Numerical Optimization
Lecture Notes #19
Quasi-Newton Methods — Symmetric-Rank-1 / Broyden Class

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Outline

1. Quasi-Newton Methods
   - Recap: DFP and BFGS
   - SR-1: Simpler Update Formulas

2. SR-1
   - Properties
   - More Properties...

3. The Broyden Class
   - A Wider Framework for Quasi-Newton Methods
   - The Restricted Broyden Class
The DFP and BFGS Methods: Rank-2 Updates

As we saw last time, the updated matrices \( H_{k+1} / B_{k+1} \) differ from their predecessors \( H_k / B_k \) by rank-2 updates, e.g. for BFGS:

\[
H_{k+1} = \left( I - \rho_k \bar{s}_k \bar{y}_k^T \right) H_k \left( I - \rho_k \bar{y}_k \bar{s}_k^T \right) + \rho_k \bar{s}_k \bar{s}_k^T, \quad \rho_k = \frac{1}{\bar{y}_k^T \bar{s}_k},
\]

or, expressed in terms of \( B_{k+1} \) and \( B_k \) (with some help from the Sherman-Morrison-Woodbury formula):

\[
B_{k+1} = B_k - \frac{B_k \bar{s}_k \bar{s}_k^T B_k}{\bar{s}_k^T B_k \bar{s}_k} + \frac{\bar{y}_k \bar{y}_k^T}{\bar{y}_k^T \bar{s}_k},
\]

where

\[
\begin{align*}
\bar{s}_k &= \bar{x}_{k+1} - \bar{x}_k \\
\bar{y}_k &= \nabla f(\bar{x}_{k+1}) - \nabla f(\bar{x}_k).
\end{align*}
\]
The Symmetric-Rank-1 (SR1) Method: A Simpler Update-Formula

We can find a much simpler update-formula, of rank 1 which maintains symmetry and satisfies the secant equation

\[ B_{k+1} \bar{s}_k = \bar{y}_k, \quad \text{or} \quad H_{k+1} \bar{y}_k = \bar{s}_k \]

We can, however, not guarantee that \( B_{k+1} \) is positive definite.

Still, stable and effective numerical algorithms based on SR1 can be developed.

The symmetric-rank-1 update has the form

\[ B_{k+1} = B_k + \sigma \bar{v} \bar{v}^T, \quad \sigma = \pm 1, \]

and \( \sigma \) and \( \bar{v} \) are chosen so that \( B_{k+1} \) satisfies the secant equation.
A Note on the Outer Product $\bar{v}\bar{v}^T$

If $\bar{v} \in \mathbb{R}^n$, then

$$A = \bar{v}\bar{v}^T = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \cdot \begin{bmatrix} \bar{v}^T \\ \bar{v}^T \\ \vdots \\ \bar{v}^T \end{bmatrix} = \begin{bmatrix} v_1 \cdot \bar{v}^T \\ v_2 \cdot \bar{v}^T \\ \vdots \\ v_n \cdot \bar{v}^T \end{bmatrix}.$$

I.e all rows of $A$ are multiples of $\bar{v}^T$, and

$$\text{eig}(A) = \{\lambda_1, 0, \ldots, 0\}, \quad \lambda_1 = \bar{v}^T\bar{v} = \|\bar{v}\|_2^2.$$

Further, the normalized eigenvector corresponding to $\lambda_1$ is

$$\bar{e}_1 = \frac{\bar{v}}{\|\bar{v}\|}.$$
The SR1 Update

Using the update, and the secant equation

\[ B_{k+1} = B_k + \sigma \bar{v} \bar{v}^T, \quad B_{k+1} \bar{s}_k = \bar{y}_k. \]

We see that

\[ \bar{y}_k = \left[ B_k + \sigma \bar{v} \bar{v}^T \right] \bar{s}_k = B_k \bar{s}_k + \sigma \bar{v} \bar{v}^T \bar{s}_k = B_k \bar{s}_k + \left[ \sigma \bar{v}^T \bar{s}_k \right] \bar{v}. \]

Since \( \sigma \bar{v}^T \bar{s}_k \) is a scalar, we have

\[ \bar{v} = \delta \left[ \bar{y}_k - B_k \bar{s}_k \right], \quad \text{for some } \delta \in \mathbb{R}. \]

We substitute this back, and get

\[ (\bar{y}_k - B_k \bar{s}_k) = \sigma \delta^2 \left[ \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \right] (\bar{y}_k - B_k \bar{s}_k). \]

A "complicated" 1
In order to satisfy

$$\sigma \delta^2 \left[ \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \right] = 1,$$

we must have

$$\sigma = \text{sign} \left( \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \right), \quad \delta = \pm \left| \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \right|^{-1/2},$$

Hence, the unique SR1 update which satisfies the secant equation is given by

$$B_{k+1} = B_k + \frac{(\bar{y}_k - B_k \bar{s}_k)(\bar{y}_k - B_k \bar{s}_k)^T}{\bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k)},$$

or equivalently, by Sherman-Morrison-Woodbury

$$H_{k+1} = H_k + \frac{(\bar{s}_k - H_k \bar{y}_k)(\bar{s}_k - H_k \bar{y}_k)^T}{\bar{y}_k^T (\bar{s}_k - H_k \bar{y}_k)}.$$
Since the terms in the denominators \( \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \) and \( \bar{y}_k^T (\bar{s}_k - H_k \bar{y}_k) \) may be negative, it is possible that \( B_{k+1} (H_{k+1}) \) is not positive definite, even though \( B_k (H_k) \) is.

This makes **SR1 updates useless for linesearch methods.**

However, for trust-region methods we can allow indefinite Hessian approximations.

The ability of the SR1 method to generate indefinite Hessian approximations is a **strength** (when leveraged right) — away from the optimum there is nothing guaranteeing that the actual Hessian, \( \nabla^2 f(\bar{x}_k) \), is positive definite.
The main problem that the SR1 method can encounter is that the denominators $\bar{s}_k^T(\bar{y}_k - B_k\bar{s}_k)$ and $\bar{y}_k^T(\bar{s}_k - H_k\bar{y}_k)$ may be zero (small).

If we look at the update for $B_{k+1}$ we have three separate cases:

1. $\bar{s}_k^T(\bar{y}_k - B_k\bar{s}_k) \neq 0$: There is a unique SR1 update (as described above).
2. $\bar{y}_k = B_k\bar{s}_k$: The only update formula satisfying the secant equation is $B_{k+1} = B_k$.
3. $\bar{s}_k \perp (\bar{y}_k - B_k\bar{s}_k)$: There is no SR1 update formula which satisfies the secant equation.

The last case is bad news! — It suggests that the SR1 method may break down.
Since SR1 may break down, maybe we should just stick with BFGS (where the updates are all SPD and safe) and call it a day?

It turns out that the SR1 method is still useful:

(i) The breakdown can be easily fixed with a simple safeguard.

(ii) The matrices generated by SR1 tend to be very good approximations of the Hessian matrices — in many cases better than the BFGS approximations. (They’re easier to compute too!)

(iii) In some cases (constrained problems, or partially separable functions) it may be impossible to satisfy the curvature condition $\bar{y}_k^T \bar{s}_k > 0$, which is required for BFGS updating.
Fixing the SR1 Breakdown

The fix is almost embarrassingly simple: “If the denominator is too small, do not update!”

In more detail, the update is only applied when

$$\bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \geq r \|\bar{s}_k\| \|\bar{y}_k - B_k \bar{s}_k\|,$$

for some $r \in (0, 1)$

A good choice is $r = \sqrt{\epsilon_{mach}} = 10^{-8}$, in our typical floating-point environments.

Not applying the update means $B_{k+1} = B_k$. 

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Algorithm: The SR1 Trust-Region Method

Given starting point $\bar{x}_0$, convergence tolerance $\epsilon > 0$, initial Hessian approximation $B_0$, trust-region radius $\Delta_0$, $\eta \in (0, 10^{-3})$ and $r \in (0, 1)$:

$k = 0$

while ($\| \nabla f(\bar{x}_k) \| > \epsilon$)

\[ \bar{s}_k = \arg \min_{\bar{s}} \nabla f(\bar{x}_k)^T \bar{s} + \frac{1}{2} \bar{s}^T B_k \bar{s}: \| \bar{s} \| \leq \Delta_k \]

\[ \bar{y}_k = \nabla f(\bar{x}_{k+1}) - \nabla f(\bar{x}_k) \]

\[ \text{ared} = f(\bar{x}_k) - f(\bar{x}_k + \bar{s}_k) \]

\[ \text{pred} = -[\nabla f(\bar{x}_k)^T \bar{s}_k + \frac{1}{2} \bar{s}_k^T B_k \bar{s}_k] \]

if (ared/pred $> \eta$) $\bar{x}_{k+1} = \bar{x}_k + \bar{s}_k$ else $\bar{x}_{k+1} = \bar{x}_k$

if (ared/pred $> 0.75$)

if ($\| \bar{s}_k \| \leq 0.8\Delta_k$) $\Delta_{k+1} = \Delta_k$ else $\Delta_{k+1} = 2 \cdot \Delta_k$

elseif ($0.1 \leq \text{ared/pred} \leq 0.75$) $\Delta_{k+1} = \Delta_k$

else $\Delta_{k+1} = \Delta_k / 2$

if ($\| \bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k) \| \geq r \| \bar{s}_k \| \| \bar{y}_k - B_k \bar{s}_k \|$)

$B_{k+1} = B_k + \frac{(\bar{y}_k - B_k \bar{s}_k)(\bar{y}_k - B_k \bar{s}_k)^T}{\bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k)}$

else $B_{k+1} = B_k$

end-while($k = k + 1$)

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Further Properties of SR1 Updating

The SR1 method generates good Hessian approximations. We take a closer look at applying the SR1 update to a quadratic objective function, with fixed step-length 1, i.e.

$$\bar{p}_k = -H_k \nabla f(\bar{x}_k), \quad \bar{x}_{k+1} = \bar{x}_k + \bar{p}_k$$

The following can be shown:

**Theorem**

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is the strongly convex function

$$f(\bar{x}) = \bar{b}^T \bar{x} + \frac{1}{2} \bar{x}^T A \bar{x},$$

where $A$ is a symmetric positive definite matrix. Then for any starting point $\bar{x}_0$ and symmetric starting matrix $H_0$, the iterates $\{\bar{x}_k\}$ generated by the SR1 updates and $\bar{p}_k = -H_k \nabla f(\bar{x}_k)$, $\bar{x}_{k+1} = \bar{x}_k + \bar{p}_k$ converges to the minimizer in at most $n$ steps, provided that $(\bar{s}_k - H_k \bar{y}_k)^T \bar{y}_k \neq 0$ for all $k$. Moreover, if $n$ steps are performed, and if the search directions $p_i$ are linearly independent, then $H_n = A^{-1}$. 
For general non-linear objectives, the SR1 updates generate good Hessian approximations as well, but the provable results is a little weaker:

**Theorem**

Suppose that $f$ is twice continuously differentiable, and the Hessian is bounded and Lipschitz continuous in a neighborhood of a point $\bar{x}^*$. Let $\{\bar{x}_k\}$ be any sequence of iterates such that $\bar{x}_k \to \bar{x}^*$ for some $\bar{x}^* \in \mathbb{R}^n$. Suppose in addition that

$$|\bar{s}_k^T (\bar{y}_k - B_k \bar{s}_k)| \geq r \|\bar{s}_k\| \|\bar{y}_k - B_k \bar{s}_k\|$$

holds for all $k$, for some $r \in (0, 1)$, and that the steps $\bar{s}_k$ are uniformly linearly independent*. Then the matrices $B_k$ generated by the SR1 updating formula satisfy

$$\lim_{k \to \infty} \|B_k - \nabla^2 f(\bar{x}^*)\| = 0.$$

* See next slide.
Note: “Uniformly Linearly Independent”

Here, “Uniformly Linearly Independent” means, roughly, that the steps do not tend to fall in a subspace of dimension less than $n$. This assumption is usually, but not always, satisfied in practice.
So far we have looked at three quasi-Newton methods: DFP, BFGS, and SR1.

There are infinitely many more quasi-Newton methods, of which the **Broyden class** is of interest.

The updates of the Broyden class takes the form

\[
B_{k+1} = B_k - \frac{B_k \bar{s}_k \bar{s}_k^T B_k}{\bar{s}_k^T B_k \bar{s}_k} + \frac{\bar{y}_k \bar{y}_k^T}{\bar{y}_k^T \bar{s}_k} + \Phi_k (\bar{s}_k^T B_k \bar{s}_k) \bar{v}_k \bar{v}_k^T,
\]

where

\[
\bar{v} = \begin{bmatrix}
\bar{y}_k \\
\bar{y}_k^T \bar{s}_k \\
\bar{y}_k^T \bar{s}_k - B_k \bar{s}_k \\
\bar{s}_k^T B_k \bar{s}_k
\end{bmatrix},
\]

and \( \Phi_k \) is a scalar.
The BFGS and DFP methods are part of the Broyden class:

<table>
<thead>
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<tr>
<td>$\Phi_k = 1$</td>
<td>DFP</td>
</tr>
</tbody>
</table>

We can view the Broyden class as a linear combination of BFGS and DFP

$$B_{k+1}^{\text{Broyden}} = (1 - \Phi_k)B_{k+1}^{\text{BFGS}} + \Phi_k B_{k+1}^{\text{DFP}}$$

Since BFGS and DFP satisfy the secant equation, so does the Broyden class.

Since BFGS and DFP preserve positive definiteness when $\bar{s}_k^T \bar{y}_k > 0$, so does the Broyden class, for $0 \leq \Phi_k \leq 1$. 
The Restricted Broyden Class, $\Phi_k \in [0, 1]$

**Theorem**

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is the strongly convex quadratic function $f(\bar{x}) = \bar{b}^T \bar{x} + \frac{1}{2} \bar{x}^T A \bar{x}$, where $A$ is SPD. Let $\bar{x}_0$ be any starting point for the iteration

$$\bar{p}_k = -B_k^{-1} \nabla f(\bar{x}_k), \quad \bar{x}_{k+1} = \bar{x}_k + \bar{p}_k$$

and $B_0$ be any SPD starting matrix, and suppose that the matrices $B_k$ are updated by the Broyden formula with $\Phi_k \in [0, 1]$. Define $\lambda_1^{(k)} \leq \lambda_2^{(k)} \leq \cdots \leq \lambda_n^{(k)}$ to be the eigenvalues of the matrix

$$A^{1/2} B_k^{-1} A^{1/2}$$

Then, for all $k$ we have

$$\min\{\lambda_i^{(k)}, 1\} \leq \lambda_i^{(k+1)} \leq \max\{\lambda_i^{(k)}, 1\}, \quad i = 1, 2, \ldots, n$$

Moreover, this is not true for $\Phi_k \not\in [0, 1]$. 
The Restricted Broyden Class: What the Theorem Means

If the eigenvalues of the matrix

\[ A^{1/2} B_k^{-1} A^{1/2} \]

are all 1, then the quasi-Newton approximation \( B_k \) is identical to the Hessian \( A \) of the quadratic objective. (This is what we want in a perfect world)

The relation

\[
\min\{\lambda_i^{(k)}, 1\} \leq \lambda_i^{(k+1)} \leq \max\{\lambda_i^{(k)}, 1\}, \quad i = 1, 2, \ldots, n
\]

tells us that the eigenvalues \( \{\lambda_i^{(k)}\} \) converge monotonically to 1.

If some \( \lambda_i^{(k)} = 0.8 \), then we know that \( \lambda_i^{(k+1)} \in [0.8, 1] \) — convergence is not strict, but at least we are not moving away from the desired result.
The theorem seems to suggest that the best update formulas belong to the restricted Broyden class. However, this has not been established.

On the contrary, computational testing and some analysis suggest that algorithms that allow $\Phi_k < 0$ may outperform BFGS.

We have already seen one example — the SR1 method

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<td>SR1</td>
</tr>
</tbody>
</table>
The Broyden Class: Properties

We know that if $B_k$ is SPD, $\bar{y}_k^T \bar{s}_k > 0$, and $\Phi_k \geq 0$, then $B_{k+1}$ is also SPD if a restricted Broyden class update is used.

It can be shown that $B_{k+1}$ is SPD for a wider range of $\Phi_k$, including some negative values; $B_{k+1}$ becomes singular (has at least one zero eigenvalue) when $\Phi_k$ takes the critical value $\Phi_k^c$

$$\Phi_k^c = \frac{1}{1 - \mu_k}, \quad \mu_k = \frac{(\bar{y}_k^T B_k^{-1} \bar{y}_k)(\bar{s}_k^T B_k \bar{s}_k)}{(\bar{y}_k^T \bar{s}_k)^2}$$

$\mu_k \geq 1$, so $\Phi_k^c \leq 0$.

Hence, if $B_0$ is SPD, $\bar{y}_k^T \bar{s}_k > 0$, and $\Phi_k > \Phi_k^c$, then $B_k$ are all SPD.

When the line search is exact, all Broyden class methods with $\Phi_k > \Phi_k^c$ generate the same sequence of iterates $\{x_k\}$. The directions $\tilde{p}_k$ differ only in length, so the exact line searches identify the same $\bar{s}_k = \alpha_k^* \tilde{p}_k$. 
Theorem

Suppose that a method of the Broyden class is applied to a strongly convex function \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), where \( \bar{x}_0 \) is the starting point and \( B_0 \) is any SPD matrix. Assume that \( \alpha_k \) is the exact step length and that \( \Phi_k \geq \Phi^c_k \) for all \( k \). Then the following statements are true:

(i) The iterates converge to the solution in at most \( n \) iterations.

(ii) The secant equation is satisfied for all previous search directions, i.e.

\[
B_k \bar{s}_j = \bar{y}_j, \quad j = 1, 2, \ldots, k - 1
\]

(iii) If the starting matrix is \( B_0 = I \), then the iterates are identical to those generated by the conjugate gradient method. In particular, the search directions are conjugate, i.e.

\[
\bar{s}_i^T A \bar{s}_j = 0, \quad \text{for } i \neq j
\]

where \( A \) is the Hessian of the quadratic function.

(iv) If \( n \) iterations are performed, then \( B_n = A \).
The results (i), (ii), and (iv) echo the result for the SR1 method applied to a strongly convex objective function.

Result (iii) may seem a little surprising?!? With an exact line search the Broyden class methods compute the conjugate gradient directions while constructing the Hessian (and/or inverse Hessian)!

If $B_0 \neq I$, then the Broyden class methods generate the iterates of the preconditioned conjugate gradient method $\text{PCG}(B_0)$.

These results are mainly theoretical curiosities, since any practical implementation would use inexact line-searches. This causes the performance to differ, sometimes dramatically.

This sort of analysis was, however, the key to development of quasi-Newton methods.
Homework #5 — Due 11/18/2016

Implement BFGS (and if you have too much time on your hands DFP and SR1).

Grab `rosenbrock_2Nd.m` from the class webpage, and use the 18-dimensional initial condition returned by `rosenbrock_2Nd(x,-1)`.

Compare against full Newton optimization — count number of “outer iterations” $x_k \rightarrow x_{k+1}$, as well as “inner iterations” (linesearches / trust-region model rebuilds).

Check the Quasi-Newton convergence criteria (from lecture #5)

$$\lim_{k \to \infty} \frac{\| (B_k - \nabla^2 f(\bar{x}_k))\bar{p}_k \|}{\| \bar{p}_k \|} = 0$$

and things that may be revealed in the future (lecture #20).