boldsymbol{u}\boldsymbol{u}^T + \beta \boldsymbol{v}\boldsymbol{v}^T$$

- Imposing the secant condition (on the inverse)

$$\begin{aligned} \boldsymbol{H}_{k+1}\boldsymbol{y}_k &= \boldsymbol{s}_k & \Rightarrow \\ \boldsymbol{H}_k\boldsymbol{y}_k + \alpha(\boldsymbol{u}^T\boldsymbol{y}_k)\boldsymbol{u} + \beta(\boldsymbol{v}^T\boldsymbol{y}_k)\boldsymbol{v} &= \boldsymbol{s}_k & \Rightarrow \\ \alpha(\boldsymbol{u}^T\boldsymbol{y}_k)\boldsymbol{u} + \beta(\boldsymbol{v}^T\boldsymbol{y}_k)\boldsymbol{v} &= \boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k \end{aligned}$$

clearly this equation has not a unique solution. A natural choice for $\boldsymbol{u}$ and $\boldsymbol{v}$ is the following:

$$\boldsymbol{u} = \boldsymbol{s}_k \qquad \boldsymbol{v} = \boldsymbol{H}_k\boldsymbol{y}_k$$

- Solving for α and β the equation

$$\alpha(\boldsymbol{s}_k^T\boldsymbol{y}_k)\boldsymbol{s}_k + \beta(\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k)\boldsymbol{H}_k\boldsymbol{y}_k = \boldsymbol{s}_k - \boldsymbol{H}_k\boldsymbol{y}_k$$

we obtain

$$\alpha = \frac{1}{\boldsymbol{s}_k^T\boldsymbol{y}_k} \qquad \beta = -\frac{1}{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}$$

- substituting in the updating formula we obtain the Davidon Fletcher and Powell (DFP) rank 2 update formula

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k} - \frac{\boldsymbol{H}_k\boldsymbol{y}_k\boldsymbol{y}_k^T\boldsymbol{H}_k}{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}$$

- Obviously this is only a possible choice and with other solution we obtain different update formulas. Next we must prove that under suitable condition the DFP update formula maintains positive definitiveness.

Positive definitiveness of DFP update

Theorem (Positive definitiveness of DFP update)

Given $\boldsymbol{H}_k$ symmetric and positive definite, then the DFP update

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k} - \frac{\boldsymbol{H}_k\boldsymbol{y}_k\boldsymbol{y}_k^T\boldsymbol{H}_k}{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}$$

produce $\boldsymbol{H}_{k+1}$ positive definite if and only if $\boldsymbol{s}_k^T\boldsymbol{y}_k > 0$.

Remark (Wolfe ⇒ DFP update is SPD)

Expanding $\boldsymbol{s}_k^T\boldsymbol{y}_k > 0$ we have $\nabla f(\boldsymbol{x}_{k+1})\boldsymbol{s}_k > \nabla f(\boldsymbol{x}_k)\boldsymbol{s}_k$. Remember that in a minimum search algorithm we have $\boldsymbol{s}_k = \alpha_k\boldsymbol{p}_k$ with $\alpha_k > 0$. But the second Wolfe condition for line-search is $\nabla f(\boldsymbol{x}_k + \alpha_k\boldsymbol{p}_k)\boldsymbol{p}_k \geq c_2 \nabla f(\boldsymbol{x}_k)\boldsymbol{p}_k$ with $0 < c_2 < 1$. But this imply:

$$\nabla f(\boldsymbol{x}_{k+1})\boldsymbol{s}_k \geq c_2 \nabla f(\boldsymbol{x}_k)\boldsymbol{s}_k > \nabla f(\boldsymbol{x}_k)\boldsymbol{s}_k \quad \Rightarrow \quad \boldsymbol{s}_k^T\boldsymbol{y}_k > 0.$$

Proof. (1/2).

Let be $s_k^T y_k > 0$: consider a $z \neq 0$ then

$$z^T H_{k+1} z = z^T \left(H_k - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k} \right) z + z^T \frac{s_k s_k^T}{s_k^T y_k} z$$
$$= z^T H_k z - \frac{(z^T H_k y_k)(y_k^T H_k z)}{y_k^T H_k y_k} + \frac{(z^T s_k)^2}{s_k^T y_k}$$

H_k is SPD so that there exists the Cholesky decomposition $LL^T = H_k$. Defining $a = L^T z$ and $b = L^T y_k$ we can write

$$z^T H_{k+1} z = \frac{(a^T a)(b^T b) - (a^T b)^2}{b^T b} + \frac{(z^T s_k)^2}{s_k^T y_k}$$

from the Cauchy-Schwartz inequality we have $(a^T a)(b^T b) \geq (a^T b)^2$ so that $z^T H_{k+1} z \geq 0$.

Proof. (2/2).

To prove strict inequality remember from the Cauchy-Schwartz inequality that $(a^T a)(b^T b) = (a^T b)^2$ if and only if $a = \lambda b$, i.e.

$$L^T z = \lambda L^T y_k \quad \Rightarrow \quad z = \lambda y_k$$

but in this case

$$\frac{(z^T s_k)^2}{s_k^T y_k} = \lambda^2 \frac{(y^T s_k)^2}{s_k^T y_k} > 0 \quad \Rightarrow \quad z^T H_{k+1} z > 0.$$

Let be $z^T H_{k+1} z > 0$ for all $z \neq \mathbf{0}$: Choosing $z = y_k$ we have

$$0 < y_k^T H_{k+1} y_k = \frac{(y^T s_k)^2}{s_k^T y_k} = s_k^T y_k$$

□

Algorithm (DFP quasi-Newton algorithm)

$k \leftarrow 0$;
x *assigned*; $g \leftarrow \nabla f(x)$; $H \leftarrow \nabla^2 f(x)^{-1}$;
while $\|g\| > \epsilon$ **do**
  — *compute search direction*
  $d \leftarrow Hg$;
  Approximate $\arg\min_{\alpha>0} f(x - \alpha d)$ *by linsearch;*
  — *perform step*
  $x \leftarrow x - \alpha d$;
  — *update* H_{k+1}
  $y \leftarrow \nabla f(x) - g$; $z \leftarrow Hy$; $g \leftarrow \nabla f(x)$;
  $H \leftarrow H - \alpha \dfrac{dd}{d^T y} - \dfrac{zz^T}{y^T z}$;
  $k \leftarrow k + 1$;
end while

Theorem (property of DFP update)

Let be $q(x) = \frac{1}{2}(x - x_\star)^T A (x - x_\star) + c$ *with* $A \in \mathbb{R}^{n\times n}$ *symmetric and positive definite. Let be* x_0 *and* H_0 *assigned. Let* $\{x_k\}$ *and* $\{H_k\}$ *produced by the sequence* $\{s_k\}$

1. $x_{k+1} \leftarrow x_k + s_k$;
2. $H_{k+1} \leftarrow H_k + \dfrac{s_k s_k^T}{s_k^T y_k} - \dfrac{H_k y_k y_k^T H_k}{y_k^T H_k y_k}$;

where $s_k = \alpha_k p_k$ *with* α_k *is obtained by exact line-search. Then for* $j < k$ *we have*

1. $g_k^T s_j = 0$; *[orthogonality property]*
2. $H_k y_j = s_j$; *[hereditary property]*
3. $s_k^T A s_j = 0$; *[conjugate direction property]*
4. *The method terminate (i.e.* $\nabla f(x_m) = \mathbf{0}$*) at* $x_m = x_\star$ *with* $m \leq n$*. If* $n = m$ *then* $H_n = A^{-1}$.

Proof. (1/4).

Points (1), (2) and (3) are proved by induction. The base of induction is obvious, let be the theorem true for $k > 0$. Due to exact line search we have:

$$\boldsymbol{g}_{k+1}^T \boldsymbol{s}_k = 0$$

moreover by induction for $j < k$ we have $\boldsymbol{g}_{k+1}^T \boldsymbol{s}_j = 0$, in fact:

$$\begin{aligned}
\boldsymbol{g}_{k+1}^T \boldsymbol{s}_j &= \boldsymbol{g}_j^T \boldsymbol{s}_j + \sum_{i=j}^{k-1} (\boldsymbol{g}_{i+1} - \boldsymbol{g}_i)^T \boldsymbol{s}_j \\
&= 0 + \sum_{i=j}^{k-1} (\boldsymbol{A}(\boldsymbol{x}_{i+1} - \boldsymbol{x}_\star) - \boldsymbol{A}(\boldsymbol{x}_i - \boldsymbol{x}_\star))^T \boldsymbol{s}_j \\
&= \sum_{i=j}^{k-1} (\boldsymbol{A}(\boldsymbol{x}_{i+1} - \boldsymbol{x}_i))^T \boldsymbol{s}_j \\
&= \sum_{i=j}^{k-1} \boldsymbol{s}_i^T \boldsymbol{A} \boldsymbol{s}_j = 0. \qquad \text{[induction + conjugacy prop.]}
\end{aligned}$$

Proof. (2/4).

By using $\boldsymbol{s}_{k+1} = -\alpha_{k+1} \boldsymbol{H}_{k+1} \boldsymbol{g}_{k+1}$ we have $\boldsymbol{s}_{k+1}^T \boldsymbol{A} \boldsymbol{s}_j = 0$, in fact:

$$\begin{aligned}
\boldsymbol{s}_{k+1}^T \boldsymbol{A} \boldsymbol{s}_j &= -\alpha_{k+1} \boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1} (\boldsymbol{A}\boldsymbol{x}_{j+1} - \boldsymbol{A}\boldsymbol{x}_j) \\
&= -\alpha_{k+1} \boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1} (\boldsymbol{A}(\boldsymbol{x}_{j+1} - \boldsymbol{x}_\star) - \boldsymbol{A}(\boldsymbol{x}_j - \boldsymbol{x}_\star)) \\
&= -\alpha_{k+1} \boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1} (\boldsymbol{g}_{j+1} - \boldsymbol{g}_j) \\
&= -\alpha_{k+1} \boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1} \boldsymbol{y}_j \\
&= -\alpha_{k+1} \boldsymbol{g}_{k+1}^T \boldsymbol{s}_j \qquad \text{[induction + hereditary prop.]} \\
&= 0
\end{aligned}$$

notice that we have used $\boldsymbol{A}\boldsymbol{s}_j = \boldsymbol{y}_j$.

Proof. (3/4).

Due to DFP construction we have

$$\boldsymbol{H}_{k+1} \boldsymbol{y}_k = \boldsymbol{s}_k$$

by inductive hypothesis and DFP formula for $j < k$ we have, $\boldsymbol{s}_k^T \boldsymbol{y}_j = \boldsymbol{s}_k^T \boldsymbol{A} \boldsymbol{s}_j = 0$, moreover

$$\begin{aligned}
\boldsymbol{H}_{k+1} \boldsymbol{y}_j &= \boldsymbol{H}_k \boldsymbol{y}_j + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T \boldsymbol{y}_j}{\boldsymbol{s}_k^T \boldsymbol{y}_k} - \frac{\boldsymbol{H}_k \boldsymbol{y}_k \boldsymbol{y}_k^T \boldsymbol{H}_k \boldsymbol{y}_j}{\boldsymbol{y}_k^T \boldsymbol{H}_k \boldsymbol{y}_k} \\
&= \boldsymbol{s}_j + \frac{\boldsymbol{s}_k 0}{\boldsymbol{s}_k^T \boldsymbol{y}_k} - \frac{\boldsymbol{H}_k \boldsymbol{y}_k \boldsymbol{y}_k^T \boldsymbol{s}_j}{\boldsymbol{y}_k^T \boldsymbol{H}_k \boldsymbol{y}_k} \qquad [\boldsymbol{H}_k \boldsymbol{y}_j = \boldsymbol{s}_j] \\
&= \boldsymbol{s}_j - \frac{\boldsymbol{H}_k \boldsymbol{y}_k (\boldsymbol{g}_{k+1} - \boldsymbol{g}_k)^T \boldsymbol{s}_j}{\boldsymbol{y}_k^T \boldsymbol{H}_k \boldsymbol{y}_k} \qquad [\boldsymbol{y}_j = \boldsymbol{g}_{j+1} - \boldsymbol{g}_j] \\
&= \boldsymbol{s}_j \qquad \text{[induction + ortho. prop.]}
\end{aligned}$$

Proof. (4/4).

Finally if $m = n$ we have $\boldsymbol{s}_j$ with $j = 0, 1, \ldots, n-1$ are conjugate and linearly independent. From hereditary property and lemma on slide 8

$$\boldsymbol{H}_n \boldsymbol{A} \boldsymbol{s}_k = \boldsymbol{H}_n \boldsymbol{y}_k = \boldsymbol{s}_k$$

i.e. we have

$$\boldsymbol{H}_n \boldsymbol{A} \boldsymbol{s}_k = \boldsymbol{s}_k, \qquad k = 0, 1, \ldots, n-1$$

due to linear independence of $\{\boldsymbol{s}_k\}$ follows that $\boldsymbol{H}_n = \boldsymbol{A}^{-1}$. □

Outline

1. Quasi Newton Method
2. The symmetric rank one update
3. The Powell-symmetric-Broyden update
4. The Davidon Fletcher and Powell rank 2 update
5. The Broyden Fletcher Goldfarb and Shanno (BFGS) update
6. The Broyden class

- Another update which maintain symmetry and positive definitiveness is the Broyden Fletcher Goldfarb and Shanno (BFGS,1970) rank 2 update.
- This update was independently discovered by the four authors.
- A convenient way to introduce BFGS is by the concept of duality.
- Duality means that if I found an update for the Hessian, say

$$\boldsymbol{B}_{k+1} \leftarrow \mathcal{U}(\boldsymbol{B}_k, \boldsymbol{s}_k, \boldsymbol{y}_k)$$

which satisfy $\boldsymbol{B}_{k+1}\boldsymbol{s}_k = \boldsymbol{y}_k$ (the secant condition on the Hessian). Then by exchanging $\boldsymbol{B}_k \rightleftharpoons \boldsymbol{H}_k$ and $\boldsymbol{s}_k \rightleftharpoons \boldsymbol{y}_k$ we obtain the update for the inverse of the Hessian, i.e.

$$\boldsymbol{H}_{k+1} \leftarrow \mathcal{U}(\boldsymbol{H}_k, \boldsymbol{y}_k, \boldsymbol{s}_k)$$

which satisfy $\boldsymbol{H}_{k+1}\boldsymbol{y}_k = \boldsymbol{s}_k$ (the secant condition on the inverse of the Hessian).

- Starting from the Davidon Fletcher and Powell (DFP) rank 2 update formula

$$\boldsymbol{H}_{k+1} \leftarrow \boldsymbol{H}_k + \frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k} - \frac{\boldsymbol{H}_k\boldsymbol{y}_k\boldsymbol{y}_k^T\boldsymbol{H}_k}{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}$$

by the duality we obtain the Broyden Fletcher Goldfarb and Shanno (BFGS) update formula

$$\boldsymbol{B}_{k+1} \leftarrow \boldsymbol{B}_k + \frac{\boldsymbol{y}_k\boldsymbol{y}_k^T}{\boldsymbol{y}_k^T\boldsymbol{s}_k} - \frac{\boldsymbol{B}_k\boldsymbol{s}_k\boldsymbol{s}_k^T\boldsymbol{B}_k}{\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k}$$

- The BFGS formula written in this way is not useful in the case of large problem. We need an equivalent formula for the inverse of the approximate Hessian. This can be done with a generalization of the Sherman-Morrison formula.

Sherman-Morrison-Woodbury formula (1/2)

Sherman-Morrison-Woodbury formula permit to explicit write the inverse of a matrix changed with a rank k perturbation

Proposition (Sherman–Morrison–Woodbury formula)

$$(\boldsymbol{A} + \boldsymbol{U}\boldsymbol{V}^T)^{-1} = \boldsymbol{A}^{-1} - \boldsymbol{A}^{-1}\boldsymbol{U}\left(\boldsymbol{I} + \boldsymbol{V}^T\boldsymbol{U}\right)^{-1}\boldsymbol{V}^T\boldsymbol{A}^{-1}$$

where

$$\boldsymbol{U} = \left[\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k\right] \qquad \boldsymbol{V} = \left[\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_k\right]$$

The Sherman–Morrison–Woodbury formula can be checked by a direct calculation.

Sherman-Morrison-Woodbury formula (2/2)

Remark

The previous formula can be written as:

$$\left(\boldsymbol{A}+\sum_{i=1}^{k}\boldsymbol{u}_i\boldsymbol{v}_i^T\right)^{-1}=\boldsymbol{A}^{-1}-\boldsymbol{A}^{-1}\boldsymbol{U}\boldsymbol{C}^{-1}\boldsymbol{V}^T\boldsymbol{A}^{-1}$$

where

$$C_{ij}=\delta_{ij}+\boldsymbol{v}_i^T\boldsymbol{u}_j\qquad i,j=1,2,\ldots,k$$

The BFGS update for $\boldsymbol{H}$

Proposition

By using the Sherman-Morrison-Woodbury formula the BFGS update for $\boldsymbol{H}$ becomes:

$$\begin{aligned}\boldsymbol{H}_{k+1}\leftarrow \boldsymbol{H}_k &-\frac{\boldsymbol{H}_k\boldsymbol{y}_k\boldsymbol{s}_k^T+\boldsymbol{s}_k\boldsymbol{y}_k^T\boldsymbol{H}_k}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\\ &+\frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\left(1+\frac{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)\end{aligned}\qquad (A)$$

Or equivalently

$$\boldsymbol{H}_{k+1}\leftarrow\left(\boldsymbol{I}-\frac{\boldsymbol{s}_k\boldsymbol{y}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)\boldsymbol{H}_k\left(\boldsymbol{I}-\frac{\boldsymbol{y}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)+\frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\qquad (B)$$

Proof. (1/3).

Consider the Sherman-Morrison-Woodbury formula with $k=2$ and

$$\boldsymbol{u}_1=\boldsymbol{v}_1=\frac{\boldsymbol{y}_k}{(\boldsymbol{s}_k^T\boldsymbol{y}_k)^{1/2}}\qquad \boldsymbol{u}_2=-\boldsymbol{v}_2=\frac{\boldsymbol{B}_k\boldsymbol{s}_k}{(\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k)^{1/2}}$$

in this way (setting $\boldsymbol{H}_k=\boldsymbol{B}_k^{-1}$) we have

$$\begin{aligned}C_{11}&=1+\boldsymbol{v}_1^T\boldsymbol{u}_1=1+\frac{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\\ C_{22}&=1+\boldsymbol{v}_2^T\boldsymbol{u}_2=-\frac{\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{H}_k\boldsymbol{B}_k\boldsymbol{s}_k}{\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k}=1-1=0\\ C_{12}&=\boldsymbol{v}_1^T\boldsymbol{u}_2\quad=\frac{\boldsymbol{y}_k^T\boldsymbol{B}_k\boldsymbol{s}_k}{(\boldsymbol{s}_k^T\boldsymbol{y}_k)^{1/2}(\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k)^{1/2}}=\frac{(\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k)^{1/2}}{(\boldsymbol{s}_k^T\boldsymbol{y}_k)^{1/2}}\\ C_{21}&=\boldsymbol{v}_2^T\boldsymbol{u}_1\quad=-C_{12}\end{aligned}$$

Proof. (2/3).

In this way the matric $\boldsymbol{C}$ has the form

$$\boldsymbol{C}=\begin{pmatrix}\beta & \alpha\\ -\alpha & 0\end{pmatrix}\qquad \boldsymbol{C}^{-1}=\frac{1}{\alpha^2}\begin{pmatrix}0 & -\alpha\\ \alpha & \beta\end{pmatrix}$$

$$\beta=1+\frac{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\qquad \alpha=\frac{(\boldsymbol{s}_k^T\boldsymbol{B}_k\boldsymbol{s}_k)^{1/2}}{(\boldsymbol{s}_k^T\boldsymbol{y}_k)^{1/2}}$$

where setting $\tilde{\boldsymbol{U}}=\boldsymbol{H}_k\boldsymbol{U}$ and $\tilde{\boldsymbol{V}}=\boldsymbol{H}_k\boldsymbol{V}$ where

$$\tilde{\boldsymbol{u}}_i=\boldsymbol{H}_k\boldsymbol{u}_i\quad\text{and}\quad\tilde{\boldsymbol{v}}_i=\boldsymbol{H}_k\boldsymbol{v}_i\qquad i=1,2$$

we have

$$\begin{aligned}\boldsymbol{H}_{k+1}\leftarrow\boldsymbol{H}_k-\boldsymbol{H}_k\boldsymbol{U}\boldsymbol{C}^{-1}\boldsymbol{V}^T\boldsymbol{H}_k&=\boldsymbol{H}_k-\tilde{\boldsymbol{U}}\boldsymbol{C}^{-1}\tilde{\boldsymbol{V}}^T\\ &=\boldsymbol{H}_k+\frac{1}{\alpha}(-\tilde{\boldsymbol{u}}_1\tilde{\boldsymbol{v}}_2^T+\tilde{\boldsymbol{u}}_2\tilde{\boldsymbol{v}}_1^T)-\frac{\beta}{\alpha^2}\tilde{\boldsymbol{u}}_2\tilde{\boldsymbol{v}}_2^T\end{aligned}$$

Proof. (3/3).

Substituting the values of α, β, $\widetilde{u}$'s and $\widetilde{v}$'s we have we have

$$H_{k+1} \leftarrow H_k - \frac{H_k y_k s_k^T + s_k y_k^T H_k}{s_k^T y_k} + \frac{s_k s_k^T}{s_k^T y_k}\left(1 + \frac{y_k^T H_k y_k}{s_k^T y_k}\right)$$

At this point the update formula (B) is a straightforward calculation.

Positive definitiveness of BFGS update

Theorem (Positive definitiveness of BFGS update)

Given H_k symmetric and positive definite, then the DFP update

$$H_{k+1} \leftarrow \left(I - \frac{s_k y_k^T}{s_k^T y_k}\right) H_k \left(I - \frac{y_k s_k^T}{s_k^T y_k}\right) + \frac{s_k s_k^T}{s_k^T y_k}$$

produce H_{k+1} positive definite if and only if $s_k^T y_k > 0$.

Remark (Wolfe $\Rightarrow$ BFGS update is SPD)

Expanding $s_k^T y_k > 0$ we have $\nabla f(x_{k+1}) s_k > \nabla f(x_k) s_k$. Remember that in a minimum search algorithm we have $s_k = \alpha_k p_k$ with $\alpha_k > 0$. But the second Wolfe condition for line-search is $\nabla f(x_k + \alpha_k p_k) p_k \geq c_2 \nabla f(x_k) p_k$ with $0 < c_2 < 1$. But this imply:

$$\nabla f(x_{k+1}) s_k \geq c_2 \nabla f(x_k) s_k > \nabla f(x_k) s_k \quad \Rightarrow \quad s_k^T y_k > 0.$$

Proof.

Let be $s_k^T y_k > 0$: consider a $z \neq 0$ then

$$z^T H_{k+1} z = w^T H_k w + \frac{(z^T s_k)^2}{s_k^T y_k} \quad \text{where} \quad w = z - y_k \frac{s_k^T z}{s_k^T y_k}$$

In order to have $z^T H_{k+1} z = 0$ we must have $w = 0$ and $z^T s_k = 0$. But $z^T s_k = 0$ imply $w = z$ and this imply $z = \mathbf{0}$.

Let be $z^T H_{k+1} z > 0$ for all $z \neq \mathbf{0}$: Choosing $z = y_k$ we have

$$0 < y_k^T H_{k+1} y_k = \frac{(s_k^T y_k)^2}{s_k^T y_k} = s_k^T y_k$$

and thus $s_k^T y_k > 0$. □

Algorithm (BFGS quasi-Newton algorithm)

$k \leftarrow 0$;
x assigned; $g \leftarrow \nabla f(x)$; $H \leftarrow \nabla^2 f(x)^{-1}$;
while $\|g\| > \epsilon$ **do**
  — compute search direction
  $d \leftarrow Hg$;
  Approximate $\arg\min_{\alpha>0} f(x - \alpha d)$ by linsearch;
  — perform step
  $x \leftarrow x - \alpha d$;
  — update H_{k+1}
  $y \leftarrow \nabla f(x) - g$; $z \leftarrow Hy$; $g \leftarrow \nabla f(x)$;
  $H \leftarrow H - \dfrac{zd^T + dz^T}{d^T y} + \left(\alpha - \dfrac{y^T z}{d^T y}\right)\dfrac{dd^T}{d^T y}$;
  $k \leftarrow k + 1$;
end while

Theorem (property of BFGS update)

Let be $\mathrm{q}(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_\star)^T \boldsymbol{A}(\boldsymbol{x}-\boldsymbol{x}_\star) + c$ *with* $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ *symmetric and positive definite. Let be* $\boldsymbol{x}_0$ *and* $\boldsymbol{H}_0$ *assigned. Let* $\{\boldsymbol{x}_k\}$ *and* $\{\boldsymbol{H}_k\}$ *produced by the sequence* $\{\boldsymbol{s}_k\}$

1. $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \boldsymbol{s}_k$;
2. $\boldsymbol{H}_{k+1} \leftarrow \left(\boldsymbol{I} - \frac{\boldsymbol{s}_k\boldsymbol{y}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)\boldsymbol{H}_k\left(\boldsymbol{I} - \frac{\boldsymbol{y}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right) + \frac{\boldsymbol{s}_k\boldsymbol{s}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}$;

where $\boldsymbol{s}_k = \alpha_k \boldsymbol{p}_k$ *with* α_k *is obtained by exact line-search. Then for* $j < k$ *we have*

1. $\boldsymbol{g}_k^T \boldsymbol{s}_j = 0$; *[orthogonality property]*
2. $\boldsymbol{H}_k \boldsymbol{y}_j = \boldsymbol{s}_j$; *[hereditary property]*
3. $\boldsymbol{s}_k^T \boldsymbol{A}\boldsymbol{s}_j = 0$; *[conjugate direction property]*
4. *The method terminate (i.e.* $\nabla \mathrm{f}(\boldsymbol{x}_m) = \boldsymbol{0}$*) at* $\boldsymbol{x}_m = \boldsymbol{x}_\star$ *with* $m \le n$. *If* $n = m$ *then* $\boldsymbol{H}_n = \boldsymbol{A}^{-1}$.

Proof. (1/4).

Points (1), (2) and (3) are proved by induction. The base of induction is obvious, let be the theorem true for $k > 0$. Due to exact line search we have:

$$\boldsymbol{g}_{k+1}^T \boldsymbol{s}_k = 0$$

moreover by induction for $j < k$ we have $\boldsymbol{g}_{k+1}^T \boldsymbol{s}_j = 0$, in fact:

$$\begin{aligned}
\boldsymbol{g}_{k+1}^T \boldsymbol{s}_j &= \boldsymbol{g}_j^T \boldsymbol{s}_j + \sum_{i=j}^{k-1} (\boldsymbol{g}_{i+1} - \boldsymbol{g}_i)^T \boldsymbol{s}_j \\
&= 0 + \sum_{i=j}^{k-1} (\boldsymbol{A}(\boldsymbol{x}_{i+1} - \boldsymbol{x}_\star) - \boldsymbol{A}(\boldsymbol{x}_i - \boldsymbol{x}_\star))^T \boldsymbol{s}_j \\
&= \sum_{i=j}^{k-1} (\boldsymbol{A}(\boldsymbol{x}_{i+1} - \boldsymbol{x}_i))^T \boldsymbol{s}_j \\
&= \sum_{i=j}^{k-1} \boldsymbol{s}_i^T \boldsymbol{A}\boldsymbol{s}_j = 0. \qquad \text{[induction + conjugacy prop.]}
\end{aligned}$$

Proof. (2/4).

By using $\boldsymbol{s}_{k+1} = -\alpha_{k+1}\boldsymbol{H}_{k+1}\boldsymbol{g}_{k+1}$ we have $\boldsymbol{s}_{k+1}^T \boldsymbol{A}\boldsymbol{s}_j = 0$, in fact:

$$\begin{aligned}
\boldsymbol{s}_{k+1}^T \boldsymbol{A}\boldsymbol{s}_j &= -\alpha_{k+1}\boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1}(\boldsymbol{A}\boldsymbol{x}_{j+1} - \boldsymbol{A}\boldsymbol{x}_j) \\
&= -\alpha_{k+1}\boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1}(\boldsymbol{A}(\boldsymbol{x}_{j+1} - \boldsymbol{x}_\star) - \boldsymbol{A}(\boldsymbol{x}_j - \boldsymbol{x}_\star)) \\
&= -\alpha_{k+1}\boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1}(\boldsymbol{g}_{j+1} - \boldsymbol{g}_j) \\
&= -\alpha_{k+1}\boldsymbol{g}_{k+1}^T \boldsymbol{H}_{k+1}\boldsymbol{y}_j \\
&= -\alpha_{k+1}\boldsymbol{g}_{k+1}^T \boldsymbol{s}_j \qquad \text{[induction + hereditary prop.]} \\
&= 0
\end{aligned}$$

notice that we have used $\boldsymbol{A}\boldsymbol{s}_j = \boldsymbol{y}_j$.

Proof. (3/4).

Due to BFGS construction we have

$$\boldsymbol{H}_{k+1}\boldsymbol{y}_k = \boldsymbol{s}_k$$

by inductive hypothesis and BFGS formula for $j < k$ we have, $\boldsymbol{s}_k^T \boldsymbol{y}_j = \boldsymbol{s}_k^T \boldsymbol{A}\boldsymbol{s}_j = 0$,

$$\begin{aligned}
\boldsymbol{H}_{k+1}\boldsymbol{y}_j &= \left(\boldsymbol{I} - \frac{\boldsymbol{s}_k\boldsymbol{y}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)\boldsymbol{H}_k\left(\boldsymbol{y}_j - \frac{\boldsymbol{s}_k^T\boldsymbol{y}_j}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\boldsymbol{y}_k\right) + \frac{\boldsymbol{s}_k\boldsymbol{s}_k^T\boldsymbol{y}_j}{\boldsymbol{s}_k^T\boldsymbol{y}_k} \\
&= \left(\boldsymbol{I} - \frac{\boldsymbol{s}_k\boldsymbol{y}_k^T}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\right)\boldsymbol{H}_k\boldsymbol{y}_j + \frac{\boldsymbol{s}_k 0}{\boldsymbol{s}_k^T\boldsymbol{y}_k} \qquad [\boldsymbol{H}_k\boldsymbol{y}_j = \boldsymbol{s}_j] \\
&= \boldsymbol{s}_j - \frac{\boldsymbol{y}_k^T\boldsymbol{s}_j}{\boldsymbol{s}_k^T\boldsymbol{y}_k}\boldsymbol{s}_k \\
&= \boldsymbol{s}_j
\end{aligned}$$

Proof. (4/4).

Finally if $m = n$ we have s_j with $j = 0, 1, \ldots, n-1$ are conjugate and linearly independent. From hereditary property and lemma on slide 8

$$H_n A s_k = H_n y_k = s_k$$

i.e. we have

$$H_n A s_k = s_k, \qquad k = 0, 1, \ldots, n-1$$

due to linear independence of $\{s_k\}$ follows that $H_n = A^{-1}$. □

Outline

1 Quasi Newton Method
2 The symmetric rank one update
3 The Powell-symmetric-Broyden update
4 The Davidon Fletcher and Powell rank 2 update
5 The Broyden Fletcher Goldfarb and Shanno (BFGS) update
6 The Broyden class

- The DFP update

$$H_{k+1}^{BFGS} \leftarrow H_k - \frac{H_k y_k s_k^T + s_k y_k^T H_k}{s_k^T y_k} + \frac{s_k s_k^T}{s_k^T y_k}\left(1 + \frac{y_k^T H_k y_k}{s_k^T y_k}\right)$$

and BFGS update

$$H_{k+1}^{DFP} \leftarrow H_k + \frac{s_k s_k^T}{s_k^T y_k} - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k}$$

maintains the symmetry and positive definitiveness.

- The following update

$$H_{k+1}^{\theta} \leftarrow (1-\theta) H_{k+1}^{DFP} + \theta H_{k+1}^{BFGS}$$

maintain for any θ the symmetry, and for $\theta \in [0,1]$ also the positive definitiveness.

Positive definitiveness of Broyden Class update

Theorem (Positive definitiveness of Broyden Class update)

Given H_k symmetric and positive definite, then the Broyden Class update

$$H_{k+1}^{\theta} \leftarrow (1-\theta) H_{k+1}^{DFP} + \theta H_{k+1}^{BFGS}$$

produce H_{k+1}^{θ} positive definite for any $\theta \in [0,1]$ if and only if $s_k^T y_k > 0$.

Theorem (property of Broyden Class update)

Let be $\mathsf{q}(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_\star)^T\boldsymbol{A}(\boldsymbol{x}-\boldsymbol{x}_\star)+c$ *with* $\boldsymbol{A}\in\mathbb{R}^{n\times n}$ *symmetric and positive definite. Let be* $\boldsymbol{x}_0$ *and* $\boldsymbol{H}_0$ *assigned. Let* $\{\boldsymbol{x}_k\}$ *and* $\{\boldsymbol{H}_k\}$ *produced by the sequence* $\{\boldsymbol{s}_k\}$

1. $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \boldsymbol{s}_k$;
2. $\boldsymbol{H}^{\theta}_{k+1} \leftarrow (1-\theta)\boldsymbol{H}^{DFP}_{k+1} + \theta\boldsymbol{H}^{BFGS}_{k+1}$;

where $\boldsymbol{s}_k = \alpha_k\boldsymbol{p}_k$ *with* α_k *is obtained by exact line-search. Then for* $j<k$ *we have*

1. $\boldsymbol{g}_k^T\boldsymbol{s}_j = 0$; *[orthogonality property]*
2. $\boldsymbol{H}_k\boldsymbol{y}_j = \boldsymbol{s}_j$; *[hereditary property]*
3. $\boldsymbol{s}_k^T\boldsymbol{A}\boldsymbol{s}_j = 0$; *[conjugate direction property]*
4. *The method terminate (i.e.* $\nabla\mathsf{f}(\boldsymbol{x}_m)=\boldsymbol{0}$*) at* $\boldsymbol{x}_m=\boldsymbol{x}_\star$ *with* $m\le n$*. If* $n=m$ *then* $\boldsymbol{H}_n=\boldsymbol{A}^{-1}$.

- The Broyden Class update canbe written as

$$\begin{aligned}\boldsymbol{H}^{\theta}_{k+1} &= \boldsymbol{H}^{DFP}_{k+1} + \theta\boldsymbol{w}_k\boldsymbol{w}_k^T\\ &= \boldsymbol{H}^{BFGS}_{k+1} + (\theta-1)\boldsymbol{w}_k\boldsymbol{w}_k^T\end{aligned}$$

where

$$\boldsymbol{w}_k = (\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k)^{1/2}\left[\frac{\boldsymbol{s}_k}{\boldsymbol{s}_k^T\boldsymbol{y}_k} - \frac{\boldsymbol{H}_k\boldsymbol{y}_k}{\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k}\right]$$

- For particular values of θ we obtain
  1. $\theta=0$, the DFP update
  2. $\theta=1$, the BFGS update
  3. $\theta=\boldsymbol{s}_k^T\boldsymbol{y}_k/(\boldsymbol{s}_k-\boldsymbol{H}_k\boldsymbol{y}_k)^T\boldsymbol{y}_k$ the SR1 update
  4. $\theta=(1\pm(\boldsymbol{y}_k^T\boldsymbol{H}_k\boldsymbol{y}_k/\boldsymbol{s}_k^T\boldsymbol{y}_k))^{-1}$ the Hoshino update

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