# 17. Quasi-Newton methods

- variable metric methods
- quasi-Newton methods
- BFGS update
- limited-memory quasi-Newton methods

# Newton method for unconstrained minimization

$$\text{minimize} \quad f(x)$$

$f$ 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 approximatian of the Hessian at $x_k$, chosen to:

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

**'Variable metric' interpretation** (EE236B, 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 $x_0 \in \operatorname{dom} f$, $H_0 \succ 0$

**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**

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

where

$$s = x_{k+1} - x_k, \qquad y = \nabla f(x_{k+1}) - \nabla f(x_k)$$

**Inverse update**

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

- note that $y^T s > 0$ 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,

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

- if $H_k \succ 0$, 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 $x_{k+1}$

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

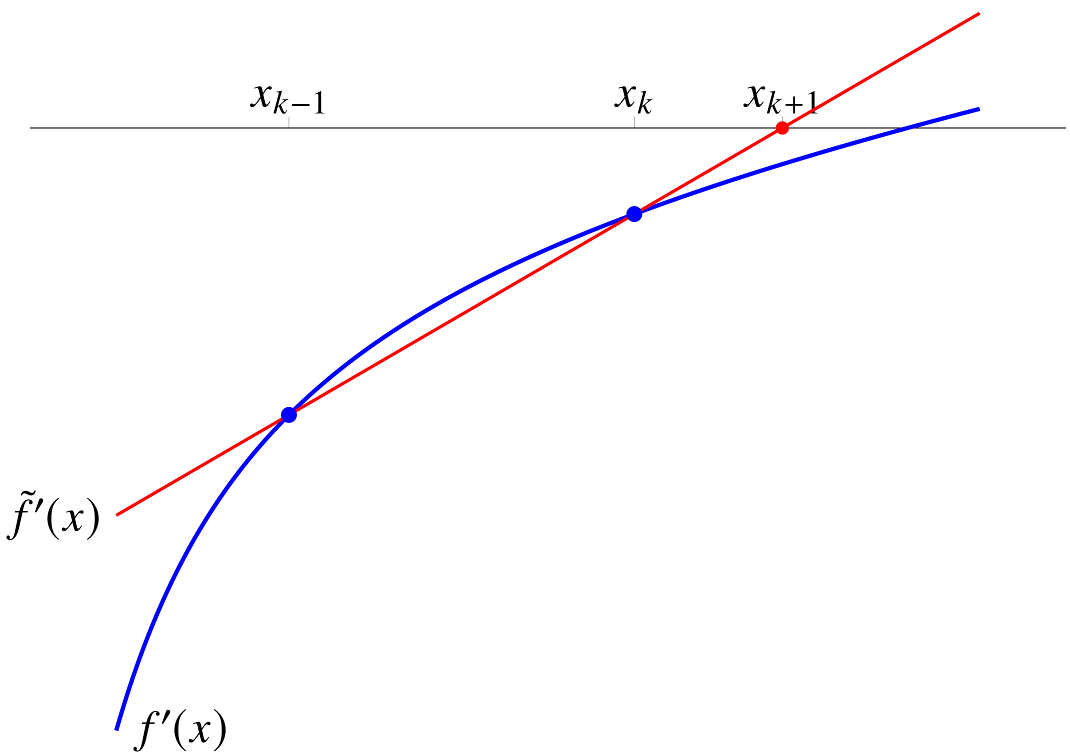
- by construction $\nabla \tilde{f}(x_{k+1}) = \nabla f(x_{k+1})$
- secant condition implies that also $\nabla \tilde{f}(x_k) = \nabla f(x_k)$:

$$\begin{aligned} \nabla \tilde{f}(x_k) &= \nabla f(x_{k+1}) + H_{k+1}(x_k - x_{k+1}) \\ &= \nabla f(x_k) \end{aligned}$$

# Secant method

for $f : \mathbf{R} \to \mathbf{R}$, BFGS with unit step size gives the secant method

$$x_{k+1} = x_k - \frac{f'(x_k)}{H_k}, \qquad H_k = \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}$$



# Convergence

**Global result**

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

**Local convergence**

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

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

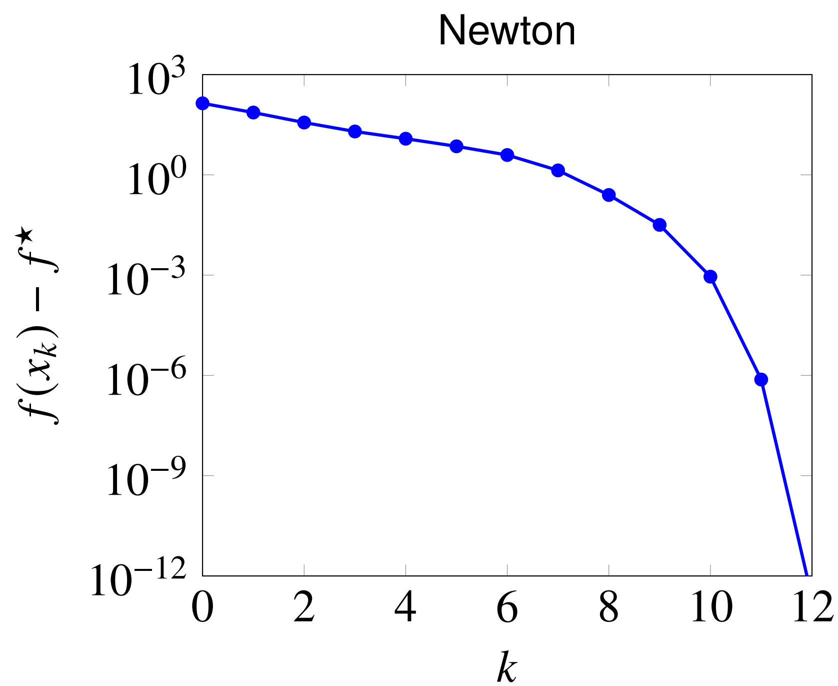
where $c_k \to 0$

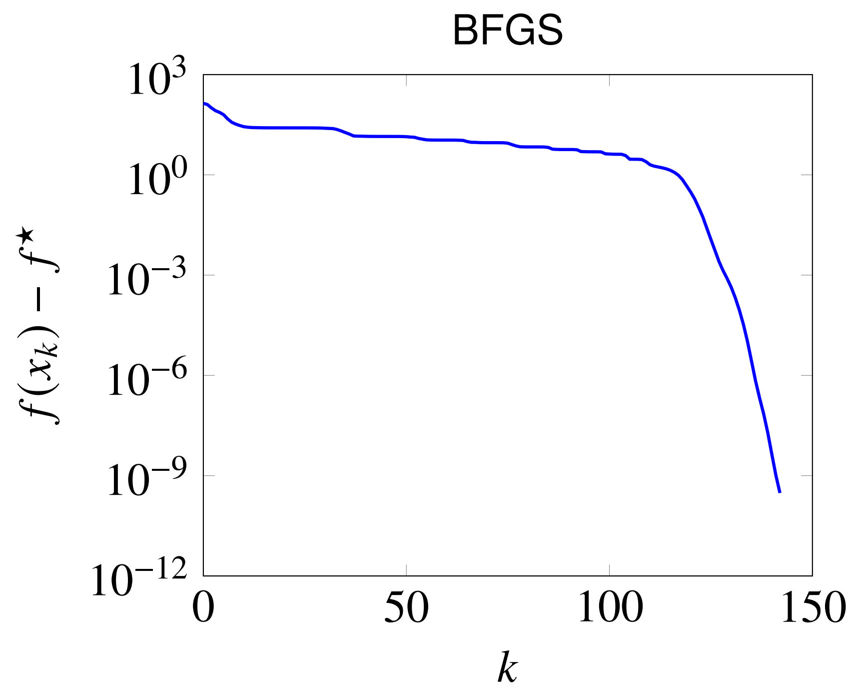
(*cf.*, quadratic local convergence of Newton method)

# Example

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

$n = 100$, $m = 500$




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

# 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

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

  where

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

- 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

$$\begin{array}{ll} \text{minimize} & \operatorname{tr}(H_k^{-1}X) - \log\det(H_k^{-1}X) - n \\ \text{subject to} & Xs = y \end{array}$$

- 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

$$X^{-1} = H_k^{-1} - \frac{1}{2}(s\nu^T + \nu s^T), \qquad Xs = y, \qquad X \succ 0$$

with

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

# Davidon–Fletcher–Powell (DFP) update

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

$$\begin{array}{ll} \text{minimize} & \operatorname{tr}(H_k X^{-1}) - \log\det(H_k X^{-1}) - n \\ \text{subject to} & Xs = y \end{array}$$

- 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

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

(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

$$s_j = x_{j+1} - x_j, \qquad y_j = \nabla f(x_{j+1}) - \nabla f(x_j)$$

- 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 17.5) if $H_0 = I$:

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

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

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

- 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


- J. E. Dennis, Jr., and R. B. Schabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations* (1996), chapter 9.
- C. T. Kelley, *Iterative Methods for Optimization* (1999), chapter 4.
- J. Nocedal and S. J. Wright, *Numerical Optimization* (2006), chapter 6 and section 7.2.