Chapter 3 – Line Search Methods

1) Choose (compute) direction p_k
2) Choose (compute) step length α

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

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: $p_k^T \nabla f_k = -\nabla f_k^T B_k^{-1} \nabla f_k < 0$

$\rightarrow$ descent direction

How about "α"?

3.1 Step Length

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

Too expensive $\rightarrow$ $f(x)$ (very) expensive

We want "sufficient" progress (reduction) for modest work

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

1) find suitable interval
2) find good choice in interval

Why "suff. decrease"?
Why is $f(x_k + \alpha_k p_k) < f(x_k)$ not good enough?

(similar problem might occur with choices of p_k)

<u>Conditions on step length</u>

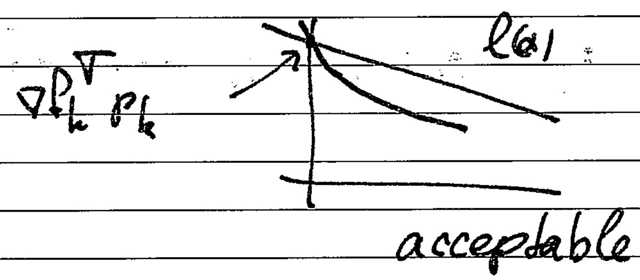
Wolfe Conditions

a) (Armijo condition)

$$f(x_k + \alpha p_k) \le f(x_k) + c_1 \alpha \nabla f_k^T p_k \quad c_1 \in (0,1)$$

reduction proportional to α and $\nabla f_k^T p_k$

$$l(\alpha) = f_k + c_1 \alpha \nabla f_k^T p_k$$



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

We don't want very short steps:

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 $\phi(\alpha)$ at α_k greater than c_2 times initial slope $\phi'(0)$. → ~~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

$$\begin{cases} f(x_k + \alpha_k p_k) \leq f(x_k) + \alpha_k c_1 \nabla f_k^T p_k \\ \nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k \end{cases}$$

with $0 < c_1 < c_2 < 1$

Alternatively, in strong Wolfe cond.s 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 curv. cond.)

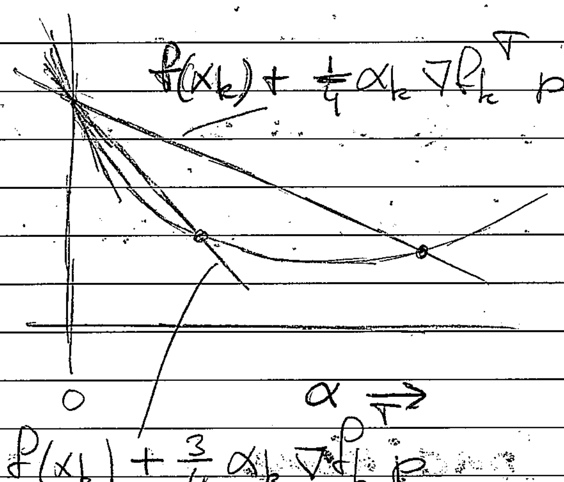
Note that Wolfe cond.s are scale invariant,

$f \to a \cdot f$ makes no difference.

Alternative, Goldstein cond.s.

$f(x_k) + (1-c)\alpha_k \nabla f_k^T p \le f(x_k + \alpha_k p_k) \le f(x_k) + \alpha_k c \nabla f_k^T p$

with $0 < c < \frac{1}{2}$



Sufficient decrease and backtracking

We can drop curv. condition (and alt.s)

if we consider large enough step and reduce

if suff. progress not satisfied.

Backtracking: Choose $\bar{\alpha} > 0$, $\rho \in (0,1)$, $c \in (0,1)$

$\alpha = \bar{\alpha}$

do until $f(x_k + \alpha_k p_k) \le f(x_k) + c\alpha_k \nabla f_k^T p$

$\quad \alpha = \rho\alpha$

end

$\alpha_k = \alpha$

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

ρ need not be constant (some choices later); however, we need $\rho \in [\rho_{lo}, \rho_{hi}]$ where $0 < \rho_{lo} < \rho_{hi} < 1$

Backtracking ensures that α_k satisfies suff. progress (by getting smaller until satisfied) but does not get too small $\}$:

either $\alpha_k = \bar{\alpha}$ or

$\alpha_k > \tilde{\alpha}\rho$ where $\tilde{\alpha}$ is largest nr. giving suff. progr. less than $\bar{\alpha}$ (check)

Convergence of Line Search Methods

Assume using Wolfe cond.s.

First prove suitable α_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 α that satisfy the Wolfe cond.s (and the strong Wolfe cond.s).

Proof

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

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

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

Therefore:

$$\nabla f(x_k + \alpha'' p_k)^T p_k = c_1 \nabla f_k^T p_k > c_2 \nabla f_k^T p_k$$

(since $c_1 < c_2$ and $\nabla f_k^T p_k < 0$)

There α'' satisfies Wolfe cond.s (with strict ineq.s) $\rightarrow$ there is neighborhood of α'' for which the Wolfe cond.s hold. $\left(\frac{f(x_k+\alpha'' p_k) - f_k}{\alpha'}\right)$

Since $\nabla f(x_k + \alpha'' p_k)^T p_k < 0$

the strong Wolfe cond.s hold as well.

To prove convergence of iteration

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

where α_k satisfies Wolfe cond.s we need conditions on p_k. (Is $\nabla f_k^T p_k < 0$ enough?)

Define θ_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. Suppose f bounded below in $\mathbb{R}^n$ and f cont. diff. in open set N containing level set $\mathcal{L} = \{x \mid f(x) \leq f(x_0)\}$, 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.

$$\|\nabla f(x) - \nabla f(\tilde{x})\| \le L \|x - \tilde{x}\| \text{ for all } x, \tilde{x} \in N.$$

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

(Does this prove conv., $\nabla f_k \to 0$?)
(There are some subtleties; e.g. $\mathcal{L}$ need not be connected. Nevertheless, the alg. never leaves $\mathcal{L}$)

Proof:

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

$$\left.\begin{array}{l}(\nabla f_{k+1} - \nabla f_k)^T p_k \geq c_2 \nabla f_k^T p_k - \nabla f_k^T p_k = (c_2 - 1)\nabla f_k^T p_k \\ (\nabla f_{k+1} - \nabla f_k)^T p_k \le \alpha_k L \|p_k\|^2\end{array}\right\} \to$$

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

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

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

$$f_{k+1} \le f_k - \frac{c_1(c_2-1)}{L} \cos^2\theta_k \|\nabla f_k\|^2$$

Summing over all indices up to k:

$$f_{k+1} \le f_0 - c \sum_{i=0}^{k} \cos^2\theta_i \|\nabla f_i\|^2$$

Since f is bounded from ~~∞~~ below

~~f_{k+1}~~ $f_0 - f_{k+1} \leq M$ ($f_0 - f_{min}$ or sup)

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

↳ Zoutendijk condition

(similar for strong Wolfe or Goldstein cond.)

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

So, if we pick p_k such that

$\cos\theta_k \geq \delta > 0$ for all k

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

$\to 0$ $\to 0$ (duh)

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

So, conv. of iteration guaranteed (to stat. pt.)

provided p_k never (too) close to orthog. to gradient.

So, steepest descent globally convergent.

Globally convergent → converging to stationary point from any starting point (satisfying reas. 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:

$$\kappa(B_k) = \|B_k\|_2 \|B_k^{-1}\|_2 \leq M \quad \text{for all } k$$

(some pos. constant M)

Then $\cos\theta_k \geq \frac{1}{M}$.

Hence $\lim_{k \to \infty} \|\nabla f_k\| = 0$

$$\cos\theta_k = \frac{-\nabla f_k^T B_k^{-1} \nabla f_k}{\|p_k\| \, \|\nabla f_k\|} = \frac{-\nabla f_k^T B_k^{-1} \nabla f_k}{\|B_k^{-1} p_k\| \, \|\nabla f_k\|}$$

$$|\cos\theta_k| \leq \frac{\|\nabla f_k\|^2 \, d_{max}^{-1}}{\|\nabla f_k\|^2 \, d_{min}^{-1}} = \frac{d_{min}}{d_{max}} = \kappa^{-1}(B_k)$$

where $d_{min} = \min \Lambda(B_k)$ — spectrum

$$d_{max} = \max \Lambda(B_k)$$

So, quasi-Newton with line search globally convergent as long as ~~po~~ SPD B_k and cond. nr. bounded.

Rate of Convergence of LS methods.

Steepest Descent

Consider simple case $f(x) = \frac{1}{2} x^T Q x - b^T x + c$

(Q SPD) with solution $x^* = Q^{-1} b$

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

Optimal step length easy in this case

~~$\frac{d}{d\alpha}\{f(x_k + \alpha b - \alpha Q x_k)\} = 0$~~

Consider (descent) direction p_k:

$f(x_k + \alpha p_k) =$

$\frac{1}{2}(x_k + \alpha p_k)^T Q (x_k + \alpha p_k) - b^T(x_k + \alpha p_k) + c =$

$\frac{1}{2}\alpha^2 p_k^T Q p_k + \alpha x_k^T Q p_k - \alpha b^T p_k + \frac{1}{2} x_k^T Q x_k - b^T x_k + c$

$$\frac{d}{d\alpha} f(x_k + \alpha p_k) = \alpha p_k^T Q p_k + x_k^T Q p_k - b^T p_k = 0$$

$$\alpha = \frac{p_k^T(b - Qx_k)}{p_k^T Q p_k} \quad \text{(opt. step)}$$

If $p_k = -\nabla f_k = b - Qx_k \rightarrow \alpha = \dfrac{+\nabla f_k^T \nabla f_k}{\nabla f_k^T Q \nabla f_k}$

(note $\alpha > 0$ in this case)

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

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

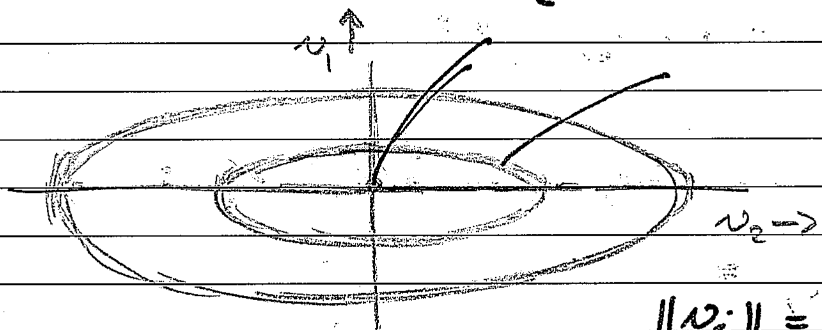
↳ residual lin. sys.

Steepest Descent Iteration:

$$x_{k+1} = x_k - \frac{\nabla f_k^T \nabla f_k}{\nabla f_k^T Q \nabla f_k} \nabla f_k$$

Contours of f are ellipsoids with axes along eigenvectors of Q and ~~[illegible]~~ axes lengths inv. proportional to eigenvalue

$-\frac{1}{2} b^T Q^{-1} b$



$d_1 > d_2$

$\|v_i\| = 1 \quad Q v_i = d_i v_i$

$$x = Q^{-1} b + \alpha v_i$$

$$f(x) = \tfrac{1}{2}(Q^{-1}b + \alpha v_i)^T Q (Q^{-1}b + \alpha v_i) - b^T(Q^{-1}b + \alpha v_i) + c$$

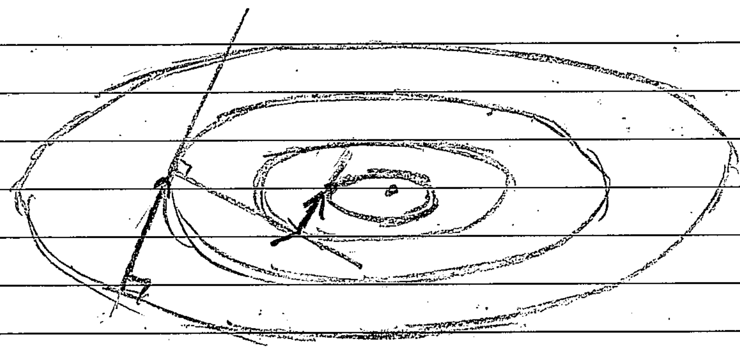
$$= \tfrac{1}{2} b^T Q^{-1} b + \cancel{\alpha b^T v_i} + \tfrac{1}{2}\alpha^2 v_i^T Q v_i - b^T Q^{-1} b - \cancel{\alpha b^T v_i} + c$$

$$= \underbrace{-\tfrac{1}{2} b^T Q^{-1} b + c}_{K} + \tfrac{1}{2}\alpha^2 d_i$$

$\frac{1}{2}\alpha^2 d_i = \gamma$ (constant)

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

$$Q^{-1} b + \alpha_1 v_1 + \alpha_2 v_2 \rightarrow K + \tfrac{1}{2}\alpha_1^2 d_1 + \tfrac{1}{2}\alpha_2^2 d_2$$



$$Q(\overbrace{x_k - x^*}^{e_k}) = Qx_k - b$$
$$= \nabla f_k$$
$$e_k = Q^{-1}\nabla f_k$$

steps ineffective if ellipses very elongated

Sol. $\min_x f(x) = x^* \iff Qx = b \Rightarrow x = Q^{-1}b$

$$x_{k+1} - x^* = x_k - x^* - \alpha\nabla f_k \qquad (\alpha \text{ steep. desc.})$$

$$\|x_{k+1} - x^*\|_Q^2 = \|x_k - x^*\|_Q^2 - 2\alpha\nabla f_k^T \underbrace{Q(x_k - x^*)}_{\nabla f_k} + \alpha^2 \nabla f_k^T Q \nabla f_k$$

$$\iff \|e_{k+1}\|_Q^2 = \|e_k\|_Q^2 - 2\alpha\nabla f_k^T\nabla f_k + \alpha^2 \nabla f_k^T Q \nabla f_k$$

$$= \|e_k\|_Q^2 - 2\frac{(\nabla f_k^T\nabla f_k)^2}{\nabla f_k^T Q \nabla f_k} + \frac{(\nabla f_k^T\nabla f_k)^2}{\nabla f_k^T Q \nabla f_k}$$

$$= \|e_k\|_Q^2 - \frac{(\nabla f_k^T\nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)\underbrace{(\nabla f_k^T Q^{-1}\nabla f_k)}_{= \|e_k\|_Q^2}} \|e_k\|_Q^2$$

<u>Note</u> $e_k^T Q e_k = \nabla f_k^T Q^{-1} Q Q^{-1}\nabla f_k = \nabla f_k^T Q^{-1}\nabla f_k$

$$\|e_{k+1}\|_Q^2 = \left(1 - \frac{(\nabla f_k^T\nabla f_k)^2}{(\nabla f_k^T Q \nabla f_k)(\nabla f_k^T Q^{-1}\nabla f_k)}\right)\|e_k\|_Q^2$$

So, convergence linear with rate $\left(1 - \frac{\cdot\cdot}{\cdot\cdot}\right)^{1/2}$

pretty miserable if Q ill-cond.

Consider $\left(1 - \frac{(x^T x)^2}{(x^T Q x)(x^T Q^{-1} x)}\right)$ for $Q \in \mathbb{R}^{2\times2}_{SPD}$

generalization not hard but cumbersome

$Q = V \Lambda V^T$ and $x = V\xi$ $\quad d_i$ eig. values
$V^T V = I$

$$1 - \frac{(\xi^T \xi)^2}{(\xi^T \Lambda \xi)(\xi^T \Lambda^{-1} \xi)}$$ ~~lower~~ upper bound so

$$\min_\xi \frac{\|\xi\|^4}{(\xi^T \Lambda \xi)(\xi^T \Lambda^{-1} \xi)} = \min_\xi \frac{1}{(\xi^T \Lambda \xi)(\xi^T \Lambda^{-1} \xi)} \text{ for } \|\xi\| = 1$$

$$\max\ (\xi^T \Lambda \xi)(\xi^T \Lambda^{-1} \xi) \to \left(\textstyle\sum_i \xi_i^2 d_i\right)\left(\textstyle\sum_i \xi_i^2 d_i^{-1}\right)$$

$Q \in \mathbb{R}^{2\times2}$ and SPD, and $d_1 < d_2$

$$\left(\xi_1^2 d_1 + (1-\xi_1^2) d_2\right)\left(\xi_1^2 d_1^{-1} + (1-\xi_1^2) d_2^{-1}\right) =$$

$$\left(\xi_1^2 + (1-\xi_1^2) d_2/d_1\right)\left(\xi_1^2 + (1-\xi_1^2) d_1/d_2\right)$$

$$d_2/d_1 = \kappa \to \left(\xi_1^2 + (1-\xi_1)^2 \kappa\right)\left(\xi_1^2 + (1-\xi_1^2)\kappa^{-1}\right)$$

$$\frac{d}{d\xi_1}(\,) = 0 \to (2\xi_1 - 2\xi_1\kappa)\left(\xi_1^2 + (1-\xi_1^2)\kappa^{-1}\right) +$$
$$(2\xi_1 - 2\xi_1\kappa^{-1})\left(\xi_1^2 + (1-\xi_1^2)\kappa\right) = 0$$

$$\Leftrightarrow \cancel{2\xi_1}\ 2\xi_1(1-\kappa)\left(\xi_1^2 + (1-\xi_1^2)\kappa^{-1}\right) +$$
$$2\xi_1(\kappa-1)\left(\xi_1^2\kappa^{-1} + (1-\xi_1)^2\right) = 0$$

$$\to \cancel{(1-\xi_1^2)}\ \xi_1^2 + (1-\xi^2)\kappa^{-1} = \xi_1^2\kappa^{-1} + (1-\xi_1^2)\xi$$

$$1 - 2\xi_1^2 = \kappa^{-1}(1-2\xi_1^2)$$

$\kappa^{-1} = 1$ $\quad$ or $\quad \xi_1^2 = \frac{1}{2} \to \xi_1 = \frac{1}{2}\sqrt{2}\ (>0)$

$(\kappa = 1 \to$ ellipses are circles, conv. in 1 step$)$

$$1 - \frac{1}{(\frac{1}{2}d_1 + \frac{1}{2}d_2)(\frac{1}{2}d_1^{-1} + \frac{1}{2}d_2^{-1})} = 1 - \frac{4}{(1 + d_2/d_1)(1 + d_1/d_2)} =$$

$$\frac{(1+\kappa)(1+\kappa^{-1})}{(1+\kappa)(1+\kappa^{-1})} - \frac{4}{(1+\kappa)(1+\kappa^{-1})} = \frac{2 + (\kappa+\kappa^{-1}) - 4}{(1+\kappa)(1+\kappa^{-1})}$$

$$= \frac{\kappa - 2 + \kappa^{-1}}{(1+\kappa)(1+\kappa^{-1})} = \frac{-(1-\kappa)(1-\kappa^{-1})}{}$$

$$1 - \frac{1}{(\frac{1}{2}d_1 + \frac{1}{2}d_2)(\frac{1}{2}d_1^{-1} + \frac{1}{2}d_2^{-1})} = 1 - \frac{4}{(d_1+d_2)(d_1^{-1}+d_2^{-1})}$$

$$= 1 - \frac{4d_1d_2}{(d_1+d_2)^2} = \frac{d_1 + 2d_1d_2 + d_2^2 - 4d_1d_2}{(d_1+d_2)^2}$$

$$= \frac{(d_1-d_2)^2}{(d_1+d_2)^2} \quad (\max)$$

$$\|e_{k+1}\|_Q^2 \le \frac{(d_2-d_1)^2}{(d_2+d_1)^2} \|e_k\|_Q^2 \quad \Leftrightarrow$$

$$\|e_{k+1}\|_Q \le \left(\frac{\kappa-1}{\kappa+1}\right) \|e_k\|_Q$$

So, if κ large ($d_1 \ll d_n$) bound suggests very slow convergence $\rightarrow$ true (bnd can be sharp)

$$\kappa = 1000 \rightarrow \frac{999}{1000} \qquad \|e_{k+10}\|_Q \le \left(\frac{999}{1000}\right)^{10} \|e_k\|_Q$$

$\hookrightarrow \simeq 0.99$

(reduction by 1%)

For general 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 $f: \mathbb{R}^n \to \mathbb{R}$ 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 $d_1 \le d_2 \le \cdots \le d_n$ are eig. val.s Hessian at x^*. Then for all k suff. large, we have

$$f(x_{k+1}) - f(x_k^{*}) \le r^2 \left(f(x_k) - f(x^*) \right)$$

$$\left(\text{note } f(x_k) - f(x^*) = \overbrace{\tfrac{1}{2} \| x_k - x^* \|_Q^2}^{\frac{1}{2}\|e_k\|_Q^2} \right)$$

Better than Steepest Descent?

Newton's Method

$$p_k^N = -\nabla^2 f_k^{-1} \nabla f_k$$

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

Theo 3.5

Suppose f twice diff. and Hessian $\nabla^2 f$ Lip. cont. in n.hood of a soluton x^* at which second order suff. cond. for local min are satisfied. Consider iter.

$x_{k+1} = x_k + p_k^N$. Then

i) if starting pt. x_0 suff. close to x^*, the seq. of iterates conv. to x^*.

ii) conv. rate of $\{x_k\}$ is quadratic

iii) seq. of grad norms $\{\|\nabla f_k\|\}$ conv. quadr. to zero

Proof:

Since $\nabla f_* = 0$: $\overbrace{x_k + p_k^N - x^*}^{e_{k+1}} = x_k - x^* - \nabla^2 f_k^{-1} \nabla f_k$

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

Taylor: $\nabla f_k - \nabla f_* = \int_0^1 \nabla^2 f(x_k + t(x^* - x_k))(x_k - x^*)\,dt$

Hence $\|\nabla^2 f(x_k)(x_k - x^*) - (\nabla f_k - \nabla f_*)\| =$

$$\left\| \int_0^1 \left[\nabla^2 f(x_k) - \nabla^2 f(x_k + t(x^* - x_k))\right](x_k - x^*)\,dt \right\|$$

$$\leq \int_0^1 \|\nabla^2 f(x_k) - \nabla^2 f(x_k + t(x^* - x_k))\| \, \|x_k - x^*\|\,dt$$

$$\leq \|x_k - x^*\| \int_0^1 L t \|x^* - x_k\|\,dt =$$

Lip const.

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

Since $\nabla^2 f(x^*)$ nonsingular and Lip. cont. there is radius $r > 0$ s.t. $\|\nabla^2 f_k^{-1}\| \leq 2\|\nabla^2 f_*^{-1}\|$

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

$$\|x_k + p_k^N - x^*\| \le L\,\|\nabla^2 f(x^*)^{-1}\|\,\|x_k - x^*\|^2$$
$$= \tilde{L}\,\|x_k - x^*\|^2$$

$x_0 \in \overline{B(\,)}$ First prove that seq. started inside $B(x^*, \min(r, \frac{1}{2\tilde{L}}))$ stays inside

$$\|x_{k+1} - x^*\| \le \tilde{L}\,\overline{\|x_k - x^*\|}^2$$

if $\|x_k - x^*\| \le \min(r, (2\tilde{L})^{-1}) \Rightarrow$

$$\|x_{k+1} - x^*\| \le \min\left(\frac{\tilde{L}}{2\tilde{L}}\,\|x_k - x^*\|, \frac{\tilde{L}}{r}\|x_k - x^*\|\right)$$
$$\le \underline{\tfrac{1}{2}\|x_k - x^*\|}$$

So, if $x_k \in B(\underline{x^*, \min(r, \frac{1}{2\tilde{L}})})$ then $x_{k+1} \in \overline{B(\,)}$

Hence if x_0 inside ball, etc (by induction).

Proves convergence. → (separate part as $\tilde{L}$ poss. large)

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

In addition, as $\nabla^2 f_k\, p_k^N + \nabla f_k = 0$,

$$\|\nabla f(x_{k+1})\| = \|\nabla f(x_{k+1}) - \nabla f_k - \nabla^2 f_k\, p_k^N\|$$
$$= \left\|\int_0^1 \nabla^2 f(x_k + t p_k^N)(x_{k+1} - x_k)\,dt - \nabla^2 f_k\, p_k^N\right\|$$

$$\leq \int_0^1 \| \nabla^2 f(x_k + t p_k^N) - \nabla^2 f(x_k) \| \, \| p_k^N \| \, dt$$

$$\leq \tfrac{1}{2} L \| p_k^N \|^2 \leq \tfrac{1}{2} L \| \nabla^2 f(x_k)^{-1} \|^2 \, \| \nabla f_k \|^2$$

$$\leq 2 L \| \nabla^2 f(x^*)^{-1} \|^2 \, \| \nabla f_k \|^2$$

↑ cond. (to zero)

So, $\|\nabla f_k\|$ 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 quadr. conv. (locally)

Quasi-Newton : $p_k = -B_k^{-1} \nabla f_k$

We assume B_k (modified to be) SPD

Theo 3.6 Let $f : \mathbb{R}^n \to \mathbb{R}$ twice cont. diff. Consider iter. $x_{k+1} = x_k + \alpha_k p_k$, where p_k descent dir. and α_k sat.s W. cond.s with $c_1 \leq \frac{1}{2}$

If $\{x_k\}$ conv. to pt. x^* s.t. $\nabla f_* = 0$, $\nabla^2 f_*$ SPD and p_k sat.s $\lim_{k \to \infty} \dfrac{\| \nabla f_k + \nabla^2 f_k p_k \|}{\| p_k \|} = 0$

then

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

(ii) if $\alpha_k = 1$ $\forall k \geq k_0$, $\{x_k\}$ conv. superlin to x^*

If $p_k = -B_k^{-1}\nabla f_k$ then

$$\|\nabla f_k + \nabla^2 f_k\, p_k\| = \|\nabla^2 f_k\, p_k - B_k p_k\| =$$
$$\|(\nabla^2 f_k - B_k)\, p_k\|$$

So, need $\displaystyle\lim_{k\to\infty} \|(\nabla^2 f_k - B_k)\, p_k\| / \|p_k\| = 0$

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

<u>Theo 3.7</u> Let $f: \mathbb{R}^n \to \mathbb{R}$ twice cont. diff.
Consider $x_{k+1} = x_k + p_k$ where $p_k = -B_k^{-1}\nabla f_k$.
Assume $\{x_k\}$ conv. to x^* s.t. $\nabla f_* = 0$ and
$\nabla^2 f_*$ SPD. Then $\{x_k\}$ conv. superlin. <u>iff</u>
$\displaystyle\lim_{k\to\infty} \|(B_k - \nabla^2 f_k)\, p_k\| / \|p_k\| = 0$

$$\begin{aligned}
p_k - p_k^N &= \nabla^2 f_k^{-1}\left(\nabla^2 f_k\, p_k + \nabla f_k\right) \\
&= \nabla^2 f_k^{-1}\left(\nabla^2 f_k - B_k\right) p_k \\
&= O\left(\|(\nabla^2 f_k - B_k)\, p_k\|\right) \quad \text{\underline{suff. close} to } x^* \\
&= o(\|p_k\|)
\end{aligned}$$

Hessian modification –

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

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

Alg 3.2 (given x_0)

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

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

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

B_k suff. pos. def

end

Solve $B_k p_k = -\nabla f_k$

$x_{k+1} = x_k + \alpha_k p_k$ where α sat.s

Wolfe, Goldstein, or Arm. back tr. cond.s

end

* B_k suff. pos. def so that cond. nr. remains bounded and hence $\angle(p_k, -\nabla f_k)$ bounded away from $\pi/2$.

Bounded modified fact. cond:

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

for all k whenever $\{\nabla^2 f_k\}_k$ is bounded.

Under these cond.s global convergence can be proved.

<u>Theo 3.8</u> f twice cont. diff. on open set D and starting pt x_0 (of alg 3.2) is such that level set $\mathcal{L} = \{x \in D : f(x) \leq f(x_0)\}$ is compact. Then if bounded mod. fact. property holds, we have $\lim_{k \to \infty} \nabla f(x_k) = 0$.

If $\nabla^2 f_*$ (suff.) pos. def. that $E_k = 0$ for large enough k (depends on strategy) then $\alpha_k = 1$ for large enough k and convergence will be quadratic.

If $\nabla^2 f_*$ close to singular, convergence linear.

Modifying $\nabla^2 f_k = Q \Lambda Q^T$ some $\lambda_i < 0$

Basic idea $\nabla^2 f_k + Q D Q^T = Q(\Lambda + \underbrace{D}_{\text{diag}}) Q^T$

s.t. $\lambda_i + d_i \geq$ tolerance > 0

(problem with comp. p_k if tolerance too small)

Simplest $\nabla^2 f_k + \tau I \rightarrow$ needs estimate of smallest (alg.) λ_i

Alg 3.3 (comp. fact of $B_k = \nabla^2 f_k + \tau I$) Chol

need this fact. to solve $B_k p_k = -\nabla f_k$

Choose tolerance β, set $\tau_0 = 0$
Guarantee diag coeff. B_k pos (nec. cond)
if not
$$\tau_0 = -\min (B_k)_{ii} + \beta$$

Try Chol. fact. $LL^T = B_k + \tau_\ell I$

If fails
$$\tau_{\ell+1} = \max(2\tau_\ell, \beta)$$

Can be expensive if mult. fact. needed.
See book for choices of β
Also possible more rapid increase of $\tau_{\ell+1}$

Alg 3.4 L unit lowertri.

Compute mod. Chol. fact. $B_k = LDL^T$ where

we modify d_i (diag) as we go

(Std) Cholesky decomp / fact.

$A = LDL^T$ L is unit lower triang.
D is diagonal (positive)

$A_1 = A$

$$A_1 = \left[\begin{array}{c|c} a_{11} & s_1^T \\ \hline s_1 & \hat{A}_1 \\ & \end{array}\right]$$

$$\left[\begin{array}{c|c} a_{11} & s_1^T \\ \hline s_1 & \hat{A}_1 \end{array}\right] = \begin{bmatrix} 1 & \\ l_1 & \hat{L}_1 \end{bmatrix} \begin{bmatrix} d_1 & \\ & \hat{D}_1 \end{bmatrix} \begin{bmatrix} 1 & l_1^T \\ & \hat{L}_1^T \end{bmatrix}$$

$(A_1)_{11} \leftarrow a_{11} = d_1$, $s_1^T = d_1 l_1^T \Rightarrow l_1 = d_1^{-1} s_1 \rightarrow d_1^{-1} (A_1)_{1,2:n}$

$\hat{A}_1 = l_1 d_1 l_1^T + \hat{L}_1 \hat{D}_1 \hat{L}_1^T \Rightarrow$

next step compute $\hat{L}_1 \hat{D}_1 \hat{L}_1^T = \underbrace{\hat{A}_1 - l_1 d_1 l_1^T}$

only update lower half (including diag)

$\in \mathbb{R}^{(n-1)\times(n-1)}$

$A_2 = \hat{A}_1 - l_1 d_1 l_1^T$, repeat

$d_2 = (A_2)_{11}$, $l_2 = d_2^{-1} (A_2)_{1,2:n-1}$

$A_3 = (A_2)_{2:n-1,2:n-1} - l_2 d_2 l_2^T$ (lower half)

In order to guarantee d_i suff. large s.t. $B_k = LDL^T$ (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.

↳ pert. called backward error

where $\|\delta A\|_2 \leq c\,\varepsilon_{mach} \|A\|_2$

Modified Cholesky: pick positive δ, β and update d_j s.t. $d_j \geq \delta$ and

$|l_{ij}| \sqrt{d_j} \leq \beta$

Modify d_j as follows:

At step j,

set $\theta_j = \max |(A_j)_{2:n-j+1,1}|$

$d_j = \max\left(|(A_j)_{11}|, \left(\frac{\theta_j}{\beta}\right)^2, \delta \right)$

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

$A_{j+1} = A_j - l_j d_j l_j^T$

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

$\rightarrow PAP^T + E = LDL^T$

E nonnegative diagonal matrix

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

$\kappa(B_k) \leq C$ (some $C > 0$) for all k,

assuming norm Hessian remains bounded.

* "growth" norm LDL^T
* "bounds" coeff. of E

Why does alg. work ?

$$LDL^T = LD^{1/2} D^{1/2} L^T = \tilde{L}\tilde{L}^T$$

let's bound smallest singular value of $\tilde{L}$ assuming diag. coeff. $\tilde{l}_{ii}$ ~~are~~ suff. large and $\tilde{l}_{ij}$ suff. small.

(Note $\lambda_m(\tilde{L}\tilde{L}^T) = \sigma^2_{min}(\tilde{L})$)

$y^T = z^T \tilde{L}$ $\quad \|z\| = 1$ s.t. $\|y\| = \min \to \sigma_{min}$

$\tilde{l}_{kk} > 0$ choose z s.t. $z_k > 0$

$$y_k = \tilde{l}_{kk} z_k + \sum_{j>k} \tilde{l}_{jk} z_j$$

Assume $|\tilde{l}_{jk}| \le \beta_k \le \beta$ for $j > k$ $(= 0 \ j < k)$

$\exists k$. s.t. $|z_k| \geqslant |z_j|$ ~~$\forall j$~~ for all j Then

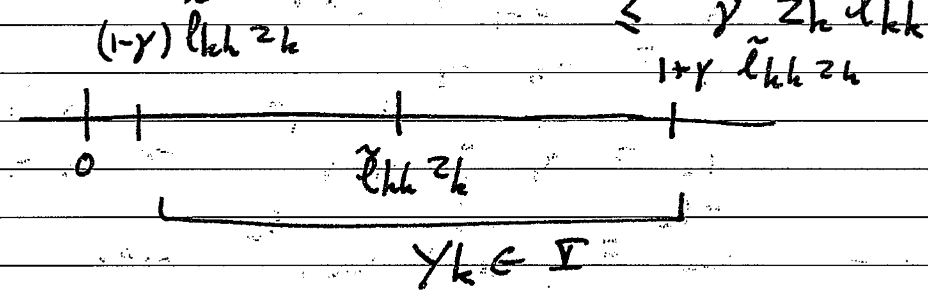
$$|y_k - \tilde{l}_{kk} z_k| = \left|\sum_{j>k} z_j \tilde{l}_{jk}\right| \le \sum_{j>k} |z_j|\,|\tilde{l}_{jk}|$$

$$\le |z_k| \sum_{j>k} |\tilde{l}_{jk}| = |z_k|\,\beta_k (n-k)$$

Now assume $\beta_k \le \frac{\gamma}{n} \tilde{l}_{kk}$ where $\gamma \in (0,1)$

Then $|y_k - \tilde{l}_{kk} z_k| \le z_k \cdot \frac{n-k}{n} \gamma \tilde{l}_{kk}$

$$\le \gamma z_k \tilde{l}_{kk}$$



We know $z_k \geqslant \sqrt{\frac{1}{n}}$,

So, if we bound $\tilde{l}_{kk} \geqslant \delta > 0$ we have minimum bound on σ_{min} ($\|y\| \geqslant |y_k|$)

$$\tilde{l}_{kk} z_k - \gamma \tilde{l}_{kk} z_k \le y_k \le \tilde{l}_{kk} z_k + \gamma \tilde{l}_{kk} z_k$$

$$(1-\gamma)\, \tilde{l}_{kk} z_k \le y_k \le (1+\gamma)\, \tilde{l}_{kk} z_k$$

$\hookrightarrow \ \ge (1-\gamma)\, \delta \sqrt{1/n}$

$\hookrightarrow$ fixed for fixed n

$$\tilde{l}_{jk} = a_{jk}^{(k)} / \tilde{l}_{kk} \longrightarrow \text{make } \tilde{l}_{kk} \text{ large enough}$$

$$|a_{jk}^{(k)}| / \tilde{l}_{kk} \le \beta_k = \gamma/n\ \tilde{l}_{kk} \Leftrightarrow$$

$$|a_{jk}^{(k)}| \le \gamma/n\ \tilde{l}_{kk}^2 = \gamma/n\ (a_{kk}^{(k)} + e_{kk}) \Rightarrow$$

$$(a_{kk}^{(k)} + e_{kk}) \ge \frac{n}{\gamma} \max_{j>k} |a_{jk}^{(k)}|$$

Also need $a_{kk}^{(n)} + e_{kk} \ge \delta^2$ $(\tilde{l}_{kk} \ge \delta)$

(some further details → Gill & Murray paper)

Step 1 $\quad A_1 = A \quad \tilde{l}_{11} = (a_{11}^{(1)} + e_{11})^{1/2}$ s.t.

$$a_{11}^{(1)} + e_{11} \ge \frac{n}{\gamma} \max_{j>1} |a_{j1}^{(1)}|$$

$$\hat{l}_1 = \tilde{l}_{11}^{-1} s_1$$

$$A_2 = \hat{A}_1 - \hat{l}_1 \hat{l}_1^T \longrightarrow \hat{L}_1 \hat{L}_1^T$$

Step 2 $\quad \tilde{l}_{22} = (a_{11}^{(2)} + e_{22})^{1/2}$ s.t.

$$a_{11}^2 + e_{22} \ge \frac{n}{\gamma} \max_{j>2} |a_{j2}^{(2)}|$$

etc

$$A_k = (a_{ij}^{(k)})$$

Result $(A+E) = \tilde{L}\tilde{L}^T = LDL^T$

bound on $d_{max}(A+E)$ follows ~~fo~~ from showing that e_{kk} remain bounded.

Note that $a_{11}^{(k)} = a_{kk} - \sum_{i=1}^{k-1} \tilde{l}_{ki}^2$

Also larger $e_{11} \cdots e_{k-1,k-1}$ make $a_{11}^{(k)}$ larger (because $\tilde{l}_{ki}^2$ are smaller) $\rightarrow$ no instability (growth of e_{kk})

~~$\|A+E\| \le$~~

max e_{kk} not much larger than smallest $a_{11}^{(k)}$ (poss. negative) that would have occurred in Chol. fact. of A. So, max e_{kk} modest multiple of $|d_{min}| \le \|A\|$

$\|A+E\| \le (2+\zeta)\|A\|$ (ζ modest if γ, β, δ well-chosen)

$\|A\|$ bounded by assumption

(Work out for fun!)

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

B block diag w. 1×1 or 2×2 blocks

1×1 pos. or neg.
2×2 pos. eigvalue and neg. eigenvalue

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

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

$F = Q\,\mathrm{diag}(\tau_i)\,Q^T$, $\tau_i = \begin{cases} 0 & \lambda_i \geq \delta \\ \delta - \lambda_i & \lambda_i < \delta \end{cases}$

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

$E = P^T L F L^T P \rightarrow$ not diag (in gen.)

Step-length Selection Algorithms.

$\phi(\alpha) = f(x_k + \alpha p_k) \qquad (\mathbb{R} \rightarrow \mathbb{R})$

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

suff. decrease: ~~$\phi(\alpha_k) \leq \phi(0) + \alpha_k \phi'(0)$~~

$$\phi(\alpha_k) \leq \phi(0) + c_1 \alpha_k \phi'(0)$$

$\uparrow$ k-th opt. step

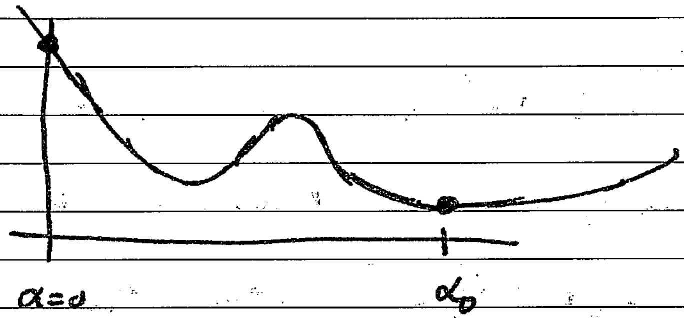
If f quadratic, $f = \frac{1}{2}x^T Q x - b^T x$

$$\Rightarrow \alpha_k = -\frac{\nabla f_k^T p_k}{p_k^T Q p_k}$$

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

more later $\leftarrow$ * Choose initial α_0 ($\alpha_0 = 1$ Newton)

Eval $\phi(\alpha_0)$



We know $\phi(0)$, $\phi'(0)$, and $\phi(\alpha_0)$ $\rightarrow$

fit quadr. poly and take min $\rightarrow \alpha_1$

if satisfied, done

Otherwise fit cubic : $\phi(0), \phi'(0), \phi(\alpha_0), \phi(\alpha_1)$

and ~~mini~~ let α_2 be min in $[0, \alpha_1]$

if necessary repeal with

$$\phi(0), \phi'(0), \underbrace{\phi(\alpha_1), \phi(\alpha_2)}_{\text{latest two points}} \quad \underline{\text{etc}}$$

if some α_i too close to 0 or α_{i-1}

take $\alpha_i = \alpha_{i-1}/2$

If ϕ' cheap to compute, we can also use ϕ' 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:

$$\alpha_0 \text{ s.t. } \alpha_0^{(k)} \nabla f_k^T p_k = \alpha^{(k-1)} \nabla f_{k-1}^T p_{k-1}$$

(ii) interpolate using previous step and current step.

$$\underline{\min} \quad \alpha_0 = \frac{2(f_{k-1} - f_k)}{\phi'(0)}$$

(if $x_k \to x^*$ superlin then

$$2/\phi'(0) \, (f_{k-1} - f_k) \to 1)$$

$$\text{altern.} \quad \alpha_0 = \min\left(1,\ 1.01 * \frac{2(f_{k-1} - f_k)}{\phi'(0)}\right)$$

Line Search for Strong Wolfe cond.s

(See book for details)

Alg. 3.5 $\to$ finds interval $[\alpha_{lo}, \alpha_{hi}]$ (bracket) that contains α satisfying SW cond.s

Alg 3.6 $\to$ finds α_j by interpol. formula or "search" and returns if α_j acceptable, otherwise adjusts the interval.

Interval (α_{i-1}, α_i) contains acc. step length if
$$\begin{cases} \alpha_i \text{ violates suff. decrease} \\ \phi(\alpha_i) \geq \phi(\alpha_{i-1}) \\ \phi'(\alpha_i) \geq 0 \end{cases}$$

$\rightarrow$ Alg 3.5.

$\rightarrow$ call zoom$(\alpha_{lo}, \alpha_{hi})$

Alg 3.6. maintains "bracket" $\rightarrow$ a interval satisf. cond.s for containing solution

a) $[\alpha_{lo}, \alpha_{hi}]$ contains α satisf. SW cond.s

b) α_{lo} ~~smallest step~~ s.t. $\phi(\alpha_{lo})$ min among all tried steps satisf. suff. decr.

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

↳ improv. of $\phi(\alpha)$ possible in interval

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

new α by interpol + (safeguarding)

suff. decrease interval size