Projected Pseudo-Transient Continuation

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Outline

Collaborators

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Newton's method

Problem: solve $F(u) = 0$
$F : R^N \to R^N$ is Lipschitz continuously differentiable.
Newton's method

$$u_+ = u_c + s.$$

The step is

$$s = -F'(u_c)^{-1} F(u_c)$$

$F'(u_c)$ is the Jacobian matrix

Implementation

Inexact formulation:

$$\|F'(u_c)s + F(u_c)\| \le \eta_c \|F(u_c)\|.$$

$\eta = 0$ for direct solvers + analytic Jacobians.
If $F(u^*) = 0$, $F'(u^*)$ is nonsingular, and u_c is close to u^*

$$\|u_+ - u^*\| = O(\eta_c \|u_c - u^*\| + \|u_c - u^*\|^2)$$

Meditation exercise: What's η?

But what if u_0 is far from u^*?

Armijo Rule: Find the least integer $m \geq 0$ such that

$$\|F(u_c + 2^{-m}s)\| \leq (1 - \alpha 2^{-m})\|F(u_c)\|$$

- $m = 0$ is Newton's method.
- Make it fancy by replacing 2^{-m}.
- $\alpha = 10^{-4}$ is standard.

Theory

If F is smooth and you get s with a direct solve or GMRES then either

- **BAD:** the iteration is unbounded, i. e. $\limsup \|u_n\| = \infty$,
- **BAD:** the derivatives tend to singularity, i. e. $\limsup \|F'(u_n)^{-1}\| = \infty$, or
- **GOOD:** the iteration converges to a solution u^* in the terminal phase, $m = 0$, and

$$\|u_{n+1} - u^*\| = O(\eta_n \|u_n - u^*\| + \|u_n - u^*\|^2).$$

Bottom line: you get an answer or an easy-to-detect failure.

Why worry?

- Stagnation at singularity of F' really happens.
    - steady flow $\longrightarrow$ shocks in CFD
- Non-physical results
    - fires go out
    - negative concentrations
- Nonsmooth nonlinearities
    - are not uncommon: flux limiters, constitutive laws
    - globalization is harder
    - finite diff directional derivatives may be wrong

Ψtc is one way to fix some of these things.

Steady-state Solutioins

Think about a PDE

$$\frac{du}{dt} = -F(u), u(0) = u_0,$$

and its solution $u(t)$.
$F(u)$ contains

- the nonlinearity,
- boundary conditions, and
- spatial derivatives.

We want the steady-state solution: $u^* = \lim_{t \to \infty} u(t)$.

What can go wrong?

If u_0 is separated from u^* by

- complex features like shocks,
- stiff transient behavior, or
- unstable equlibria,

the Newton-Armijo iteration can

- stagnate at a singular Jacobian, or
- find a solution of $F(u) = 0$ that is not the one you want.

A Questionable Idea

One way to guarantee that you get u^* is

- Find a high-quality temporal integration code.
- Set the error tolerances to very small values.
- Integrate the PDE to steady state.
  - Continue in time until $u(t)$ isn't changing much.
- Then apply Newton to make sure you have it right.

Problem: you may not live to see the results.

Ψtc

Integrate

$$\frac{du}{dt} = -F(u)$$

to steady state in a stable way with increasing time steps.
Equation for Ψtc Newton step:

$$\left(\delta_c^{-1} I + F'(u_c)\right) s = -F(u_c),$$

or

$$\| \left(\delta_c^{-1} I + F'(u_c)\right) s + F(u_c)\| \leq \eta_c \|F(u_c)\|.$$

Ψtc as an Integrator

Implicit Euler for $y' = -F(y)$

$$u_{n+1} = u_n + \delta F(u_{n+1})$$

u_{n+1} is the solution of

$$G(u) = u - u_n + \delta F(u) = 0.$$

Since $G'(u) = I + \delta F'(u)$, a single Newton iterate from $u_c = u_n$ is

$$\begin{aligned} u_+ &= u_c - (I + \delta F'(u_c))^{-1}(u_c - u_n + \delta F(u_c)) \\ &= u_c - (\delta^{-1} I + F'(u_c))^{-1} F(u_c), \end{aligned}$$

since $u_c - u_n = 0$.

Ψtc as an Integrator

- Low accuracy PECE integration
  - Trivial predictor
  - Backward Euler corrector + one Newton iteration
  - 1st order Rosenbrock method
    High order possible, Luo, K, Liao, Tam 06
- Begin with small "time step" δ. Resolve transients.
- Grow the "time step" near u^*. Turn into Newton.

Is this stable?

Time Step Control

Grow the time step with switched evolution relaxation (SER)

$$\delta_n = \min(\delta_0 \|F(u_0)\| / \|F(u_n)\|, \delta_{max}).$$

If $\delta_{max} = \infty$ then $\delta_n = \delta_{n-1} \|F(u_{n-1})\| / \|F(u_n)\|$.
Alternative with no theory (SER-B):

$$\delta_n = \delta_{n-1} / \|u_n - u_{n-1}\|$$

Temporal Truncation Error (TTE)

Estimate local truncation error by

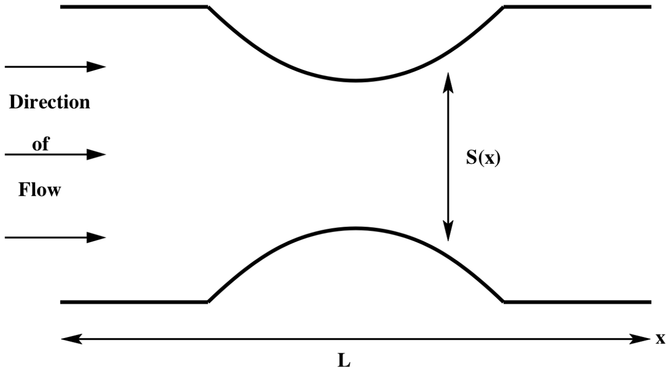
$$\tau = \frac{\delta_n^2 (u)_i''(t_n)}{2}$$

and approximate $(u)_i''$ by

$$\frac{2}{\delta_{n-1} + \delta_{n-2}} \left[\frac{((u)_i)_n - ((u)_i)_{n-1}}{\delta_{n-1}} - \frac{((u)_i)_{n-1} - ((u)_i)_{n-2}}{\delta_{n-2}} \right]$$

Adjust step so that $\tau = .75$.

Numerical Example: Flow through a Nozzle



Euler Equations

unknowns density, velocity, energy.

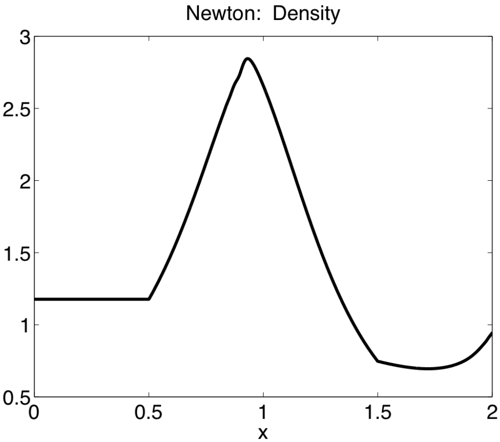
$$\nabla \cdot (\rho \mathbf{v}) = 0$$

$$\nabla \cdot (\rho \mathbf{v}\mathbf{v} + pI) = 0$$

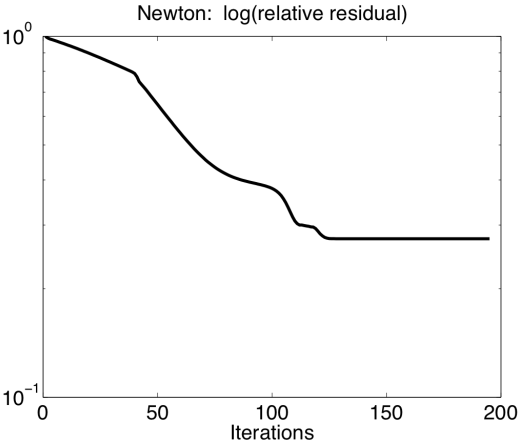
$$\nabla \cdot ((\rho e + p)\mathbf{v}) = 0$$

Ideal gas law $p = \rho(\gamma - 1)(e - |\mathbf{v}|^2/2)$, where γ is the ratio of specific heats.
Use nonsmooth slope limiter to get second order accuracy.

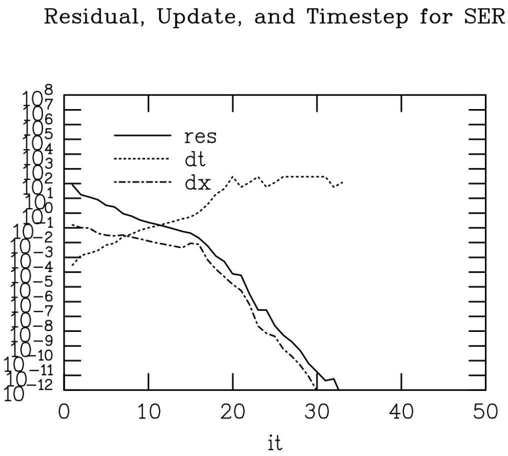
Trouble with Newton: density



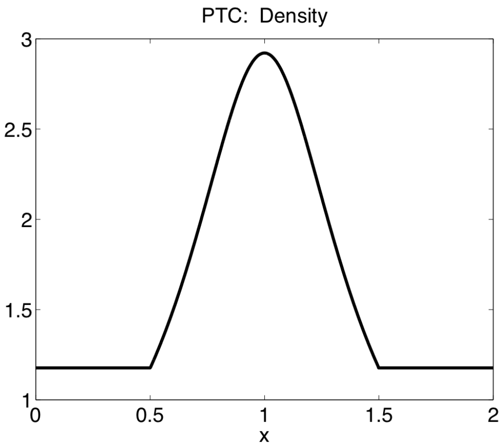
Trouble with Newton: convergence



Ψtc with SER


Residual, Update, and Timestep for SER
res
dt
dx
10^{8}
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
0
10
20
30
40
50
it

And Ψtc gets it right!



But F is not smooth

Typical Euler equation approach

- Discretize with 2nd order scheme with slope limiter. Slope limiters can be nonsmooth, but Lipschitz continuous.
- Use Jacobian of a (smooth) 1st order scheme.

Modified method: $u_+ = u_c + s$ where

$$\| \left(\delta_c^{-1} I + J_c\right) s + F(u_c) \| \le \eta_c \| F(u_c) \|,$$

and J_c is the Jacobian of the smooth, low-order discretization. Folwer-K and Liao-Qi-K results explain this.

Constraints

$$\frac{du}{dt} = -F(u), u(0) = u_0 \in \Omega.$$

$u(t) \in \Omega$, $F(u) \in \mathcal{T}(u)$ (tangent to Ω).
Examples:

- Ω has interior: bound constrained optimization
- Ω smooth manifold: inverse singular value problem

Problem: Ψtc will drift away from Ω.

Projected Ψtc

$$u_+ = \mathcal{P}(u_c - \left(\delta_c^{-1} I + H(u_c)\right)^{-1} F(u_c))$$

where

- $\mathcal{P}$ is map-to-nearest $R^N \to \Omega$
  $\|\mathcal{P}'(u)\| = 1$ for $u \in \Omega$.
- $H(u_c)$ makes Newton-like method fast.

General Method

Liao-Qi-K, 2006

F Lipschitz (no smoothness assumptions)

$$u_+ = \mathcal{P}(u_c - (\delta^{-1} I + H(u_c))^{-1} F(u_c)),$$

where H is an approximate Jacobian.

Theory: H bounded, other assumptions imply $u_n \to u^*$ and

$$u_{n+1} = u^N_{n+1} + O(\delta_n^{-1} + \eta_n) \| u_n - u^* \|$$

where

$$u^N_{n+1} = u_n - H(u_n)^{-1} F(u_n)$$

which is as fast as the underlying method.

What are those assumptions?

- $u(t) \to u^*$
- δ_0 is sufficiently small.
- $\|\mathcal{P}'(u)\| = 1$ or Lip const of $\mathcal{P} = 1$
- u^* is dynamically stable
- $H(u)$ is uniformly well-conditioned near $\{u(t) \,|\, t \geq 0\}$
- $u_+ = u_c - H(u_c)^{-1}F(u_c)$ is rapidly locally convergent near u^*

A word about dynamics

$$\frac{du}{dt} = -F(u), u(0) = u_0$$

implies $u(t) \to u^*$ if $F = \nabla f$ and

- f is real analytic,
- the Lojasiewicz inequality

$$\|\nabla f(u)\| \geq c|f(u) - f(u^*)|$$

  holds, or
- f has bounded level sets and finitely many critical points.

But none of this implies that u^* is dynamically stable.

Fixing TTE and SER-B

If the underlying problem is minimization of f and ...

- you reduce δ until f is reduced,
- δ_0 is sufficiently small, and
- u^* is the unique root of F.

Then either $\delta_n \to 0$ or you converge to u^*.

Bound Constrained Optimization

$$\min_{u \in \Omega} f(u)$$

$$\Omega = \{u \,|\, L_i \leq (u)_i \leq U_i\}$$

$$\mathcal{P}(u)_i = \begin{cases} L_i & \text{if } (u)_i \leq L_i \\ (u)_i & \text{if } L_i < (u)_i < U_i \\ U_i & \text{if } (u)_i \geq U_i \end{cases}$$

Necessary Conditions:

$$F(u) \equiv u - \mathcal{P}(u - \nabla f(u)) = 0.$$

Construction of H

Identify binding constraints

$$\begin{aligned}\mathcal{B}(u) &= \{ i \,|\, (u)_i = L_i \text{ and } (\nabla f(u))_i < 0 \text{ or} \\ & (u)_i = U_i \text{ and } (\nabla f(u))_i > 0 \}.\end{aligned}$$

with an over estimate to get fast convergence.
σ-binding set

$$\begin{aligned}\mathcal{B}^\sigma(u) &= \{ i \,| \quad U_i - (u)_i \le \sigma \text{ and } (\nabla f(u))_i < -\sqrt{\sigma} \text{ or} \\ & (u)_i - L_i \le \sigma \text{ and } (\nabla f(u))_i > \sqrt{\sigma} \}.\end{aligned}$$

Approximate Reduced Hessian

Set $\sigma(u) = \|F(u)\|$ and

$$H(u)_{ij} = \begin{cases} \nabla^2 f(u)_{ij} & i \notin \mathcal{B}^\sigma(u) \\ \delta_{ij} & i \in \mathcal{B}^\sigma(u) \end{cases}$$

Then it all works.

Linear Algebra Problem

Chu, 92 ...

Find $c \in R^N$ so that the $M \times N$ matrix

$$B(c) = B_0 + \sum_{k=1}^{N} c_k B_k$$

has prescribed singular values $\{\sigma_i\}_{i=1}^N$.
Data: Frobenius orthogonal $\{B_i\}_{i=1}^N$, $\{\sigma_i\}_{i=1}^N$.

Formulation

Least squares problem

$$\min F(U,V) \equiv \|R(U,V)\|_F^2$$

where

$$R(U,V) = U\Sigma V^T - B_0 - \sum_{k=1}^{N} < U\Sigma V^T, B_k >_F B_k$$

Manifold constraints: U is orthogonal $M \times M$ and V is orthogonal $N \times N$

Dynamic Formulation

$$\Omega = \{ \begin{pmatrix} U \\ V \end{pmatrix} \in R^{M \times M} \oplus R^{N \times N} \mid U \text{ and } V \text{ orthogonal} \}$$

Projected gradinet:

$$g(U,V) = \frac{1}{2} \begin{pmatrix} (R(U,V) V \Sigma^T U^T - U \Sigma V^T R(U,V)^T) U \\ (R(U,V)^T U \Sigma V^T - V \Sigma^T U^T R(U,V)) V \end{pmatrix}.$$

ODE:

$$\dot{u} = \begin{pmatrix} \dot{U} \\ \dot{V} \end{pmatrix} = -F(u) \equiv -g(U,V).$$

Projection onto Ω

Higham 86, 04

Projection of square matrix onto orthogonal matrices

$$A \rightarrow U_P.$$

where $A = U_P H_P$ is the polar decomposition.
Compute U_P via the SVD $A = U \Sigma V^T$

$$U_P = U V^T.$$

Projection of

$$w = \begin{pmatrix} A \\ B \end{pmatrix}$$

onto Ω is

$$\mathcal{P}(w) = \begin{pmatrix} U_P^A \\ U_P^B \end{pmatrix}.$$

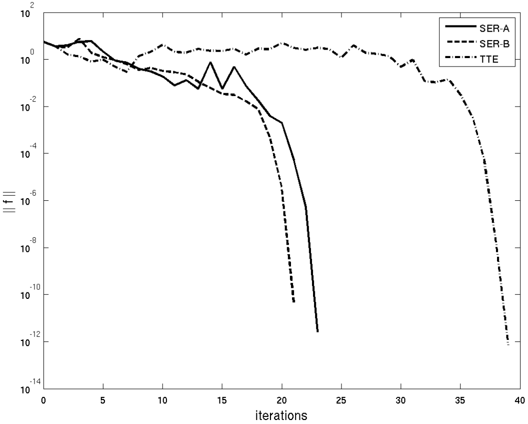
The local method

Given $u \in \Omega$ let $P_T(u) = \mathcal{P}'(u)$ be the projection onto the tangent space to Ω at u. Let

$$H = (I - P_T(u)) + P_T(u)F'(u)P_T(u)$$

Locally (very locally) superlinearly convergent if Ω is OK near u^*.

Inverse Singular Value Problem



Optimization Example I

Parameter ID: Find c and k for simple harmonic oscillator

$$w'' + cw' + kw = 0; w(0) = w_0, w'(0) = 0,$$

by sampling output of `ode15s` with

$$rtol = atol = 10^{-6}$$

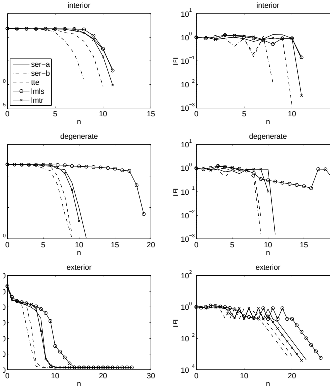
and comparing to exact solution $(c = k = 1)$ at 100 equally spaced points.
$u = (c, k)^T, \ M = 100, \ N = 2.$

$$R(u)_i = w^{exact}(t_i) - w_i(u)$$

Results from three cases

Bounds: $u \le u_0 = (10, 10)$ in all cases
Interior: $(0, 0) \le u$, zero residual Exterior: $(2, 0) \le u$, non-zero residual Exterior: $(1, 0) \le u$, zero residual, degenerate.

Computations



Conclusions

- Ψtc computes steady-state solutions.
  - Can succeed when traditional methods fail.
  - It is not a general nonlinear solver!
- Theory and practice for many problems
  - ODEs, DAEs
  - Nonsmooth F
- Tempting idea for optimization