

Lecture 19: The Inexact Newton-Krylov Algorithm

COMP5930M Scientific Computation

Today

Iterative linear algebra

Convergence

Inexact Newton-Krylov

Summary

Case studies

Porous medium equation

Newton's method + iterative linear solver

- ▶ We now have 2 levels of iteration
 - ▶ An **outer iteration** for the nonlinear system:
Newton's Method
 - ▶ An **inner iteration** for the linear system
at each nonlinear step:
Preconditioned Krylov-subspace iterations
- ▶ It is important to consider the effect of
approximate solution of the (**inner**) linear system
on the (**outer**) nonlinear system solution

Convergence control

- ▶ Iterative solution of the linear system is approximate
 - ▶ We monitor the residual norm $R_i = ||\mathbf{r}_i||$
- ▶ The Newton iteration is also approximate
 - ▶ We monitor the nonlinear function norm $F_k = ||\mathbf{F}(\mathbf{U}_k)||$
- ▶ While F_k is large we do not require R_i to be completely converged
 - ▶ We require **sufficient** accuracy
- ▶ We do not have this flexibility with direct solution

Inexact Newton method

Exact Newton iteration: find δ_k s.t.

$$\begin{aligned}J(\mathbf{x}_k)\delta_k &= -\mathbf{F}(\mathbf{x}_k) \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha\delta_k\end{aligned}$$

where $\alpha > 0$ is found through a line-search procedure

Inexact Newton iteration: for given $0 \leq \eta_k < 1$, find δ_k s.t.

$$\begin{aligned}\|J(\mathbf{x}_k)\delta_k + \mathbf{F}(\mathbf{x}_k)\| &\leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\| \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \delta_k\end{aligned}$$

Inexact Newton method

Exact Newton iteration: find δ_k s.t.

$$\begin{aligned}J(\mathbf{x}_k)\delta_k &= -\mathbf{F}(\mathbf{x}_k) \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha\delta_k\end{aligned}$$

where $\alpha > 0$ is found through a line-search procedure

Inexact Newton iteration: for given $0 \leq \eta_k < 1$, find δ_k s.t.

$$\begin{aligned}\|\mathbf{J}(\mathbf{x}_k)\delta_k + \mathbf{F}(\mathbf{x}_k)\| &\leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\| \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \delta_k\end{aligned}$$

Inexact Newton method

Exact Newton iteration: find δ_k s.t.

$$\begin{aligned}\mathbf{J}(\mathbf{x}_k)\delta_k &= -\mathbf{F}(\mathbf{x}_k) \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha\delta_k\end{aligned}$$

where $\alpha > 0$ is found through a line-search procedure

Inexact Newton iteration: for given $0 \leq \eta_k < 1$, find δ_k s.t.

$$\begin{aligned}\|\mathbf{r}_k\| &\leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\| && \text{(linear residual)} \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \delta_k\end{aligned}$$

Theorem: With some mild assumptions, the inexact Newton iteration converges linearly. If $\eta_k \rightarrow 0$, convergence is superlinear.

Inexact Newton method

Exact Newton iteration: find δ_k s.t.

$$\begin{aligned} \mathbf{J}(\mathbf{x}_k)\delta_k &= -\mathbf{F}(\mathbf{x}_k) \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha\delta_k \end{aligned}$$

where $\alpha > 0$ is found through a line-search procedure

Inexact Newton iteration: for given $0 \leq \eta_k < 1$, find δ_k s.t.

$$\begin{aligned} \|\mathbf{r}_k\| &\leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\| && \text{(linear residual)} \\ \mathbf{x}_{k+1} &= \mathbf{x}_k + \delta_k \end{aligned}$$

Theorem: With some mild assumptions, the inexact Newton iteration converges linearly. If $\eta_k \rightarrow 0$, convergence is superlinear.

Implementation

At inexact Newton iteration step k , the linear system is solved to the tolerance $\|\mathbf{r}_k\| \leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\|$ using iterative linear solvers.

Standard choices of η_k :

- ▶ Eisenstat-Walker: $\eta_k = C \frac{\|\mathbf{F}(x_k)\|^2}{\|\mathbf{F}(x_{k-1})\|^2}$, where $0 < C \leq 1$
- ▶ Kelley:

$$\eta_k = \min \left\{ \eta_{\max}, \max \left(\eta_k^{\text{safe}}, C \frac{\|\mathbf{F}(x_k)\|^2}{\|\mathbf{F}(x_{k-1})\|^2} \right) \right\}$$

where $\eta_{\max} < 1$ and η_k^{safe} is chosen to ensure that the η_k do not approach 0 too rapidly

(for details, see Kelley CT. Solving nonlinear equations with Newton's method. SIAM, 2003)

Implementation

At inexact Newton iteration step k , the linear system is solved to the tolerance $\|\mathbf{r}_k\| \leq \eta_k \|\mathbf{F}(\mathbf{x}_k)\|$ using iterative linear solvers.

Standard choices of η_k :

- ▶ **Eisenstat-Walker:** $\eta_k = C \frac{\|\mathbf{F}(x_k)\|^2}{\|\mathbf{F}(x_{k-1})\|^2}$, where $0 < C \leq 1$
- ▶ **Kelley:**

$$\eta_k = \min \left\{ \eta_{\max}, \max \left(\eta_k^{\text{safe}}, C \frac{\|\mathbf{F}(x_k)\|^2}{\|\mathbf{F}(x_{k-1})\|^2} \right) \right\}$$

where $\eta_{\max} < 1$ and η_k^{safe} is chosen to ensure that the η_k do not approach 0 too rapidly

(for details, see Kelley CT. Solving nonlinear equations with Newton's method. SIAM, 2003)

The Inexact Newton-Krylov Algorithm

- ▶ $k = 0$
- ▶ Specify or compute \mathbf{U}_0
- ▶ Compute $\mathbf{F}_0 = \mathbf{F}(\mathbf{U}_0)$
- ▶ While $|\mathbf{F}_k| > Tol$
 - ▶ Compute $\mathbf{J}_k = \mathbf{J}(\mathbf{U}_k)$
 - ▶ Assemble preconditioner matrix \mathbf{M}_k
 - ▶ Solve $\mathbf{J}_k \delta_k = -\mathbf{F}_k$ to tolerance $tol = \eta_k \|\mathbf{F}_k\|$ using Krylov-subspace iterative method and preconditioner \mathbf{M}_k
 - ▶ Update $\mathbf{U}_{k+1} = \mathbf{U}_k + \delta_k$
 - ▶ Compute $\mathbf{F}_{k+1} = \mathbf{F}(\mathbf{U}_{k+1})$
 - ▶ $k = k + 1$

Convergence of residuals: exact vs. inexact Newton

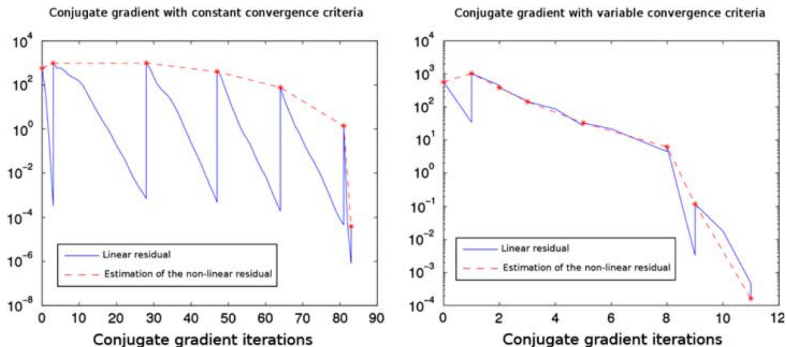


Figure 1. Illustration of the oversolving phenomenon.

Summary

The combination of:

- ▶ Newton's method;
- ▶ inexact solution of the linear system;
- ▶ preconditioned Krylov-subspace iterative techniques;
- ▶ matrix-permutation algorithms;
- ▶ approximate matrix factoring algorithms;

enables the efficient solution of very large, sparse, highly-nonlinear systems

Case study: Porous-medium equation

$u(x, y)$ represents concentration of some property

$$\frac{\partial}{\partial x} \left(g(u) \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(g(u) \frac{\partial u}{\partial y} \right) = 0$$

where

$$g(u) = 1 + \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2$$

Defined on a spatial region Ω with boundary conditions
 $u = U_1(x, y)$ on boundary $\partial\Omega$

Spatial approximation

- ▶ A linear triangular finite element method is used (equivalent to FDM in 1-D)
- ▶ The resulting Jacobian is sparse and symmetric positive definite and can be approximated analytically

Numerical method

- ▶ A Newton-Krylov solution strategy
- ▶ Preconditioned Conjugate Gradient iterations for the Jacobian system
- ▶ A state-of-the-art multigrid preconditioner¹ was tested for the CG iterations

¹Recall idea of using multiple levels of discrete grids to find initial conditions, can also be used here to generate efficient preconditioners

Timing results

| Equations N | Newton iterations | Sparse direct Time (s) | CG iterations Time (s) |
|----------------|----------------------|---------------------------|---------------------------|
| 9^2 | 10 | 0.9 | 0.1 |
| 17^2 | 12 | 21.6 | 0.6 |
| 33^2 | 13 | 382.6 | 2.7 |
| 65^2 | 15 | - | 12.7 |
| 129^2 | 17 | - | 57.1 |
| 257^2 | 19 | - | 261.6 |