Methods for Underdetermined systems

11/22/2006

(11)

Problem: Given $F : \mathbb{R}^{\bar{n}} \longrightarrow \mathbb{R}^{n}$

find $\bar{x}_*$ such that $F(\bar{x}_*) = 0$

Assume $\bar{n} \geq n$

Example: Bratu problem $\left(\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)$

$$\Delta u + \lambda e^{u} = 0 \quad \text{in} \quad D = [0,1] \times [0,1]$$

$$u = 0 \quad \text{on} \quad \partial D$$

$\lambda \leq 0 \implies$ no solution

$0 < \lambda < \lambda_* \in (6,7) \implies$ at least two solutions

$\lambda = \lambda_* \implies$ at least one solution

$\lambda > \lambda_* \implies$ no known solutions

- Discretizing this and treating λ as unknown gives system of n equations (n = # of grid points) in $n+1$ unknowns (approximate u-values on grid points + λ)
- Might want to trace out whole solution curve with a continuation methods

Another application: Finding periodic solutions

suppose have $\left\{ \begin{array}{l} y' = Y(y) \\ y(0) = x \end{array} \right\}$ IVP (initial value problem)

- suppose we want periodic solution: $y(x) = x$
- need particular x and t
- denote solution of IVP by $y(t,x)$
- define $F(\bar{x}) = x - y(t,x)$, $\bar{x} = \binom{x}{t}$

want $\bar{x}_*$ such that $F(\bar{x}_*) = 0$

Back to general problem

Suppose have $\bar{x}$

Reasoning with Newton's method:

want $\bar{s}$ satisfying

$$F(\bar{x}) + F'(\bar{x})\bar{s} = 0$$

If $\bar{n} > n$, this is underdetermined linear system

(assume F' is of full rank n)

$\Rightarrow$ infinitely many solutions (s in range of F')

How to specify $\bar{s}$ uniquely?

- **Augmented Jacobian approach**
- need $\bar{n}-n$ additional linear conditions
- express these as <u>orthogonality</u> conditions

$$V\bar{s} = 0 \quad , \quad V \in \mathbb{R}^{(\bar{n}-n)\times\bar{n}}$$

clearly want $\left\{\begin{array}{l} F'\bar{s} = -F \\ V\bar{s} = 0 \end{array}\right\}$ to have unique solution

i.e. want $\begin{pmatrix} F' \\ V \end{pmatrix} \in \mathbb{R}^{\bar{n}\times\bar{n}}$ nonsingular

Augmented Jacobian method

given $\bar{x}$ and $V \in \mathbb{R}^{(\bar{n}-n)\times\bar{n}}$

until termination, do

solve $\begin{pmatrix} F'(\bar{x}) \\ V \end{pmatrix} \bar{s} = \begin{pmatrix} -F(\bar{x}) \\ 0 \end{pmatrix}$

update $\bar{x} \leftarrow \bar{x} + s$

One issue:

want $\begin{pmatrix} F'(x) \\ V \end{pmatrix}$ nonsingular & not ill-conditioned in region of interest

So rows of $\bar{V}$ should be "sufficiently linearly independent" and scaled to reflect scaling of F'. May be hard to achieve

Another issue:

Have $\bar{x}_k = \bar{x}_0 + \sum_{j=0}^{k-1} \bar{s}_j$

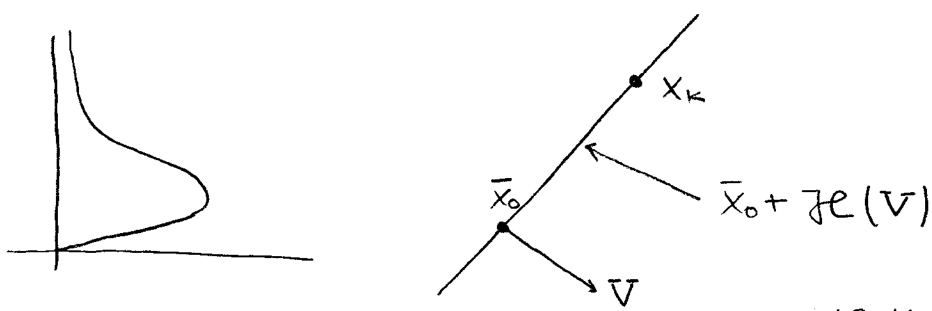
$$\Rightarrow \quad \bar{V}\bar{x}_k = \bar{V}\bar{x}_0 + \cancelto{0}{\sum_{j=0}^{k-1} \bar{V}\bar{s}_j} = \bar{V}\bar{x}_0$$

so $\bar{x}_k \in \bar{x}_0 + \mathcal{N}(\bar{V})$ (affine subspace)

$\mathcal{N}(\bar{V}) \equiv \{\bar{y} : \bar{V}\bar{y} = 0\}$ (null-space)

Then can't possibly find a solution if solution set doesn't intersect $\bar{x}_0 + \mathcal{N}(\bar{V})$

Example:



we missed solution entirely

Normal flow approach

choose $\bar{s} = -F'(x)^{+} F(\bar{x})$

where "+" denotes <u>pseudo-inverse</u>

i.e. $\bar{s}$ = minimal norm solution

Assume $\|\cdot\| = \|\cdot\|_2$ for convenience

Characterize $\bar{s}$

projection theorem $\Rightarrow$ can write any $\bar{s}$ as

$\bar{s} = \bar{n} + \bar{t}$ where $\bar{n} \in \mathcal{N}(F') \equiv \{\bar{v} : F'\bar{v} = 0\}$ and

$\bar{t} \in \mathcal{N}(F')^{\perp}$ (orthogonal complement of null space)

Suppose $F'\bar{s}_1 = -F$ and $F'\bar{s}_2 = -F$

$\Rightarrow F'(\bar{s}_1 - \bar{s}_2) = 0 \Rightarrow \bar{s}_1 - \bar{s}_2 \in \mathcal{N}(F')$

So have $\bar{s}_1 = \bar{u}_1 + t$ and $\bar{s}_2 = \bar{u}_2 + \bar{t}$ for some $\bar{t} \in \mathcal{N}(F')^\perp$

If $\bar{s} = \bar{u} + \bar{t} \in \mathcal{N}(F')$ then $\|\bar{s} + \bar{t}\|^2$

$$\|\bar{s}\|^2 = \|\bar{u} + \bar{t}\|^2 = \|\bar{u}\|^2 + \|\bar{t}\|^2 \geq \|\bar{t}\|^2$$

$\Rightarrow \bar{t}$ is the pseudo-inverse solution

See: pseudo-inverse solution is:

$\#$ denote $J = F'$

$$\bar{s} = J^T \underbrace{(JJ^T)^{-1}}_{n \times n} (-F)$$

nonsingular since J is full rank

why?

to verify that, show that it is solution and orthogonal to null-space

(1) $J\bar{s} = JJ^T(JJ^T)^{-1}(-F) = -F$ so it is solution

(2) $\bar{u} \in \mathcal{N}(J) \Rightarrow \bar{u}^T\bar{s} = \underbrace{\bar{u}^T J^T}_{(J\bar{u})^T = 0}(JJ^T)^{-1}(-F) = 0$ $\Rightarrow$ orthogonal to null-space

Normal flow method

given $\bar{x}$

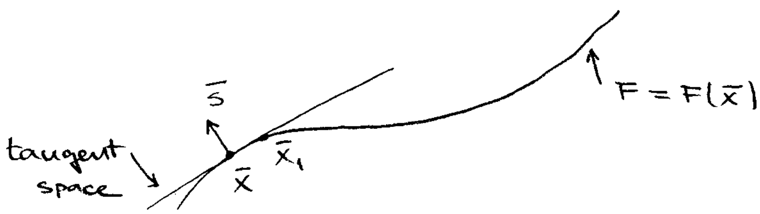
until termination do

compute $\bar{s} = -F'(\bar{x})^+ F(\bar{x})$

update $\bar{x} \leftarrow \bar{x} + \bar{s}$

See: No "scaling" issue associated with auxiliary orthogonality conditions

- Iterates are not restricted to any affine subspace
- step directions are orthogonal (normal) to surfaces $F = \text{const}$



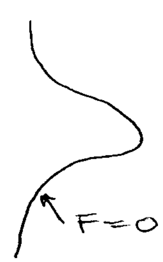
$$F(\bar x_1) = \cancel{F(\bar x)}$$
$$\|$$
$$\cancel{F(\bar x)} + F'(\bar x)(\bar x_1 - \bar x) + o(\|\bar x_1 - \bar x\|)$$
$$\Rightarrow \quad F'(\bar x)(\bar x_1 - \bar x) \approx 0$$

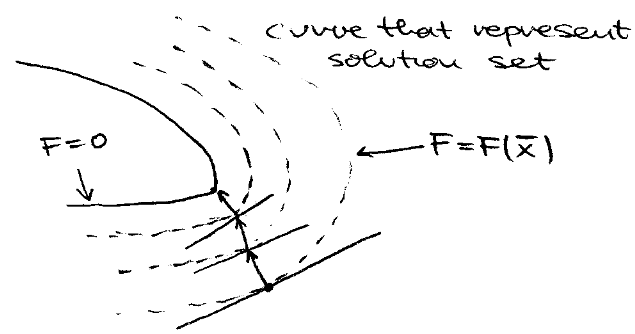
see: tangent space of $(\bar n - n)$ dimensional surface

$$\{\bar y : F(\bar y) = F(\bar x)\} \text{ is just } \mathcal{N}(F'(\bar x))$$
$$\equiv \{\bar v : F'(\bar x)\bar v = 0\}$$

so $\bar s = -F'(\bar x)^+ F(\bar x)$ is orthogonal to this tangent space

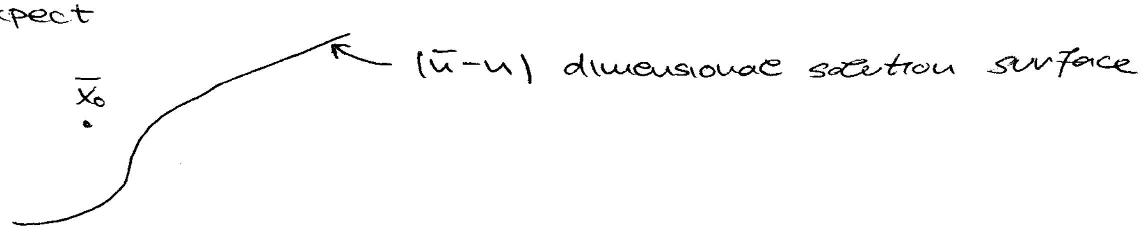
Advantage:





Local convergence analysis

expect



In general solutions are not isolated, so can't predict in advance any solution $\bar{x}_*$ such that $\bar{x}_k \to \bar{x}_*$

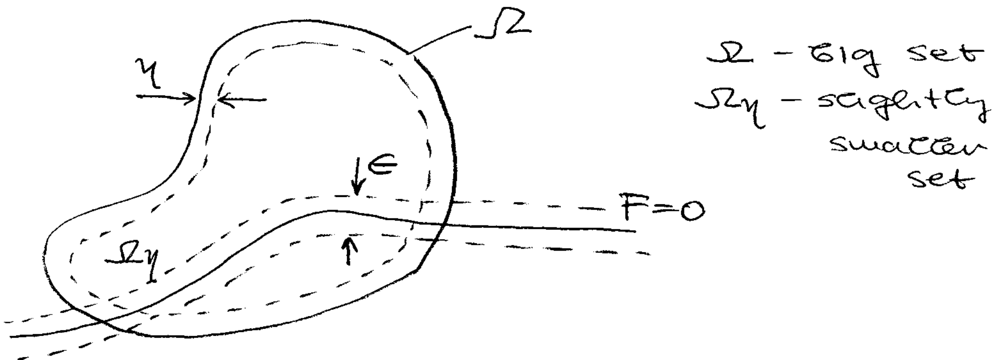
Need Kantorovich-type analysis

will assume $\|F(x_0)\|$ small, $\|F^+(\bar{x})\|$ bounded nearby and F' is Lipschitz nearby

$$\Rightarrow \bar{x}_k = \bar{x}_* \text{ such that } F(\bar{x}_*) = 0$$

From Walker-Watson SINUM 1990

Hypothesis 1



suppose F is differentiable and rank n in Ω and

i) $\|F'(\bar{y}) - F'(\bar{x})\| \le \gamma \|\bar{y} - \bar{x}\|$ for $\bar{x}, \bar{y} \in \Omega$

Lipschitz continuous

ii) $\|F'(\bar{x})^+\| \le \mu$ for $\bar{x} \in \Omega$ (pseudo-inverse is bounded)

For $\eta > 0$ define

$$\Omega_\eta = \{\bar{x} \in \Omega : \|\bar{y} - \bar{x}\| < \eta \Rightarrow \bar{y} \in \Omega\}$$

Theorem: Suppose hypothesis 1 holds in Ω and have Ω_η for some $\eta > 0$. Then $\exists\, \epsilon > 0$ depending only on γ, μ and η such that if $\|F(\bar{x}_0)\| < \epsilon$ then normal flow iterates remain in Ω and converge quadratically to $\bar{x}_* \in \Omega$ such that $F(\bar{x}_*) = 0$

Can apply this to show local convergence of Augmented Jacobian method.

Hypothesis 2: F is differentiable and $\begin{pmatrix} F'(\bar{x}) \\ V \end{pmatrix}$ is nonsingular in Ω and

i) $\| F'(\bar{y}) - F'(x) \| \leq \gamma \| \bar{y} - \bar{x} \|$ for $\bar{x}, \bar{y}$ in Ω

ii) $\left\| \begin{pmatrix} F'(\bar{x}) \\ V \end{pmatrix} \right\| \leq \bar{\mu}$

Theorem: Suppose Hypothesis 2 holds and have Ω_η for some $\eta > 0$. Then $\exists \epsilon > 0$ depending only on $\gamma, \bar{\mu}$ and η. Such that if $\bar{x}_0 \in \Omega_\eta$ and $\| F(\bar{x}_0) \| < \epsilon$. Then augmented Jacobian iterates converge quadratically to $\bar{x}_* \in \Omega$ such that $F(\bar{x}_*) = 0$

proof idea: Define $\bar{F}(\bar{x}) = \begin{pmatrix} F(\bar{x}) \\ V(\bar{x} - \bar{x}_0) \end{pmatrix}$

then $\bar{F}'(\bar{x}) = \begin{pmatrix} F'(\bar{x}) \\ V \end{pmatrix}$

and Augmented Jacobian iterates are just the Newton iterates for $\bar{F}$, which are the normal flow iterates for $\bar{F}$.

Applying previous theorem

if $\bar{s} = J^T (J^T J)^{-1} (-F)$ and $\bar{u} = u$ then

$\bar{s} = J^T (J^T)^{-1} J^{-1} (-F) = - J^{-1} F$

Apply normal flow to find periodic solution of

clarinet reed model (Lord Rayleigh) $\left\{ x'' = ax' + b(x')^3 - kx \right.$ $\quad a = 5$, $b = 4$, $k = 5$

rewrite as $y' = \varphi(y)$

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \qquad \begin{matrix} y_1 = x \\ y_2 = x' \end{matrix} \qquad \varphi(y) = \begin{pmatrix} y_2 \\ a y_2 - b y_2^3 - k y_1 \end{pmatrix}$$

MATLAB: periodic (@vdfun, (2;2), 3)
(3;3), 4

- How to set up periodic-solution problem as $F(\bar{x}) = 0$ & apply normal flow method.

Denote solution by $y(t,x)$

set $F(\bar{x}) = x - y(t,x)$, $\bar{x} = \begin{pmatrix} x \\ t \end{pmatrix}$ $\quad \bar{n} = n+1$

have $F'(\bar{x}) = [F_x, F_t]$

see $F_t = \frac{\partial}{\partial t}\left(x - y(t,x)\right) = -\frac{\partial}{\partial t} y(t,x) = -\varphi(y(t))$

$F_x = I - y_x(t,x)$, where $y_x = \frac{\partial}{\partial x} y(t,x)$

have $y'(t,x) = \varphi(y(t,x))$
$y(0,x) = x$

$$\Rightarrow \left.\begin{matrix} y_x'(t,x) = \varphi'(y(t,x))\, y_x \\ y_x(0,x) = I \end{matrix}\right\} \text{ IVP for } y_x$$

So can find $y_x(t,x)$ by integrating this along with IVP for y

$y' = \varphi(y)$ ... n equations

$y_x' = \varphi'(y) \cdot y_x$ ... n^2 equations

system gets big very quickly

General remarks on computing $\bar{s} = -F'(\bar{x})^{+} F(\bar{x})$

(note: $J = F'(\bar{x})$)

prof Walker's favourit way (OK if $\bar{n}, n$ not too large)

$$\underset{\bar{n}\times n}{J^T} = \underset{\bar{n}\times n}{Q}\,\underset{n\times n}{R}$$

want $J\bar{s} = -F$

$$R^T Q^T \bar{s} = -F$$

1) solve $R^T y = -F$

2) set $\bar{s} = Q\cdot y$

Then verify that:

(1) is solution

$$J\bar{s} = R^T \underbrace{Q^T Q}_{I_n} \cdot y = R^T y = -F$$

(2) verify that is min. norm solution $\Leftrightarrow$ orthogonal to null-space of J

$$\bar{\eta} = \mathcal{N}(J) \quad \text{i.e.} \quad J\bar{n} = 0$$

$$\Rightarrow \bar{n}^T \bar{s} = \bar{n}\, Q\cdot y = (Q^T \bar{n})^T y = (\underbrace{\underbrace{R^T Q^T}_{J}\, \bar{n}}_{J\cdot\bar{n} \,=\, 0})^T R^{-1} y = 0$$

Path following methods

- Suppose have $F(\bar{x}) : \mathbb{R}^{(n+1)} \longrightarrow \mathbb{R}^n$
- want to follow curve of solution $F(\bar{x}) = 0$
- usual $\bar{x} = \begin{pmatrix} x \\ \lambda \end{pmatrix}$

example: $\Delta u + \lambda e^u = 0$ in D

$u = 0$ on ∂D

λ "normal" parameter $\Rightarrow$ continuation methods

Also there are "artificial parameter" – homotopy method

Suppose have $\underset{\substack{\uparrow \\ \text{hard}}}{G(x) = 0}$; $G: \mathbb{R}^n \to \mathbb{R}^n$

given x_0, solving

$$H(x) = G(x) - G(x_0) = 0$$

Homotopy idea:

set $F(x,t) = (1-t)H(x) + t\,G(x)$

and follow solution curve

$$F(x,t) = 0 \quad , \quad 0 \le t \le 1$$

Assume $F'(\bar{x})$ is full-rank n always

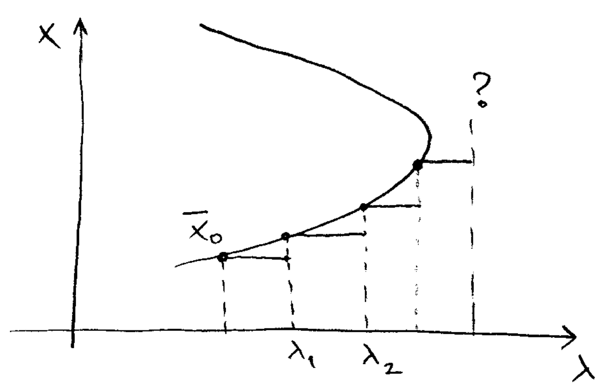
First thought: Start with $\bar{x}_0 = \begin{pmatrix} x_0 \\ \lambda_0 \end{pmatrix}$, $F(\bar{x}_0) = 0$

choose $\Delta\lambda$

given $\bar{x}_i$ with $F(\bar{x}_i) = 0$

set $\lambda_{i+1} = \lambda_i + \Delta\lambda$ and iterate to solve

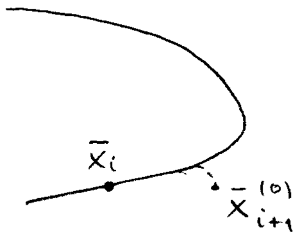
$F(x_{i+1}, \lambda_{i+1}) = 0$



you can't go pass the turn

Second thought: Given $\bar{x}_i = \begin{pmatrix} x_i \\ \lambda_i \end{pmatrix}$ "predict" $\bar{x}_{i+1}^{(0)}$ and

iterate to find $\bar{x}_{i+1} \approx$ on curve

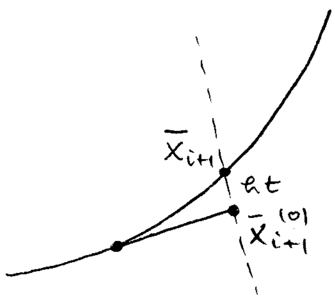


simple predictor / corrector idea

predict $\bar{x}_{i+1} = \bar{x}_i + h\bar{t}_i$

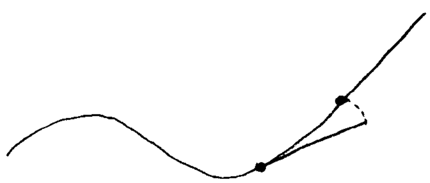
$\bar{t}_i$ = (approximate) tangent

corrector iterations can be either augmented Jacobian iterations $(\bar{V} = \bar{t}_i^{+})$ or normal flow iterat.



augmented Jacobian

(at the sharp turn, augmented Jacobian may not be able to get to the curve)



normal flow

Note: normal flow may succeed near "turning point" where augmented Jacobian may fail.

More sophisticated predictor:

Hermit cubic predictor based on $\bar{x}_{i-1}$, $\bar{x}_i$ and $\bar{t}_{i-1}$, $\bar{t}_i$

- can either each $\bar{t}_i$ accumulate

or use $\dfrac{\bar{x}_i - \bar{x}_{i-1}}{\| \bar{x}_i - \bar{x}_{i-1} \|} = \bar{t}_i$