A Tuned Preconditioner for Inexact Inverse Iteration for Generalised Eigenvalue Problems

Alastair Spence

Department of Mathematical Sciences
University of Bath, United Kingdom

IWASEP VI
May 22-25, 2006
Pennsylvania State University, University Park

Joint work with: Melina Freitag and Eero Vainikko

Outline

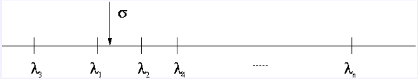
Motivation

- $Ax = \lambda M x$
- (λ_1, x_1): $Ax_1 = \lambda_1 M x_1$
- Large sparse nonsymmetric matrices
- Stability calculations for linearised N-S using Mixed FEM
- Hopf bifurcation: λ complex
- Simple eigenvalues
- Inverse Iteration with iterative solves for shifted linear systems
- Jacobi-Davidson, Arnoldi,...
- TODAY: costs of system solves

Outline

Inexact inverse iteration (an inner-outer iteration)

- $Ax = \lambda Mx, \quad (A - \sigma M)^{-1} Mx = \frac{1}{\lambda - \sigma} x$
- Fixed shift, $x^{(0)}$, $c^H x^{(0)} = 1$



for $i = 1$ to $\ldots$ **do**

  choose $\tau^{(i)}$

  solve

$$\|(A - \sigma M)y^{(i)} - Mx^{(i)}\| \leq \tau^{(i)},$$

  update eigenvector $x^{(i+1)} = \dfrac{y^{(i)}}{c^H y^{(i)}}$,

  update eigenval $\lambda^{(i+1)}$ =Ray Quot.

  e-value residual $r^{(i+1)} = (A - \lambda^{(i+1)} M)x^{(i+1)}$.

end for

PDE Example

Consider

$$-\Delta u + 5u_x + 5u_y = \lambda x$$

and its

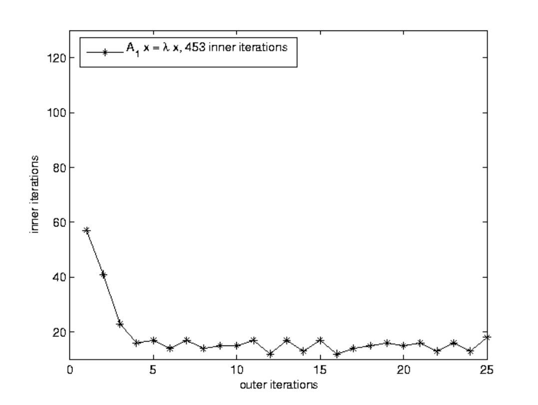
- Finite Difference Discretisation: $A_1 x = \lambda x$
- Finite Element Discretisation: $A_2 x = \lambda M_2 x$

Apply inexact inverse iteration with fixed shift σ and decreasing tolerance:

$$(A_1 - \sigma I)y^{(i)} = x^{(i)}, \quad (A_2 - \sigma M_2)y^{(i)} = M_2 x^{(i)},$$

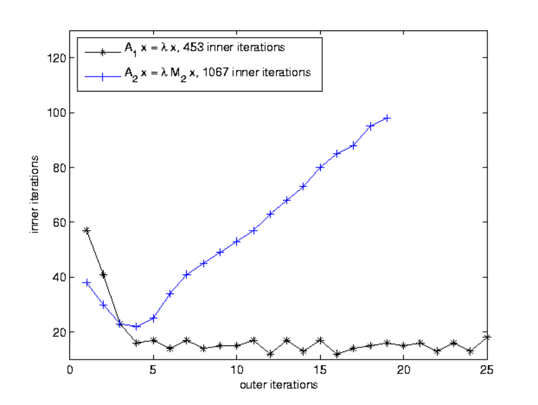
PDE Example: Numerics

Inner v. outer iterations



PDE Example: Numerics

Inner v. outer iterations



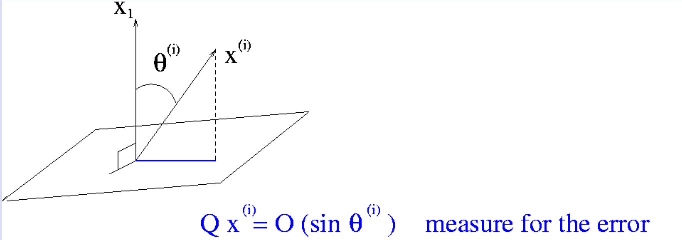
Questions

For decreasing solve tolerances

- Since the linear systems are being solved more and more accurately, why isn't the # inner iterations increasing with i for $A_1 x = \lambda x$?
- Why is the inner iteration behaviour different for the two discretizations?
- Can we achieve no increase in # inner iterations for $A_2 x = \lambda M_2 x$? (Yes: 'tuning')
- What implications are there for preconditioned iterative solvers?
- Next talk......

Convergence Analysis

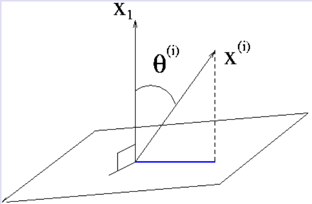
$Ax_1 = \lambda_1 x_1$, A symmetric (see Parlett's book)



- $C|\sin\theta^{(i)}| \le \|r^{(i)}\| \le C'|\sin\theta^{(i)}|, \quad r^{(i)} = (A - \lambda^{(i)} M)x^{(i)}$
- Nonsymmetric: $Ax = \lambda Mx$ [Golub/Ye (2000); Berns-Müller/Sp (2006)]
- If $\tau^{(i)} = C\|r^{(i)}\|$ then LINEAR convergence

Convergence Analysis

$Ax_1 = \lambda_1 x_1$, A symmetric (see Parlett's book)



$Q x^{(i)} = O(\sin\theta^{(i)})$ measure for the error

- $C|\sin\theta^{(i)}| \le \|r^{(i)}\| \le C'|\sin\theta^{(i)}|, \quad r^{(i)} = (A - \lambda^{(i)} M)x^{(i)}$
- Nonsymmetric: $Ax = \lambda Mx$ [Golub/Ye (2000); Berns-Müller/Sp (2006)]
- If $\tau^{(i)} = C\|r^{(i)}\|$ then LINEAR convergence

Outline

Krylov solvers for $By = b$

- $B = (A - \sigma I)$ and $b = x$
- (later $B = (A - \sigma M)$ and $b = Mx$)
- $\|b - By_k\| = \min \|p_k(B)b\| \leq C\rho^k \|b\|, \quad (0 < \rho < 1).$
- If $\|b - By_k\| \leq \tau$ then

$$k \geq C_1 + C_2 \log \frac{\|b\|}{\tau}$$

- Bound on k increases as τ decreases

Krylov solvers for $By = b$

- $B = (A - \sigma I)$ and $b = x$
- (later $B = (A - \sigma M)$ and $b = Mx$)
- $\|b - By_k\| = \min \|p_k(B)b\| \leq C\rho^k \|b\|, \quad (0 < \rho < 1).$
- If $\|b - By_k\| \leq \tau$ then

$$k \geq C_1 + C_2 \log \frac{\|b\|}{\tau}$$

- Bound on k increases as τ decreases

Krylov solvers for $By = b$: sophisticated analysis

- for a well-separated eigenvalue
- For $B = (A - \sigma I)$ then $Bx_1 = (\lambda_1 - \sigma)x_1$
- $$\|b - By_k\| = \min\|p_k(B)b\| \leq \|p_{k-1}(B)q_1(B)b\|$$
- $$\|b - By_k\| \leq \|p_{k-1}(B)q_1(B)Qb\|$$
- to achieve $\|b - By_k\| \leq \tau$ then
$$k \geq C_3 + C_4 \log \frac{\|Qb\|}{\tau}$$
- Bound on k depends on $\frac{\|Qb\|}{\tau}$

Krylov solvers for $By = b$: sophisticated analysis

- for a well-separated eigenvalue
- For $B = (A - \sigma I)$ then $Bx_1 = (\lambda_1 - \sigma)x_1$
- $$\|b - By_k\| = \min\|p_k(B)b\| \leq \|p_{k-1}(B)q_1(B)b\|$$
- $$\|b - By_k\| \leq \|p_{k-1}(B)q_1(B)Qb\|$$
- to achieve $\|b - By_k\| \leq \tau$ then
  $$k \geq C_3 + C_4 \log \frac{\|Qb\|}{\tau}$$
- Bound on k depends on $\frac{\|Qb\|}{\tau}$

Krylov solvers for $By = b$: sophisticated analysis

- for a well-separated eigenvalue
- For $B = (A - \sigma I)$ then $Bx_1 = (\lambda_1 - \sigma)x_1$
- $$\|b - By_k\| = \min \|p_k(B)b\| \leq \|p_{k-1}(B)q_1(B)b\|$$
- $$\|b - By_k\| \leq \|p_{k-1}(B)q_1(B)Qb\|$$
- to achieve $\|b - By_k\| \leq \tau$ then
$$k \geq C_3 + C_4 \log \frac{\|Qb\|}{\tau}$$
- Bound on k depends on $\frac{\|Qb\|}{\tau}$

Some answers for $\tau^{(i)} = C\|r^{(i)}\| = \mathcal{O}(\sin\theta^{(i)})$

$(A - \sigma I)y^{(i)} = x^{(i)}$

- $b = x^{(i)}$ and $\|Qx^{(i)}\| = \mathcal{O}(\sin\theta^{(i)})$
- Hence $\|Qb\|/\tau = \mathcal{O}(1)$ and the bound on k doesn't increase
- Consistent with numerics for $A_1 x = \lambda x$

$(A - \sigma M)y^{(i)} = Mx^{(i)}$

- $b = Mx^{(i)}$ and $\|QMx^{(i)}\| = \mathcal{O}(1)$
- Hence $\|Qb\|/\tau = \mathcal{O}(\sin\theta^{(i)})^{-1}$ and the bound on k increases
- Consistent with numerics for $A_2 x = \lambda M_2 x$

Outline

For $(A - \sigma M)y^{(i)} = Mx^{(i)}$

Introduce the "tuning matrix" $\mathbb{T}$ and consider (think preconditioning)

$$\mathbb{T}^{-1}(A - \sigma M)y^{(i)} = \mathbb{T}^{-1}Mx^{(i)}$$

- Key Condition: $\mathbb{T}^{-1}Mx^{(i)} = x^{(i)}$
- Re-arrange to:

$$Mx^{(i)} = \mathbb{T}x^{(i)}$$

- Implement by rank-one change to Identity:

$$\mathbb{T} := I + (Mx^{(i)} - x^{(i)})c^H \quad (c^H x^{(i)} = 1)$$

- Use Sherman-Morrison to get action of $\mathbb{T}^{-1}$

For $(A - \sigma M)y^{(i)} = Mx^{(i)}$

Introduce the “tuning matrix” $\mathbb{T}$ and consider (think preconditioning)

$$\mathbb{T}^{-1}(A - \sigma M)y^{(i)} = \mathbb{T}^{-1}Mx^{(i)}$$

- Key Condition: $\mathbb{T}^{-1}Mx^{(i)} = x^{(i)}$
- Re-arrange to:

$$Mx^{(i)} = \mathbb{T}x^{(i)}$$

- Implement by rank-one change to Identity:

$$\mathbb{T} := I + (Mx^{(i)} - x^{(i)})c^H \quad (c^H x^{(i)} = 1)$$

- Use Sherman-Morrison to get action of $\mathbb{T}^{-1}$

For $(A - \sigma M)y^{(i)} = Mx^{(i)}$

Introduce the "tuning matrix" $\mathbb{T}$ and consider (think preconditioning)

$$\mathbb{T}^{-1}(A - \sigma M)y^{(i)} = \mathbb{T}^{-1}Mx^{(i)}$$

- Key Condition: $\mathbb{T}^{-1}Mx^{(i)} = x^{(i)}$
- Re-arrange to:

$$Mx^{(i)} = \mathbb{T}x^{(i)}$$

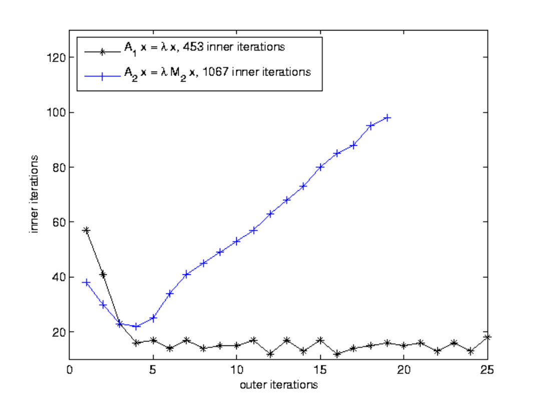
- Implement by rank-one change to Identity:

$$\mathbb{T} := I + (Mx^{(i)} - x^{(i)})c^H \quad (c^H x^{(i)} = 1)$$

- Use Sherman-Morrison to get action of $\mathbb{T}^{-1}$

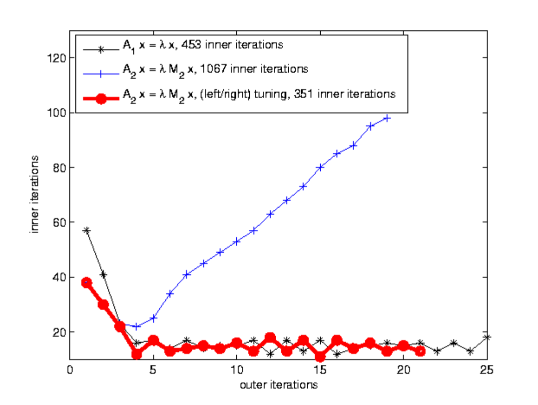
PDE Example: Numerics

Inner v. outer iterations



PDE Example: Numerics

Inner v. outer iterations



Outline

Flow past a circular cylinder (incompressible Navier-Stokes)

- $Re = 25$, $\lambda \approx \pm 10i$
- Mixed FEM: $Q_2 - Q_1$ elements
- Elman preconditioner: 2-level additive Schwarz
- ≈ 54000 degrees of freedom

Flow past a circular cylinder (incompressible Navier-Stokes)

Figure: Fixed Shift

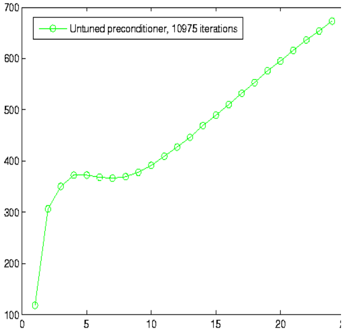
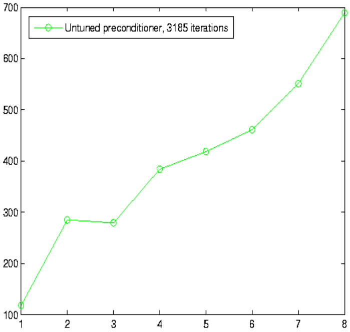


Figure: Rayleigh Quotient Shift



Tuning the preconditioner

- Preconditioned iterates should behave as in unpreconditioned standard EVP case
- right preconditioned system $(A - \sigma M)P_S^{-1}\tilde{y}^{(i)} = Mx^{(i)}$
- theory of Krylov solver for $By = b$ indicates that $Mx^{(i)}$ should be close to eigenvector of $(A - \sigma M)P_S^{-1}$
- Introduce a tuned preconditioner $\mathbb{P}$ so that we solve

$$(A - \sigma M)\mathbb{P}^{-1}\tilde{y}^{(i)} = Mx^{(i)}$$

- Remember $Ax_1 = \lambda_1 Mx_1$, so condition $\mathbb{P}x^{(i)} \approx \lambda^{(i)}Mx^{(i)}$?
- Take

$$\mathbb{P}x^{(i)} = Ax^{(i)}$$

since then

$$\mathbb{P}x^{(i)} = \lambda^{(i)}Mx^{(i)} + (Ax^{(i)} - \lambda^{(i)}Mx^{(i)})$$

Tuning the preconditioner

- Preconditioned iterates should behave as in unpreconditioned standard EVP case
- right preconditioned system $(A - \sigma M)P_S^{-1}\tilde{y}^{(i)} = Mx^{(i)}$
- theory of Krylov solver for $By = b$ indicates that $Mx^{(i)}$ should be close to eigenvector of $(A - \sigma M)P_S^{-1}$
- Introduce a tuned preconditioner $\mathbb{P}$ so that we solve

$$(A - \sigma M)\mathbb{P}^{-1}\tilde{y}^{(i)} = Mx^{(i)}$$

- Remember $Ax_1 = \lambda_1 Mx_1$, so condition $\mathbb{P}x^{(i)} \approx \lambda^{(i)}Mx^{(i)}$?
- Take

$$\mathbb{P}x^{(i)} = Ax^{(i)}$$

since then

$$\mathbb{P}x^{(i)} = \lambda^{(i)}Mx^{(i)} + (Ax^{(i)} - \lambda^{(i)}Mx^{(i)})$$

Tuning the preconditioner

- Preconditioned iterates should behave as in unpreconditioned standard EVP case
- right preconditioned system $(A - \sigma M)P_S^{-1}\tilde{y}^{(i)} = Mx^{(i)}$
- theory of Krylov solver for $By = b$ indicates that $Mx^{(i)}$ should be close to eigenvector of $(A - \sigma M)P_S^{-1}$
- Introduce a tuned preconditioner $\mathbb{P}$ so that we solve

$$(A - \sigma M)\mathbb{P}^{-1}\tilde{y}^{(i)} = Mx^{(i)}$$

- Remember $Ax_1 = \lambda_1 Mx_1$, so condition $\mathbb{P}x^{(i)} \approx \lambda^{(i)}Mx^{(i)}$?
- Take

$$\mathbb{P}x^{(i)} = Ax^{(i)}$$

since then

$$\mathbb{P}x^{(i)} = \lambda^{(i)}Mx^{(i)} + (Ax^{(i)} - \lambda^{(i)}Mx^{(i)})$$

Implementation of $\boxed{\mathbb{P}x^{(i)} = Ax^{(i)}}$

- Given P_S
- Evaluate $u^{(i)} = Ax^{(i)} - P_S x^{(i)}$
- Rank-one update: $\boxed{\mathbb{P} = P_S + u^{(i)} c^H}$

$$\mathbb{P}x^{(i)} = P_S x^{(i)} + u^{(i)} c^H x^{(i)} = P_S x^{(i)} + u^{(i)} = Ax^{(i)}$$

- Use Sherman-Morrison - one extra backsolve per outer iteration

Implementation of $\boxed{\mathbb{P}x^{(i)} = Ax^{(i)}}$

- Given P_S
- Evaluate $u^{(i)} = Ax^{(i)} - P_S x^{(i)}$
- Rank-one update: $\boxed{\mathbb{P} = P_S + u^{(i)} c^H}$

$$\mathbb{P}x^{(i)} = P_S x^{(i)} + u^{(i)} c^H x^{(i)} = P_S x^{(i)} + u^{(i)} = Ax^{(i)}$$

- Use Sherman-Morrison - one extra backsolve per outer iteration

Example

Figure: Fixed Shift

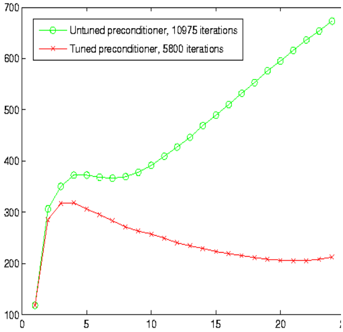
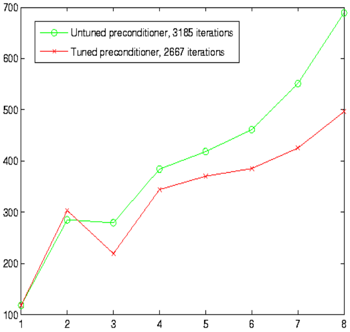


Figure: Rayleigh Quotient Shift



Conclusion

- When preconditioning an eigenvalue problem think of adding the property

$$\mathbb{P}x^{(i)} = Ax^{(i)}$$

  to your favourite preconditioner
- This can be achieved by a simple and cheap rank one modification

M. A. Freitag and A. Spence, *Convergence rates for inexact inverse iteration with application to preconditioned iterative solves*, 2006.
Submitted to BIT.

———, *A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems*, 2006.
Submitted to IMA J. Numer. Anal.