Broyden's Method

Secant method : $x_{n+1} = x_n - b_n^{-1} f(x_n)$

$$\text{where } b_n = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Newton : $x_{n+1} = x_n - F'(x_n)^{-1} F(x_n)$

replace $F'(x_n)$ by approximation B_n that satisfies the secant condition (equation): $B_n(x_n - x_{n-1}) = F(x_n) - F(x_{n-1})$

Broyden's method : $x_{n+1} = x_n - d_n B_n^{-1} F(x_n)$

where d_n comes from linesearch.

Next we update $B_{n+1} = B_n + \dfrac{(y - B_n s)s^T}{s^T s}$ $\rightarrow$ minimum norm update satisfying secant condition!

where $y = F(x_{n+1}) - F(x_n)$

and $s = x_{n+1} - x_n = d_n d_n$

So, $B_{n+1} s = B_n s + (y - B_n s) \dfrac{s^T s}{s^T s} = y = F(x_{n+1}) - F(x_n)$

Convergence

We consider a slightly more general iteration :

$x_{n+1} = x_n - B_n^{-1} F(x_n)$

where the sequence B_n is generated by some (arbitrary) method. Let $B_n = F'(x^*) + E_n \simeq F'(x^*)$

Given the steps $s_n = x_{n+1} - x_n$ and the "Jacobian errors" $E_n = B_n - F'(x^*)$,

Dennis-Moré condition: $\lim_{n\to\infty} \frac{\|E_n s_n\|}{\|s_n\|} = 0$

<u>Theo:</u> Std. assumptions, B_n sequence of $N \times N$ matrices (nonsingular), $x_0 \in \mathbb{R}^N$, $\{x_n\}_{n=1}^{\infty}$ def'd by iteration ($x_n \neq x^*$)

Then $x_n \to x^*$ q-superlinearly if and only if $x_n \to x^*$ and Dennis-Moré condition holds

1) (assume cond.s and superlin. conv.)

$-F(x_n) = B_n s_n = F'(x^*) s_n + E_n s_n \iff$

$E_n s_n = -F'(x^*) s_n - F(x_n)$

$s_n = x_{n+1} - x_n = x_{n+1} - x^* - x_n + x^* = e_{n+1} - e_n$

$E_n s_n = -F'(x^*) e_{n+1} + F'(x^*) e_n - F(x_n)$

$F(x_n) = \int_0^1 F'(x^* + t e_n) e_n \, dt \quad \Rightarrow$

$F'(x^*) e_n - F(x_n) = \int_0^1 \left(F'(x^*) - F'(x^* + t e_n)\right) e_n \, dt \Rightarrow$

$\|F'(x^*) e_n - F(x_n)\| \le \frac{\gamma}{2} \|e_n\|^2$

$\|E_n s_n\| \le \|F'(x^*) e_n\| + \frac{\gamma}{2} \|e_n\|^2$

If $x_n \to x^*$ superlinearly $\left(\frac{\|e_{n+1}\|}{\|e_n\|} \to 0 \right)$

then for n large enough $\frac{\|s_n\|}{2} \le \|e_n\| \le 2\|s_n\|$

Since $x_n \ne x^*$ any n, define $\nu_n = \frac{\|e_{n+1}\|}{\|e_n\|} \to 0$

$$\|e_{n+1}\| = \nu_n \|e_n\| \le 2\nu_n \|s_n\|$$

$$\|E_n s_n\| \le \|F'(x^*) e_{n+1}\| + \frac{\gamma}{2}\|e_n\|^2$$

$$\le \|F'(x^*)\| \, \|e_{n+1}\| + \frac{\gamma}{2}\|e_n\|^2$$

$$\le \left(2\|F'(x^*)\|\nu_n + \gamma\|e_n\|\right)\|s_n\| \iff$$

$$\frac{\|E_n s_n\|}{\|s_n\|} \le 2\|F'(x^*)\|\,\nu_n + \gamma\|e_n\| \to 0 \quad (n \to \infty)$$

2) Assume $x_n \to x^*$ and $\frac{\|E_n s_n\|}{\|s_n\|} \to 0$

$$\mu_n = \frac{\|E_n s_n\|}{\|s_n\|}$$

Since $x_{n+1} = x_n - B_n^{-1} F(x_n)$ we have

$$B_n(x_{n+1} - x_n) = B_n s_n = -F(x_n)$$

$$E_n s_n = (B_n - F'(x^*)) s_n = -F(x_n) - F'(x^*) s_n$$

$$\|F'(x^*) s_n\| = \|E_n s_n + F(x_n)\| \le \|E_n s_n\| + \|F(x_n)\|$$

$$F'(x^*)^{-1} F'(x^*) s_n = s_n \Rightarrow$$

$$\|s_n\| \le \|F'(x^*)^{-1}\| \cdot \|F'(x^*) s_n\| \Rightarrow$$

$$\Rightarrow$$

$$\|F'(x^*)^{-1}\|^{-1} \|s_n\| \le \|F'(x^*) s_n\| \le \|E_n s_n\| + \|F(x_n)\|$$

$$= \mu_n \|s_n\| + \|F(x_n)\|$$

Since $\mu_n \to 0$, for n suff. large

$\mu_n \le \|F'(x^*)^{-1}\|^{-1}/2$

For such n

$$\|s_n\| \, \|F'(x^*)^{-1}\|^{-1} \le \mu_n \|s_n\| + \|F(x_n)\|$$

$$\le \|s_n\| \, \|F'(x^*)^{-1}\|^{-1}/2 + \|F(x_n)\| \iff$$

$$\|s_n\| \, \|F'(x^*)^{-1}\|^{-1}/2 \le \|F(x_n)\| \iff$$

$$\|s_n\| \le 2\|F'(x^*)^{-1}\| \, \|F(x_n)\|$$

$$\|F(x_n) + F'(x_n) s_n\| \le \underbrace{\|F(x_n) + F'(x^*) s_n\|} + \|(F'(x^*) - F'(x_n)) s_n\|$$

$$\le \|E_n s_n\| + \gamma \|x^* - x_n\| \, \|s_n\|$$

$$\le \mu_n \|s\|_n + \gamma \|e_n\| \, \|s_n\| =$$

$$(\mu_n + \gamma \|e_n\|) \|s_n\|$$

let $\eta_n = 2\|F'(x^*)^{-1}\| (\mu_n + \gamma\|e_n\|)$

Since $x_n \to x^*$, $\eta_n \to 0$

Now $\|F(x_n) + F'(x_n) s_n\| \le (\mu_n + \gamma\|e_n\|) \|s_n\|$

$$\le (\mu_n + \gamma\|e_n\|) \cdot 2\|F'(x^*)^{-1}\| \, \|F(x_n)\|$$

$$= \eta_n \|F(x_n)\|$$

Inexact Newton condition (satisfied by x_n, x_{n+1}, etc)

Since $\eta_n \to 0$ we have superlinear convergence

A useful lemma (pert. iter.)

let $0 < \hat{\theta} < 1$ and $\{\theta_n\}_{n=0}^{\infty} \subset (\hat{\theta}, 2-\hat{\theta})$

let $\{\varepsilon_n\}_{n=0}^{\infty} \subset \mathbb{R}^N$ s.t. $\sum_n \|\varepsilon_n\| < \infty$, and

let $\{\eta_n\}_{n=0}^{\infty} \subseteq \mathbb{R}^N$ s.t. $\|\eta_n\| = 0$ or $\|\eta_n\| = 1$ for all n

Let $\varphi_0 \in \mathbb{R}^N$ given. If $\{\varphi_n\}_{n=1}^{\infty}$ given by

$$\varphi_{n+1} = \varphi_n - \theta_n (\eta_n^T \varphi_n)\eta_n + \varepsilon_n$$

Then $\lim_{n\to\infty} \eta_n^T \varphi_n = 0$ ([IMLNE] pp 116–118)

also $\|\varphi_{n+1}\|^2 \le \|\varphi_n\|^2$

Bounded deterioration: Theo

let std ass. hold. Let $x_c \in \Omega$ and B_c nonsingular given.

$$x_+ = x_c - B_c^{-1} F(x_c) = x_c + s \in \Omega$$

$$B_+ = B_c + \frac{(y - B_c s)s^T}{s^T s} = B_c + \frac{F(x_+)s^T}{s^T s}$$

where $y = F(x_+) - F(x_c)$, $s = x_+ - x_c$

Then $\|E_+\|_2 \le \|E_c\| + \gamma(\|e_c\|_2 + \|e_+\|_2)/2$

Proof: $E_c s = -F(x_+) + (F(x_+) - F(x_c) - F'(x^*)s)$

$$= -F(x_+) + \int_0^1 (F'(x_c + ts) - F'(x^*))s\,dt \iff$$

$$F(x_+) = -E_c s + \int_0^1 (\cdots)s\,dt$$

$$E_+ = E_c(I - P_s) + \frac{(\Delta_c s)s^T}{\|s\|_2^2} \qquad \left(P_s = \frac{ss^T}{\|s\|_2^2}\right)$$

$$\Delta_c = \int_0^1 (F'(x_c + ts) - F'(x^*))s\,dt$$

$$\|\Delta_c\| \le \frac{\gamma}{2}(\|e_c\|_2 + \|e_+\|_2)$$

Hence $\|E_+\|_2 \leq \|E_c\|_2 + \|\Delta_c\|_2$

<u>Theo local q-linear convergence</u> (IMLNE p.122)

Std. assumptions. let $r \in (0,1)$ given. Then there are δ and δ_B s.t. if $x_0 \in B(\delta)$ and $\|E_0\| < \delta_B$ the Broyden sequence for data (F, x_0, B_0) exists and $x_n \to x^*$ q-linearly with q-fact. at most r

<u>Theo Chord method</u>: let std. assump. hold. Then there are $K_A > 0$, $\delta > 0$, $\delta_1 > 0$ s.t. if $x_0 \in B(\delta)$ and $\|A - F'(x^*)\| < \delta_1$ then (IMLNE p.77)

$$x_{n+1} = x_n - A^{-1}F(x_n)$$

converges q-linearly to x^* and

$$\|e_{n+1}\| \leq K_A \big(\underbrace{\|e_0\|}_{\delta} + \underbrace{\|A - F'(x^*)\|}_{\delta_1}\big)\, \|e_n\|$$

let δ, δ_1 s.t. Theo Chord method holds and

$$K_A(\delta + \delta_1) \leq r$$

δ suff. small s.t. $\delta_2 = \dfrac{\gamma(1+r)\delta}{2(1-r)} < \delta_1$

and set $\delta_B = \delta_1 - \delta_2$

Then $\|E_n\| \leq \delta_1$ by induction.

$\|E_0\| < \delta_B < \delta_1$ (by assumption)

Assume $\|E_k\| < \delta_1 \quad 0 \le k \le n$

By theo bounded deterioration

$$\left.\begin{array}{l} \|E_{n+1}\|_2 \le \|E_n\| + \frac{\gamma}{2}\left(\|e_n\| + \|e_{n+1}\|\right) \\ \|E_n\| < \delta_1 , \ \|e_{n+1}\| \le r\|e_n\| \end{array}\right\} \Rightarrow$$

$$\|E_{n+1}\| \le \|E_n\| + \frac{\gamma}{2}(1+r)\|e_n\| \le \|E_n\| + \gamma(1+r)r^n\delta/2$$

Same for $\|E_n\|, \|E_{n-1}\|, \ldots$

$$\|E_{n+1}\| \le \|E_0\| + \frac{\gamma}{2}(1+r)\delta \cdot \sum_{j=0}^{n} r^j$$
$$\le \delta_B + \frac{\gamma(1+r)\delta}{2(1-r)} = \delta_1$$

<u>Theo local q-superlinear convergence</u> (IMLNE p. 123)

(we established convergence, next we use the Dennis-Moré condition to prove superlinear convergence)

Let std. assump. hold. There are δ and δ_B s.t. if $x_0 \in B(\delta)$ $(N(x^*, \delta))$ and $\|E_0\| < \delta_B$ the Broyden sequence for the data (F, x_0, B_0) exists and $x_n \to x^*$ superlinearly.

Proof: let δ and δ_B be such that theo. local q-linear convergence holds.

$$P_n = \frac{s_n s_n^T}{\|s_n\|^2} \quad \text{and} \quad \Delta_n = \int_0^1 \left(F'(x_n + ts_n) - F'(x^*)\right) dt$$

$$\phi \in \mathbb{R}^N \text{ (arbitr.)} \Rightarrow E_{n+1}^T \phi = (I - P_n) E_n^T \phi + P_n \Delta_n^T \phi$$

Consider Lemma (perl. iter) with

$\psi_n = E_n^T \phi$; $\eta_n = s_n / \|s_n\|$; and $\varepsilon_n = P_n \Delta_n^T \phi$

$\sum_n \|\varepsilon_n\| < \infty$ by theo. local q-linear conv. and std. assumptions give $\|\Delta_n\| \le \frac{\gamma}{2}(1+r) r^n \delta$

Hence lemma implies

$$\eta_n^T \psi_n = \frac{(E_n^T \phi)^T s_n}{\|s_n\|} = \phi^T \frac{E_n s_n}{\|s_n\|} \to 0$$

Since ϕ arbitrary $\to$ $\dfrac{\|E_n s_n\|}{\|s_n\|} \to 0$

which implies the Dennis-Moré condition hence q-superlinear convergence.

Broyden ("dense" case)

Each step compute $B_n^{-1} F(x_n)$

and $B_{n+1} = B_n + \frac{(y - B_n s) s^T}{s^T s}$

In principle we use factorization of B_n

recomputing fact. for B_{n+1} (from scratch) is waste of comp. time $\to$ update "B_n^{-1}"

Several ways:

Assume we have $B_n = Q_n R_n$ (QR decomp.)

$$B_{n+1} = Q_n R_n + u v^T \qquad \text{typ. dense}$$

$$= Q_n (R_n + Q_n^T u v^T) = Q_n (R_n + \tilde{u} v^T)$$

Sequence of Givens rotations

$$Q_n G_1^T G_2^T \cdots G_{N-1}^T G_{N-1} G_{N-2} \cdots G_1 (R_n + \tilde{u} v^T)$$

s.t. $G_{N-1} \cdots G_1 \tilde{u} = \alpha e_1$

$$G_i = \begin{pmatrix} I & & & \\ & c_i & s_i & \\ & -s_i & c_i & \\ & & & I \end{pmatrix}$$

$$G_1 \tilde{u} = \begin{pmatrix} I & & \\ & c & s \\ & -s & c \end{pmatrix} \begin{pmatrix} \vdots \\ \tilde{u}_{N-1} \\ \tilde{u}_N \end{pmatrix} = \begin{pmatrix} \tilde{u}_1 \\ \vdots \\ \tilde{u}_{N-2} \\ \tilde{u}'_{N-1} \\ 0 \end{pmatrix} \quad \underline{\text{etc}}$$

$$G_{N-1} G_{N-2} \cdots G_1 R_n = \begin{pmatrix} x & x & \cdots & x \\ x & x & & \vdots \\ & x & \ddots & \\ & & & x\ x \end{pmatrix}$$

$$G_1 R_n \Rightarrow \begin{pmatrix} I & & \\ & c & s \\ & -s & c \end{pmatrix} \begin{pmatrix} \times & - & - & \times \\ & \ddots & & \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \end{pmatrix} \to \begin{pmatrix} \diagdown & & & | \\ & \times & \times & \times \\ & & * & * \\ & & * & * \end{pmatrix}$$

$$G_2 (G_1 R_n) \to \begin{pmatrix} I & & \\ & \begin{matrix} c & s \\ -s & c \end{matrix} & \\ & & 1 \end{pmatrix} \begin{pmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & & * & * \\ & & * & * \end{pmatrix} \to \begin{pmatrix} \times & - & - & \times \\ & \diagdown & & | \\ & \times & \times & \times \\ & * & * & * \\ & * & * & * \\ & & * & * \end{pmatrix}$$

$\underline{\text{etc}}$

$$\underbrace{(Q_n G_1^T \cdots G_{N-1}^T)}_{\tilde{Q}_{n+1}} \underbrace{\left[\begin{pmatrix} * & \cdots & * \\ * & \cdots & * \\ & * \cdots & * \\ & \diagdown & | \\ & * & * \end{pmatrix} + \begin{pmatrix} * & * & \cdots & * \\ 0 & - & - & 0 \\ | & & & | \\ 0 & - & - & 0 \end{pmatrix} \right]}_{\tilde{H}_{n+1}}$$

$\tilde{H}_{n+1}$ → still upper Hessenberg

↳ not uppertri.

Now apply second set of rotations to turn

$\tilde{H}_{n+1} \to R_{n+1}$

$$\tilde{Q}_{n+1} \tilde{G}_1^T \cdots \tilde{G}_{N-1}^T \tilde{G}_{N-1} \cdots \tilde{G}_1 \tilde{H}_{n+1}$$

$$\tilde{G}_1 \tilde{H}_{n+1} = \begin{pmatrix} \begin{matrix} c & s \\ -s & c \end{matrix} & \\ & I \end{pmatrix} \begin{pmatrix} * & - & - & * \\ * & * & - & * \\ & * & * & * \\ & & \diagdown & | \\ & & * & * \end{pmatrix} \to \begin{pmatrix} \times & - & - & \times \\ 0 & * & - & * \\ & * & - & * \\ & & | & \end{pmatrix}$$

$O(N^2)$ work instead of $O(N^3)$

Alternative use Sherman-Morrison and "preconditioning"

Inverse of rank-one update to I

$$(I + uv^T)^{-1} = I - \alpha uv^T$$

$$(I + uv^T)(I - \alpha uv^T) = I$$

$$\cancel{I} + uv^T - \alpha uv^T - \alpha v^T u\, uv^T = \cancel{I}$$

$$uv^T(1 - \alpha - \alpha v^T u) = 0 \text{ (matrix)} \rightarrow$$

$$1 - \alpha(1 + v^T u) = 0 \quad \text{(scalar)} \iff \alpha = \frac{1}{1 + v^T u}$$

So, if $v^T u = -1$: $(I + uv^T)^{-1} = I - \frac{1}{1 + v^T u} uv^T$

More general (Woodbury)

$$(I + UV^T)^{-1} = I - U(I + V^T U)^{-1} V^T$$

$\hookrightarrow$ if exists $-1 \notin \lambda(V^T U)$

$$A + uv^T = A(I + (A^{-1}u)v^T)$$

$$(A + uv^T)^{-1} = (I + (A^{-1}u)v^T)^{-1} A^{-1}$$

$$= \Big(I - \underbrace{\frac{1}{1 + v^T A^{-1} u}}_{\alpha} (A^{-1}u)v^T\Big) A^{-1} = A^{-1} - \alpha A^{-1} u v^T A^{-1}$$

if we have factorization (LU) of A we can apply $(A + uv^T)^{-1}$ at <u>quadratic</u> cost

"Trick" Let $A \simeq F'(x^*)$ and factorize A

Solve preconditioned problem

$G(x) = A^{-1}F(x) = 0 \qquad G'(x) \simeq I$ (broad minded)

So, we take $B_0 = I$

$$B_1 = I + u_0 v_0^T \quad \text{where} \begin{cases} u_0 = (y_0 - B_0 s_0)/\|s_0\| \\ v_0 = s_0/\|s_0\| \end{cases}$$

$$B_1^{-1} = I - \frac{1}{1+v_0^T u_0} u_0 v_0^T = I - w_0 v_0^T$$

where $w_0 = u_0 / 1+v_0^T u_0$

"hypothesize"

$$B_k^{-1} = (I - w_{k-1} v_{k-1}^T)(I - w_{k-2} v_{k-2}^T) \cdots (I - w_0 v_0^T)$$

$k = 1 .. n$ (true for B_1^{-1})

"induct"

$$B_{n+1} = B_n (I + B_n^{-1} u_n v_n^T)$$

$$B_{n+1}^{-1} = (I - \alpha_n B_n^{-1} u_n v_n^T) B_n^{-1}$$

$$= (I - w_n v_n^T)(I - w_{n-1} v_{n-1}^T) \cdots (I - w_1 v_1^T)$$

where $\alpha_n = (v_n^T B_n^{-1} u_n + 1)^{-1}$

$$w_n = \alpha_n B_n^{-1} u_n$$

(done)

So, applying B_n^{-1} costs k dot products + k vector updates $(x + \gamma y)$

$\rightarrow$ linear

However, computing w_k takes products, so total ~~cost~~ cost still quadratic.

Save cost by restarting or keeping only limited number of factors

$$\left(I - w_k v_k^T\right) \qquad \begin{array}{c} k = l \ldots m \\ (m-l+1) \le C \end{array}$$

$$d_{n+1} = -B_{n+1}^{-1} F(x_{n+1}) =$$

$$-\left(I - \frac{w_n s_n^T}{\|s_n\|}\right) B_n^{-1} F(x_{n+1})$$

$$= -\frac{\|s_n\|^2 B_n^{-1} F(x_{n+1}) - (1-d_n) s_n^T B_n^{-1} F(x_{n+1}) s_n}{\|s_n\|^2 + d_n s_n^T B_n^{-1} F(x_{n+1})}$$