- So far: Newton's method
  - local convergence
  - some variants of globalization (backtracking, TR)

- Tonight: **Quasi-Newton method**

  Sometimes, this refers to anything of form
  $$x_+ = x - B^{-1}F(x)$$
  for some B. Here assume, successive Bs are obtained by <u>secant</u> updating.

  In practice need to globalize.

  Here, consider on "local" form above.

- Began with method propose by W. Davidon (Argonne labs report in 1959) Later published by Davidon, Fletcher, Powell (1964)

  Original published in 1st edition of SIOPT

- Field gained momentum in 1960's; flourished in 70's matured in early 80's, slacked off after that. Now still important but less fundamental.

  Recall Newton: $x_+ = x - J^{-1}(x) F(x)$

  Forming $J(x) \sim O(n^2)$ function evaluation, may be expensive or impossible

  solving $Js = -F \sim O(n^3)$ arithmetic operations in general

  Goal: Develop methods that avoid most of these difficulties.

  General methods will require no evaluations of J and only $O(n^2)$ arithmetic operations.

  Won't enjoy quadratic local convergence but will have superlinear local convergence.

- Recall secant method for $f: \mathbb{R}^1 \to \mathbb{R}^1$

$$x_+ = x - \left[\frac{f(x) - f(x_-)}{x - x_-} \right]^{-1} f(x)$$

This has desired form with $B = \dfrac{f(x) - f(x_-)}{x - x_-}$

with no f'-evaluations and superlinear local convergence.

- Suggests that in our general method

$$x_+ = x - B^{-1} F(x)$$

B_+ = "next" B should satisfy

$$B_+ s = y \quad \text{--- } (*) \text{ secant equation}$$

where: $s = x_+ - x$

$y = F(x_+) - F(x)$

for $n=1$ case, this reduces to secant method

(say B_+ is secant update of B)

See: This determines B_+ uniquely $\Leftrightarrow n=1$

What to do when $n>1$?

- Least-change principle: Make least possible change in B to get B_+ satisfying $(*)$

- What does least-change mean?

Original interpretation - "minimum rank" interpretation

A rank-one update of B has the form

$$B_+ = B + uv^T \quad \text{for } u, v \in \mathbb{R}^n$$

To satisfy $(*)$ must have

$$\left.\begin{array}{l} y = B_+ s = Bs + uv^T s \\ \Rightarrow \quad v^T s\, u = y - Bs \Rightarrow u = \dfrac{y - Bs}{v^T s} \end{array}\right\} \Rightarrow B_+ = B + \frac{(y - Bs)v^T}{v^T s}$$

work for any v such that $v^T s \neq 0$

Of all choices of v, most succesful in practice is $v = s$

$$B_+ = B + \frac{(y - Bs)s^T}{s^T s}$$

the **Broyden** update

Introduced in 1965 but still the most successful update for general nonlinear equations.

$$s \leftarrow \lambda s \quad \Rightarrow \quad B_+ = B + \frac{(y - \lambda Bs)\lambda s^T}{\lambda^2 s^T s}$$

$$y = F(x+\lambda s) - F(x) = F'(x)\lambda s + o(\lambda)$$

- Shortcomings of minimum-rank interpretation
  - provides no basis for distinguishing Broyden update from others
  - provides no basis for understanding / analyzing method behavior
  - isn't suitable when some "auxiliary conditions" (esp. specific sparsity pattern) are imposed in addition to $(*)$

- Modern interpretation: Make the least change in B as measured in some $\|.\|$ on $\mathbb{R}^{n\times n}$ to get B_+ satisfying $(*)$

More precisely

$$B_+ = \underset{\bar{B}s = y}{\operatorname{argmin}} \{ \|\bar{B} - B\| \}$$

denote

$$Q(y,s) = \{ \bar{B} \in \mathbb{R}^{n\times n} : \bar{B}s = y \}$$

and consider

$$\mathcal{H} = \{ H \in \mathbb{R}^{n\times n} : Hs = 0 \}$$ H-matrices "annihilators" of s

Claim $\mathcal{H}$ is a subspace of $\mathbb{R}^{n\times n}$

Why? If H_1, H_2 are in $\mathcal{H}$ then for scalars $\alpha_1\ \alpha_2$

$$(\alpha_1 H_1 + \alpha_2 H_2) s = \alpha_1 \underbrace{H_1 s}_{=0} + \alpha_2 \underbrace{H_2 s}_{=0} = 0$$

$$\Rightarrow \alpha_1 H_1 + \alpha_2 H_2 \in \mathcal{H}$$

Suppose $M \in Q(y,s)$ and $H \in \mathcal{H}$

Then $(M+H)s = Ms + Hs = y + 0$

$\Rightarrow$ $M+H$ also in Q

If M_1, M_2 are in Q then

$$(M_1 - M_2)s = M_1 s - M_2 s = y - y = 0$$

$\Rightarrow$ $M_1 - M_2$ is in $\mathcal{H}$

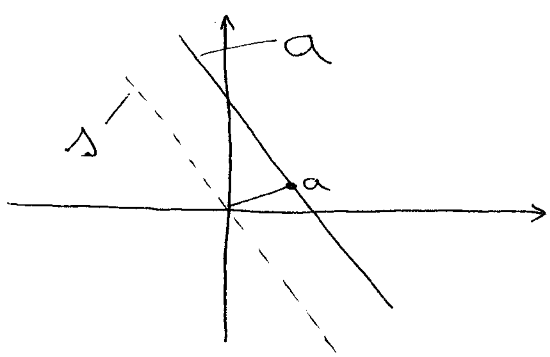
So $Q(y,s)$ is an affine subspace of $\mathbb{R}^{n\times n}$ with parallel subspace $\mathcal{H}$

- Affine subspace – a translate of a subspace.

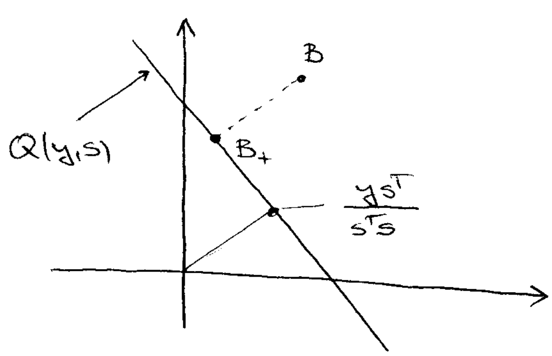
General form

$$\mathcal{a} = a + \mathcal{S}$$

a ↑ vector, $\mathcal{S}$ ↖ subspace



so have

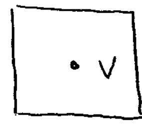


so want B_+ to be the closest element of Q to B as measured by $\|\cdot\|$

- For general $\|\cdot\|$, "closest" may not uniquely define B_+

- Example:

$\|\cdot\|_\infty$ on $\mathbb{R}^n$



← all points on boundary are equally close to v in $\|\cdot\|_\infty$

$\|\cdot\|_1$ on $\mathbb{R}^n$

same situation in $\|\cdot\|_1$

$\Rightarrow$ closest point is not uniquely defined

- For some norms "closest" may uniquely defined but not easy to compute

- Assume $\|\cdot\|$ is an inner-product norm on $\mathbb{R}^{n\times n}$ i.e. $\|M\| = \sqrt{\langle M, M\rangle}$

Then can characterize B_+ as an orthogonal projection of B onto Q

- For now, take $\|\cdot\|$ - Frobenius norm, define by

$$\langle A, B\rangle = \sum_{1\le i,j\le n} A_{ij} B_{ij} = \text{trace}\{A B^T\}$$

$\#$ trace$\{M\} = \sum_i M_{ii}$ $\#$

so

$$\|A\| = \langle A, A\rangle^{1/2} = \sqrt{\sum_{1\le i,j\le n} A_{ij}^2} = \text{trace}\{AA^T\}$$

Know $Q(y,s)$ is an affine subspace with parallel subspace $\mathcal{H}$. Indeed

$$Q(y,s) = \frac{ys^T}{s^Ts} + \mathcal{H}$$

see $\frac{ys^T}{s^Ts}\cdot s = y$

where $\frac{ys^T}{s^Ts}$ is the normal element

i.e. $\frac{ys^T}{s^Ts} \in Q(y,s) \cap \mathcal{H}^\perp$

Why? See $\frac{ys^T}{s^Ts} \in Q$ and if $H \in \mathcal{H}$ then

$$\left\langle \frac{ys^T}{s^Ts}, H \right\rangle = \text{trace} \left\langle \frac{ys^T}{s^Ts} H^T \right\rangle = \text{trace} \left\{ \frac{y\,(\overbrace{Hs}^{\overset{0}{\shortparallel}})^T}{s^Ts} \right\} = 0$$

with $\langle \cdot, \cdot \rangle$ can say B_+ = orthogonal projection of B onto Q, i.e. the unique element of Q such that $(B_+ - B) \in \mathcal{H}^\perp$

i.e. $B_+ = P_Q \cdot B$

where P_Q = orthogonal projection onto Q

In general, if a is an affine subspace with normal element a_n and parallel subspace $\mathcal{S}$ then

$$\underset{\substack{\uparrow \\ \text{orthogonal} \\ \text{projection} \\ \text{onto } a}}{P_a \cdot v} = a_n + \underset{\substack{\uparrow \\ \text{orthogonal} \\ \text{projection} \\ \text{onto } \mathcal{S}}}{P_{\mathcal{S}} v}$$

Why?

(1) $$P_a(P_a \cdot v) = a_n + P_{\mathcal{S}}(P_a \cdot v)$$
$$= a_n + P_{\mathcal{S}}(a_n + P_{\mathcal{S}} v)$$
$$= a_n + \underbrace{\cancel{P_{\mathcal{S}} a_n}}_{\substack{0 \\ \text{since } a_n \perp \mathcal{S}}} + \underbrace{P_{\mathcal{S}}(P_{\mathcal{S}} v)}_{\substack{\shortparallel \\ P_{\mathcal{S}} v \text{ since } \mathcal{S} \text{ is on} \\ \text{projection}}}$$

(2) clearly $P_a \cdot v = a_n + P_{\mathcal{S}} v \in a$

for all $v \Rightarrow$ range $(P_a) \leq a$

Also if $v \in a \Rightarrow v - a_n \in \mathcal{S}$

$$\Rightarrow P_{\mathcal{S}}(v - a_n) = v - a_n$$

$$\Rightarrow v = a_n + P_{\mathcal{S}}(v - a_n)$$

$$v \in \text{range}\,(P_{\mathcal{A}})$$

$$\mathcal{A} \subseteq \text{range}\,(P_{\mathcal{A}})$$

$$\text{so range}\,(P_{\mathcal{A}}) = \mathcal{A}$$

Then (1) & (2) show that $P_{\mathcal{A}}$ is an <u>algebraic</u> projection

Also have for any v and any $w \in \mathcal{S}$

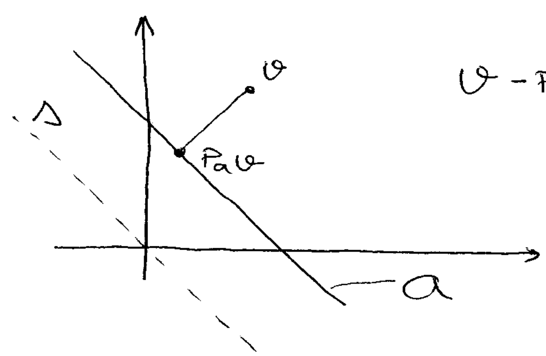
$$\langle v - P_{\mathcal{A}} v, w \rangle = \langle v - a_n - P_{\mathcal{S}} v, w \rangle$$

$$= \underbrace{\langle v - P_{\mathcal{S}} v, w \rangle}_{\overset{\shortparallel}{0}} - \underbrace{\langle a_n, w \rangle}_{\overset{\shortparallel}{0}} = 0$$

since $a_n \perp \mathcal{S}$

since $P_{\mathcal{S}}$ is orthogonal projection onto $\mathcal{S}$ and therefore $v - P_{\mathcal{S}} v \perp \mathcal{S}$

So $P_{\mathcal{A}}$ is orthogonal projection onto Q



$$v - P_{\mathcal{A}} v \perp \mathcal{S}$$

So have

normal element

$$Q(y,s) = \frac{ys^T}{s^Ts} + \mathcal{H}$$

so

$$B_+ = P_Q B = \frac{ys^T}{s^Ts} + P_{\mathcal{H}} B$$

In general, if $\mathcal{S}$ is a subspace, then P is orthogonal projection onto $\mathcal{S}$ $\Leftrightarrow$

(1) $P^2 = P$
(2) range $P = \mathcal{S}$ } algebraic projection
(3) for all v and all $s \in \mathcal{S}$ $\langle v - P_{\mathcal{S}} v, s \rangle = 0$ } orthogonal projection

Note : Since Δ is a subspace

(3) holds $\iff$ $\langle P_\Delta v, w\rangle = \langle v, P_\Delta w\rangle$ ... (3')

for all v, w

Claim : $P_{\mathcal{H}} B = B\left[I - \frac{ss^T}{s^Ts}\right]$

Why ? Verify that (1), (2), (3) or (3') hold

So

$$B_+ = \frac{ys^T}{s^Ts} + B\left[I - \frac{ss^T}{s^Ts}\right]$$

$$= B + \frac{(y-Bs)s^T}{s^Ts}$$

Broyden update again !

Properties of Broyden's method

Doesn't require $J(x)$ at each step

$$X_+ = X - B^{-1}F(x) \qquad \text{(But often } B_0 = J(X_0) \text{ in practice)}$$

$$B_+ = B + \frac{(y-Bs)s^T}{s^Ts}$$

Solving $Bs = -F(x)$ appears to require $O(n^3)$ arithmetic

In fact, since B_+ = rank one update of B, can implement

only $O(n^2)$ arithmetic

One way (original way)

Sherman - Morrison - Woodbury formula

If A nonsingular and u, v vectors, the $A + uv^T$

is nonsingular $\iff$ $\sigma = 1 + v^TA^{-1}u \neq 0$ in which case

$$(A+uv^T)^{-1} = A^{-1} - \frac{1}{\sigma}A^{-1}uv^TA^{-1}$$

(Note $\exists$ generalization to the rank k update case

- see Golub - Van Loan)

For Broyden, then can form B_0^{-1} using $O(n^3)$ arithmetic

If we ever have to do inverse
$$\left\{\begin{array}{l} \text{Factor } B_0 = LU \quad \sim O(n^3) \\ \text{for } j = 1, \dots, n \\ \qquad \text{solve } B_0 c_j = e_j \quad \sim O(n^2) \qquad (e_j = j^{th} \text{ column of } I) \\ \text{then } B_0^{-1} = (c_1, \dots, c_n) \end{array}\right.$$

Then define

$$B_{k+1}^{-1} = B_k^{-1} - \frac{1}{\sigma_k} B_k^{-1} \frac{(y - B_k s) s^T}{s_k^T s_k} B_k^{-1} \quad \text{with } O(n^2) \text{ arithmetic}$$

Preferred way (more complicated but occasionally better numerically)

Form $B_0 = Q_0 R_0$

Then update Q_k & R_k to get Q_{k+1} & R_{k+1} in $O(n^2)$ arit

- Originated by Gill - Murray (1972)
- Can show

Theorem: (Broyden - Dennis - Moré 1971)
Suppose F is Lipschitz continuously differentiable at x_* such that $F(x_*) = 0$ and $F'(x_*)$ nonsingular. Then for x_0 sufficiently near x_* and B_0 sufficiently near $F'(x_*)$, $\{x_k\}$ produced by Broyden's method is well-defined and $x_k \to x_*$ superlinearly.

Moreover $\{B_k\}$ and $\{B_k^{-1}\}$ are bounded.

- Suppose we want to impose structure* on B_k's reflecting that of $J(x_k)$

* e.g. symmetry, particular sparsity etc.

Can extend least-change secant update approach to do this

(1) Suppose have $\langle \cdot , \cdot \rangle$ and $\| \cdot \|$ on $\mathbb{R}^{n \times n}$
(Frobenious norm or weighted Frobenious norm)

$$\langle A, B \rangle = \operatorname{trace}\{ A W B^T \}$$

where W = SPD weight matrix

(2) an affine subspace $\mathcal{A} \subseteq \mathbb{R}^{n \times n}$ of matrices having the desired structure

Then, given B take

$$B_+ = \underset{\bar{B} \in \mathcal{A} \cap Q}{\operatorname{argmin}} \| \bar{B} - B \|$$ = least-change secant update at B in $\mathcal{A}$

Assuming $\mathcal{A} \cap Q \neq 0$ have

$$B_+ s = y$$

since $B_+ \in Q$

Also if $\mathcal{A} \cap Q \neq 0$ can show $\mathcal{A} \cap Q$ is an affine subspace: If $\mathcal{A} = a_n + \Delta$ and $Q = \frac{y s^T}{s^T s} + \mathcal{H}$ then

$$\mathcal{A} \cap Q = \eta + \Delta \cap \mathcal{H}$$

so some $\eta \in (\mathcal{A} \cap Q) \cap \mathcal{H}^{\perp}$

Then

$$B_+ = P_{\mathcal{A} \cap Q} B = \eta \, P_{\Delta \cap \mathcal{H}} B$$

Usually $\mathcal{A} \cap Q \neq 0$

Proposition: If $J(x) \in \mathcal{A}$ for all x of interest then $\mathcal{A} \cap Q \neq 0$

proof: $y = F(x_*) - F(x)$

$$= \int_0^1 \frac{d}{dt} F(x+ts)\,dt = \underbrace{\int_0^1 J(x+ts)\,dt}_{\in \mathcal{Q}} \cdot s$$

This machinery can actually be applied to derive updates. slides 99–102 in short course notes for derivation of the Powell, symmetric Broyden update in which $\mathcal{Q}$ = subspace of symmetric matrices

- See slides 104–107 for many updates that can be derived using this approach.
- See slide 108 for "theorem" giving local superlinear convergence for all of these.
- see slide 109 for recommendations