Chapter 3 - Line Search Methods

1) Choose (compute) direction $p_k$

2) Choose (compute) step length $\alpha$

$$x_{k+1} = x_k + \alpha p_k$$

$p_k$ should be descent direction: $p^T \nabla f_k < 0$

Often $p_k = -B_k^{-1} \nabla f_k$ for some

symm. nonsingular $B_k$

Ex. $B_k = I$ (steepest descent)

$B_k = \nabla^2 f_k$ (Newton)

If $B_k$ SPD: $\nabla f_k = \nabla^2 f_k B_k^{-1} \nabla f_k < 0$

→ descend direction

How about "$\alpha$"?

3.1 Step Length

Ideally min. $\phi(\alpha) = f(x_k + \alpha p_k), \alpha > 0$

Too expensive → $f(x)$ (very) expensive
We want "sufficient" progress (reduction) for modest work.

Two phases: 1) bracketing phase  
2) function/interpol. phase

1) find suitable interval

2) find good choice in interval

Why "suff. decrease"?

Why is $F(x_k + a_k p_k) < F(x_k)$ not good enough?

(similar problem might occur with choices of $p_k$)

Conditions on step length

Wolfe Conditions

a) (Armijo condition)

\[ F(x_k + a p_k) \leq F(x_k) + c_1 a \nabla F_k \cdot p_k, \quad c_1 \in (0, 1) \]

reduction proportional to $a$ and $\nabla F_k \cdot p_k$

\[ l(a) = F_k + c_1 a \nabla F_k \cdot p_k \]

\[ \frac{\nabla F_k \cdot p_k}{l(a)} \]

acceptable
Condition often quite weak \((c_1 = 10^{-4}, \text{book})\)
c_1 \text{ small}

We don't want very short steps:

\[
\text{curvature cond.: } \nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k
\]

For some constant \(c_2 \in (c_1, 1)\)

the slope of \(\phi(x)\) at \(x_k\) greater than \(c_2\) times initial slope \(\phi'(a)\) → progress

rate of progress is decreasing.

Typical values \(c_2 = 0.9\) for Newton
or quasi-Newton directions; \(c_2 = 0.1\) for
nonlinear Conj. Grad.

Together the 2 conditions are known as
the Wolfe conditions

\[
\begin{align*}
\phi(x_k + \alpha_k p_k) & \leq \phi(x_k) + \alpha_k c_1 \nabla f_k^T p_k \\
\nabla f(x_k + \alpha_k p_k)^T p_k & \geq c_2 \nabla f_k^T p_k
\end{align*}
\]

with \(0 < c_1 < c_2 < 1\)

Alternatively, in strong Wolfe cond. replace curvature cond. by

\[
| \nabla f(x_k + \alpha_k p_k)^T p_k | \leq c_2 | \nabla f_k^T p_k |
\]

(which also implies curvature cond.)
Note that Wolfe conditions are scale invariant, 

\( f \rightarrow a \cdot f \) makes no difference.

Alternative, Goldstein cond. 

\[
p(x_k) + (1-c) \alpha_k \nabla f_k^T p \leq p(x_k + \alpha_k p_k) \leq p(x_k) + \alpha_k c \nabla f_k^T p
\]

with \( 0 < c < \frac{1}{2} \)

\[
p(x_k) + \frac{1}{c} \alpha_k k \nabla f_k^T p
\]

Sufficient decrease and backtracking

We can drop curv. condition (and all\'s) 
if we consider large enough step and reduce 
if suff. progress not satisfied.

Backtracking: choose \( \bar{\alpha} > 0, \ p \in (0,1), \ c \in (0,1) \)

\[
\alpha = \frac{\bar{\alpha}}{p}
\]
do until \( p(x_k + \alpha_k p_k) \leq p(x_k) + c \alpha_k \nabla f_k^T p \)

end

\( \alpha_k = \alpha \)
Typically $\bar{a} = 1$ in Newton or quasi-Newton (other choices in CG or steepest descent).

$p$ need not be constant (some choices later);
however, we need $p \in [\Phi_0, \Phi_1]$ where $0 < \Phi_0 < \Phi_1 < 1$.

Backtracking ensures that $\alpha_k$ satisfies sufficient progress (by getting smaller until satisfied) but does not get too small:

- either $\alpha_k = \bar{\alpha}$, or
- $\alpha_k > \bar{\alpha} \beta p$ where $\bar{\alpha}$ is largest $\alpha$ giving sufficient progress less than $\bar{\alpha}$ (check)
Convergence of Line Search Methods

Assume using Wolfe conds.

First prove suitable $\alpha_k$ exists. We assume $f$ bounded from below along $\{x_k + \alpha p_k \mid \alpha > 0\}$ (why okay?).

Lemma 3.1: Let $f: \mathbb{R}^n \to \mathbb{R}$ be cont. diff. Let $p_k$ be a descent direction at $x_k$, and $f$ bounded from below on $\{x_k + \alpha p_k \mid \alpha > 0\}$. Then if $0 < c_1 < c_2 < 1$, there exist intervals for $\alpha$ that satisfy the Wolfe conds. (and the strong Wolfe conds).

Proof

Since $0 < c_1 < 1$, the line $l(\alpha) = p_k + \alpha g_k^T p_k$ is strict monot. decreasing. So, there exists a smallest $\alpha' > 0$ s.t. $f(x_k + \alpha' p_k) = p_k + \alpha' g_k^T p_k$

Hence suff. decrease holds for $\alpha \leq \alpha'$.

By Mean Value Theorem, there exists $\alpha'' \in (0, \alpha')$ s.t. $f(x_k + \alpha' p_k) - f_k = \alpha' g_k^T (x_k + \alpha'' p_k) p_k$

Therefore:

$\nabla f(x_k + \alpha'' p_k)^T p_k = c_1 g_k^T p_k > c_2 g_k^T p_k$
(since $c_1 < c_2 \beta$ and $\nabla f^T P_k < 0$)

There $\alpha^*$ satisfies Wolfe cond. (with strict
meq. $s$) \( \Rightarrow \) there is neighborhood of $\alpha^*$ for
which the Wolfe cond. is hold.

\[
\frac{\frac{\partial f(x_k + \alpha^* P_k)}{\partial \alpha}}{\frac{\partial f(x_k)}{\partial \alpha}} < 0
\]

Since $\nabla f(x_k + \alpha^* P_k)^T P_k < 0$ \( \Rightarrow \)
the strong Wolfe cond. hold as well.

To prove convergence of iteration

\[ x_{k+1} = x_k + \alpha_k P_k \]

where $\alpha_k$ satisfies Wolfe cond. we need
conditions on $P_k$. (Is $\nabla f^T P_k < 0$ enough?)

Define $\theta_k$ angle between $P_k$ and $-\nabla f_k$:

\[
\cos \theta_k = \frac{-\nabla f_k^T P_k}{\|\nabla f_k\| \|P_k\|}
\]

Consider:

Theo 3.2: For given iter., where $P_k$ is descent
dir. and $\alpha_k$. Suppose $f$ bounded below in $\mathbb{R}^n$
and $f$ cont. diff. in open set $N$ containing
level set $R = \{ x | f(x) \leq f(x_0) \}$, where $x_0$ is
starting pt. iter. In addition, assume
gradient of $f$ Lipschitz continuous on $N$
That is, there exist $L > 0$ s.t.
\[ \| \nabla f(x) - \nabla f(\bar{x}) \| \leq L \| x - \bar{x} \| \quad \text{for all } x, \bar{x} \in \mathbb{N}. \]

Then \( \sum_{k \geq 0} \cos^2 \theta_k \| \nabla f_k \|^2 < \infty. \)

(Does this prove conv., $\nabla f_k \rightarrow 0$?)

(There are some subtleties, e.g., $P$ need not be connected. Nevertheless, the alg. never leaves

\[\text{Proof:} \quad (P) \]

From $x_{k+1} = x_k + \alpha_k p_k$ and curr. cond.

\[
\begin{align*}
(\nabla f_{k+1} - \nabla f_k)^T p_k \geq c_2 \nabla f_k^T p_k - \nabla f_k^T p_k = (c_2 - 1) \nabla f_k^T p_k \\
(\nabla f_{k+1} - \nabla f_k)^T p_k \leq \alpha_k L \| p_k \|^2
\end{align*}
\]

Intermezzo: \( \| \nabla f(x_{k+1}) - \nabla f(x_k) \| \leq L \| \alpha_k p_k \| = \alpha_k L \| p_k \| \)

\[\alpha_k \geq \frac{c_2 - 1}{L} \frac{\nabla f_k^T p_k}{\| p_k \|^2} \quad \text{(bounded const. $x$ \norm grad.)} \]

First Wolfe cond: $f_{k+1} \leq f_k - \frac{c_1 (c_2 - 1)}{L} (\nabla f_k^T p_k)^2 / \| p_k \|^2$

\[
\begin{align*}
f_{k+1} \leq f_k - \frac{c_1 (c_2 - 1)}{L} \cos^2 \theta_k \| \nabla f_k \|^2
\end{align*}
\]

Summing over all indices up to $k$:

\[
f_{k+1} \leq f_0 - \left( \sum_{i=0}^{k} \cos^2 \theta_i \| \nabla f_i \|^2 \right)
\]
Since $f$ is bounded from below

$$\beta_k f_0 - f_k \leq M \quad (f_0 - f_{\text{min or sup}})$$

Hence

$$\sum_{k=0}^{\infty} \cos^2 \theta_k \| \nabla f_k \|^2 < \infty$$

$\Rightarrow$ Zoutendijk condition

(similar for strong Wolfe or Goldstein cond.)

Obviously 2. cond: $\cos^2 \theta_k \| \nabla f_k \| \rightarrow 0$

So, if we pick $p_k$ such that

$$\cos \theta_k \geq \delta > 0 \quad \text{for all } k$$

$$\cos^2 \theta_k \| \nabla f_k \| \geq \delta \| \nabla f_k \| \geq 0$$

$\rightarrow 0 \quad \rightarrow 0$ (duh)

So, $\delta \| \nabla f_k \| \rightarrow 0 \Rightarrow \| \nabla f_k \| \rightarrow 0$

So, conv. of iteration guaranteed (to stat. pt.) provided $p_k$ never (too) close to orthogonal to gradient.

So, steepest descent globally convergent.

Globally convergent $\rightarrow$ converging to stationary point from any starting point (satisfying res. conditions).

Convergence to local min requires some extra steps.
Consider iteration
\[ x_{k+1} = x_k + \alpha_k p_k \quad \text{where} \]
\[ p_k = -B_k^{-1} \nabla f_k \]

Assume \( B_k \) are (all) symm. pos. def.
and condition number uniformly bounded:
\[ \kappa(B_k) = \frac{\|B_k\_2\|\|B_k^{-1}\_2\|}{\|B_k\|\_2\|B_k^{-1}\|_2} \leq M \quad \text{for all } k \]
(some pos. constant \( M \))

Then \( \cos \theta_k \geq \frac{1}{M} \).
Hence \( \lim_{k \to \infty} \|\nabla f_k\| = 0 \)

\[ \cos \theta_k = \frac{-\nabla f_k^T B_k^{-1} \nabla f_k}{\|\nabla f_k\| \|B_k^{-1} \nabla f_k\|} = \frac{-\nabla f_k^T B_k^{-1} \nabla f_k}{\|B_k\|_2 \|\nabla f_k\|_2 \|B_k^{-1} \nabla f_k\|_2} \]

\[ |\cos \theta_k| \leq \frac{\|\nabla f_k\|_2^2 \text{dmax}}{\|\nabla f_k\|_2^2 \text{dmin}^2} = \frac{\text{dmin}}{\text{dmax}} = \kappa^{-1}(B_k) \]

where \( \text{dmin} = \min \Lambda(B_k) \quad \text{spectrum} \)
\( \text{dmax} = \max \Lambda(B_k) \)

So, quasi-Newton with line search globally convergent as long as \( B_k \) SPD and cond. nr. bounded.
Rate of Convergence of LS methods

Steepest Descent

Consider simple case \( f(x) = \frac{1}{2}x^TQx - b^Tx + c \) (Q SPD) with solution \( x^* = Q^{-1}b \)

\( \nabla f(x) = Qx - b \)

Optimal step length easy in this case

\[ \nabla f(x_k + \alpha p_k) = 0 \]

Consider (descent) direction \( p_k : \)

\[
\begin{align*}
\frac{d}{d\alpha} f(x_k + \alpha p_k) &= \alpha p_k^TQp_k + x_k^TQp_k - b^Tp_k + \frac{1}{2}x_k^TQx_k - b^Tx_k + c \\\frac{d}{d\alpha} f(x_k + \alpha p_k) &= \alpha p_k^TQp_k + x_k^TQp_k - b^Tp_k = 0 \\alpha &= \frac{p_k^T(b - Qx_k)}{p_k^TQp_k} \quad \text{(opt. step)}
\end{align*}
\]

\( \nabla p_k = -\nabla f_k = b - Qx_k \rightarrow \alpha = \frac{+\nabla p_k^T \nabla f_k}{\nabla p_k^T \nabla p_k} \) 

(note \( \alpha \geq 0 \) in this case)

Note \( \nabla f = 0 \iff Qx = b \) (sol. linear system)

\[ \alpha = \frac{r_k^T r_k}{r_k^T Q r_k} \quad \text{where} \quad r_k = b - Qx_k \]

\text{residual lin. sys.}
Steepest Descent Iteration:

\[ x_{k+1} = x_k - \frac{\nabla f_k^T \nabla f_k}{\nabla f_k^T \nabla^2 f_k \nabla f_k} \nabla f_k \]

Contours of \( f \) are ellipsoids with axes along eigenvectors of \( \nabla^2 f \) and axes lengths proportional to eigenvalue \(-\frac{1}{\varepsilon} b^T a^{-1} b\)

\[ \|v_i\| = 1 \quad \alpha v_i = d_i v_i \]

\[ x = \alpha^{-1} b + \alpha v_i \]

\[ f(x) = \frac{1}{2} (\alpha^{-1} b + \alpha v_i)^T \alpha (\alpha^{-1} b + \alpha v_i) - b^T (\alpha^{-1} b + \alpha v_i) + c \]

\[ = \frac{1}{2} b^T \alpha^{-1} b + \alpha b^T v_i + \frac{1}{2} \alpha^2 v_i^T \alpha v_i - b^T \alpha^{-1} b - \alpha b v_i + c \]

\[ = -\frac{1}{2} b^T \alpha^{-1} b + c + \frac{1}{2} \alpha^2 d_i \]

\[ \frac{1}{2} \alpha^2 d_i = \gamma \text{ (constant)} \]

\[ \alpha = \pm \left( \frac{2 \gamma}{d_i} \right)^{1/2} \]

\[ \alpha v_i b + \alpha v_i + \alpha v_i \rightarrow K + \frac{1}{2} \alpha^2 d_1 + \frac{1}{2} \alpha^2 d_2 \]
\[
\begin{align*}
\theta(x_k - x^*) &= \theta x_k - b \\
&= \nabla P_k \\
e_k &= \theta^{-1} \nabla P_k
\end{align*}
\]

steps ineffective if ellipses very elongated

So, \( \min \frac{p(x)}{x} = x^* \) \( \implies \theta x = b \implies x = \theta^{-1} b \)

\[
x_{k+1} - x^* = x_k - x^* - \alpha \nabla P_k \quad \text{(a step. desc.)}
\]

\[
\|x_{k+1} - x^*\|_\theta^2 = \|x_k - x^*\|_\theta^2 - 2\alpha \nabla P_k^T (x_k - x^*) + \alpha^2 \nabla P_k^T \theta \nabla P_k
\]

\[
\|e_{k+1}\|_\theta^2 = \|e_k\|_\theta^2 - 2 \frac{(\nabla P_k^T \nabla P_k)^2}{\nabla P_k^T \theta \nabla P_k} + \frac{(\nabla P_k^T \nabla P_k)^2}{\nabla P_k^T \theta \nabla P_k}
\]

\[
\|e_{k+1}\|_\theta^2 = \|e_k\|_\theta^2 - \frac{(\nabla P_k^T \nabla P_k)^2}{\nabla P_k^T \theta \nabla P_k}
\]

Note \( e_k^T \theta e_k = \nabla P_k^T \theta ^{-1} \nabla P_k = \nabla P_k^T \theta ^{-1} \nabla P_k \)

\[
\|e_{k+1}\|_\theta^2 = (1 - \frac{(\nabla P_k^T \nabla P_k)^2}{\nabla P_k^T \theta \nabla P_k}) \|e_k\|_\theta^2
\]

So, convergence linear with rate \( (1 - ...) \frac{1}{2} \)

pretty miserable if \( \theta \) ill-cond.
Consider \( \left( 1 - \frac{(x^T x)^2}{(x^T A x)(x^T A^T x)} \right) \) for \( A \in \mathbb{R}^{2 \times 2} \) and \( \mathbf{x} = V \xi \) leading to eigenvalues.

\( V^T V = \Sigma \)

\[
1 - \frac{(\xi^T \xi)^2}{(\xi^T A \xi)(\xi^T A^T \xi)}
\]

upper bound so

min \( \frac{\| \xi \|^2}{(\xi^T A \xi)(\xi^T A^T \xi)} \) = min \( \frac{1}{\xi^T (\xi^T A \xi)(\xi^T A^T \xi) \xi} \) for \( \| \xi \| = 1 \)

\[
\max (\xi^T A \xi)(\xi^T A^T \xi) \rightarrow (\sum \xi_i^2 d_i)(\sum \xi_i^2 d_i^{-1})
\]

\( \xi \in \mathbb{R}^{2 \times 2} \) and \( \Sigma \), and \( d_1 \leq d_2 \)

\[
(\xi^2 d_1 + (1 - \xi^2) d_2 ) (\xi^2 d_1^{-1} + (1 - \xi^2) d_2^{-1})
\]

\[
(\xi^2 + (1 - \xi^2) d_1 d_2^{-1}) (\xi^2 + (1 - \xi^2) d_1 d_2^{-1})
\]

\[
d_2/d_1 = k \rightarrow (\xi^2 + (1 - \xi^2) k)(\xi^2 + (1 - \xi^2) k^{-1})
\]

\[
\frac{d}{d\xi} (\cdot) = 0 \rightarrow (2\xi - 2\xi k)(\xi^2 + (1 - \xi^2) k^{-1}) + (2\xi - 2\xi k^{-1})(\xi^2 + (1 - \xi^2) k) = 0
\]

\[
\Rightarrow \frac{2\xi^2}{2\xi}(1 - k)(\xi^2 + (1 - \xi^2) k^{-1}) + 2\xi(1 - \xi k)(\xi^2 + (1 - \xi^2) k^{-1}) = 0
\]

\[
\Rightarrow 2\xi^2(1 - \xi k)(\xi^2 + (1 - \xi^2) k^{-1}) = 0
\]

\[
\Rightarrow k = (2\xi^2 + (1 - \xi^2) k^{-1}) = 0
\]

\[
1 - 2\xi^2 = x^2(1 - 2\xi^2)
\]

\( \xi \sim 1 \Rightarrow 2 \xi^2 = \frac{1}{2} \Rightarrow \xi = \frac{1}{2} \sqrt{2} \) (> 0)

\( (k = 1 \rightarrow \text{ellipses are circles, conv. in 1 step}) \)
\[ 1 - \frac{1}{\left(\frac{d_1 + \frac{1}{2} d_2}{d_1} + \frac{1}{2} d_2^{-1}\right)\left(\frac{d_1 + \frac{1}{2} d_2}{d_2} + \frac{1}{2} d_1^{-1}\right)} = 1 - \frac{y}{(d_1 + d_2)(d_1^{-1} + d_2^{-1})} = 1 - \frac{y d_1 d_2}{(d_1 + d_2)^2} = \frac{d_1 + 2 d_1 d_2 + d_2^2}{(d_1 + d_2)^2} - y d_1 d_2 \]

\[ = \frac{(d_1 - d_2)^2}{(d_1 + d_2)^2} \quad \text{(max)} \]

\[ \| e_{k+1} \|_Q^2 \leq \frac{(d_2 - d_1)^2}{(d_2 + d_1)^2} \| e_k \|_Q^2 \]

\[ \| e_{k+1} \|_Q \leq \frac{k-1}{k+1} \| e_k \|_Q \]

So, if \( k \) large (\( d_1 \ll d_n \)) bound suggests very slow convergence \( \Rightarrow \) true (and can be sharp)

\[ k = 1000 \rightarrow \frac{999}{1000} \| e_{k+1} \|_Q \leq \frac{(999)^2}{1000^2} \| e_k \|_Q \]

\[ L \approx 0.99 \]

For nonlinear functions similar behavior

So, convergence steepest descent in general very poor \( \Rightarrow \)

Guaranteed global conv not so useful.
Note non-optimal step lengths will generally not improve conv.

**Theo 3.4** Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ twice cont. diff. and iterates by steepest descent with exact optimal line search converge to $x^*$ and Hessian $\nabla^2 f(x^*)$ SPD. Let $r$ be any scalar satisfying $r \in \left( \frac{d_n-d_1}{d_n+d_1}, 1 \right)$ where $d_1 < d_2 < \ldots < d_n$ are eig. vals. Hessian at $x^*$. Then for all $k$ suff. large, we have

$$f(x_k^+) - f(x_k^*) \leq r^2 \left( f(x_k) - f(x^*) \right)$$

(note $f(x_k) - f(x^*) = \frac{1}{2} \| x_k - x^* \|_2^2$)

Better than Steepest Descent?

Newton's Method

$$p_k^N = x_k - \nabla^2 f(x_k)^{-1} \nabla f(x_k)$$

(assuming Hessian SPD we discuss later what to do if this is not the case)

**Theo 3.5**

Suppose $f$ twice diff. and Hessian $\nabla^2 f$ lip. cont. in nhood of a solution $x^*$ at which second order suff. cond. for local
\[
\min \text{ are satisfied. Consider iter.}
\]
\[
x_{kn} = x_k + p_k. \text{ Then}
\]
\[
i) \text{ if starting pt. } x_0 \text{ suff. close to } x^*, \text{ the}
\]
\[
\text{seq. of iterates conv. to } x^*
\]
\[
ii) \text{ conv. rate of } \{x_k\} \text{ is quadratic}
\]
\[
iii) \text{ seq. of grad norms } \{\|\nabla f_k\|\} \text{ conv. quadr. to zero}
\]

**Proof:** \[
\frac{e_{kn}}{k}
\]

Since \(\nabla^2 f_k = 0\): \[
x_k + p_k - x^* = x_k - x^* - \nabla^2 f_k \nabla f_k
\]

\[
= \nabla^2 f_k^{-1} \left( \nabla^2 f_k (x_k - x^*) - (\nabla f_k - \nabla f_k) \right)
\]

Taylor: \[
\nabla^2 f_k - \nabla f_k = \int \nabla^2 f(x_k + t(x^* - x_k))(x_k - x^*)d\tau
\]

Hence \[
\| \nabla^2 f_k(x_k)(x_k - x^*) - (\nabla f_k - \nabla f_k) \| =
\]

\[
\int \| \nabla^2 f_k(x_k) - \nabla^2 f_k(x_k + t(x^* - x_k)) \| (x_k - x^*) d\tau\]

\[
\leq \| x_k - x^* \| \int \| \nabla^2 f_k(x_k) - \nabla^2 f_k(x_k + t(x^* - x_k)) \| d\tau
\]

\[
\leq \| x_k - x^* \| \int \| x^* - x_k \| d\tau = \text{Lip const.}
\]

\[
\leq L \| x_k - x^* \|^2 \cdot \left[ \frac{1}{2} t^2 \right]_0^1 = \frac{1}{2} L \| x_k - x^* \|^2
\]

Since \(\nabla^2 f(x^*)\) nonsingular and Lip. cont.,

there is radius \(r > 0\) s.t. \(\|\nabla^2 f_k^{-1}\| \leq 2 \|\nabla^2 f_k\|\)

for all \(x_k \in \mathcal{B}(x^*, r)\)

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\[ \|x_k + P_k^{N} - x^*\| \leq L \left\| \nabla^2 f(x^*)^{-1} \right\| \|x_k - x^*\|^2 \]

\[ = \tilde{L} \|x_k - x^*\|^2 \]

First prove that seq. started inside $B(x^*, \min(\gamma, \frac{1}{\tilde{L}}))$ stays inside $B(x^*, \min(\gamma, \frac{1}{\tilde{L}}))$

\[ \|x_{k+1} - x^*\| \leq \tilde{L} \|x_k - x^*\|^2 \]

\[ \iff \|x_k - x^*\| \leq \min(\gamma, \frac{1}{\tilde{L}}) \Rightarrow \]

\[ \|x_{k+1} - x^*\| \leq \left( \frac{\tilde{L}}{\gamma} \|x_k - x^*\|, \frac{\tilde{L}}{\gamma} \|x_k - x^*\| \right) \]

\[ \leq \frac{1}{\gamma} \|x_k - x^*\| \]

So, if $x_k \in B(x^*, \min(\gamma, \frac{1}{\tilde{L}}))$ then $x_{k+1} \in B(x^*, \min(\gamma, \frac{1}{\tilde{L}}))$

Hence if $x_0$ inside ball, etc (by induction) proves convergence, \( \text{in pos. large} \)

Moreover, $\|x_{k+1} - x^*\| \leq \tilde{L} \|x_k - x^*\|^2$ so conv.

is quadratic.

In addition, as $\nabla^2 f_k P_k^{N} + \nabla f_k = 0$,

\[ \|\nabla f(x_{k+1})\| = \|\nabla f(x_{k+1}) - \nabla f_k - \nabla^2 f_k P_k^{N}\| \]

\[ = \|\int_0^1 \nabla^2 f(x_k + tP_k^{N})(x_{k+1} - x_k) \, dt - \nabla^2 f_k P_k^{N}\| \]
\[ \leq \int \| \nabla^2 f(x_k + \epsilon p_k^N) - \nabla^2 f(x_k) \| \| p_k^N \| \, d\epsilon \]
\[ \leq \frac{1}{2} \| p_k^N \|^2 \leq \frac{1}{2} \| \nabla^2 f(x_k)^{-1} \| \| \nabla f(x_k) \|^2 \]
\[ \leq 2 \| \nabla^2 f(x_k)^{-1} \| \| \nabla f(x_k) \|^2 \]

So, \( \| \nabla f(x_k) \| \) converges quadratically as well.

So, if using Newton with LS (w. cond.s) and some modif. if Hessian not SPD, only need to show that close to \( x^* \) line search alg. pick \( \alpha = 1 \) to obtain quad. conv. (locally)

**Quasi-Newton:** \( p_k = -B_k^{-1} \nabla f_k \)

We assume \( B_k \) (modified to be) SPD.

**Theo.6** Let \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) twice cont. diff. Consider iter.

\( x_{k+1} = x_k + \alpha_k p_k \), where \( p_k \) descent dir. and \( \alpha_k \) sat.s W. cond.s with \( c_1 \leq \frac{1}{2} \)

\( \nabla f \{ x_k \} \) conv. to pl. \( x^* \) s.t. \( \nabla f(x^*) = 0 \), \( \nabla^2 f(x^*) \) SPD and \( p_k \) sat.s \( \lim_{k \to \infty} \| \nabla f_k + \nabla^2 f_k p_k \| = 0 \)

then

(i) \( \alpha_k = 1 \) admiss. for all \( k > k_0 \) (some \( k_0 \))

(ii) \( \left\{ \alpha_k \right\} \) conv superlin to \( x^* \)
If \( p_k = -B_k^{-1}/\nabla p_k \) then
\[
\| \nabla p_k + \nabla^2 p_k p_k^* \| = \| \nabla^2 p_k p_k^* - B_k p_k^* \| = \\
\| (\nabla^2 p_k - B_k) p_k^* \|
\]
So, need \( \lim_{k \to \infty} \| (\nabla^2 p_k - B_k) p_k^* \| / \| p_k^* \| = 0 \)

Hence \( B_k \to \nabla^2 p_k^* \) not necessary,
just suff. accurate along \( p_k^* \)

Theo 37. Let \( f: \mathbb{R}^n \to \mathbb{R} \) twice condl. diff.
Consider \( x_{k+n} = x_k + p_k^* \) where \( p_k = -B_k^{-1}/\nabla p_k \).
Assume \( \{ x_k \} \) conv. to \( x^* \) s.t. \( \nabla f_{x^*} = 0 \) and \( \nabla^2 f_{x^*} \) SPD. Then \( \{ x_k \} \) conv. superlin. iff
\[
\lim_{k \to \infty} \| (B_k - \nabla^2 p_k) p_k^* \| / \| p_k^* \| = 0
\]

\[
p_k^* - p_k^* = \nabla^2 p_k^{-1} (\nabla^2 p_k p_k^* + \nabla \nabla p_k)
= \nabla^2 p_k^{-1} (\nabla^2 p_k - B_k) p_k^*
= \theta(\| (\nabla^2 p_k - B_k) p_k^* \|) \text{ suff. close to } x^*
= \theta(\| p_k^* \|)
\]
Hessian modification –

What if $\nabla^2 f_k$ not SPD? (same for $B_k$)

Modify $\nabla^2 f_k$ s.t. (suff.) pos. def.

\[ \text{Alg 3.2 (given } x_k) \]

for $k = 0, 1, 2, \ldots$

if $\nabla^2 f_k$ suff. pos. def. $B_k = \nabla^2 f_k$

else find $B_k = \nabla^2 f_k + E_k$ s.t.

$B_k$ suff. pos. def

end

Solve $B_k p_k = -\nabla f_k$

$x_{kn} = x_k + \alpha_k p_k$ where $\alpha$ sats.

Wolfe, Goldstein, or Arm. backtr. cond.s

end

* $B_k$ suff. pos. def so that cond. nr.

remains bounded and hence $\Delta(p_k, -\nabla f_k)$

bounded away from $\delta/2$.

Bounded modified 2nd. cond.:

$\kappa(B_k) = \|B_k\|_2 \|B_k^{-1}\|_2 \leq C \ (C > 0)$

for all $k$

whenever $\{\nabla^2 f_k\}_k$ is bounded.
Under these conditions, global convergence can be proved.

**Theorem 3.8** If twice continuously differentiable on open set \( D \) and starting point \( x_0 \) (of alg 3.2) is such that level set \( L = \{ x \in D : f(x) \leq f(x_0) \} \) is compact. Then if bounded modulus, fact property holds, we have \( \lim_{k \to \infty} \nabla f(x_k) = 0 \).

If \( \nabla^2 f(x) \) (suff.) pos. def. that \( F_k = 0 \) for large enough \( k \) (depends on strategy) then \( x_k = 1 \) for large enough \( k \) and convergence will be quadratic.

If \( \nabla^2 f(x) \) close to singular, convergence linear.

Modifying \( \nabla^2 f_k = A \Lambda A^T \) some \( d_i < 0 \)

Basic idea \( \nabla^2 f_k + A D A^T = A (\Lambda + D) A^T \) is diagonal

s.t. \( d_i + d_i > \text{tolerance} > 0 \)

(problem with computation \( p_k \) if tolerance too small)

Simplest \( \nabla^2 f_k + T I \rightarrow \) needs estimate of smallest (alg.) \( d_i \)
Alg 3.3  (comp. fact of $B_k = V^2(I + D_k I)$)

need this fact to solve $B_k P_k = -Q_k$

Choose tolerance $\rho$, set $\omega_0 = 0$

Guarantee diag coeff. $B_k \rho > 0$  (nec. cond)

if not

$\omega_0 = - \min (B_k)_{ii} + \rho$

Try Chol. fact. $B_k L L^T = B_k + \epsilon_k I$

If fails

$\epsilon_{mh} = \max (2 \epsilon_k, \rho)$

Can be expensive if mult. fact. needed.

See book for choices of $\rho$

Also possible more rapid increase of $\epsilon_{mh}$

Alg 3.4

$L$ unit lowertri.

Compute mod. Chol. fact. $B_k = L D L^T$ where

we modify $d_i$ (diag) as we go

(Std) Cholesky decomp./Fact

$A = L D L^T$

$L$ is unit lower trian.

$D$ is diagonal (positive)

$A_1 = A$

$A_1 = \begin{bmatrix} a_{11} & s_1^T \\ s_1 & A_1 \end{bmatrix}$
\[
\begin{bmatrix}
    a_{ii} & s_{i}^T \\
    s_{i} & A_{i}
\end{bmatrix} = \begin{bmatrix}
    d_{i} & e_{i}^T \\
    e_{i} & L_{i}
\end{bmatrix}
\]

\( (A_{i})_{ii} - a_{ii} = d_{i}, \quad s_{i}^T = d_{i} e_{i}^T \Rightarrow e_{i} = d_{i}^{-1} s_{i} \rightarrow d_{i} (A_{i})_{1:2:n} \)

\( \hat{A}_{i} = e_{i} d_{i} e_{i}^T + L_{i} \tilde{D}_{i} L_{i}^T \Rightarrow \)

next step compute \( \hat{L}_{i} \hat{D}_{i} \hat{L}_{i}^T = \hat{A}_{i} - e_{i} d_{i} e_{i}^T \)

\( e \in \mathbb{R}^{(n-1) \times (n-1)} \quad \text{only update lower half} \quad (\text{including diag}) \)

\( A_{2} = \hat{A}_{i} - e_{i} d_{i} e_{i}^T , \quad \text{repeat} \)

\( d_{2} = (A_{2})_{ii} , \quad \hat{l}_{2} = d_{2}^{-1} (A_{2})_{1:2:n-1} \)

\( A_{3} = (A_{2})_{2:n-1,2:n-1} - l_{2} d_{2} l_{2}^T \quad (\text{lower half}) \)

In order to guarantee \( d_{i} \) sufficiently large s.t. \( B_{k} = \hat{L} \hat{D} \hat{L}^T \) (but modified), we update \( d_{i} \) as we go.

For a SPD \( L, D \) always exist (no pivoting needed) and \( D \) guaranteed to be positive

* Proof? (by induction)

* In practice computed result satisfies

\( (A + \delta A) = \tilde{L} \tilde{D} \tilde{L}^T \rightarrow \tilde{L}, \tilde{D} \) computed quant

\( \Leftrightarrow \) perh. called backward error

where \( \| \delta A \|_2 \leq C \epsilon \max \| A \|_2 \)

www.rollingstimelapse.com
Modified Cholesky: pick positive $\delta$, $\beta$ and update $d_j$ s.t. $d_j \geq \delta$ and $\frac{1}{\beta} \geq \frac{1}{\sqrt{d_j} \delta}$.

\[ |l_{ij}| \sqrt{d_j} \leq \beta \]

Modify $d_j$ as follows:

At step $j$, set

\[ \theta_j = \max_{j \neq i} \left( \frac{\theta_i}{\beta^2}, d_j \right) \]

\[ d_j = \max \left( \|A_j\|_1, \left( \frac{\theta_j}{\beta} \right)^2, \delta \right) \]

\[ l_j = d_j^{-1} (A_j)_{2:n-j+1,1} \]

\[ A_{j+1} = A_j - l_j d_j l_j^T \]

Pivoting (rows and columns in same way) can be used to reduce size of modification.

\[ \rightarrow P A P^T + E = L D L^T \]

$E$ nonnegative diagonal matrix

This alg. leads to $B_k = L D L^T$ s.t.

\[ \kappa(B_k) \leq C \quad (\text{some } C > 0) \quad \text{for all } k, \]

assuming norm Hessian remains bounded.

* "growth" norm $L D L^T$

* "bounds" coeff of $E$
Why does alg. work?

\[ LD L^T = L D^{1/2} D^{1/2} L^T = \tilde{\Sigma} \tilde{L} \tilde{L}^T \]

Let's bound smallest singular value of \( \tilde{L} \) assuming diag. coeff. \( \bar{d}_i \) are suff.
Large and \( \tilde{b}_{ij} \) suff. small.

(Note \( \text{dim} (\tilde{L} L^T) = \sigma_{\text{min}} (\tilde{L}) \))

\( y = z L \perp \|z\| = 1 \quad \text{s.t.} \quad \|y\| = \min \rightarrow \sigma_{\text{min}} \)

\( \tilde{b}_{kh} > 0 \)

\[ y_k = \tilde{\ell}_{hh} z_k + \sum_{j > k} \tilde{\ell}_{jh} z_j \]

Choose \( z \)

3. Let

Assume \( |\tilde{\ell}_{jk}| < \beta_k < \beta \) for \( j > k \)

\( \beta_k > 0 \)

\[ \exists k \text{ s.t. } |z_k| > |z_j| \quad \forall j \text{ for all } j \]

Then

\[ |y_k - \tilde{\ell}_{hh} z_k| = \epsilon \sum_{j > k} |z_j| \tilde{\ell}_{jh} \ln \sum_{j > k} |z_j| \tilde{\ell}_{jh} \]

\[ \leq |z_k| \sum_{j > k} |\tilde{\ell}_{jh}| = |z_k| \beta_k (n - k) \]

Now assume \( \beta_k < \frac{\epsilon}{n \tilde{\ell}_{hh}} \) where \( y \in (0, 1) \)

Then

\[ |y_k - \tilde{\ell}_{hh} z_k| \leq \beta_k \frac{n - k}{n} \] \( y \tilde{\ell}_{hh} \)

\[ (1 - y) \tilde{\ell}_{hh} z_k \leq y \tilde{\ell}_{hh} \frac{n - k}{n} \]

\[ 0 \leq \tilde{\ell}_{hh} z_k \]

\[ y_k \leq 1 \]

We know \( z_k > \sqrt{\frac{\epsilon}{n}} \)

So, if we bound \( \tilde{\ell}_{hh} > \delta > 0 \) we have:

minimum bound on \( \sigma_{\text{min}} (\|y\|) \geq |y_k| \)}
\[ \ell_{kk} z_k - y \ell_{kk} z_k \leq Y_k \leq \ell_{kk} z_k + y \ell_{kk} z_k \]

\[ \left(1 - y \right) \ell_{kk} z_k \leq Y_k \leq \left(1 + y \right) \ell_{kk} z_k \]

\[ L \Rightarrow \left(1 - y \right) \delta \sqrt{n} \]

\[ \Rightarrow \text{fixed for fixed } n \]

\[ \ell_{jk} = a_{jk}^{(k)} / \ell_{kk} \Rightarrow \text{make } \ell_{kk} \text{ large enough} \]

\[ \left| a_{jk}^{(k)} \right| / \ell_{kk} \leq \beta_k = \frac{Y_k}{\ell_{kk}} \Rightarrow \left| a_{jk}^{(k)} \right| \leq \frac{Y_k}{\ell_{kk}} \ell_{kk} = Y_k / \ell_{kk} \Rightarrow \]

\[ \left( a_{kk}^{(k)} + e_{kk} \right) \]

\[ \left( a_{kk}^{(k)} + e_{kk} \right)^2 \geq \frac{n}{\delta} \max_{j > h} \left| a_{jk}^{(k)} \right| \]

Also need \[ \left( a_{kk}^{(k)} + e_{kk} \right) \geq \delta \left( \ell_{kk} \geq \delta \right) \]

(some further details \( \Rightarrow \) Gill & Murray paper)

**Step 1**

\[ A_1 = A \quad \ell_{11} = \left( a_{11}^{(1)} + e_{11} \right)^{1/2} \quad \text{s.t.} \]

\[ a_{11}^{(1)} + e_{11} \geq \frac{n}{\delta} \max_{j > 1} \left| a_{j1}^{(1)} \right| \]

\[ \ell_{11} = \ell_{11} \quad s.t. \]

\[ A_2 = \hat{A}_1 - \hat{\ell}_1 \hat{\ell}_1^T \rightarrow \hat{L}_1 \hat{L}_1^T \]

**Step 2**

\[ \ell_{22} = \left( a_{11}^{(2)} + e_{22} \right)^{1/2} \quad \text{s.t.} \]

\[ a_{11}^{(2)} + e_{22} \geq \frac{n}{\delta} \max_{j > 2} \left| a_{j2}^{(2)} \right| \]

\[ A_{kk} = \left( a_{kk}^{(k)} \right) \]

\[ etc. \]
Result \( (A+E) = LL^T = LDL^T \)

bound on \( \max_k (A+E) \) follows from showing that \( e_k \) remain bounded.

Note that \( a_{ii}^{(k)} = a_{kk}^{(k)} - \sum_{l=1}^{k-1} \ell_{ki}^2 \)

Also larger \( e_j \ldots e_j \) make \( a_{ii}^{(k)} \) larger (because \( \ell_{ki}^2 \) are smaller) \( \rightarrow \) no instability (growth of \( e_{kk} \))

max \( e_{kk} \) not much larger than smallest \( a_{ii}^{(k)} \) (poss. negative) that would have occurred in Chol. fac. of \( A \). So

max \( e_{kk} \) modest multiple of \( \| \min s \| \| A \| \)

\( \| A+E \| \leq (2+\delta) \| A \| \) (\( \delta \) modest if \( \gamma, \beta, \delta \) well-chosen)

\( \| A \| \) bounded by assumption

(Work out for fun!)

---

www.rollabindsystems.com
Alternative approach computes sym. indef factorization: $PAP^T = LBL^T$

$B$ block diag w/ $1 \times 1$ or $2 \times 2$ blocks

$1 \times 1$ pos. or neg.

$2 \times 2$ pos.eigenvalue and neg. eigenvalue

$\Lambda(\Sigma)$ easy/cheap to compute $B = A \Lambda A^T$

F s.t. $L(B+F)L^T$ supp. pos. def.

$F = \Omega \text{ diag } (\Sigma_i) \Omega^T$, $\Sigma_i = \begin{cases} 0 & \lambda_i > \delta \\ \delta - \lambda_i & \lambda_i < \delta \end{cases}$

$\rightarrow P(A+E)P^T = L(B+F)L^T$, where

$E = P^TLFLTP \rightarrow$ not diag (in gen.)

---

Step-length Selection Algorithms.

$\phi(x) = f(x_k + \alpha k^m)$ ($IR \rightarrow IR$)

for $p_k$ descent direction $\rightarrow \phi'(0) < 0$

supp. decrease: $\phi(x) \leq \phi(x) + c_1 \alpha_k \phi'(0)$

$\rightarrow \phi_k \leq\phi_k + c_1 \alpha_k \phi'(x)$

$k$-th opt. step

$P^T f$ quadratic, $f = \frac{1}{2} x^T A x - b^T x$

$\rightarrow \alpha_k = \frac{\langle P^T \nabla f, -P_k \rangle}{P_k^T A P_k}$

www.rollabindsystems.com
sup. decrease: \( \phi(a_k) \leq \phi(x_0) + \varepsilon a_k \phi'(x_0) \)

more \( \leftarrow \) * Choose initial \( x_0 \) (\( x_0 = 1 \) Newton)

Eval \( \phi(x_0) \)

\[ \begin{array}{c}
\alpha = 0 \\
\alpha_0
\end{array} \]

We know \( \phi(0), \phi'(0), \) and \( \phi(x_0) \rightarrow \)

Fit quad. poly. and take min \( \rightarrow \alpha_1 \)

if satisfied, done

otherwise Fit cubic: \( \phi(0), \phi'(0), \phi(x_0), \phi(x_1) \)

and min let \( x_2 \) be min in \([0, x_1]\)

if necessary repeat with \( \phi(0), \phi'(0), \phi(x_1), \phi(x_2) \) etc

[ latest two points

if some \( x_i \) too close to \( 0 \) or \( x_{i-1} \)

take \( x_i = x_{i-1}/2 \)

If \( \phi' \) cheap to compute, we can also use \( \phi' \) at new points
See book 3.5 for cubic interpolation formula's

Starting values:

(i) make (try to) first order improvement same as in previous step,

\[ \alpha_0 \text{ s.t. } \alpha_0 \nabla \phi^T \mathbf{p}_k = \alpha^{(k-1)} \nabla \phi^T \mathbf{p}_{k-1} \]

(ii) interpolate using previous step and current step.

\[ \min \alpha_0 = \frac{2(P_{k-1} - P_k)}{\phi'(0)} \]

(of \( x_k \to x^* \) superlin then

\[ \frac{2}{\phi'(0)} P_{k-1} - P_k \to 1 \]

altern. \( \alpha_0 = \min \left(1, 1.01 + \frac{2(P_{k-1} - P_k)}{\phi'(0)} \right) \)

Line Search for Strong Wolfe conds.

(See book for details)

Alg. 3.5 \to finds interval \([\alpha_{lo}, \alpha_{hi}]\) that contains \( \alpha \) satisfying SW conds.

Alg 3.6 \to finds \( \alpha \) by interpol. formula or "search" and returns if \( \alpha \) acceptable, otherwise adjusts the interval.
Interval \((a_{i-1}, a_i)\) contains acc. step

length if \(a_i\) violates suff. decrease

\[
\begin{align*}
\phi(a_i) &\geq \phi(a_{i-1}) \\
\phi'(a_i) &> 0
\end{align*}
\]

\(\rightarrow\) call zoom\((a_{lo}, a_{hi})\)

Alg 3.6: maintains "bracket" \(\rightarrow\) interval
satisf. cond.s for containing solution

a) \([a_{lo}, a_{hi}]\) contains a satisf. SW cond.s
b) \(a_{lo}\) is a step s.t. \(\phi(a_{lo})\) min among all tried steps satisf. suff. decr.

c) \(a_{hi}\) s.t. \(\phi'(a_{lo})(a_{hi} - a_{lo}) < 0\)

\(\rightarrow\) emp. of \(\phi(a)\) possible in interval

\(\rightarrow\) get new \(a\) (interpol), decrease interval or accept.

new \(a\) by interpol + (safeguarding)
suff. decrease interval size