15. Quasi-Newton methods

- variable metric methods
- quasi-Newton methods
- BFGS update
- limited-memory quasi-Newton methods
Newton method for unconstrained minimization

minimize \( f(x) \)

\( f \) convex, twice continously differentiable

Newton method

\[ x_{k+1} = x_k - t_k \nabla^2 f(x_k)^{-1} \nabla f(x_k) \]

- advantages: fast convergence, robustness, affine invariance
- disadvantages: requires second derivatives and solution of linear equation

can be too expensive for large scale applications
Variable metric methods

\[ x_{k+1} = x_k - t_k H_k^{-1} \nabla f(x_k) \]

the positive definite matrix \( H_k \) is an approximation of the Hessian at \( x_k \), chosen to:

- avoid calculation of second derivatives
- simplify computation of search direction

“Variable metric” interpretation (236B, lecture 10, page 11)

\[ \Delta x = -H^{-1} \nabla f(x) \]

is the steepest descent direction at \( x \) for the quadratic norm

\[ \|z\|_H = \left( z^T H z \right)^{1/2} \]
Quasi-Newton methods

given: starting point $x_0 \in \text{dom } f$, $H_0 > 0$

for $k = 0, 1, \ldots$

1. compute quasi-Newton direction $\Delta x_k = -H_k^{-1}\nabla f(x_k)$

2. determine step size $t_k$ (e.g., by backtracking line search)

3. compute $x_{k+1} = x_k + t_k \Delta x_k$

4. compute $H_{k+1}$

- different update rules exist for $H_{k+1}$ in step 4
- can also propagate $H_k^{-1}$ or a factorization of $H_k$ to simplify calculation of $\Delta x_k$
Broyden–Fletcher–Goldfarb–Shanno (BFGS) update

**BFGS update**

\[
H_{k+1} = H_k + \frac{yy^T}{y^Ts} - \frac{H_k s s^T H_k}{s^T H_k s} \\
\]

where

\[
s = x_{k+1} - x_k, \quad y = \nabla f(x_{k+1}) - \nabla f(x_k) \]

**Inverse update**

\[
H^{-1}_{k+1} = \left( I - \frac{sy^T}{y^Ts} \right) H^{-1}_k \left( I - \frac{ys^T}{y^Ts} \right) + \frac{ss^T}{y^Ts} \\
\]

- note that $y^Ts > 0$ for strictly convex $f$; see page 1.8
- cost of update or inverse update is $O(n^2)$ operations
Positive definiteness

- if $y^T s > 0$, BFGS update preserves positive definitess of $H_k$
- this ensures that $\Delta x = -H_k^{-1} \nabla f(x_k)$ is a descent direction

**Proof:** from inverse update formula,

$$v^T H_k^{-1} v = \left( v - \frac{s^T v}{s^T y} y \right)^T H_k^{-1} \left( v - \frac{s^T v}{s^T y} y \right) + \frac{(s^T v)^2}{y^T s}$$

- if $H_k > 0$, both terms are nonnegative for all $v$
- second term is zero only if $s^T v = 0$; then first term is zero only if $v = 0$
Secant condition

the BFGS update satisfies the *secant condition*

\[ H_{k+1} s = y \]

where \( s = x_{k+1} - x_k \) and \( y = \nabla f(x_{k+1}) - \nabla f(x_k) \)

**Interpretation:** we define a quadratic approximation of \( f \) around \( x_{k+1} \)

\[
\tilde{f}(x) = f(x_{k+1}) + \nabla f(x_{k+1})^T (x - x_{k+1}) + \frac{1}{2} (x - x_{k+1})^T H_{k+1} (x - x_{k+1})
\]

- by construction \( \nabla \tilde{f}(x_{k+1}) = \nabla f(x_{k+1}) \)
- secant condition implies that also \( \nabla \tilde{f}(x_k) = \nabla f(x_k) \):

\[
\nabla \tilde{f}(x_k) = \nabla f(x_{k+1}) + H_{k+1} (x_k - x_{k+1})
= \nabla f(x_k)
\]
Secant method

for \( f: \mathbb{R} \rightarrow \mathbb{R} \), BFGS with unit step size gives the secant method

\[
x_{k+1} = x_k - \frac{f'(x_k)}{H_k}, \quad H_k = \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}
\]
Convergence

Global result

if $f$ is strongly convex, BFGS with backtracking line search (EE236B, lecture 10-6) converges from any $x_0, H_0 > 0$

Local convergence

if $f$ is strongly convex and $\nabla^2 f(x)$ is Lipschitz continuous, local convergence is superlinear: for sufficiently large $k$,

$$\|x_{k+1} - x^*\|_2 \leq c_k \|x_k - x^*\|_2$$

where $c_k \to 0$

(cf., quadratic local convergence of Newton method)
**Example**

\[
\text{minimize} \quad c^T x - \sum_{i=1}^{m} \log(b_i - a_i^T x)
\]

\[
n = 100, \quad m = 500
\]

- cost per Newton iteration: \(O(n^3)\) plus computing \(\nabla^2 f(x)\)
- cost per BFGS iteration: \(O(n^2)\)

Quasi-Newton methods
Square root BFGS update

To improve numerical stability, propagate $H_k$ in factored form $H_k = L_k L_k^T$

- if $H_k = L_k L_k^T$ then $H_{k+1} = L_{k+1} L_{k+1}^T$ with

$$L_{k+1} = L_k \left( I + \frac{\alpha \tilde{y} - \tilde{s}}{\tilde{s}^T \tilde{s}} \tilde{s}^T \right),$$

where

$$\tilde{y} = L_k^{-1} y, \quad \tilde{s} = L_k^T s, \quad \alpha = \left( \frac{\tilde{s}^T \tilde{s}}{y^T s} \right)^{1/2}$$

- if $L_k$ is triangular, cost of reducing $L_{k+1}$ to triangular form is $O(n^2)$
Optimality of BFGS update

$X = H_{k+1}$ solves the convex optimization problem

$$\begin{align*}
\text{minimize} & \quad \text{tr} \left( H_k^{-1} X \right) - \log \det \left( H_k^{-1} X \right) - n \\
\text{subject to} & \quad Xs = y
\end{align*}$$

- cost function is nonnegative, equal to zero only if $X = H_k$
- also known as relative entropy between densities $N(0, X), N(0, H_k)$
- BFGS update is a least-change secant update

Optimality result follows from KKT conditions: $X = H_{k+1}$ satisfies

$$X^{-1} = H_k^{-1} - \frac{1}{2} (sv^T + vs^T), \quad Xs = y, \quad X > 0$$

with

$$v = \frac{1}{s^T y} \left( 2H_k^{-1} y - \left( 1 + \frac{y^T H_k^{-1} y}{y^T s} \right) s \right)$$
Davidon–Fletcher–Powell (DFP) update

switch $H_k$ and $X$ in objective on previous page

$$\text{minimize} \quad \text{tr} \left( H_k X^{-1} \right) - \log \det \left( H_k X^{-1} \right) - n$$
$$\text{subject to} \quad X s = y$$

- minimize relative entropy between $N(0, H_k)$ and $N(0, X)$
- problem is convex in $X^{-1}$ (with constraint written as $s = X^{-1}y$)
- solution is ‘dual’ of BFGS formula

$$H_{k+1} = \left( I - \frac{ys^T}{s^Ty} \right) H_k \left( I - \frac{ys^T}{s^Ty} \right) + \frac{yy^T}{s^Ty}$$

(known as DFP update)

predates BFGS update, but is less often used
Limited memory quasi-Newton methods

main disadvantage of quasi-Newton method is need to store $H_k$, $H_k^{-1}$, or $L_k$

**Limited-memory BFGS** (L-BFGS): do not store $H_k^{-1}$ explicitly

- instead we store up to $m$ (e.g., $m = 30$) values of

\[ s_j = x_{j+1} - x_j, \quad y_j = \nabla f(x_{j+1}) - \nabla f(x_j) \]

- we evaluate $\Delta x_k = H_k^{-1} \nabla f(x_k)$ recursively, using

\[
H_{j+1}^{-1} = \left( I - \frac{s_j y_j^T}{y_j^T s_j} \right) H_j^{-1} \left( I - \frac{y_j s_j^T}{y_j^T s_j} \right) + \frac{s_j s_j^T}{y_j^T s_j}
\]

for $j = k - 1, \ldots, k - m$, assuming, for example, $H_{k-m} = I$

- an alternative is to restart after $m$ iterations
- cost per iteration is $O(nm)$, storage is $O(nm)$
Interpretation of CG as restarted BFGS method

first two iterations of BFGS (page 15.5) if $H_0 = I$:

$$
x_1 = x_0 - t_0 \nabla f(x_0), \quad x_2 = x_1 - t_1 H_1^{-1} \nabla f(x_1)
$$

where $H_1$ is computed from $s = x_1 - x_0$ and $y = \nabla f(x_1) - \nabla f(x_0)$ via

$$
H_1^{-1} = I + \left(1 + \frac{y^T y}{s^T y} \right) \frac{ss^T}{y^T s} - \frac{ys^T + sy^T}{y^T s}
$$

- if $t_0$ is determined by exact line search, then $\nabla f(x_1)^T s = 0$
- quasi-Newton step in second iteration simplifies to

$$
-H_1^{-1} \nabla f(x_1) = -\nabla f(x_1) + \frac{y^T \nabla f(x_1)}{y^T s} s
$$

this is the Hestenes–Stiefel conjugate gradient update

nonlinear CG can be interpreted as L-BFGS with $m = 1$
References