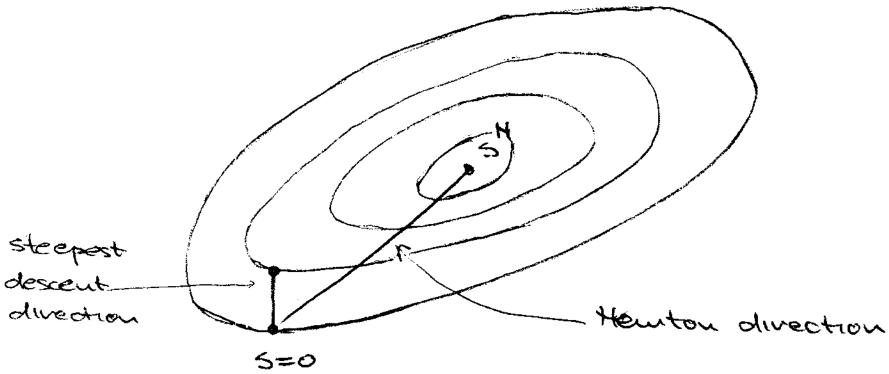
More on globalization

- Backtracking from Newton step may have shortcomings
- If F is "badly behaved"
  - many steplength reductions may be required
  - reduction in $\|F\|$ may be small relative to that given by other steps of same length (but different direction)

Badly behaved? May be

- highly nonlinear or may have ill-conditioned Jacobian (write $J(x)$ for $F'(x)$)

  picture $(\|.\| = \|.\|_2)$ of level sets $\|F + Js\| \equiv c$ in S-space



Eccentricity is directly related to $K(J) = \|J\| \|J^{-1}\|$

- If J is very badly conditioned, Newton direction and steepest descent direction may be nearly orthogonal
- can show for an unfortunate choice of F and J can have

$$\left(\frac{\nabla f}{\|\nabla f\|_2}\right)\left(\frac{s^N}{\|s^N\|_2}\right) \approx \frac{1}{K_2(J)} \quad \text{where } f = \tfrac{1}{2}\|F\|^2$$

Also, in this case, J is "nearly singular" $\Rightarrow s^N$ is likely to be long

$\Rightarrow$ many steplength reductions may be required to deal with nonlinearity

$\Rightarrow$ short step λs^N

Since s^N is nearly orthogonal to steepest descent direction, an equally short step in (or near) the steepest descent direction might give much greater reduction in $\|F\|$

- Trust region methods

Idea: At each step, have a trust region

$$H_\delta(x) = \{ y : \|y - x\| \le \delta \}$$

about current x defined by trust region radius $\delta > 0$ such that we "trust"

$$F(x) + J(x)\cdot s \approx F(x+s)$$

for $\|s\| < \delta$

Then choose $s = \underset{\|w\| \le \delta}{\operatorname{argmin}} \|F + Jw\|$ (ideally)

finding exact solution is real challenge

Test s

unacceptable $\Rightarrow$ reduce δ, find new s

$s = \underset{\|w\| \le \delta}{\operatorname{argmin}} \|F + Jw\|$, repeat the test

acceptable $\Rightarrow$ update $x \leftarrow x + s$, consider adjusting δ for next step

- General TR method is a long way from a practical algorithm
- Biggest issue: finding satisfactory $s \approx \underset{\|w\| \le \delta}{\operatorname{argmin}} \|F + Jw\|$

- Develop some properties of ideal s

Proposition: If J is nonsingular and $s = \arg\min_{\|w\| \leq \delta} \|F + Jw\|$

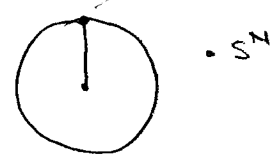
then:

i) $\|s^N\| < \delta \Rightarrow s = s^N$

ii) $\|s^N\| \geq \delta \Rightarrow \|s\| = \delta$

i)

ii)



some point on the boundary but not necessarily in Newton direction

proof: i) clear since $\|F + Js^N\|$

ii) if $\|s\| < \delta$ can find h such that

$$Jh = -\epsilon[F + Js]$$

where $0 < \epsilon < 1$ so small that $\|s + h\| < \delta$. Then

$$\|F + J(s+h)\| = \|F + Js - \epsilon[F+Js]\|$$
$$= \|(1-\epsilon)(F + Js)\|$$
$$= (1-\epsilon)\|F+Js\| < \|F + Js\|$$

contradiction!

In general TR method can have breakdown in while-loop if J is singular

Example: $F(x) = 1 + x^2$

At $x = 0$, $J = 0 \Rightarrow \|F + Js\| = \|F\|$

for every $s \Rightarrow$ pred $= 0$ (acceptable)

but ared $= F(0) - F(0+s) = 1 - (1+s^2) = -s^2 < 0$

Can never have ared $\geq t$ pred for $s \neq 0$

But don't have breakdown if J nonsingular

Proposition: Suppose F is continuously differentiable near x and $J(x)$ nonsingular. Then for

$$s = \underset{\|w\| \leq \delta}{\operatorname{argmin}} \| F + Jw \|$$

have

$$\text{ared} \geq \left[1 - \omega(\delta) \| J(x)^{-1} \|\right] \text{pred}$$

where

$$\omega(\delta) = \max_{\|u\| \leq \delta} \| J(x+u) - J(x) \|$$

So since $\omega(\delta) \to 0$ as $\delta \to 0$ will have ared $\geq$ pred when δ is so small that

$$1 - \omega(\delta) \| J(x)^{-1} \| \geq t$$

i.e.,

$$\omega(\delta) \leq \frac{1-t}{\| J^{-1} \|}$$

proof:

$$\begin{aligned} \text{ared} &= \|F\| - \|F(x+s)\| \\ &= \|F\| - \|F(x+s) - F - Js + F + Js\| \\ &\geq \underbrace{\|F\| - \|F+Js\|}_{\text{pred}} - \|F(x+s) - F - Js\| \end{aligned}$$

If $\quad \|F(x+s) - F - Js\| \leq \omega(\delta) \| J^{-1} \| \cdot \text{pred}$, then done

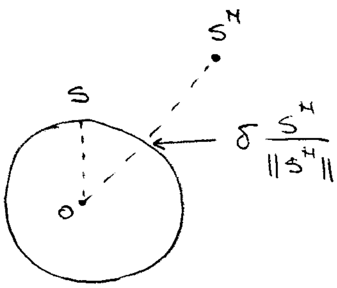
(assume $\|s^N\| > \delta \Rightarrow \|s\| = \delta$)

Handy Lemma (VI) $\Rightarrow \|F(x+s) - F - Js\| \leq \omega(\|s\|) \|s\|$
$$= \omega(\delta) \cdot \delta$$

so need only to show $\quad \delta \leq \| J^{-1} \|$ pred subtract something bigger so that you can get something smaller

Have $\quad pred = \|F\| - \|F + Js\|$

$$\geq \|F\| - \underbrace{\left\| F + J\left(\delta \frac{s^N}{\|s^N\|}\right)\right\|}_{\left\| \left(1 - \frac{\delta}{\|s^N\|}\right) F + \frac{\delta}{\|s^N\|} \underbrace{(F + Js^N)}_{=0} \right\|}$$



$$= \|F\| - \left(1 - \frac{\delta}{\|s^N\|}\right)\|F\|$$

$$= \frac{\delta}{\|s^N\|}\|F\| \quad , \quad \|s^N\| = -J^{-1}F$$

note $\frac{\delta}{\|s^N\|} \leq 1$

$$\geq \frac{\delta}{\|J^{-1}\| \, \cancel{\|F\|}} \cancel{\|F\|} = \frac{\delta}{\|J^{-1}\|}$$

Nice: 1) $pred = \|F\| - \|F + Js\| \geq 0$

2) J nonsingular and $F \neq 0 \implies pred > 0$

If $s = s^N$, $pred = \|F\| > 0$

If $\|s\| = \delta < \|s^N\|$, then

$$pred \geq \|F\| - \left\|F + J\left(\delta \frac{s^N}{\|s^N\|}\right)\right\|$$

$$= \|F\| - \left(1 - \frac{\delta}{\|s^N\|}\right)\|F\|$$

$$= \frac{\delta}{\|s^N\|}\|F\| > 0$$

3) If $\|v\| = \langle v, v \rangle^{1/2}$, then s is a descent direction for $\|F\|$ at x

i.e. $\langle \nabla \|F\|, s \rangle < 0$

proof: $f(x) = \frac{1}{2}\|F(x)\|^2$

$$\frac{d}{d\theta} f(x + \theta s)\Big|_{\theta=0} = \langle F(x+\theta s), J(x+\theta) s \rangle \Big|_{\theta=0}$$

$$= \langle F, Js \rangle$$

$$= \langle F, F+Js \rangle - \langle F, F \rangle$$

$$\leq \|F\| \, \|F+Js\| - \|F\|^2$$

$$= - \|F\| \text{ pred} < 0$$

Def: x is a stationary point of $\|F\|$ if

$$\|F+Js\| \geq \|F\| \quad \text{for every step}$$

(traditional def. of stationary point, point where $\nabla f = 0$)

Note: Suppose $\|v\| = \langle v, v \rangle^{1/2}$

Then $\|F\| \leq \|F+Js\|$

$$\Rightarrow \quad \|F\|^2 \leq \|F+Js\|^2 = \|F\| + 2\langle F, Js \rangle + \|Js\|^2$$

this holds for all s only if $\langle F, Js \rangle = 0$ for all s

$$\Rightarrow \quad \langle J^* F, s \rangle = 0 \quad \text{for all } s$$

(J^*: adjoint operation)

$$\Rightarrow \quad J^* F = 0$$

If $\|\cdot\| = \|\cdot\|_2$ then $0 = J^* F = J^T F = \nabla\left(\frac{1}{2}\|F\|^2\right)$

Theorem: Suppose $\{x_k\}$ is produced by General Trust region method

Then every limit point is a stationary point of $\|F\|$.

backtracking doesn't guarantee this

If x_* is a limit point such that $F'(x_*)$ is nonsingular, then $F(x_*) = 0$, $x_k \to x_*$, and $s_k = x_{k+1} - x_k = -J(x_k)^{-1} F(x_k)$ for all sufficiently large k

(Th. 4.4. of Eisenstat - Walker 1994)

$\exists$ examples for which Newton + backtracking iterates converge to non-stationary points

- For a practical algorithm, specify many details as with backtracking

choose t small (e.g. 10^{-4}) — so that any step that reduces the norm is acceptable

$\theta_{min} = 0.1$ $\quad \theta_{max} = 0.5$

choosing $\theta \in [\theta_{min}, \theta_{max}]$

- First if $\|s\| < \delta$ then reduce δ to $\|s\|$
- Once $\|s\| = \delta$, choose θ as before to minimize an interpolating quadratic or cubic

(requires $\|v\| = \langle v, v \rangle^{1/2}$ inner-product norm)

Details similar to backtracking see Dennis & Schnabel

- Final step: possibly adjusting δ for next step

As in Dennis & Schnabel:

i) $\delta \leftarrow 2\delta$ if good agreement

ii) $\delta \leftarrow \delta$ if so-so agreement

iii) $\delta \leftarrow \delta/2$ if poor agreement

for i) test ared $\geq u \cdot$ pred for $t \leq u \leq 1$

ii) test $v \cdot$ pred $\leq$ ared $< u \cdot$ pred

for $t \leq v \leq u < 1$

iii) test ared $< v \cdot$ pred

Dennis - Schnabel $\quad u = 0.75$

$v = 0.1$

with $t = 10^{-4}$

Computing the TR step

$$s = \underset{\|w\| \leq \delta}{\operatorname{argmin}} \|F + Jw\|$$

- computing s exactly is not practical
- want to approximate adequately at reasonable cost
- work toward a more refined characterization of s

(assume $\|\cdot\| = \|\cdot\|_2$ throughout, for convenience only any inner-product norm will work)

Lemma: If J is nonsingular then

$$s = s(\mu) \equiv -\left[J^T J + \mu I\right]^{-1} J^T F$$

for a unique $\mu \geq 0$ as follows

$\|s^N\| \leq \delta \Rightarrow \mu = 0$

$\|s^N\| > 0 \Rightarrow \mu > 0$ and uniquely determined by $\|s(\mu)\| = \delta$

proof: If $\|s^N\| \leq \delta$ then $s = s^N = -J^{-1}F = -[J^T J]^{-1} J^T F$ and $\mu = 0$

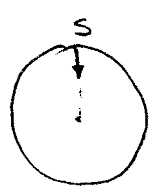
suppose $\|s^N\| > \delta$

set $e(s) = \frac{1}{2}\|F + Js\|^2$

have $\nabla e(s) = J^T(F + Js) = J^T F + J^T J s \neq 0$

since $s \neq s^N$ = unique point where $\nabla e = 0$

(s - step on the boundary of trust region but not in a Newton direction, so grad $\neq 0$)



since s minimizes e over TR, must have $\nabla e(s)$ pointing inside TR and orthogonal to the boundary

$\Rightarrow \nabla e(s) = -\mu s$ for some $\mu > 0$

Then $-\mu s = J^T F + J^T J s$

$$(J^T J + \mu I) s = -J^T F$$

so have existance of $\mu > 0$, uniqueness follows from Proposition and Corrolory below

Proposition:

i) $s(\mu)$ is differentiable and $s'(\mu) = -\left[J^T J + \mu I\right]^{-1} s(\mu)$

ii) $\varphi(\mu) \equiv \|s(\mu)\|^2$ is differentiable and

(*) $$\varphi'(\mu) = 2 s(\mu)^T s'(\mu)$$
$$= -2 s(\mu)^T \left[J^TJ + \mu I\right]^{-1} s(\mu)$$

Corollary: $\| s(\mu) \|$ is monotone strictly in μ with $\| s(0) \| = \| s^N \|$ and $\lim_{\mu \to \infty} \| s(\mu) \| = 0$

proof of corollary:

(*) $\Rightarrow \varphi'(\mu) < 0$ since $[J^TJ + \mu I]$ is SPD

$\Rightarrow \| s(\mu) \|$ strictly monotone decreasing

Also know: $s(0) = s^N$

Finally: $s(\mu) = -[J^TJ + \mu I]^{-1} J^T F \approx -\frac{1}{\mu} J^T F$

for large $\mu \to 0$ as $\mu \to \infty$

proof of proposition:

suppose $A(\mu)$ is some differentiable function of μ and that $A(\mu)$ is invertible. Then $A(\mu + \Delta)$ is invertible for small Δ and

$$\frac{1}{\Delta}\left[A(\mu+\Delta)^{-1} - A(\mu)^{-1}\right] = A(\mu+\Delta)^{-1}\left[\frac{A(\mu) - A(\mu+\Delta)}{\Delta}\right] A^{-1}(\mu)$$

$$\longrightarrow -A(\mu)^{-1} A'(\mu) A(\mu)^{-1}$$

$$\Rightarrow \frac{d}{d\mu} A(\mu)^{-1} = -A(\mu)^{-1} A'(\mu) A(\mu)^{-1}$$

Have $s(\mu) = -\underbrace{\left[J^TJ + \mu I\right]}_{\substack{A(\mu) \\ A'(\mu) I}}{}^{-1} J^T F$

$$\Rightarrow s'(\mu) = -\left[J^TJ + \mu I\right]^{-1} I \underbrace{\left[J^TJ + \mu I\right]^{-1} J^T F}_{-s(\mu)} = -\left[J^TJ + \mu I\right]^{-1} s(\mu)$$

For $\varphi(\mu) = \| s(\mu) \|^2 = s(\mu)^T s(\mu)$

$$\Rightarrow \varphi'(\mu) = 2 s(\mu)^T s'(\mu) = -2 s(\mu)^T \left[J^TJ + \mu I\right]^{-1} s(\mu)$$