Inexact Newton Methods, Newton-Krylov Methods, and Extensions for Large-Scale Underdetermined Systems

Homer Walker DOE Office of Advanced Scientific Computing and

Worcester Polytechnic Institute

Includes joint work with Roger Pawlowski (SNL), John Shadid (SNL), and Joseph Simonis (WPI/Boeing).

Supported in part by the DOE ASC program and Office of Science MICS program, Sandia National Laboratories CSRI, and the DOE-funded University of Utah C-SAFE.

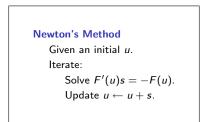
IN/NK Methods & Extensions Oak Ridge National Laboratory

August 22, 2008

Slide 1/37

Classical Newton's Method

Problem: F(u) = 0, $F : \mathbb{R}^n \to \mathbb{R}^n$ continuously differentiable.



Guiding application: discretized nonlinear PDEs.

Typically ...

- quadratic, mesh-independent <u>local</u> convergence \Rightarrow globalize,
- n is very large, F'(u) is sparse and may be infeasible to evaluate/store ⇒ Krylov subspace method.

イロト 不得下 イヨト イヨト 二日

Globalizations of Newton's Method

We can't guarantee convergence to a solution

... but we can make it more likely.

We can't guarantee convergence to a solution

... but we can make it more likely.

Idea: Repeat as necessary ...

- *Test* a step for acceptable progress.
- ▶ If unacceptable, *modify* it and test again.

We can't guarantee convergence to a solution

... but we can make it more likely.

Idea: Repeat as necessary ...

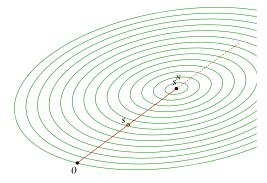
- *Test* a step for acceptable progress.
- If unacceptable, modify it and test again.

Major approaches:

- *Backtracking* (linesearch, damping).
- Trust region.

Backtracking (Linesearch, Damping) Globalization

- $s \leftarrow \theta s^N$ for an appropriate $\theta > 0$.
 - s^N is a *descent direction* for ||F|| at x
 - \Rightarrow s is acceptable for sufficiently small $\theta > 0$.



Red: feasible s Green: level curves of ||F(u) + F'(u)s||

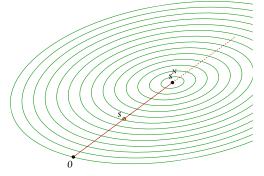
IN/NK Methods & Extensions Oak Ridge National Laboratory

August 22, 2008

▲□→ ▲ □→ ▲ □→

Backtracking (Linesearch, Damping) Globalization

- $s \leftarrow \theta s^N$ for an appropriate $\theta > 0$.
 - s^N is a *descent direction* for ||F|| at x
 - \Rightarrow *s* is acceptable for sufficiently small $\theta > 0$.
- s^N may be only a "weak" descent direction if F'(u) is ill-conditioned.

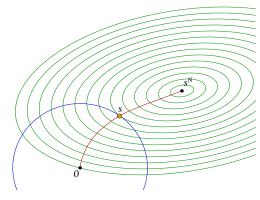


Red: feasible s Green: level curves of ||F(u) + F'(u)s||

→ ∃ → < ∃ →</p>

Trust-Region Globalization

•
$$s = \arg \min_{\|w\| < \delta} \|F(u) + F'(u)w\|.$$



Red: feasible s Green: level curves of ||F(u) + F'(u)s||Blue: trust region boundary

IN/NK Methods & Extensions Oak Ridge National Laboratory

August 22, 2008

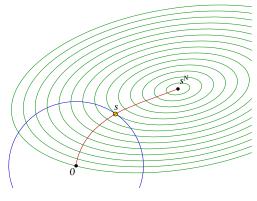
э

<ロ> <同> <同> < 回> < 回>

Trust-Region Globalization

•
$$s = \arg \min_{\|w\| \leq \delta} \|F(u) + F'(u)w\|.$$

• Computing *s* accurately may be problematic.



Red: feasible s Green: level curves of ||F(u) + F'(u)s||Blue: trust region boundary

IN/NK Methods & Extensions Oak Ridge National Laboratory

August 22, 2008

э

(a)

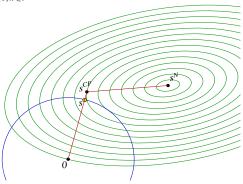
The Dogleg Step

Define

• Cauchy point $s^{CP} \equiv \underset{0 \le \lambda < \infty}{\arg \min} \|F(u) - F'(u)\lambda \nabla f(u)\|, f(u) \equiv \frac{1}{2} \|F(u)\|^2$

• dogleg curve
$$\Gamma^{DL}: 0 \to s^{CP} \to s^N$$

• dogleg step
$$s = \underset{\|w\| \le \delta, w \in \Gamma^{DL}}{\arg \min} \|F(u) + F'(u)w\|$$



- 34

- 4 回 2 - 4 三 2 - 4 三 2

Use a Krylov subspace method to approximately solve F'(u) s = -F(u).

For solving $Ax = b \dots$

Krylov Subspace Method Given x_0 , determine ... $x_k = x_0 + z_k$, $z_k \in \mathcal{K}_k \equiv \operatorname{span} \{r_0, Ar_0, \dots, A^{k-1}r_0\}$,

A few examples ...

CG/CR, GMRES, BCG, CGS, QMR, TFQMR (QMRCGS), QMR-squared, BiCGSTAB, BiCGSTAB2, BiCGSTAB(ℓ), QMRCGSTAB, Arnoldi (FOM/IOM), GMRESR, GCR, GMBACK, MINRES, SYMMLQ, ORTHODIR, ORTHOMIN, ORTHORES, Axelsson, SYMMBK, CGNR, CGNE, LSQR,....

イロト 不同下 イヨト イヨト

Special appeal of Krylov subspace methods:

- Most require only products of F'(u) with vectors ⇒ "matrix-free" implementations.
- They have desirable *optimality properties*.
 - GMRES and other "minimum residual" methods minimize the linear residual norm ||F(u) + F'(u) s|| (the *linear model norm*) over each \mathcal{K}_k .
 - ▶ For optimization, say $\min_{u \in \mathbb{R}^n} f(u)$, $f : \mathbb{R}^n \to \mathbb{R}^1$,
 - CG minimizes the local quadratic model $q(s) \equiv f(u) + \nabla f(u)^T s + \frac{1}{2} s^T \nabla^2 f(u) s$ over each \mathcal{K}_k .
 - The first CG step is the steepest descent step.

・ 同 ト ・ ヨ ト ・ ヨ ト

Inexact Newton methods (Dembo-Eisenstat-Steihaug 1982) provide a framework for analysis and implementation.

```
Inexact Newton Method

Given an initial u.

Iterate:

Find <u>some</u> \eta \in [0, 1) and s that satisfy

\|F(u) + F'(u) s\| \le \eta \|F(u)\|.

Update u \leftarrow u + s.
```

(E)

Regard Newton-Krylov methods as a special case

- Choose $\eta \in [0, 1)$.
- Apply the Krylov solver to F'(u) s = -F(u) until

 $\|F(u)+F'(u)s\|\leq \eta\|F(u)\|.$

< 🗇 >

A B M A B M

Regard Newton-Krylov methods as a special case

- Choose $\eta \in [0, 1)$.
- Apply the Krylov solver to F'(u) s = -F(u) until

 $\|F(u)+F'(u)s\|\leq \eta\|F(u)\|.$

The issue of when to stop the linear iterations becomes the issue of choosing the "forcing term" η .

12 N 4 12 N

Dembo–Eisenstat–Steihaug (1982): Local convergence is controlled by the forcing terms.

Theorem: Suppose $F(u_*) = 0$ and $F'(u_*)$ is invertible. If $\{u_k\}$ is an inexact Newton sequence with u_0 sufficiently near u_* , then

• $\eta_k \leq \eta_{\max} < 1 \implies u_k \rightarrow u_*$ linearly in the norm $\|w\|_{F'(u_*)} \equiv \|F'(u_*)w\|$,

•
$$\eta_k \to 0 \implies u_k \to u_*$$
 superlinearly.

If also F' is Hölder continuous with exponent p at u_* , then

•
$$\eta_k = O(||F(u_k)||^p) \implies u_k \to u_* \text{ with } q \text{-order } 1 + p.$$

More on forcing terms later ...

イロト 不得下 イヨト イヨト 二日

Present a subset of results in

R. P. PAWLOWSKI, J. P. SIMONIS, J. N. SHADID, HW, *Globalization techniques for Newton–Krylov methods and applications to the fully coupled solution of the Navier–Stokes equations*, SIREV, 48 (2006), 700–721.

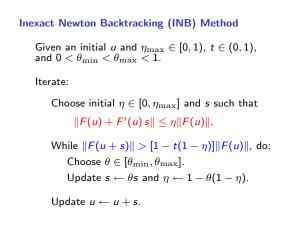
• Describe two representative Newton-Krylov globalizations:

- a backtracking method,
- a dogleg trust-region method.
- Outline their theoretical support and discuss a few implementational details.
- Report on numerical experiments.

4 E N 4 E N

The Backtracking Method

The backtracking method (Eisenstat-HW 1994) is



A B M A B M

Theorem: If $\{u_k\}$ produced by the INB method has a limit point u_* such that $F'(u_*)$ is nonsingular, then $F(u_*) = 0$ and $u_k \rightarrow u_*$. Furthermore, the initial s_k and η_k are accepted for all sufficiently large k.

Possibilities:

- $||u_k|| \to \infty$.
- $\{u_k\}$ has limit points, and F' is singular at each one.
- $\{u_k\}$ converges to u_* such that $F(u_*) = 0$, $F'(u_*)$ is nonsingular, and asymptotic convergence is determined by the initial η_k 's.

(4回) (注) (注) (注)

The Dogleg Method



```
Given an initial u and \eta_{\max} \in [0, 1), t \in (0, 1), 0 < \theta_{\min} < \theta_{\max} < 1, and 0 < \delta_{\min} \le \delta.
```

Iterate:

```
Choose \eta \in [0, \eta_{\max}] and s^{IN} such that
\|F(u) + F'(u) s^{IN}\| \le \eta \|F(u)\|.
```

Evaluate s^{CP} and determine $s \in \Gamma^{DL}$: $0 \rightarrow s^{CP} \rightarrow s^{IN}$.

```
 \begin{array}{l} \mbox{While ared} < t \cdot pred \mbox{ do:} \\ \mbox{Choose } \theta \in [\theta_{\min}, \theta_{\max}]. \\ \mbox{Update } \delta \leftarrow \max\{\theta\delta, \delta_{\min}\}. \\ \mbox{Redetermine } s \in \Gamma^{DL}. \end{array}
```

Update $u \leftarrow u + s$ and update δ .

12 N 4 12 N

Dogleg Details

• Sufficient decrease is based on the inexact Newton condition and

 $ared \equiv ||F(u)|| - ||F(u+s)||$ (actual reduction) $pred \equiv ||F(u)|| - ||F(u) + F'(u)s||$ ("predicted" reduction)

• Update δ a la Dennis–Schnabel (1983).

- Determine $s \in \Gamma^{DL}$ by the "standard strategy":
 - If $||s^{IN}|| \leq \delta$, then $s = s^{IN}$;
 - else, if $\|s^{CP}\| \ge \delta$, then $s = (\delta/\|s^{CP}\|) s^{CP}$;
 - ► else, $s = (1 \tau)s^{CP} + \tau s^{IN}$, where $\tau \in (0, 1)$ is uniquely determined so that $||s|| = \delta$.
- Alternative dogleg strategies and refinements are given in R. P. PAWLOWSKI, J. P. SIMONIS, HW, J. N. SHADID, *Inexact Newton dogleg methods*, SINUM, 46 (2007-2008), 2112-2132.

August 22, 2008

Recall: *u* is a *stationary point* of $||F|| \iff ||F(u)|| \le ||F(u) + F'(u)s||$ for all *s*.

Theorem: If u_* is a limit point of $\{u_k\}$ produced by the INDL method, then u_* is a stationary point of ||F||. If additionally $F'(u_*)$ is nonsingular, then $F(u_*) = 0$ and $u_k \to u_*$; furthermore, $s_k = s_k^{IN}$ for all sufficiently large k.

Possibilities:

- $||u_k|| \to \infty$.
- $\{u_k\}$ has limit points, and each is a stationary point of F.
- $\{u_k\}$ converges to u_* such that $F(u_*) = 0$, $F'(u_*)$ is nonsingular, and asymptotic convergence is determined by the initial η_k 's.

イロト 不得 とくき とくき とうき

Two typical procedures were used in the numerical experiments (see Dennis–Schnabel (1983)).

- Choose θ to minimize a quadratic p(t) that satisfies $p(0) = \frac{1}{2} ||F(u)||^2$, $p(1) = \frac{1}{2} ||F(u+s)||^2$, and $p'(0) = \frac{d}{dt} \frac{1}{2} ||F(u+ts)||^2 \Big|_{t=0}$.
- Choose θ to minimize
 - a quadratic on the first reduction,
 - a cubic on subsequent reductions.

-

・ 同 ト ・ ヨ ト ・ ヨ ト

Choosing the Forcing Terms

Two choices were used in the numerical experiments.

- Small constant forcing terms: $\eta_k = 10^{-4}$ for each k \Rightarrow fast local linear convergence.
- Adaptive forcing terms: "Choice 1" from (Eisenstat-HW 1996)

$$\eta_{k} = \min \left\{ \frac{\left| \|F(u_{k})\| - \|F(u_{k-1}) + F'(u_{k-1}) s_{k-1}\|\right|}{\|F(u_{k-1})\|}, \eta_{\max} \right\}.$$

Theorem: Suppose $F(u_*) = 0$ and $F'(u_*)$ is invertible. Let $\{u_k\}$ be an inexact Newton sequence with each η_k given as above. If u_0 is sufficiently near u_* , then $u_k \rightarrow u_*$ with

$$||u_{k+1} - u_*|| \le \beta ||u_k - u_*|| \cdot ||u_{k-1} - u_*||, \qquad k = 1, 2, \dots$$

for a constant β independent of k.

Numerical Experiments

- Test problems: Three benchmark flow problems in 2D and 3D ...
 - lid-driven cavity,
 - thermal convection,
 - backward-facing step.
- PDEs: Low Mach number Navier–Stokes equations with heat transport as appropriate.
- Discretization: Pressure stabilized streamline upwind Petrov-Galerkin FEM.
- Algorithms and software: Newton-GMRES implementations in the Sandia NOX nonlinear solver suite, with GMRES and domain-based (overlapping Schwarz) ILU preconditioners from the Sandia Aztec package. The simulation driver was the Sandia MPSalsa parallel reacting flow code.
- Problem sizes: 25,263 to 1,042,236 unknowns.
- Machines: 8 CPUs on a 16-node, 32-CPU IBM Linux cluster; 100 CPUs on Sandia's 256-node, 512-CPU Institutional Cluster.

- N

2D and 3D Thermal Convection	Ra =	10 ³ , 10 ⁴ , 10 ⁵ , 10 ⁶
2D and 3D Backward Facing Step	Re =	100, 200,, 700, 750, 800
2D Lid Driven Cavity	Re =	1000, 2000,, 10, 000
3D Lid Driven Cavity	Re =	100, 200,, 1000

Total numbers of failures:

Method	Forcing Term	2D Problems		3D Problems		All Problems	
Backtracking, Quadratic Only	Adaptive	0	10	0	0	0	10
	10 ⁻⁴	10		0		10	
Dogleg	Adaptive	0	10	0	0	0	10
	10 ⁻⁴	10		0		10	
No Globalization	Adaptive	15	33	4	14	19	47
	10 ⁻⁴	18		10		28	

2

<ロ> <同> <同> < 回> < 回>

Efficiency

2D Thermal Convection	Ra =	10 ³ , 10 ⁴ , 10 ⁵
3D Thermal Convection	Ra =	10 ³ , 10 ⁴ , 10 ⁵ , 10 ⁶
2D and 3D Backward Facing Step	Re =	100, 200,, 700
2D and 3D Lid Driven Cavity	Re =	100, 200,, 1000

Method	Forcing Term	Inexact Newton Steps	Backtracks per INS	GMRES Iterations per INS	Normalized Time
Backtracking,	Adaptive	16.0	0.13	62.2	0.77
Quadratic Only	10 ⁻⁴	9.23	0.18	163	1.0 (REF)
Dogleg	Adaptive	17.0	NA	85.3	0.83
Dogleg	10-4	10.7	NA	168	1.01

 $\longleftarrow \qquad {\sf Geometric Means} \quad \longrightarrow \quad$

IN/NK Methods & Extensions Oak Ridge National Laboratory

August 22, 2008

2

<ロ> <同> <同> < 回> < 回>

• These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.

< 🗇 🕨

- These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.
- Causes of failure in our experiments:
 - Fatal near-stagnation: 26/33 backtracking/linesearch failures; 10/10 dogleg failures.
 - ▶ Globalization failure: 7/33 backtracking/linesearch failures.

< 🗇 🕨

- These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.
- Causes of failure in our experiments:
 - Fatal near-stagnation: 26/33 backtracking/linesearch failures; 10/10 dogleg failures.
 - ▶ Globalization failure: 7/33 backtracking/linesearch failures.
- Backtracking with quadratic minimization and adaptive forcing terms seems to be a clear first choice for implementation.

4 A >

- These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.
- Causes of failure in our experiments:
 - Fatal near-stagnation: 26/33 backtracking/linesearch failures; 10/10 dogleg failures.
 - ▶ Globalization failure: 7/33 backtracking/linesearch failures.
- Backtracking with quadratic minimization and adaptive forcing terms seems to be a clear first choice for implementation.
- No globalization or choice of forcing terms is always best.

< 🗇 🕨

A B M A B M

- These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.
- Causes of failure in our experiments:
 - Fatal near-stagnation: 26/33 backtracking/linesearch failures; 10/10 dogleg failures.
 - ▶ Globalization failure: 7/33 backtracking/linesearch failures.
- Backtracking with quadratic minimization and adaptive forcing terms seems to be a clear first choice for implementation.
- No globalization or choice of forcing terms is always best.
- *Many* factors contribute to success: problem formulation, discretization, preconditioning, variable scaling, accuracy, ...

- 4 回 ト 4 ヨ ト 4 ヨ ト

- These globalizations have good theoretical support and are effective on these test problems, especially with adaptive forcing terms.
- Causes of failure in our experiments:
 - Fatal near-stagnation: 26/33 backtracking/linesearch failures; 10/10 dogleg failures.
 - ▶ Globalization failure: 7/33 backtracking/linesearch failures.
- Backtracking with quadratic minimization and adaptive forcing terms seems to be a clear first choice for implementation.
- No globalization or choice of forcing terms is always best.
- Many factors contribute to success: problem formulation, discretization, preconditioning, variable scaling, accuracy, ...
- For more, see the SIREV and SINUM papers.

・ 同 ト ・ ヨ ト ・ ヨ ト

Problem: Given $F : \mathbb{R}^m \to \mathbb{R}^n$ with m > n, find u_* such that $F(u_*) = 0$.

Assume F is continuously differentiable throughout.

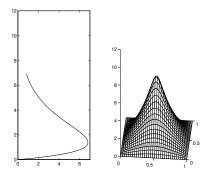
Examples:

- Parameter-dependent problems with unknown parameters.
- Time-dependent problems with periodic solutions.
- Nonlinear eigenvalue problems.

(人間) シスヨン スヨン

The Bratu (Gelfand) Problem

In 2D, this is
$$\Delta u + \lambda e^u = 0$$
 in $\mathcal{D} \equiv [0, 1] \times [0, 1]$,
 $u = 0$ on $\partial \mathcal{D}$.



Left: ||u|| vs. λ . Right: solution at final λ value.

The Model Algorithm

Extend Newton's method with

Algorithm NU: Newton's Method (Underdetermined) Given u_0 . For k = 0, 1, ...Find $s_k \in I\!\!R^m$ such that $F'(u_k)s_k = -F(u_k), \quad s_k \perp \mathcal{N}(F'(u_k)).$ Set $u_{k+1} = u_k + s_k$.

Appeal:

- This *pseudo-inverse* characterization of s_k is optimally conditioned.
- The algorithm has local convergence (up to quadratic) like that of Newton's method (HW–Watson 1990, Levin–Ben Israel 2001).

Extend inexact Newton methods with

```
Algorithm INU: Inexact Newton Method (Underdetermined)

Given u_0.

For k = 0, 1, ...

Find \eta_k \in [0, 1) and s_k \in I\!\!R^m such that

\|F(u_k) + F'(u_k)s_k\| \le \eta_k \|F(u_k)\|, \quad s_k \perp \mathcal{N}(F'(u_k)).

Set u_{k+1} = u_k + s_k.
```

イヨト・イヨト

Local Convergence Analysis

Hypothesis: The following hold in an open, convex $\Omega \subseteq \mathbb{R}^m$:

- F' is full-rank in Ω.
- ▶ There are $\gamma \ge 0$ and $p \in (0, 1]$ such that $||F'(\tilde{u}) F'(u)|| \le \gamma ||\tilde{u} u||^p$ for all $u, \tilde{u} \in \Omega$.
- There is a μ such that $||F'(u)^+|| \le \mu$ for all $u \in \Omega$.

For $\rho > 0$, set $\Omega_{\rho} \equiv \{ u \in \Omega : \| \tilde{u} - u \| \le \rho \Rightarrow \tilde{u} \in \Omega \}.$

Local Convergence Analysis

Hypothesis: The following hold in an open, convex $\Omega \subseteq \mathbb{R}^m$:

- F' is full-rank in Ω.
- ▶ There are $\gamma \ge 0$ and $p \in (0, 1]$ such that $||F'(\tilde{u}) F'(u)|| \le \gamma ||\tilde{u} u||^p$ for all $u, \tilde{u} \in \Omega$.
- There is a µ such that ||F'(u)⁺|| ≤ µ for all u ∈ Ω.

For $\rho > 0$, set $\Omega_{\rho} \equiv \{ u \in \Omega : \| \tilde{u} - u \| \le \rho \Rightarrow \tilde{u} \in \Omega \}.$

Theorem: Suppose that this hypothesis holds and that $\rho > 0$ is given. Assume that $\eta_k \leq \eta_{\max} < 1$ for all k. Then there exists an $\epsilon > 0$ depending only on γ , p, μ , ρ , and η_{\max} such that if $u_0 \in \Omega_{\rho}$ and $||F(u_0)|| \leq \epsilon$, then the iterates $\{u_k\}$ determined by Algorithm INU are well-defined and converge to $u_* \in \Omega$ such that $F(u_*) = 0$. Moreover, if $u_k \neq u_*$ for all k, then

$$\limsup_{k \to \infty} \frac{\|F'(u_*)(u_{k+1} - u_*)\|}{\|F'(u_*)(u_k - u_*)\|} \le \eta_{\max}.$$
 (*)

Additionally, if $\eta_k \to 0$, then the convergence is q-superlinear, and if $\eta_k = O(||F(u_k)||^p)$, then the convergence is of q-order 1 + p.

イロト 不得 とくき とくき とうき

Hypothesis: The following hold in an open, convex $\Omega \subseteq \mathbb{R}^m$:

- F' is full-rank in Ω.
- ▶ There are $\gamma \ge 0$ and $p \in (0, 1]$ such that $||F'(\tilde{u}) F'(u)|| \le \gamma ||\tilde{u} u||^p$ for all $u, \tilde{u} \in \Omega$.
- There is a μ such that $||F'(u)^+|| \le \mu$ for all $u \in \Omega$.

For $\rho > 0$, set $\Omega_{\rho} \equiv \{ u \in \Omega : \| \tilde{u} - u \| \le \rho \Rightarrow \tilde{u} \in \Omega \}.$

Theorem: Suppose that this hypothesis holds and that $\rho > 0$ is given. Assume that $\eta_k \leq \eta_{\max} < 1$ for all k. Then there exists an $\epsilon > 0$ depending only on γ , p, μ , ρ , and η_{\max} such that if $u_0 \in \Omega_{\rho}$ and $||F(u_0)|| \leq \epsilon$, then the iterates $\{u_k\}$ determined by Algorithm INU are well-defined and converge to $u_* \in \Omega$ such that $F(u_*) = 0$. Moreover, if $u_k \neq u_*$ for all k, then

$$\limsup_{k \to \infty} \frac{\|F'(u_*)(u_{k+1} - u_*)\|}{\|F'(u_*)(u_k - u_*)\|} \le \eta_{\max}.$$
 (*)

Additionally, if $\eta_k \to 0$, then the convergence is q-superlinear, and if $\eta_k = O(||F(u_k)||^p)$, then the convergence is of q-order 1 + p.

Remark: One can show that $||F'(u_*)(u_k - u_*)|| \ge C||u_k - u_*||$ for all large k. Then it follows from (*) that $u_k \to u_*$ r-linearly.

Extend the INB method with

$$\begin{split} & \textbf{Algorithm INBU:} \\ & \textbf{Given } u_0 \text{ and } t \in (0,1), \ \eta_{\max} \in [0,1), \text{ and } 0 < \theta_{\min} < \theta_{\max} < 1. \\ & \textbf{For } k = 0 \text{ step } 1 \text{ until } \infty \text{ do:} \\ & \textbf{Find initial } \eta_k \in [0, \eta_{\max}] \text{ and } s_k \text{ such that} \\ & \|F(u_k) + F'(u_k)s_k\| \leq \eta_k \|F(u_k)\|, \quad s_k \perp \mathcal{N}(F'(u_k)). \\ & \textbf{Evaluate } F(u_k + s_k). \\ & \textbf{While } \|F(u_k + s_k)\| > [1 - t(1 - \eta_k)] \|F(u_k)\|, \text{ do} \\ & \textbf{Choose } \theta \in [\theta_{\min}, \theta_{\max}]. \\ & \textbf{Update } s_k \leftarrow \theta s_k \text{ and } \eta_k \leftarrow 1 - \theta(1 - \eta_k). \\ & \textbf{Evaluate } F(u_k + s_k). \\ & \textbf{Set } u_{k+1} = u_k + s_k. \end{split}$$

3.0

3 1 4

A 10

Theorem: Suppose that $\{u_k\}$ is generated by Algorithm INBU. If u_* is a limit point of $\{u_k\}$ such that $F'(u_*)$ is full-rank, then $F(u_*) = 0$ and $u_k \rightarrow u_*$. Furthermore, the initial η_k and u_k are accepted without modification in the while-loop for all sufficiently large k.

Possibilities:

- $\blacktriangleright \|u_k\| \to \infty.$
- $\{u_k\}$ has limit points, and F' is rank-deficient at each.
- ► $\{u_k\}$ converges to u_* such that $F(u_*) = 0$, $F'(u_*)$ is full-rank, and asymptotic convergence is determined by the initial η_k 's.

Note: By taking $\eta_{\rm max} = 0$ in Algorithm INBU, we obtain a bactracking extension of Algorithm NU, to which this theorem applies.

Solving for *s*_k

Extend the technique in (SISC, 2000) for adapting Krylov subspace methods.

Set $\ell = m - n$. Let $\{v_1, \ldots, v_\ell\}$ be an orthonormal basis of $\mathcal{N}(F'(u_k))$.

For $i = 1, ..., \ell$, Obtain a Householder P_i such that $P_i ... P_1 v_i = e_{n-i+1} \in \mathbb{R}^m$.

• Set
$$Q = P_1 \dots P_\ell \begin{pmatrix} I_n \\ 0 \end{pmatrix} \in \mathbb{R}^{m \times n}$$
.

Apply the Krylov subspace method to approximately solve

$$F'(u_k)Q\tilde{s}_k = -F(u_k)$$

▶ Set $s_k = Q\tilde{s}_k \in \mathbb{R}^m$.

Cost:

- ► O(ℓ²m) flops and O(ℓm) storage for P₁, ..., P_ℓ.
- $O(\ell m)$ flops for each Q-product.

For $i = 1, \ldots, \ell$,

- Obtain an initial v_i orthogonalized against v₁, ..., v_{i-1} and normalized.
- ► Obtain Δv_i such that $F'(u_k)(v_i + \Delta v_i) = 0$ and $\Delta v_i \perp v_1, \ldots, v_i$. (Take $P_{i+1} = \ldots = P_{\ell} = I_m$ in forming Q.)

• Update
$$v_i \leftarrow (v_i + \Delta v_i) / ||v_i + \Delta v_i||$$
.

Cost: $O(\ell^2 m)$ flops plus ℓ solves.

・ 同 ト ・ ヨ ト ・ モ ト ・

Implementation details:

- MATLAB code.
- Parameters: $t = 10^{-4}$, $\eta_{max} = .9$, $[\theta_{min}, \theta_{max}] = [.1, .9]$.
- Krylov solver: Restarted GMRES applied as just outlined.
- Forcing terms: "Choice 1" from (Eisenstat–W 1996), with $\eta_0 = \eta_{\rm max} = .9$.
- Backtracking: $\theta \in [\theta_{\min}, \theta_{\max}]$ chosen to minimize an interpolating quadratic.

4 **A** N A **B** N A **B** N

PDEs on $\mathcal{D} = [0,1] \times [0,1]$.

2D Bratu Problem: $\Delta u + \lambda e^u = 0$ in \mathcal{D} , u = 0 on $\partial \mathcal{D}$

- Unknowns u, λ ; $u_0 = 2\sin(\pi u)\sin(\pi y)$, $\lambda_0 = 7.0$.
- Centered differences, 50×50 grid $\Rightarrow n = 2500$, m = 2501.
- GMRES(20), up to 3 restarts, Poisson-solver right preconditioning.

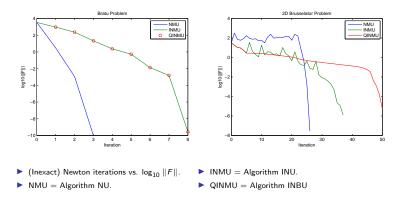
2D Brusselator Problem:

$$\begin{aligned} \partial u/\partial t &= \alpha \Delta u + 1 + u^2 v - 4.4u \text{ in } \mathcal{D} \\ \partial v/\partial t &= \alpha \Delta v + 1 + 3.4u - u^2 v \text{ in } \mathcal{D} \\ \partial u/\partial n &= \partial v/\partial n = 0 \text{ on } \partial \mathcal{D} \end{aligned}$$

- $\alpha = .002 \Rightarrow$ periodic solution.
- Unknowns u, v, T (period); $u_0 = 0.5 + y$, $v_0 = 1 + 5x$, T = 7.5.
- Centered differences, 21×21 grid $\Rightarrow n = 882$, m = 883.
- GMRES(50), up to 10 restarts, Poisson-solver right preconditioning.

(人間) システン イラン

Test Results: Bratu and Brusselator Problems



Note: On the Brusselator problem, the Algorithm NU iterates converged to the trivial solution (with zero period).

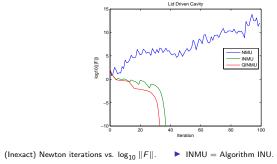
A

Test Results: Lid-Driven Cavity Problem

2D Lid-Driven Cavity Problem: $\frac{1}{\text{Re}}\Delta^2 u - (u_y\Delta u_x + u_x\Delta u_y) = 0$ in \mathcal{D} ,

with u = 0 on ∂D , $u_n = 0$ on the sides and bottom, and $u_n = 1$ on the top.

- Unknowns u, Re; $u_0 = 0$, Re₀ = 1000.
- Centered differences, 40×40 staggered grid $\Rightarrow n = 1600$, m = 1601.
- GMRES(50), up to 10 restarts, biharmonic-solver right preconditioning.



NMU = (exact) Newton's method.

QINMU = Algorithm INBU

We have:

- extended inexact Newton methods to underdetermined systems;
- provided local and global convergence results;
- reported results of limited numerical experiments.

Still needed:

- extensions to trust-region methods for underdetermined systems;
- *much* more testing.