09/21/2006

(2)

"pure" methods for finding x_* such that

$$f(x_*)=0 \quad , \quad f: \mathbb{R}^1 \longrightarrow \mathbb{R}^1$$

- bisection ~ r-linear convergence ; 1-function eval/iter.
- Newton's method ~ q-quadratic local convergence
  1-function eval/iter + 1-f' eval./iter
- secant ~ q-order $\frac{1+\sqrt{5}}{2}$ local convergence
  1-function eval./iter.

For secant method can also show

suppose: f is continuously differentiable near x_* such that $f(x_*)=0$, $f'(x_*) \neq 0$

suppose that:

$$|f'(x) - f'(x_*)| \leq L\,|x - x_*|$$

If x_0, x_- are sufficiently near x_*, then secant iterates $\{x_k\}$ converges to x_* with

$$|x_{k+1} - x_*| \leq \Delta\,|x_k - x_*|\,|x_{k-1} - x_*|$$

follows that

$$|x_{k+1} - x_*| \leq c_k\,|x_k - x_*|$$

$$\text{for } c_k = \Delta\,|x_{k-1} - x_*| \longrightarrow 0 \quad \text{(superlinear convergence)}$$

Can also show $\exists\, \gamma \in (0,1)$ such that

$$|x_k - x_*| \leq \gamma^{r^k} \quad \text{where} \quad r = \frac{1+\sqrt{5}}{2}$$

since $\gamma^{r^k} \longrightarrow 0$ with q order $\frac{1+\sqrt{5}}{2}$ follows that

$x_k \longrightarrow x_*$ with r order $\frac{1+\sqrt{5}}{2}$

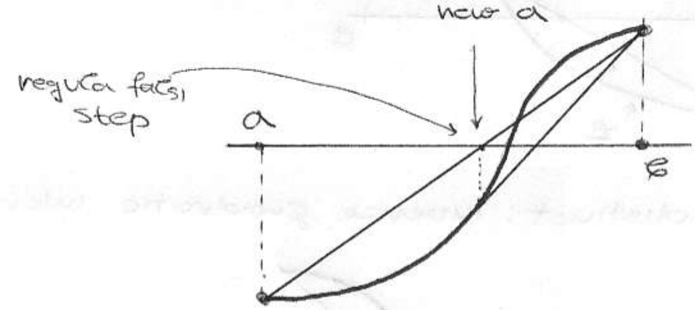
see Ralston & Rabinowitz

Practical "hybrid" methods

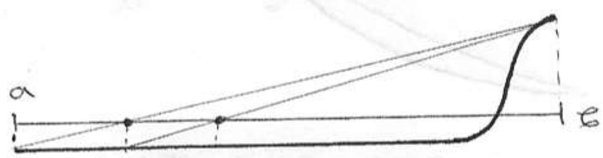
Idea: Combine features of different "pure" methods
To retain advantages, avoid disadvantages

Classical: regula falsi (false position)

suppose have $f(a) \cdot f(b) < 0$



Often works well but not always



More effective idea: Brent's algorithm
(from work of Dekker (1969) & Brent (1973))

Operation:

Begins with

i) a, b such that $f(a) \cdot f(b) < 0$

ii) tolerance δ (algorithm returns approximate solution with 2δ of a solution)

Maintains at each iteration a, b, c (initially $c = a$) such that:

i) $f(a) \cdot f(b) \leq 0$

ii) $|f(b)| \leq |f(c)| \Rightarrow b$ is current approximate solution

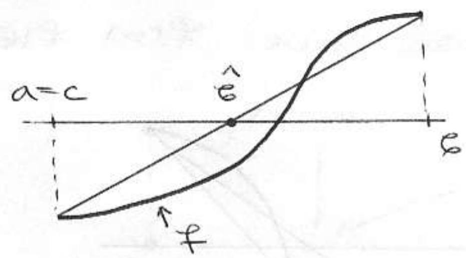
iii) either a is distinct from b and c, or $a = c$ and is imediate past value of b

Iteration:

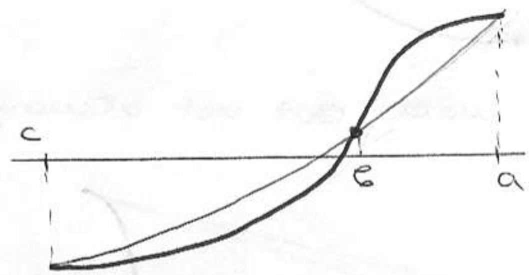
1) if $|b-a| \le \delta$, return $b \approx x_*$

2) else, determine a trial $\hat{b}$:

i) $a = c$: linear interpolation



ii) a, b, c distinct: inverse quadratic interpolation



Have a, b, c and $f(a), f(b), f(c)$

Determine:

$$p(y) = \alpha + \beta y + \gamma y^2$$

such that

$$p(f(a)) = a \quad p(f(b)) = b \; ; \; p(f(c)) = c$$

Then take $\hat{b} = p(0) = \alpha$

iii) obtain final b by adjusting $\hat{b}$ if necessary so it's neither too long nor too short (and occasionally force a bisection step)

iv) use a, b, c and final $\hat{b}$ to choose new a, b, c according to complicated rules

good ref: Forsythe, Malcolm, Moler

MATLAB ex:

```
fzero(@(x) 4*x+tan(x), 2\pi+.01)
```

ans: pi/2

```
options = optimset('Display', 'iter')
```

Newton's method for systems

Consider a general system problem

find x_* such that $F(x_*)=0$

Here: $F: \mathbb{R}^n \to \mathbb{R}^m$ (usually $m=n$)

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n \qquad F(x) = \begin{pmatrix} F_1(x) \\ \vdots \\ F_m(x) \end{pmatrix} \in \mathbb{R}^m$$

example:

$$x_1^2 + x_1 x_2^3 = 9$$
$$3x_1^2 x_2 - x_2^3 = 4$$

here: $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ $\quad F(x) = \begin{pmatrix} x_1^2 + x_1 x_2^3 - 9 \\ 3x_1^2 x_2 - x_2^3 - 4 \end{pmatrix}$

Preliminaries:

$$\mathbb{R}^n = \left\{ x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} : x_i \in \mathbb{R}^1, \text{ for } 1 \le i \le n \right\}$$

$$\mathbb{R}^{m\times n} = \left\{ A = \begin{pmatrix} a_{11} \cdots a_{1n} \\ \vdots \\ a_{m1} \cdots a_{mn} \end{pmatrix} : a_{ij} \in \mathbb{R}^1, \text{ for } \begin{matrix} 1 \le i \le m \\ 1 \le j \le n \end{matrix} \right\}$$

These are vector spaces under usual vector and matrix addition and scalar multiplication

Def: A norm $\|\cdot\|$ is a non-negative function such that for all vectors v, u and scalar α

i) $\|v\| > 0$, with $\|v\| = 0 \Leftrightarrow v = 0$

ii) $\|\alpha v\| = |\alpha| \, \|v\|$

iii) $\|v+u\| \le \|v\| + \|u\|$ (triangle inequality)

Examples: on $\mathbb{R}^n$, $v = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$

i) $\|v\|_1 = \sum_{i=1}^{n} |v_i|$

ii) $\|v\|_\infty = \max \{ |v_i| , 1 \leq i \leq n \}$

iii) $\|v\|_p = \left[\sum_i |v_i|^p \right]^{1/p}$

$p = 2 \Rightarrow$ Euclidian norm

Any norm $\|.\|$ on $\mathbb{R}^n$ induces a norm $\|.\|$ on $\mathbb{R}^{m\times n}$ by:

$$\|A\| = \max_{\|v\|=1} \|Av\| = \max_{v \neq 0} \frac{\|Av\|}{\|v\|}$$

Note: If $A \in \mathbb{R}^{m\times p}$, $B \in \mathbb{R}^{p\times n}$ then

$$\|AB\| \leq \|A\| + \|B\|$$

Examples:

i) $\|.\|_1$ on $\mathbb{R}^n$ defines

$$\|A\|_1 = \max_j \sum_{i=1}^{m} |a_{ij}|$$

ii) $\|.\|_\infty$ on $\mathbb{R}^n$ defines

$$\|A\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$$

Not all matrix norms are induced

Ex: Forbenius norm

$$\|A\|_F = \left\{ \sum_{ij} |a_{ij}|^2 \right\}^{1/2} = \left\{ \text{trace} \{AA^T\} \right\}^{1/2}$$

Note: this comes from the inner product on $\mathbb{R}^{m\times n}$

$$\langle A, B \rangle_F = \text{trace} \{AB^T\} = \sum_{i,j} a_{ij} b_{ij}$$

Fact: Any two norms on a finite-dimensional vector space (such as $\mathbb{R}^n$ or $\mathbb{R}^{m \times n}$) are equivalent, i.e. if $\|.\|$ and $|||.|||$ are any two norms, then $\exists\ c_1 > 0$ and $c_2 > 0$ such that

$$c_1 \|v\| \leq |||v||| \leq c_2 \|v\| \quad \text{for all } v$$

Def: $\{x_k\}$ converges to x_* if $\|x_k - x_*\| \to 0$

On a finite dimension space, by norm-equivalence convergence in <u>any</u> norm implies convergence in <u>every</u> norm. Convergence is norm independent.

Rate of convergence:

Say $x_k \to x_*$

- q-linearly if $\exists\ \lambda \in (0,1)$ such that

$$\|x_k - x_*\| \leq \lambda \|x_k - x_*\|$$

- q-superlinearly if

$$\|x_{k+1} - x_*\| \leq c_k \|x_k - x_*\| \quad , c_k \to 0$$

- q-order p, $1 < p < \infty$ if

$$\|x_{k+1} - x_k\| \leq \Delta \|x_k - x_*\|^p$$

Can show: q-superlinear and q-order p $(1<p<\infty)$ convergence are <u>norm</u> independent but q-linear convergence is norm dependent

Say $x_k \to x_*$ r-linearly (r-superlinearly, r-order p) if $\|x_k - x_*\| \leq \Delta_k$, where $\Delta_k \to 0$ q-linearly (q-superlinearly, q-order p)

Suppose X, Y are vector spaces with norms $\|\cdot\|_X$, $\|\cdot\|_Y$

Then $F: X \to Y$ is continuous at $x \in X$ if for every $\epsilon > 0$, $\exists \delta > 0$ that

$$\|y - x\|_X < \delta \Rightarrow \|F(y) - F(x)\|_Y < \epsilon$$

Continuity can be subtle

ex: $F: \mathbb{R}^2 \to \mathbb{R}^1$

$$F(x) = \begin{cases} \dfrac{x_1 x_2}{x_1^2 + x_2^2}, & x \neq 0 \\ 0, & x = 0 \end{cases}$$

continuous everywhere except at ϕ

Along any ray $x = r\begin{pmatrix}\cos\theta \\ \sin\theta\end{pmatrix}$ with $\cos\theta\sin\theta \neq 0$

$$F(x) = \cos\theta \sin\theta \not\to F(0) = 0$$

but if either x_1 or x_2 is fixed, $F(x)$ is continuous in the other

Def: $F: X \to Y$ is Lipschitz continuous at x if $\exists L$ such that

$$\|F(y) - F(x)\|_Y \leq L\|y - x\|_X$$

see: Lipschitz continuity $\Rightarrow$ continuity

Suppose: $F: \mathbb{R}^n \to \mathbb{R}^m$ given by

$$F(x) = \begin{pmatrix} F_1(x) \\ \vdots \\ F_m(x) \end{pmatrix}$$

If $\dfrac{\partial F_i}{\partial x_j}$ exists for each i, j write

$$F'(x) = \begin{pmatrix} \partial F_1/\partial x_1 & \cdots & \partial F_1/\partial x_n \\ \vdots & & \\ \partial F_m/\partial x_1 & \cdots & \partial F_1/\partial x_n \end{pmatrix}$$ Jacobian matrix sometimes denote by $J(x)$

If $F'(x)$ exists and $F(y) = F(x) + F'(x)(y-x) + o(y-x)$ then F is (Frechet) differentiable at x and $F'(x)$ is the (Frechet) derivative of F at x

Here $\dfrac{o(y-x)}{\|y-x\|} \to 0$ as $y \to x$

Recall: If $m=n=1$ then $F'(x)$ exist $\Leftrightarrow$ F is differentiable

Jacobian matrix can exist without function being differentiable

Note: F differentiable at $x \Rightarrow F$ continuous at x

Ex: (i) $F(x) = \dfrac{x_1 x_2}{x_1^2 + x_2^2}$ see $F'(0) = (0,0)$

but F not even continuous at $x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

(ii) $F(x) = \dfrac{x_1 x_2}{\sqrt{x_1^2 + x_2^2}}$

continuous at $x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $F'(0) = (0,0)$

but on a ray $x = r\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ with $\cos\theta \sin\theta \neq 0$

$F(x) = r\cos\theta\sin\theta \sim O(x)$ but not $o(x)$

$\Rightarrow$ not differentiable at $x = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

Note: F differentiable at $x \Rightarrow F$ Lipschitz continuous at x

Newton's method (assume $m = n$)

Suppose F continuously differentiable near x_* such that $F(x_*) = 0$

Then

$$0 = F(x_*) = F(x) + F'(x)(x_* - x) + o(x_* - x)$$

$$\Rightarrow \quad x_* = x - F'(x)^{-1} F(x) - \underbrace{F'(x)^{-1} o(x_* - x)}_{o(x - x_*)}$$

provided $F'(x)$ is invertible

So have

$$x_* \approx x_+ \equiv x - F'(x)^{-1} F(x)$$

and

$$\frac{\| x_+ - x_* \|}{\| x - x_* \|} \longrightarrow 0 \quad \text{as} \quad x \longrightarrow x_*$$

approximation gets better and better

given initial x
until termination do

$$x \leftarrow x - F'(x)^{-1} F(x) \quad \text{- - - -} \quad (*)$$

Remarks:

(1) $(*)$ is better phrased as

solve $F'(x) \cdot s = -F(x)$
update $x \leftarrow x + s$

(2) method breaks down if $F'(x)$ is singular
- numerical difficulties may occur if $F'(x)$ is ill-conditioned

(3) solving $F'(x) \cdot s = -F(x)$ takes up to $O(n^3)$ arithmetic operations in general

(4) evaluating $F'(x)$ requires up to n^2 scalar function evaluations

(5) "until termination" much as before:

Termination criteria

$$\| F(x) \| \leq tol_F$$

$$\| x_+ - x \| \leq tol_x$$

it. number $\geq$ ITMAX

as before must choose tol_F and tol_x with eye toward scales of F and x

(6) new complication: different components of F and x may have different scales

Might want to use diagonal scaling matrices D_F, D_x and use

$$\| D_F \, F(x) \| \leq tol_F$$

$$\| D_x \; x \| \leq tol_x$$

(7) convergence issues are much as before

Iterates may diverge in general but usually converge rapidly (typically quadratic) if initial guess is near solution

$$x_1^2 + x_1 x_2^3 = 9$$

$$3x_1^2 x_2 + x_2^3 = 4$$