Numerical Optimization
Lecture Notes #18
Quasi-Newton Methods — The BFGS Method

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Outline

1. Quasi-Newton Methods
   - Introduction
   - The BFGS Method

2. BFGS Variants
   - Limited-memory BFGS
Quasi-Newton methods require **only the gradient** (like steepest descent) of the objective to be computed at each iterate.

By successive measurements of the gradient, Quasi-Newton methods build a quadratic model of the objective function which is sufficiently good that **superlinear** convergence is achieved.

Quasi-Newton methods are much faster than steepest descent (and coordinate descent) methods.

Since second derivatives (the Hessian) are not required, quasi-Newton methods are **sometimes** more efficient (as measured by total work / “wall-clock computational time”) than Newton methods, especially when Hessian evaluation is slow/expensive.
The BFGS method is named for its discoverers: Broyden-Fletcher-Goldfarb-Shanno, and is the most popular quasi-Newton method.

We first derive the DFP method (a close relative; named after Davidon-Fletcher-Powell) and then the BFGS method; and look at some properties and practical implementation details.

The derivation starts with the quadratic model

\[ m_k(p) = f(x_k) + \nabla f(x_k)^T p + \frac{1}{2} p^T B_k p \]

at the current iterate \( x_k \). \( B_k \) is a symmetric positive definite matrix (model Hessian) that will be updated in every iteration.
Given this convex quadratic model, we can write down the minimizer $\bar{p}_k$ explicitly as

$$
\bar{p}_k = -B_k^{-1}\nabla f(\bar{x}_k).
$$

We can compute the search direction $\bar{p}_k$ using e.g. the Cholesky factorization, or a (P)CG-iteration; once we have $\bar{p}_k$ we find the new iterate:

$$
\bar{x}_{k+1} = \bar{x}_k + \alpha_k \bar{p}_k,
$$

where we require that the step length $\alpha_k$ satisfies e.g. the Wolfe conditions:

$$
f(\bar{x}_k + \alpha \bar{p}_k) \leq f(\bar{x}_k) + c_1 \alpha \bar{p}_k^T \nabla f(\bar{x}), \quad c_1 \in (0, 1)
$$

$$
\bar{p}_k^T \nabla f(\bar{x}_k + \alpha \bar{p}_k) \geq c_2 \bar{p}_k^T \nabla f(\bar{x}_k), \quad c_2 \in (c_1, 1).
$$
So far we have not really done anything new — the key difference compared with the linesearch Newton method is that we are using an approximate Hessian $B_k \neq \nabla^2 f(\bar{x}_k)$.

Instead to computing a completely new $B_k$ in each iteration, we will update

$$B_{k+1} = B_k + \text{“something,”}$$

using partial about the curvature at step $\neq k$. Thus we get a new model

$$m_{k+1}(\bar{p}) = f(\bar{x}_{k+1}) + \nabla f(\bar{x}_{k+1})^T \bar{p} + \frac{1}{2} \bar{p}^T B_{k+1} \bar{p}.$$  

Clearly, for this to make sense we must impose some conditions on the update.
We impose two conditions on the new model $m_{k+1}(\bar{p})$:

1. $m_{k+1}(\bar{p})$ must match the gradient of the objective function in $\bar{x}_k$ and $\bar{x}_{k+1}$.

The second condition is satisfied by construction, since

$$\nabla m_{k+1}(\bar{p}) = \nabla f(\bar{x}_{k+1}).$$

The first condition gives us

$$\nabla m_{k+1}(-\alpha_k \bar{p}_k) = \nabla f(\bar{x}_{k+1}) - \alpha_k B_{k+1} \bar{p}_k = \nabla f(\bar{x}_k).$$

With a little bit of re-arrangement we get

$$\alpha_k B_{k+1} \bar{p}_k = \nabla f(\bar{x}_{k+1}) - \nabla f(\bar{x}_k).$$
We clean up the notation by introducing \((\bar{x}_k, \text{ and } \bar{y}_k)\):

\[
\begin{align*}
\bar{s}_k &= \bar{x}_{k+1} - \bar{x}_k \\
\bar{y}_k &= \nabla f(\bar{x}_{k+1}) - \nabla f(\bar{x}_k).
\end{align*}
\]

We can now express the condition on \(B_{k+1}\) in terms of \(\bar{s}_k\) and \(\bar{y}_k\):

**Secant Equation**

\[
B_{k+1} \bar{s}_k = \bar{y}_k.
\]

By pre-multiplying the secant equation by \(\bar{s}_k^T\) we get the **Curvature Condition**

\[
\bar{s}_k^T B_{k+1} \bar{s}_k = \bar{s}_k^T \bar{y}_k \implies \bar{s}_k^T \bar{y}_k > 0.
\]

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If we impose the Wolfe, or strong Wolfe condition on the line search procedure, the curvature condition will always hold, since

\[ \nabla f(\bar{x}_{k+1})^T \bar{s}_k \geq c_2 \nabla f(\bar{x}_k)^T \bar{s}_k, \]

by the (curvature) Wolfe condition, and therefore

\[ \bar{y}_k^T \bar{s}_k \geq (c_2 - 1) \alpha_k \nabla f(\bar{x}_k)^T \bar{p}_k, \]

where the right-hand-side is positive since \( c_2 < 1 \) and \( \bar{p}_k \) is a descent direction.

**When the curvature condition is satisfied, the secant equation always has at least one solution \( B_{k+1} \).**
It turns out that there are infinitely many symmetric positive definite matrices $B_{k+1}$ which satisfy the secant equation.

<table>
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<th>Degrees of Freedom</th>
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<td>$n(n + 1)/2$ — Symmetric</td>
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To determine $B_{k+1}$ uniquely we must impose additional conditions — we will select the $B_{k+1}$ that is closest to $B_k$ in some sense:

Matrix-Minimization-Problem

$$B_{k+1} = \arg \min_B \| B - B_k \|_{\text{some-norm}}$$

subject to $B = B^T$, $B\bar{s}_k = \bar{y}_k$. 
Each choice of matrix norm in this matrix-minimization-problem (MMP) gives rise to a different quasi-Newton method.

The **weighted Frobenius norm**

\[
\| A \|_W = \| W^{1/2} AW^{1/2} \|_F = \| C \|_F = \sqrt{\sum_{i=0}^{n} \sum_{j=0}^{n} c_{ij}^2}
\]

allows easy solution of the MMP, and gives rise to a scale-invariant optimization method.

The matrix \( W \) is chosen to be the inverse \( G_k^{-1} \) of the **average Hessian**

\[
G_k = \int_0^1 \nabla^2 f(\bar{x}_k + \tau \alpha_k \bar{p}_k) d\tau.
\]
A positive semi-definite matrix, $M$ has a unique positive semi-definite square root, $R = M^{1/2}$.

When $M = XX^{-1} \equiv Q\Lambda Q^T$, let $R = QSQ^T$, and

$$R^2 = (QSQ^T)^2 = QSQ^TQSQ^T = QSSQ^T = QS^2Q^T = M,$$

showing that

$$S = \Lambda^{1/2}, \quad \text{and therefore} \quad R = Q\Lambda^{1/2}Q^T$$

∃ other approaches.
With this weighting matrix and norm, the unique solution of the MMP is

\[ B_{k+1} = \left( I - \gamma_k \bar{y}_k \bar{s}_k^T \right) B_k \left( I - \gamma_k \bar{s}_k \bar{y}_k^T \right) + \gamma_k \bar{y}_k \bar{y}_k^T, \quad \gamma_k = \frac{1}{\bar{y}_k^T \bar{s}_k}. \]

Note that \( \gamma_k \) is a scalar, and \( \bar{y}_k \bar{s}_k^T, \bar{s}_k \bar{y}_k^T, \) and \( \bar{y}_k \bar{y}_k^T \) are rank-one matrices.

This is the original Davidon-Fletcher-Powell (DFP) method suggested by W.C. Davidon in 1959.

The original paper describing this revolutionary idea — *the first quasi-Newton method* — was not accepted for publication. It later appeared in 1991 in the first issue the the SIAM Journal on Optimization.

Fletcher and Powell demonstrated that this algorithm was much faster and more reliable than existing methods (at the time). This revolutionized the field of non-linear optimization.
The inverse of $B_k$ is useful for the implementation of the method, since it allows the search direction $\bar{p}_k$ to be computed using a simple matrix-vector product. We let

$$H_k = B_k^{-1}$$

and use

**Sherman-Morrison-Woodbury formula**

If $A \in \mathbb{R}^{n \times n}$ is non-singular and $\bar{a}, \bar{b} \in \mathbb{R}^n$, and if

$$B = A + \bar{a}\bar{b}^T$$

then

$$B^{-1} = A^{-1} - \frac{A^{-1}\bar{a}\bar{b}^T A^{-1}}{1 + \bar{b}^T A^{-1}\bar{a}}.$$
With a little bit of linear algebra we end up with

\[ H_{k+1} = H_k - \frac{H_k \bar{y}_k \bar{y}_k^T H_k}{\bar{y}_k^T H_k \bar{y}_k} \bar{s}_k \bar{s}_k^T. \]

Both the update terms are rank-one matrices; so that \( H_k \) undergoes a rank-2 modification in each iteration.

This is the fundamental idea of quasi-Newton updating: instead of recomputing the matrix (-inverse) from scratch each time around, we apply a simple modification which combines the more recently observed information about the objective with existing knowledge embedded in the current Hessian approximation.
The DFP method is quite effective, but once the quasi-Newton idea was accepted by the optimization community is was quickly superseded by the BFGS method.

BFGS updating is derived by instead of imposing conditions on the Hessian approximations $B_k$, we impose conditions directly on the inverses $H_k$.

The updated approximation must be symmetric positive definite, and must satisfy the secant equation in the form

$$H_{k+1} \bar{y}_k = \bar{s}_k,$$

**compare:**

$$B_{k+1} \bar{s}_k = \bar{y}_k.$$ 

We get a slightly different matrix minimization problem...
The BFGS Matrix Minimization Problem

\[
H_{k+1} = \arg \min_H \| H - H_k \|_{\text{some-norm}}
\]
subject to \( H = H^T, \ H\bar{y}_k = \bar{s}_k \)

If we again choose the weighted Frobenius norm (with the same weight), then we get the unique update

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

which translated back to the Hessian approximation yields

\[
B_{k+1} = B_k - \frac{B_k \bar{s}_k \bar{s}_k^T B_k}{\bar{s}_k^T B_k \bar{s}_k} + \frac{\bar{y}_k \bar{y}_k^T}{\bar{y}_k^T \bar{s}_k}.
\]
BFGS vs. DFP Updates

**BFGS Update —**

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

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

**DFP Update —**

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

\[
H_{k+1} = H_k - \frac{H_k \bar{y}_k \bar{y}_k^T H_k}{\bar{y}_k^T H_k \bar{y}_k} + \frac{\bar{s}_k \bar{s}_k^T}{\bar{y}_k^T \bar{s}_k}.
\]
The initial value for the iteration can be selected in different ways

- A finite difference approximation at $\bar{x}_0$.

- $H_0 = I$, the identity matrix.

- $H_0 = \text{diag}(s_1, s_2, \ldots, s_n)$, where $\bar{s}$ captures the scaling of the variables (if known).
The BFGS Method: Algorithm

Algorithm: The BFGS Method

Given starting point $\bar{x}_0$, convergence tolerance $\varepsilon > 0$, and initial inverse Hessian approximation $H_0$:

$k = 0$

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

$\bar{p}_k = -H_k \nabla f(\bar{x}_k)$

$\bar{x}_{k+1} = \text{linesearch}(\bar{p}_k, \ldots)$

$\bar{s}_k = \bar{x}_{k+1} - \bar{x}_k$

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

$\rho_k = \frac{1}{\bar{y}_k^T \bar{s}_k}$

$H_{k+1} = \left( I - \rho_k \bar{s}_k \bar{y}_k^T \right) H_k \left( I - \rho_k \bar{y}_k \bar{s}_k^T \right) + \rho_k \bar{s}_k \bar{s}_k^T$

$k = k + 1$

end-while
The BFGS Method: Summary

The cost per iteration is

- $O(n^2)$ arithmetic operations
- function evaluation
- gradient evaluation

The convergence rate is

- Super-linear

Newton’s method converges quadratically, but the cost per iteration is higher — it requires the solution of a linear system. In addition Newton’s method requires the calculation of second derivatives whereas the BFGS method does not.
If at some point $\rho_k = 1/\bar{y}_k^T \bar{s}_k$ becomes large, i.e. $\bar{y}_k^T \bar{s}_k \sim 0$, then from the update formula

$$H_{k+1} = \left( I - \rho_k \bar{s}_k \bar{y}_k^T \right) H_k \left( I - \rho_k \bar{y}_k \bar{s}_k^T \right) + \rho_k \bar{s}_k \bar{s}_k^T$$

we see that $H_{k+1}$ becomes large.

If for this, or some other, reason $H_k$ becomes a poor approximation of $[\nabla^2 f(\bar{x}_k)]^{-1}$ for some $k$, is there any hope of correcting it?

It has been shown that the BFGS method has self-correcting properties. — If $H_k$ incorrectly estimates the curvature of the objective function, and if this estimate slows down the iteration, then the Hessian approximation will tend to correct itself within a few steps.
The self-correcting properties stand and fall with the quality of the line search! — The Wolfe conditions ensure that the model captures appropriate curvature information.

The DFP method is less effective at self-correcting bad Hessian approximations.

**Practical Implementation Details:**

- The linesearch should always test $\alpha = 1$ first, because this step length will eventually be accepted, thus creating super-linear convergence.
- The linesearch can be somewhat “sloppy:” $c_1 = 10^{-4}$ and $c_2 = 0.9$ are commonly used values in the Wolfe conditions.
- The initial matrix $H_0$ should not be too large, if $H_0 = \beta I$, then the first step is $\bar{p}_0 = -\beta \nabla f(\bar{x}_0)$ which may be too long if $\beta$ is large, often $H_0$ is rescaled before the update $H_1$ is computed:

$$H_0 \leftarrow \frac{\bar{y}_k^T \bar{s}_k}{\bar{y}_k^T \bar{y}_k} I.$$
L-BFGS

Forming the $n \times n$ dense matrix $H_k$ can be quite expensive for large problems. L-BFGS stores a limited history of the BFGS update vectors $\bar{s}_k$ and $\bar{y}_k$ (which are size $n$), and use these to “implicitly” form the matrix operations.

In standard BFGS, the current $H_k$ contains updates all the way back to initial step $\{\bar{s}_j, \bar{y}_j\}_{j=0}^{k-1}$, whereas L-BFGS only uses a limited number of “recent” updates; so that the action of $\tilde{H}_k$ is formed by application of $\{\bar{s}_j, \bar{y}_j\}_{j=\max(0,k-m)}^{k-1}$.
L-BFGS

"Two Loop Recursion"

Given a local initial positive definite model for the Hessian, $\tilde{H}_k$:

1. $\bar{v} = \nabla f(\bar{x}_k)$
2. $\alpha_j = \rho_j \bar{s}_j^T \bar{v}$, \quad $\bar{v} = \bar{v} - \alpha_j \bar{y}_j$, \quad $j = k - 1, \ldots, k - m$.
3. $\bar{w} = \tilde{H}_k \bar{v}$
4. $\beta_j = \rho_j \bar{y}_j^T \bar{w}$, \quad $\bar{w} = \bar{w} + \bar{s}_j (\alpha_j - \beta_j)$, \quad $j = k - m, \ldots, k - 1$
5. Now, use $\bar{p}_k = -\bar{w}$ \quad ($\approx -H_k \nabla f(\bar{x}_k)$).

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