

Quasi-Newton methods

Basic idea (§11.1)

- Newton's method:
 - Fast convergence if we start close enough to solution.
 - Requires Hessian inverse (which may be large).
- Quasi-Newton methods: approximate the Hessian inverse using only gradient information.

- Basic quasi-Newton algorithm:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha_k \mathbf{H}_k \mathbf{g}^{(k)},$$

where \mathbf{H}_k takes the place of the true Hessian inverse in Newton's algorithm.

- The matrix \mathbf{H}_{k+1} is computed using $\mathbf{x}^{(k)}$, $\mathbf{x}^{(k+1)}$, $\mathbf{g}^{(k)}$, $\mathbf{g}^{(k+1)}$, and \mathbf{H}_k .
- \mathbf{H}_k is supposed to “mimic” $\mathbf{F}(\mathbf{x}^{(k)})^{-1}$.
- What properties of $\mathbf{F}(\mathbf{x}^{(k)})^{-1}$ should it mimic?
- At least \mathbf{H}_k should be symmetric.
- Another property that \mathbf{H}_k should mimic is the “secant” property.
- To explain this property, assume that f is quadratic, with Hessian \mathbf{Q} .

- Note that \mathbf{Q} satisfies

$$\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)} = \mathbf{Q}(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}),$$

or

$$\mathbf{Q}^{-1}(\mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}) = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}.$$

- Let

$$\begin{aligned} \Delta \mathbf{g}^{(k)} &\triangleq \mathbf{g}^{(k+1)} - \mathbf{g}^{(k)}, \\ \Delta \mathbf{x}^{(k)} &\triangleq \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}. \end{aligned}$$

- At any k , \mathbf{Q}^{-1} satisfies:

$$\mathbf{Q}^{-1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

- To mimic \mathbf{Q}^{-1} , we want \mathbf{H}_{k+1} to also satisfy

$$\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

- The above is called the quasi-Newton (or secant) condition.

Summary of quasi-Newton algorithm

- Form of algorithm:

$$\begin{aligned} \mathbf{d}^{(k)} &= -\mathbf{H}_k \mathbf{g}^{(k)} \\ \alpha_k &= \arg \min_{\alpha \geq 0} f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)}) \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}, \end{aligned}$$

where the matrices $\mathbf{H}_0, \mathbf{H}_1, \dots$ are symmetric.

- In the quadratic case, the above matrices are required to satisfy

$$\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

- Theorem (11.1): Any quasi-Newton algorithm is a conjugate direction algorithm.
- Specifically, suppose the quasi-Newton (secant) condition holds: for $0 \leq k < n - 1$,

$$\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

For $0 \leq k < n - 1$, if $\alpha_i \neq 0, 0 \leq i \leq k$, then $\mathbf{d}^{(0)}, \dots, \mathbf{d}^{(k+1)}$ are \mathbf{Q} -conjugate.

Proof of theorem:

- We use induction.
- For $k = 0$, we have

$$\begin{aligned} \mathbf{d}^{(1)T} \mathbf{Q} \mathbf{d}^{(0)} &= -\mathbf{g}^{(1)T} \mathbf{H}_1 \mathbf{Q} \mathbf{d}^{(0)} \\ &= -\mathbf{g}^{(1)T} \mathbf{H}_1 \frac{\mathbf{Q} \Delta \mathbf{x}^{(0)}}{\alpha_0} \\ &= -\mathbf{g}^{(1)T} \frac{\mathbf{H}_1 \Delta \mathbf{g}^{(0)}}{\alpha_0} \\ &= -\mathbf{g}^{(1)T} \frac{\Delta \mathbf{x}^{(0)}}{\alpha_0} \\ &= -\mathbf{g}^{(1)T} \mathbf{d}^{(0)} \\ &= 0 \end{aligned}$$

because of our choice of α_0 .

- Suppose the result is true for $k - 1$; i.e., $\mathbf{d}^{(0)}, \dots, \mathbf{d}^{(k)}$ are \mathbf{Q} -conjugate.
- We now prove the result for k ; i.e., that $\mathbf{d}^{(0)}, \dots, \mathbf{d}^{(k+1)}$ are \mathbf{Q} -conjugate.

- It suffices to show that $\mathbf{d}^{(k+1)T} \mathbf{Q} \mathbf{d}^{(i)} = 0$, $0 \leq i \leq k$.

- Given i , $0 \leq i \leq k$, we have

$$\begin{aligned}
 \mathbf{d}^{(k+1)T} \mathbf{Q} \mathbf{d}^{(i)} &= -\mathbf{g}^{(k+1)T} \mathbf{H}_{k+1} \mathbf{Q} \mathbf{d}^{(i)} \\
 &= -\mathbf{g}^{(k+1)T} \mathbf{H}_{k+1} \frac{\mathbf{Q} \Delta \mathbf{x}^{(i)}}{\alpha_i} \\
 &= -\mathbf{g}^{(k+1)T} \frac{\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)}}{\alpha_i} \\
 &= -\mathbf{g}^{(k+1)T} \frac{\Delta \mathbf{x}^{(i)}}{\alpha_i} \\
 &= -\mathbf{g}^{(k+1)T} \mathbf{d}^{(i)}.
 \end{aligned}$$

- Since $\mathbf{d}^{(0)}, \dots, \mathbf{d}^{(k)}$ are \mathbf{Q} -conjugate by assumption, by the “expanding subspace” lemma, we have $\mathbf{g}^{(k+1)T} \mathbf{d}^{(i)} = 0$.
- By the previous theorem, we conclude that if we apply a quasi-Newton algorithm to a quadratic, it terminates in at most n steps.
- How do we generate the matrices \mathbf{H}_k in such a way that it satisfies the quasi-Newton condition?
- There are several update formulas available for computing \mathbf{H}_{k+1} based on \mathbf{H}_k , $\Delta \mathbf{g}^{(k)}$, and $\Delta \mathbf{x}^{(k)}$.
- Methods for generating the \mathbf{H}_k :
 - Rank one formula
 - DFP formula
 - BFGS formula
- All have the form:

$$\mathbf{H}_{k+1} = \mathbf{H}_k + \mathbf{U}_k$$

where \mathbf{U}_k is an update (correction) term that depends on \mathbf{H}_k , $\Delta \mathbf{g}^{(k)}$, and $\Delta \mathbf{x}^{(k)}$.

Descent Property

- We want the descent property to hold.
- Recall that to have the descent property, the search direction $\mathbf{d}^{(k)} = -\mathbf{H}_k \mathbf{g}^{(k)}$ must have positive inner product with $-\mathbf{g}^{(k)}$:

$$\mathbf{g}^{(k)T} \mathbf{H}_k \mathbf{g}^{(k)} > 0.$$

- Prop. (11.1): If $\mathbf{H}_k > 0$, then the algorithm has the descent property.

Rank one correction formula (§11.3)

- The rank one formula has the form

$$\mathbf{U}_k = a_k \mathbf{z}^{(k)} \mathbf{z}^{(k)T},$$

where $a_k \in \mathbb{R}$ and $\mathbf{z}^{(k)} \in \mathbb{R}^n$.

- Note that

$$\text{rank } \mathbf{z}^{(k)} \mathbf{z}^{(k)T} = \text{rank} \left(\begin{bmatrix} z_1^{(k)} \\ \vdots \\ z_n^{(k)} \end{bmatrix} \begin{bmatrix} z_1^{(k)} & \dots & z_n^{(k)} \end{bmatrix} \right) = 1.$$

Hence the name *rank one* correction.

- Note: if we start with a symmetric matrix \mathbf{H}_0 , then the \mathbf{H}_k remain symmetric.
- What should a_k and $\mathbf{z}^{(k)}$ be? We need the quasi-Newton condition to hold.
- Answer: The quasi-Newton condition holds if and only if

$$\mathbf{U}_k = \frac{(\Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)})(\Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)})^T}{(\Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)})^T \Delta \mathbf{g}^{(k)}},$$

which can be expressed as:

$$\begin{aligned} a_k &= \frac{1}{(\Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)})^T \Delta \mathbf{g}^{(k)}}, \\ \mathbf{z}^{(k)} &= \Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)}. \end{aligned}$$

- Name: Rank one update formula.
- Derivation: tedious, but straightforward.
- Note that for each k ,

$$\begin{aligned} \mathbf{H}_{k+1} \Delta \mathbf{g}^{(k)} &= \mathbf{H}_k \Delta \mathbf{g}^{(k)} + \mathbf{U}_k \Delta \mathbf{g}^{(k)} \\ &= \mathbf{H}_k \Delta \mathbf{g}^{(k)} + \Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)} \\ &= \Delta \mathbf{x}^{(k)}. \end{aligned}$$

- What about $\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)}$ for all $i = 0, \dots, k$?

Theorem (11.2): The rank one formula satisfies the quasi-Newton condition.

Proof:

- Need to show that for each k ,

$$\mathbf{H}_{k+1}\Delta\mathbf{g}^{(i)} = \Delta\mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

Use induction.

- For $k = 0$, we know it is true (because we have already seen that $\mathbf{H}_{k+1}\Delta\mathbf{g}^{(k)} = \Delta\mathbf{x}^{(k)}$ for each k).
- Assume true for $k - 1$; i.e., that $\mathbf{H}_k\Delta\mathbf{g}^{(i)} = \Delta\mathbf{x}^{(i)}$, $i < k$.

- We now show it is true for k .

- Since we already know that $\mathbf{H}_{k+1}\Delta\mathbf{g}^{(k)} = \Delta\mathbf{x}^{(k)}$, it remains to show that $\mathbf{H}_{k+1}\Delta\mathbf{g}^{(i)} = \Delta\mathbf{x}^{(i)}$ for $i < k$.

- Fix $i < k$. We have

$$\mathbf{H}_{k+1}\Delta\mathbf{g}^{(i)} = \mathbf{H}_k\Delta\mathbf{g}^{(i)} + \mathbf{U}_k\Delta\mathbf{g}^{(i)}.$$

- By the induction hypothesis, $\mathbf{H}_k\Delta\mathbf{g}^{(i)} = \Delta\mathbf{x}^{(i)}$.
- Hence, enough to show that the $\mathbf{U}_k\Delta\mathbf{g}^{(i)} = 0$. For this, it is enough that

$$\begin{aligned} (\Delta\mathbf{x}^{(k)} - \mathbf{H}_k\Delta\mathbf{g}^{(k)})^T \Delta\mathbf{g}^{(i)} \\ = \Delta\mathbf{x}^{(k)T} \Delta\mathbf{g}^{(i)} - \Delta\mathbf{g}^{(k)T} \mathbf{H}_k\Delta\mathbf{g}^{(i)} = 0. \end{aligned}$$

- We have

$$\begin{aligned} \Delta\mathbf{g}^{(k)T} \mathbf{H}_k\Delta\mathbf{g}^{(i)} &= \Delta\mathbf{g}^{(k)T} (\mathbf{H}_k\Delta\mathbf{g}^{(i)}) \\ &= \Delta\mathbf{g}^{(k)T} \Delta\mathbf{x}^{(i)} \end{aligned}$$

by the induction hypothesis.

- Since $\Delta\mathbf{g}^{(k)} = \mathbf{Q}\Delta\mathbf{x}^{(k)}$, we have

$$\Delta\mathbf{g}^{(k)T} \mathbf{H}_k\Delta\mathbf{g}^{(i)} = \Delta\mathbf{x}^{(k)T} \mathbf{Q}\Delta\mathbf{x}^{(i)} = \Delta\mathbf{x}^{(k)T} \Delta\mathbf{g}^{(i)}.$$

- Hence,

$$\begin{aligned} (\Delta\mathbf{x}^{(k)} - \mathbf{H}_k\Delta\mathbf{g}^{(k)})^T \Delta\mathbf{g}^{(i)} \\ = \Delta\mathbf{x}^{(k)T} \Delta\mathbf{g}^{(i)} - \Delta\mathbf{x}^{(k)T} \Delta\mathbf{g}^{(i)} = 0, \end{aligned}$$

which completes the proof.

Drawbacks of rank one formula

- The \mathbf{H}_k may not be positive definite (because a_k may be negative), and hence $\mathbf{d}^{(k)} = -\mathbf{H}_k \mathbf{g}^{(k)}$ may not be a descent direction.
- There may be numerical problems if

$$\Delta \mathbf{g}^{(k)T} (\Delta \mathbf{x}^{(k)} - \mathbf{H}_k \Delta \mathbf{g}^{(k)}) \approx 0.$$

- We seek more sophisticated update formulas that avoid the above problems.
- We study two other formulas: DFP and BFGS.

The DFP Algorithm (§11.4)

- DFP update formula:

$$\mathbf{U}_k = \frac{\Delta \mathbf{x}^{(k)} \Delta \mathbf{x}^{(k)T}}{\Delta \mathbf{x}^{(k)T} \Delta \mathbf{g}^{(k)}} - \frac{\mathbf{H}_k \Delta \mathbf{g}^{(k)} \Delta \mathbf{g}^{(k)T} \mathbf{H}_k}{\Delta \mathbf{g}^{(k)T} \mathbf{H}_k \Delta \mathbf{g}^{(k)}}.$$

- Davidson, 1959; Fletcher and Powell, 1963.
- Also called *variable metric algorithm*.
- Has two “rank one” terms.

Theorem (11.3): The DFP algorithm satisfies the quasi-Newton condition.

Proof:

- Need to show $\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}$, $0 \leq i \leq k$.
- For $i = k$:

$$\begin{aligned} \mathbf{H}_{k+1} \Delta \mathbf{g}^{(k)} &= \mathbf{H}_k \Delta \mathbf{g}^{(k)} + \mathbf{U}_k \Delta \mathbf{g}^{(k)} \\ &= \Delta \mathbf{x}^{(k)}. \end{aligned}$$

- For general case, use induction.
- For $k = 0$, already showed it is true.
- Assume true for $k - 1$: $\mathbf{H}_k \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}$, $0 \leq i \leq k - 1$.
- To show true for k , remains to consider the case $i < k$.

- We have

$$\begin{aligned} \mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} &= \Delta \mathbf{x}^{(i)} \\ &+ \frac{\Delta \mathbf{x}^{(k)}}{\Delta \mathbf{x}^{(k)T} \Delta \mathbf{g}^{(k)}} (\Delta \mathbf{x}^{(k)T} \Delta \mathbf{g}^{(i)}) \\ &- \frac{\mathbf{H}_k \Delta \mathbf{g}^{(k)}}{\Delta \mathbf{g}^{(k)T} \mathbf{H}_k \Delta \mathbf{g}^{(k)}} (\Delta \mathbf{g}^{(k)T} \Delta \mathbf{x}^{(i)}). \end{aligned}$$

- Now,

$$\begin{aligned} \Delta \mathbf{x}^{(k)T} \Delta \mathbf{g}^{(i)} &= \Delta \mathbf{x}^{(k)T} \mathbf{Q} \Delta \mathbf{x}^{(i)} \\ &= \alpha_k \alpha_i \mathbf{d}^{(k)T} \mathbf{Q} \mathbf{d}^{(i)} \\ &= 0 \end{aligned}$$

by the induction hypothesis and the conjugate direction property.

- Similarly, $\Delta \mathbf{g}^{(k)T} \Delta \mathbf{x}^{(i)} = 0$.
- Hence,

$$\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)},$$

and the proof is completed.

- Theorem (11.4): Suppose $\mathbf{g}^{(k)} \neq \mathbf{0}$. In the DFP algorithm, if \mathbf{H}_k is positive definite, then so is \mathbf{H}_{k+1} .
- Proof: Tedious but straightforward.
- DFP algorithm better than rank one algorithm.
- DFP algorithm may have problems in some cases (getting stuck).

The BFGS Algorithm (§11.5)

- BFGS update algorithm:

$$\begin{aligned} \mathbf{U}_k &= \left(1 + \frac{\Delta \mathbf{g}^{(k)T} \mathbf{H}_k \Delta \mathbf{g}^{(k)}}{\Delta \mathbf{g}^{(k)T} \Delta \mathbf{x}^{(k)}} \right) \frac{\Delta \mathbf{x}^{(k)} \Delta \mathbf{x}^{(k)T}}{\Delta \mathbf{x}^{(k)T} \Delta \mathbf{g}^{(k)}} \\ &- \frac{\mathbf{H}_k \Delta \mathbf{g}^{(k)} \Delta \mathbf{x}^{(k)T} + (\mathbf{H}_k \Delta \mathbf{g}^{(k)} \Delta \mathbf{x}^{(k)T})^T}{\Delta \mathbf{g}^{(k)T} \Delta \mathbf{x}^{(k)}}. \end{aligned}$$

- Broyden, Fletcher, Goldfarb, and Shanno, 1970.

- The BFGS formula is derived from the DFP formula using a technique called *complementarity*.
- Consider the quasi-Newton condition:

$$\mathbf{H}_{k+1} \Delta \mathbf{g}^{(i)} = \Delta \mathbf{x}^{(i)}, \quad 0 \leq i \leq k.$$

- Consider a modified condition in which the roles of $\Delta \mathbf{g}^{(i)}$ and $\Delta \mathbf{x}^{(i)}$ are interchanged:

$$\mathbf{B}_{k+1} \Delta \mathbf{x}^{(i)} = \Delta \mathbf{g}^{(i)}, \quad 0 \leq i \leq k.$$

Call the above the “complementary quasi-Newton” condition.

- Think of \mathbf{B}_k as an approximation to the Hessian (instead of inverse Hessian).
- Given: an update equation for \mathbf{H}_k that satisfies the quasi-Newton condition.
- If we interchange $\Delta \mathbf{x}^{(k)}$ and $\Delta \mathbf{g}^{(k)}$ in the equation, and replace \mathbf{H}_k by \mathbf{B}_k , then the resulting formula satisfies the complementary quasi-Newton condition.
- Based on the DFP formula,

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\Delta \mathbf{g}^{(k)} \Delta \mathbf{g}^{(k)T}}{\Delta \mathbf{g}^{(k)T} \Delta \mathbf{x}^{(k)}} - \frac{\mathbf{B}_k \Delta \mathbf{x}^{(k)} \Delta \mathbf{x}^{(k)T} \mathbf{B}_k}{\Delta \mathbf{x}^{(k)T} \mathbf{B}_k \Delta \mathbf{x}^{(k)}}$$

- The above formula satisfies the complementary quasi-Newton condition.
- The previous formula for updating \mathbf{B}_k is not immediately useful because what we need is the inverse Hessian.
- What we need is an update formula for \mathbf{B}_k^{-1} .
- The previous formula is of the form:

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \mathbf{u}_1 \mathbf{v}_1^T + \mathbf{u}_2 \mathbf{v}_2^T.$$

- Hence,

$$\mathbf{B}_{k+1}^{-1} = (\mathbf{B}_k + \mathbf{u}_1 \mathbf{v}_1^T + \mathbf{u}_2 \mathbf{v}_2^T)^{-1}.$$

- Lemma (11.1): Let \mathbf{A} be a nonsingular matrix. Let \mathbf{u} and \mathbf{v} be column vectors and assume that $1 + \mathbf{v}^T \mathbf{A}^{-1} \mathbf{u} \neq 0$. Then, $\mathbf{A} + \mathbf{u} \mathbf{v}^T$ is nonsingular, and

$$(\mathbf{A} + \mathbf{u} \mathbf{v}^T)^{-1} = \mathbf{A}^{-1} - \frac{(\mathbf{A}^{-1} \mathbf{u})(\mathbf{v}^T \mathbf{A}^{-1})}{1 + \mathbf{v}^T \mathbf{A}^{-1} \mathbf{u}}.$$

- Proof: by verification.

- Name: *Sherman-Morrison formula*. Very useful!
- Note form:

$$(\mathbf{A} + \mathbf{u}\mathbf{v}^T)^{-1} = \mathbf{A}^{-1} + \mathbf{x}\mathbf{y}^T.$$

- Apply the Sherman-Morrison formula twice to

$$\mathbf{B}_{k+1}^{-1} = (\mathbf{B}_k + \mathbf{u}_1\mathbf{v}_1^T + \mathbf{u}_2\mathbf{v}_2^T)^{-1}.$$

- We obtain an update formula of the form:

$$\mathbf{B}_{k+1}^{-1} = \mathbf{B}_k^{-1} + \mathbf{u}_3\mathbf{v}_3^T + \mathbf{u}_4\mathbf{v}_4^T.$$

- If we now replace \mathbf{B}_k^{-1} by the symbol \mathbf{H}_k , we obtain the BFGS formula!
- BFGS is the “complementary” formula to DFP.
- By the nature of complementarity, the BFGS formula inherits the properties of DFP.
- Theorem: The BFGS formula satisfies the quasi-Newton condition.
- Theorem: Suppose $\mathbf{g}^{(k)} \neq \mathbf{0}$. In the BFGS algorithm, if \mathbf{H}_k is positive definite, then so is \mathbf{H}_{k+1} .