New Preconditioning Strategies for Eigenvalue Problems

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joint work with Howard Elman (Maryland) and Alastair Spence (Bath)

Outline

Problem and iterative methods

Find a small number of eigenvalues and eigenvectors of:

$$Ax = \lambda x, \quad \lambda \in \mathbb{C}, x \in \mathbb{C}^n$$

- A is large, sparse, nonsymmetric

Problem and iterative methods

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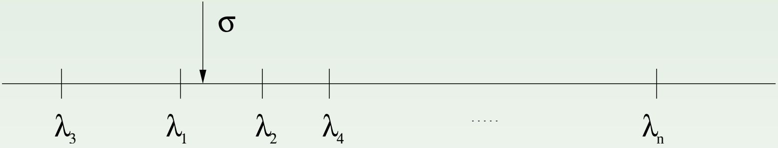
$$Ax = \lambda x, \quad \lambda \in \mathbb{C}, x \in \mathbb{C}^n$$

- A is large, sparse, nonsymmetric
- Iterative solves
  - Power method
  - Simultaneous iteration
  - Arnoldi method
  - Jacobi-Davidson method
- Usually involves repeated application of the matrix A to a vector
- Generally convergence to largest/outlying eigenvector

Outline

Shift-invert strategy

- Wish to find an eigenvalue close to a shift σ



Shift-invert strategy

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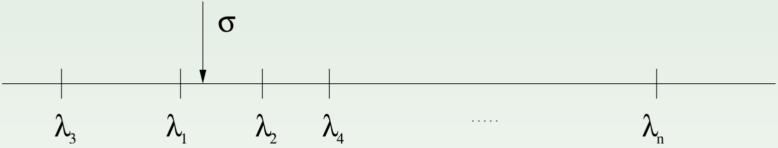

- Problem becomes
$$(A-\sigma I)^{-1}x = \frac{1}{\lambda-\sigma}x$$
- each step of the iterative method involves repeated application of $(A-\sigma I)^{-1}$ to a vector
- Inner iterative solve:
$$(A-\sigma I)y = x$$
using Krylov method for linear systems.
- leading to inner-outer iterative method.

Shift-invert strategy

This talk:
Inner Iteration and preconditioning
fixed shifts only.

Outline

1. The problem
2. Inverse iteration and Shift-invert Arnoldi method
3. Inexact inverse iteration
4. Inexact Shift-invert Arnoldi method
5. Conclusions

The algorithm

Inexact inverse iteration

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

choose $\tau^{(i)}$

solve

$$\|(A-\sigma I)y^{(i)} - x^{(i)}\| = \|d^{(i)}\| \leq \tau^{(i)},$$

Rescale $x^{(i+1)} = \dfrac{y^{(i)}}{\|y^{(i)}\|}$,

Update $\lambda^{(i+1)} = {x^{(i+1)}}^H A x^{(i+1)}$,

Test: eigenvalue residual $r^{(i+1)} = (A - \lambda^{(i+1)} I)x^{(i+1)}$.

end for

Convergence rates

If

$$\tau^{(i)} = C\|r^{(i)}\|$$

then convergence rate is linear (same convergence rate as for exact solves).

The inner iteration for $(A - \sigma I)y = x$

Standard GMRES theory for $y_0 = 0$ and A diagonalisable

$$\|x - (A - \sigma I)y_k\| \leq \kappa(W) \min_{p \in \mathcal{P}_k} \max_{j=1,\ldots,n} |p(\lambda_j)| \|x\|$$

where λ_j are eigenvalues of $A - \sigma I$ and $(A - \sigma I) = W \Lambda W^{-1}$.

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Number of inner iterations

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

for $\|x - (A - \sigma I)y_k\| \leq \tau$.

The inner iteration for $(A - \sigma I)y = x$

More detailed GMRES theory for $y_0 = 0$

$$\|x - (A - \sigma I)y_k\| \leq \tilde{\kappa}(W)\frac{|\lambda_2 - \lambda_1|}{\lambda_1} \min_{p \in \mathcal{P}_{k-1}} \max_{j=2,\dots,n} |p(\lambda_j)| \|\mathcal{Q}x\|$$

where λ_j are eigenvalues of $A - \sigma I$.

Number of inner iterations

$$k \geq C_1' + C_2' \log \frac{\|\mathcal{Q}x\|}{\tau},$$

where $\mathcal{Q}$ projects onto the space *not* spanned by the eigenvector.

The inner iteration for $(A - \sigma I)y = x$

Good news!

$$k^{(i)} \geq C_1' + C_2' \log \frac{C_3 \|r^{(i)}\|}{\tau^{(i)}},$$

where $\tau^{(i)} = C\|r^{(i)}\|$. Iteration number approximately constant!

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Bad news :-(

For a standard preconditioner P

$$(A-\sigma I)P^{-1}\tilde{y}^{(i)} = x^{(i)} \qquad P^{-1}\tilde{y}^{(i)} = y^{(i)}$$

$$k^{(i)} \geq C_1'' + C_2'' \log \frac{\|\tilde{\mathcal{Q}} x^{(i)}\|}{\tau^{(i)}} = C_1'' + C_2'' \log \frac{C}{\tau^{(i)}},$$

where $\tau^{(i)} = C\|r^{(i)}\|$. Iteration number increases!

The inner iteration for $(A - \sigma I)P^{-1}\tilde{y} = x$

How to overcome this problem

- Use a different preconditioner, namely one that satisfies

$$\mathbb{P}_i x^{(i)} = Ax^{(i)}, \quad \mathbb{P}_i := P + (A - P)x^{(i)}{x^{(i)}}^H$$

- minor modification and minor extra computational cost,
- $[A\mathbb{P}_i^{-1}]Ax^{(i)} = Ax^{(i)}$.

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Why does that work?

Assume we have found eigenvector x_1

$$A x_1 = \mathbb{P} x_1 = \lambda_1 x_1 \quad \Rightarrow \quad (A - \sigma I)\mathbb{P}^{-1} x_1 = \frac{\lambda_1 - \sigma}{\lambda_1} x_1$$

and convergence of Krylov method applied to $(A - \sigma I)\mathbb{P}^{-1}\tilde{y} = x_1$ in one iteration. For general $x^{(i)}$

$$k^{(i)} \geq C_1'' + C_2'' \log \frac{C_3 \| r^{(i)} \|}{\tau^{(i)}}, \quad \text{where} \quad \tau^{(i)} = C \| r^{(i)} \|.$$

Convection-Diffusion operator

Finite difference discretisation on a 32×32 grid of the convection-diffusion operator

$$-\Delta u + 5u_x + 5u_y = \lambda u \quad \text{on} \quad (0,1)^2,$$

with homogeneous Dirichlet boundary conditions (961×961 matrix).

- smallest eigenvalue: $\lambda_1 \approx 32.18560954$,
- Preconditioned GMRES with tolerance $\tau^{(i)} = 0.01\|r^{(i)}\|$,
- standard and tuned preconditioner (incomplete LU).

Convection-Diffusion operator

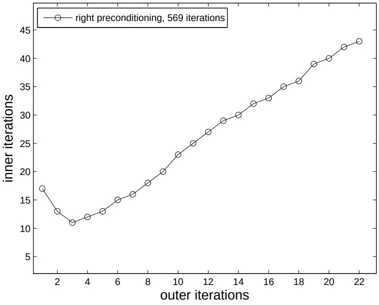

Figure: Inner iterations vs outer iterations

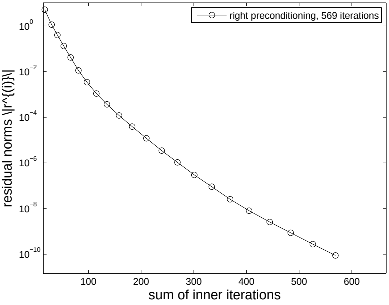

Figure: Eigenvalue residual norms vs total number of inner iterations

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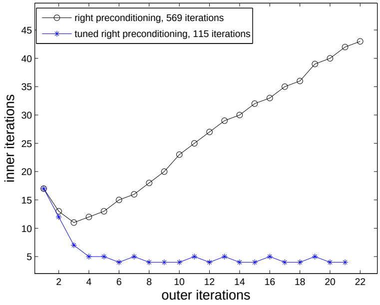

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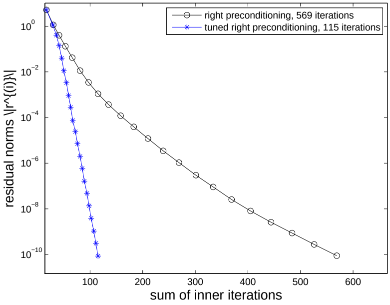

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Outline

The algorithm

Shift-invert Arnoldi-method

- Arnoldi method constructs an orthogonal basis of k-dimensional Krylov subspace

$$\mathcal{K}^{(i)}(\mathcal{A}, q^{(1)}) = \text{span}\{q^{(1)}, \mathcal{A}q^{(1)}, \mathcal{A}^2 q^{(1)}, \ldots, \mathcal{A}^{i-1} q^{(1)}\},$$

$$\mathcal{A}Q^{(i)} = Q^{(i)} H^{(i)} + q^{(i+1)} h^{(i+1,i)} e_i^H, \quad (Q^{(i)})^H Q^{(i)} = I.$$

- at each step, application of $\mathcal{A}$ to $q^{(i)}$
- Eigenvalues of $H^{(i)}$ are eigenvalue approximation of (outlying) eigenvalues of $\mathcal{A}$
- Shift-Invert $\mathcal{A} := (A - \sigma I)^{-1}$

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Inexact solves

The solve tolerance can be relaxed! (Simoncini 2005)

$$\|q^{(i)} - (A - \sigma I)\tilde{q}^{(i+1)}\| = \|d^{(i)}\|, \quad \|d^{(i)}\| = C \frac{1}{\|r^{(i)}\|}.$$

The inner iteration for $A\tilde{q} = q$ $(\sigma = 0)$

Tuning for Arnoldi's method (consider $\sigma = 0$)

Solve

$$AP^{-1}\tilde{\tilde{q}} = q, \quad P^{-1}\tilde{\tilde{q}} = \tilde{q}$$

using a tuned preconditioner

$$\mathbb{P}_i Q^{(i)} = AQ^{(i)}; \quad \text{given by} \quad \mathbb{P}_i = P + (A - P)Q^{(i)}{Q^{(i)}}^H$$

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Theorem (Properties of the tuned preconditioner)

Let P with $P = A + E$ be a preconditioner for A and assume i steps of Arnoldi's method have been carried out; then i eigenvalues of $A\mathbb{P}_i^{-1}$ are equal to one:

$$[A\mathbb{P}_i^{-1}]AQ^{(i)} = AQ^{(i)}$$

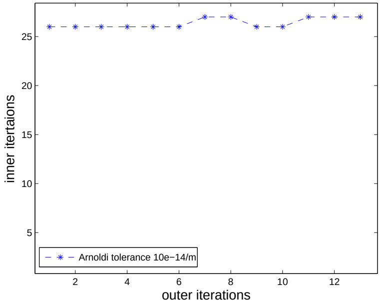
and $n - i$ eigenvalues are perturbations one, close to the eigenvalues of AP^{-1}.

Numerical Example

`sherman5.mtx` matrix from the Matrix Market library (3312×3312).

- smallest eigenvalue: $\lambda_1 \approx 4.69 \times 10^{-2}$,
- Preconditioned GMRES as inner solver (fixed tolerance and relaxation strategy),
- standard and tuned preconditioner (incomplete LU).

No tuning and standard preconditioner



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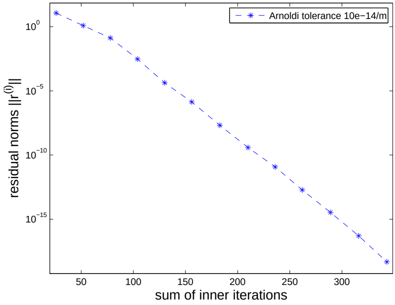
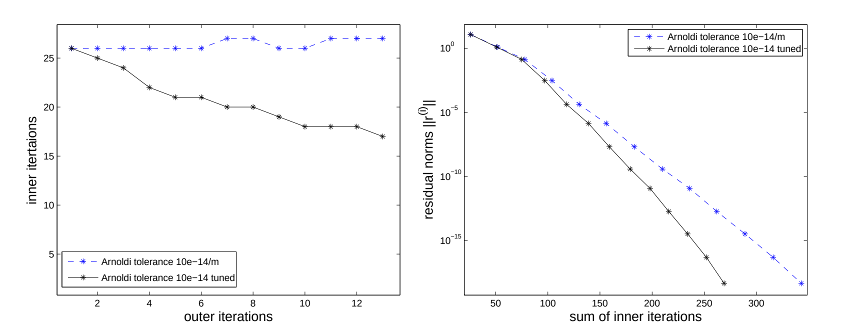


Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning



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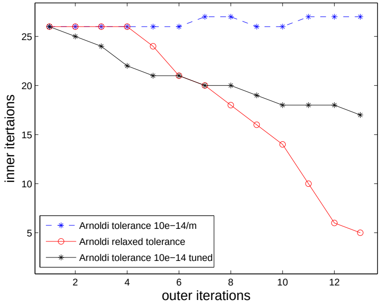
Relaxation



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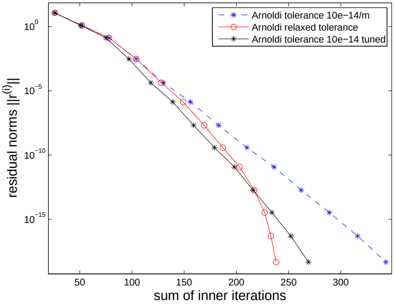

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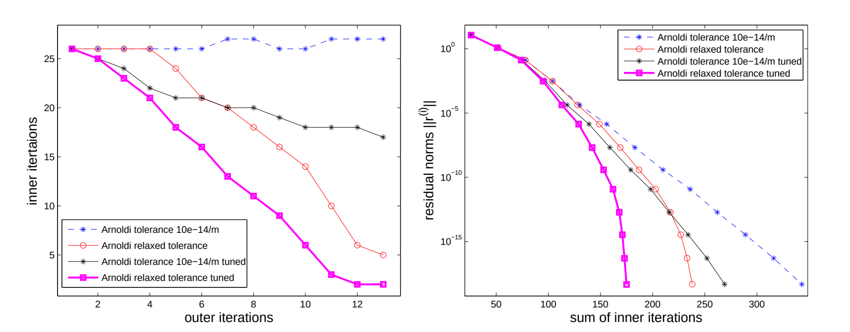
Tuning and relaxation strategy



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Outline

Conclusions

- Inexact solves for Inverse iteration and Krylov subspace methods
- Inner iteration depends on preconditioner
- For eigencomputations it is advantageous to consider modified preconditioners (works for any preconditioner)
- Extension to restarted methods is possible

M. A. Freitag and H. C. Elman, *Inexact preconditioned arnoldi's method and implicit restarts for eigenvalue computations*, 2007.
In preparation.

M. A. Freitag and A. Spence, *Convergence theory for inexact inverse iteration applied to the generalised nonsymmetric eigenproblem*, 2006.
To appear in ETNA.

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

——, *Convergence rates for inexact inverse iteration with application to preconditioned iterative solves*, BIT, 47 (2007), pp. 27–44.