A Tuned Preconditioner for Inexact Inverse Iteration for Generalised Eigenvalue Problems

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Joint work with: Melina Freitag and Eero Vainikko
1 Motivation

2 Inexact Inverse Iteration

3 Costs in Krylov solvers

4 Tuning the right-hand side

5 Tuning and Preconditioning for a N-S problem
Outline

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Motivation

- \( Ax = \lambda M x \)
- \( (\lambda_1, x_1): \quad Ax_1 = \lambda_1 M x_1 \)
- Large sparse nonsymmetric matrices
- Stability calculations for linearised N-S using Mixed FEM
- Hopf bifurcation: \( \lambda \) complex
- Simple eigenvalues
- Inverse Iteration with \textit{iterative} solves for \textit{shifted} linear systems
- Jacobi-Davidson, Arnoldi,...
- TODAY: costs of system solves
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Inexact inverse iteration (an inner-outer iteration)

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

\[
\begin{array}{cccccc}
\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \ldots & \lambda_n
\end{array}
\]

\[
\sigma
\]

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For $i = 1$ to \ldots do

choose $\tau^{(i)}$

solve

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

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

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

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

end for
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 \(\sigma\) 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

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**Inner v. outer iterations**

![Graph showing inner v. outer iterations](image)
PDE Example: Numerics

Inexact inverse iteration and tuned preconditioning

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Inner v. outer iterations

A₁ \ x = \lambda \ x, 453 inner iterations
A₂ \ x = \lambda \ M₂ \ x, 1097 inner iterations
Questions

For decreasing solve tolerances

- Since the linear systems are being solved more and more accurately, why isn’t the number of inner iterations increasing with $i$ for $A_1x = \lambda x$?

- Why is the inner iteration behaviour different for the two discretizations?

- Can we achieve no increase in the number of inner iterations for $A_2x = \lambda M_2x$? (Yes: ‘tuning’)

- What implications are there for preconditioned iterative solvers?

- Next talk......
Convergence Analysis

\[ Ax_1 = \lambda_1 x_1, \ A \text{ symmetric (see Parlett's book)} \]

\[ Q x^{(i)} = O (\sin \theta^{(i)}) \quad \text{measure for the error} \]

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

\[ Ax_1 = \lambda_1 x_1, \ A \text{ symmetric (see Parlett's book)} \]

\[ Q \cdot x^{(i)} = O \left( \sin \theta^{(i)} \right) \text{ measure for the error} \]

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

- $B = (A - \sigma I)$ and $b = x$
- (later $B = (A - \sigma M)$ and $b = Mx$)
- $\|b - By_k\| = \min \|p_k(B)b\| \leq C\rho^k\|b\|$, $(0 < \rho < 1)$.
- If $\|b - By_k\| \leq \tau$ then
  $$k \geq C_1 + C_2 \log \frac{\|b\|}{\tau}$$

- Bound on $k$ increases as $\tau$ decreases
Krylov solvers for $B y = b$

- $B = (A - \sigma I)$ and $b = x$
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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 \( \frac{\|Qb\|}{\tau} \)
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Krylov solvers for $By = b$: sophisticated analysis

- for a well-separated eigenvalue
- For $B = (A - \sigma I)$ then $Bx_1 = (\lambda_1 - \sigma)x_1$

\[\|b - By_k\| = \min\|p_k(B)b\| \leq \|p_{k-1}(B)q_1(B)b\|\]

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Krylov solvers for $By = b$: sophisticated analysis

- for a well-separated eigenvalue

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  k \geq C_3 + C_4 \log \frac{\|Qb\|}{\tau}
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- Bound on $k$ depends on $\frac{\|Qb\|}{\tau}$
Some answers for $\tau^{(i)} = C \|r^{(i)}\| = O(\sin \theta^{(i)})$

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

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

Introduce the “tuning matrix” \(T\) and consider (think preconditioning)

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

- **Key Condition:** \(T^{-1}Mx^{(i)} = x^{(i)}\)
- **Re-arrange to:**
  \[ Mx^{(i)} = Tx^{(i)} \]
- **Implement by rank-one change to Identity:**
  \[ T := I + (Mx^{(i)} - x^{(i)})c^H \quad (c^Hx^{(i)} = 1) \]
- **Use Sherman-Morrison to get action of** \(T^{-1}\)
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Inner v. outer iterations

![Graph showing inner vs. outer iterations]

- $A_1 x = \lambda x$, 453 inner iterations
- $A_2 x = \lambda M_2 x$, 1097 inner iterations
PDE Example: Numerics

Inner v. outer iterations

- $A_1 x = \lambda x$, 453 inner iterations
- $A_2 x = \lambda M_2 x$, 1067 inner iterations
- $A_3 x = \lambda M_2 x$, (left/right) tuning, 351 inner iterations
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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
- $\approx 54000$ degrees of freedom
Flow past a circular cylinder (incompressible Navier-Stokes)

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**Figure:** Fixed Shift

**Figure:** Rayleigh Quotient Shift
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 \(P\) so that we solve

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

Remember \(Ax_1 = \lambda_1 Mx_1\), so condition \(Px^{(i)} \approx \lambda^{(i)} Mx^{(i)}\) ?

Take

\[Px^{(i)} = Ax^{(i)}\]

since then

\[Px^{(i)} = \lambda^{(i)} Mx^{(i)} + (Ax^{(i)} - \lambda^{(i)} Mx^{(i)})\]
Tuning the preconditioner

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

- Remember \(Ax_1 = \lambda_1 Mx_1\), so condition \(Px(i) \approx \lambda(i) Mx(i)\)
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Tuning the preconditioner

- Preconditioned iterates should behave as in unpreconditioned standard EVP case
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  since then
  \[
  Px^{(i)} = \lambda^{(i)} Mx^{(i)} + (Ax^{(i)} - \lambda^{(i)} Mx^{(i)})
  \]
Implementation of $\mathbf{Px}^{(i)} = A\mathbf{x}^{(i)}$

- **Given** $P_S$
- **Evaluate** $u^{(i)} = A\mathbf{x}^{(i)} - P_S\mathbf{x}^{(i)}$
- **Rank-one update:**
  \[ \mathbf{P} = P_S + u^{(i)}c^H \]

\[ \mathbf{Px}^{(i)} = P_S\mathbf{x}^{(i)} + u^{(i)}c^H\mathbf{x}^{(i)} = P_S\mathbf{x}^{(i)} + u^{(i)} = A\mathbf{x}^{(i)} \]

- Use Sherman-Morrison - one extra backsolve per outer iteration
Implementation of $\mathbb{P}x^{(i)} = Ax^{(i)}$

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

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

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

**Figure:** Fixed Shift

**Figure:** Rayleigh Quotient Shift
When preconditioning an eigenvalue problem think of adding the property

\[ \mathbb{P} x^{(i)} = A x^{(i)} \]

to your favourite preconditioner

This can be achieved by a simple and cheap rank one modification
Submitted to BIT.

———, *A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems*, 2006.