

Numerical Optimization

Lecture Notes #18

Quasi-Newton Methods — The BFGS Method

Fall 2019

Outline

1 Quasi-Newton Methods

- Introduction
- The BFGS Method

2 BFGS Variants

- Limited-memory BFGS

Quasi-Newton Methods

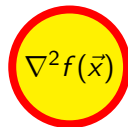
The Sales Pitch!

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

By successively measuring 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: Introduction

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The most popular quasi-Newton algorithm is the BFGS method. 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

$$m_k(\bar{\mathbf{p}}) = f(\bar{\mathbf{x}}_k) + \nabla f(\bar{\mathbf{x}}_k)^T \bar{\mathbf{p}} + \frac{1}{2} \bar{\mathbf{p}}^T B_k \bar{\mathbf{p}}$$

at the current iterate $\bar{\mathbf{x}}_k$. B_k is a symmetric positive definite matrix (model Hessian) that will be **updated** in every iteration.

The BFGS Method: Introduction

Standard Stuff

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Given this convex quadratic model, we can write down the minimizer $\bar{\mathbf{p}}_k$ explicitly as

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

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

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

where we require that the step length α_k satisfies e.g. the Wolfe conditions:

$$\begin{aligned} f(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k) &\leq f(\bar{\mathbf{x}}_k) + c_1 \alpha \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}), & c_1 &\in (0, 1) \\ \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k) &\geq c_2 \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k), & c_2 &\in (c_1, 1). \end{aligned}$$

The BFGS Method: Introduction

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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 $B_k \neq \nabla^2 f(\bar{\mathbf{x}}_k)$.

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

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

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

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

Clearly, for this to make sense we must impose some conditions on the update.

The BFGS Method: Conditions on B_{k+1}

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We impose two conditions on the new model $m_{k+1}(\bar{\mathbf{p}})$:

[1,2] The gradient of $m_{k+1}(\bar{\mathbf{p}})$ must match the gradient of the objective function in $\bar{\mathbf{x}}_k$ and $\bar{\mathbf{x}}_{k+1}$.

The second condition is satisfied by construction, since

$$\nabla m_{k+1}(\bar{\mathbf{0}}) = \nabla f(\bar{\mathbf{x}}_{k+1}).$$

The first condition gives us

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

With a little bit of re-arrangement we get

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

The BFGS Method: Conditions on B_{k+1}

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We simplify the notation by introducing $(\bar{\mathbf{x}}_k$, and $\bar{\mathbf{y}}_k)$:

$$\begin{aligned}\bar{\mathbf{s}}_k &= \bar{\mathbf{x}}_{k+1} - \bar{\mathbf{x}}_k && \equiv \alpha_k \bar{\mathbf{p}}_k \\ \bar{\mathbf{y}}_k &= \nabla f(\bar{\mathbf{x}}_{k+1}) - \nabla f(\bar{\mathbf{x}}_k).\end{aligned}$$

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

Secant Equation

$$\mathbf{B}_{k+1} \bar{\mathbf{s}}_k = \bar{\mathbf{y}}_k.$$

By pre-multiplying the secant equation by $\bar{\mathbf{s}}_k^T$ we get the

Curvature Condition

$$\underbrace{\bar{\mathbf{s}}_k^T \mathbf{B}_{k+1} \bar{\mathbf{s}}_k}_{>0} = \bar{\mathbf{s}}_k^T \bar{\mathbf{y}}_k \quad \Rightarrow \quad \bar{\mathbf{s}}_k^T \bar{\mathbf{y}}_k > 0.$$

The BFGS Method: Conditions on B_{k+1}

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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

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

by the (curvature) Wolfe condition, and therefore

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

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

When the curvature condition is satisfied, the secant equation always has at least one solution B_{k+1} .

The BFGS Method: More Conditions on B_{k+1}

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It turns out that there are infinitely many symmetric positive definite matrices B_{k+1} which satisfy the secant equation.

Degrees of Freedom of B_{k+1}	Conditions Imposed
$n(n+1)/2$ — Symmetric	n — The Secant Equation n — Principal minors positive (PD)

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

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

$$\text{subject to } B = B^T, B\bar{s}_k = \bar{y}_k.$$

The BFGS Method: More Conditions on B_{k+1}

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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**

$$G_k = \int_0^1 \nabla^2 f(\bar{\mathbf{x}}_k + \tau \alpha_k \bar{\mathbf{p}}_k) d\tau.$$

Square Roots of SPD Matrices

[SUPPLEMENTAL]

- A positive semi-definite matrix, M has a unique positive semi-definite square root, $R = M^{1/2}$.

- When $M = X\Lambda X^{-1} \stackrel{\text{SPD}}{=} Q\Lambda Q^T$, let $R = QSQ^T$, and

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

showing that

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

- \exists other approaches.

The DFP Method

With this weighting matrix and norm, the unique solution of the MMP is

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

Note that γ_k is a scalar, and $\bar{\mathbf{y}}_k \bar{\mathbf{s}}_k^T$, $\bar{\mathbf{s}}_k \bar{\mathbf{y}}_k^T$, and $\bar{\mathbf{y}}_k \bar{\mathbf{y}}_k^T$ 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 *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 DFP Method: Cleaning Up

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The inverse of B_k is useful for the implementation of the method, since it allows the search direction $\bar{\mathbf{p}}_k$ 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 $\bar{\mathbf{a}}, \bar{\mathbf{b}} \in \mathbb{R}^n$, and if

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

then

$$B^{-1} = A^{-1} - \frac{A^{-1}\bar{\mathbf{a}}\bar{\mathbf{b}}^T A^{-1}}{1 + \bar{\mathbf{b}}^T A^{-1}\bar{\mathbf{a}}}.$$

The DFP Method: Cleaning Up

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With a little bit of linear algebra we end up with

$$H_{k+1} = H_k - \underbrace{\frac{H_k \bar{\mathbf{y}}_k \bar{\mathbf{y}}_k^T H_k}{\bar{\mathbf{y}}_k^T H_k \bar{\mathbf{y}}_k}}_{\text{Update \#1}} + \underbrace{\frac{\bar{\mathbf{s}}_k \bar{\mathbf{s}}_k^T}{\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k}}_{\text{Update \#2}}.$$

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.

Improving on DFP — The BFGS Method

The DFP method is quite effective, but once the quasi-Newton idea was accepted by the optimization community it 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

$$\mathbf{H}_{k+1}\bar{\mathbf{y}}_k = \bar{\mathbf{s}}_k, \quad \text{compare:} \quad B_{k+1}\bar{\mathbf{s}}_k = \bar{\mathbf{y}}_k.$$

We get a slightly different matrix minimization problem...

The BFGS Matrix Minimization Problem

Matrix-Minimization-Problem (BFGS)

$$H_{k+1} = \arg \min_H \|H - H_k\|_{\text{some-norm}}$$

$$\text{subject to } H = H^T, \quad H\bar{\mathbf{y}}_k = \bar{\mathbf{s}}_k$$

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

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

which translated back to the Hessian approximation yields

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k \bar{\mathbf{s}}_k \bar{\mathbf{s}}_k^T \mathbf{B}_k}{\bar{\mathbf{s}}_k^T \mathbf{B}_k \bar{\mathbf{s}}_k} + \frac{\bar{\mathbf{y}}_k \bar{\mathbf{y}}_k^T}{\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k}.$$

BFGS vs. DFP Updates

BFGS Update —

$$H_{k+1} = (I - \rho_k \bar{\mathbf{s}}_k \bar{\mathbf{y}}_k^T) H_k (I - \rho_k \bar{\mathbf{y}}_k \bar{\mathbf{s}}_k^T) + \rho_k \bar{\mathbf{s}}_k \bar{\mathbf{s}}_k^T, \quad \rho_k = \frac{1}{\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k},$$

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

DFP Update —

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

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

The BFGS Method: Starting — $H_0 = ???$

The initial value for the iteration can be selected in different ways

- A finite difference approximation at $\bar{\mathbf{x}}_0$.
- $H_0 = I$, the identity matrix.
- $H_0 = \mathbf{diag}(s_1, s_2, \dots, s_n)$, where $\bar{\mathbf{s}}$ captures the scaling of the variables (if known).

The BFGS Method: Algorithm

Algorithm: The BFGS Method

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

$k = 0$

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

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

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

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

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

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

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

$$k = k + 1$$

end-while

The BFGS Method: Summary

The cost per iteration is

- $\mathcal{O}(n^2)$ 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.

The BFGS Method: Stability and Self-Correction

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If at some point $\rho_k = 1/\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k$ becomes large, i.e. $\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k \sim 0$, then from the update formula

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

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

If for this, or some other, reason H_k becomes a poor approximation of $[\nabla^2 f(\bar{\mathbf{x}}_k)]^{-1}$ 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 BFGS Method: Stability and Self-Correction

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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 $\bar{\mathbf{p}}_0 = -\beta \nabla f(\bar{\mathbf{x}}_0)$ which may be too long if β is large, often H_0 is rescaled before the update H_1 is computed:

$$H_0 \leftarrow \frac{\bar{\mathbf{y}}_k^T \bar{\mathbf{s}}_k}{\bar{\mathbf{y}}_k^T \bar{\mathbf{y}}_k} I.$$

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 $\bar{\mathbf{s}}_k$ and $\bar{\mathbf{y}}_k$ (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 $\{\bar{\mathbf{s}}_j, \bar{\mathbf{y}}_j\}_{j=0}^{k-1}$, whereas L-BFGS only uses a limited number of “recent” updates; so that the action of \tilde{H}_k is formed by application of $\{\bar{\mathbf{s}}_j, \bar{\mathbf{y}}_j\}_{j=\max(0, k-m)}^{k-1}$.

L-BFGS

"Two Loop Recursion"

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

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

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