Preconditioned inverse iteration and shift-invert Arnoldi method

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CSC Seminar
Max-Planck-Institute for Dynamics of Complex Technical Systems
Magdeburg
3rd May 2011

joint work with 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

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  - Power method
  - Simultaneous iteration
  - Arnoldi method
  - Jacobi-Davidson method
- repeated application of the matrix A to a vector
- Generally convergence to largest/outlying eigenvector

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- Iterative solves
  - Power method
  - Simultaneous iteration
  - Arnoldi method
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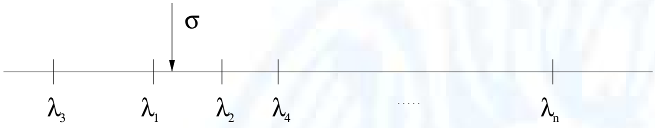
- The first three of these involve repeated application of the matrix A to a vector
- Generally convergence to largest/outlying eigenvector

Shift-invert strategy

- Wish to find a few eigenvalues close to a shift σ



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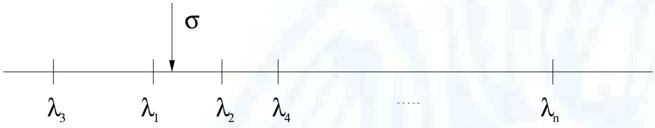

- Problem becomes

$$(A - \sigma I)^{-1} x = \frac{1}{\lambda - \sigma} x$$

- each step of the iterative method involves repeated application of $\mathcal{A} = (A - \sigma I)^{-1}$ 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

Inverse iteration and Arnoldi method

Outline

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

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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

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

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 $y_0 = 0$

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

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

Number of inner iterations

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

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!

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

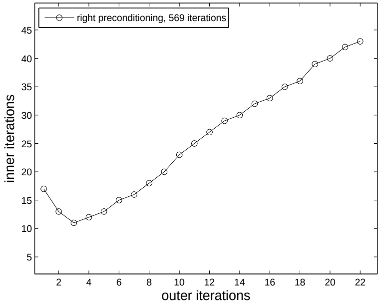

Figure: Inner iterations vs outer iterations

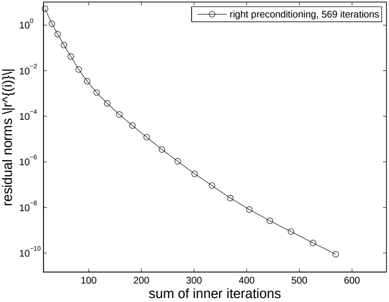

Figure: Eigenvalue residual norms vs total number of inner iterations

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

$$Ax_1 = \mathbb{P}x_1 = \lambda_1 x_1 \quad \Rightarrow \quad (A - \sigma I)\mathbb{P}^{-1}x_1 = \frac{\lambda_1 - \sigma}{\lambda_1}x_1$$

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

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

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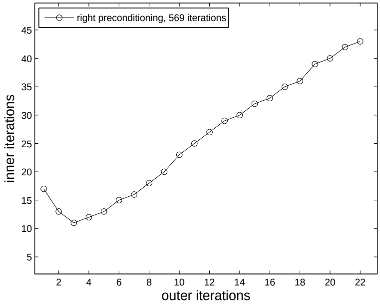

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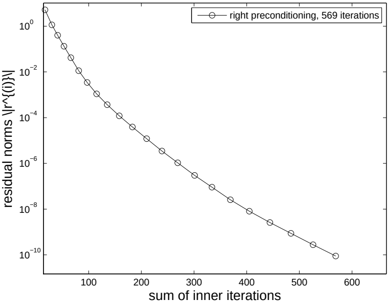

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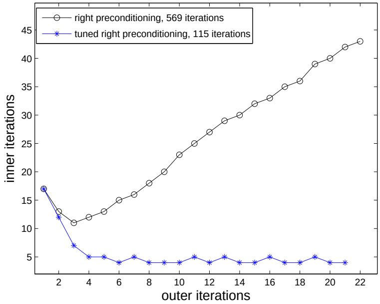

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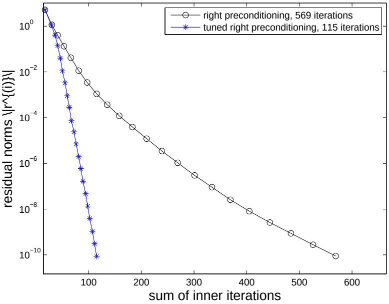

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Outline

The algorithm

Arnoldi's method

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

$$\mathcal{K}_k(\mathcal{A}, q^{(1)}) = \mathrm{span}\{q^{(1)}, \mathcal{A}q^{(1)}, \mathcal{A}^2 q^{(1)}, \ldots, \mathcal{A}^{k-1} q^{(1)}\},$$

$$\mathcal{A}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H = Q_{k+1} \begin{bmatrix} H_k \\ h_{k+1,k} e_k^H \end{bmatrix}$$

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- Eigenvalues of H_k are eigenvalue approximations of (outlying) eigenvalues of $\mathcal{A}$

$$\|r_k\| = \|\mathcal{A}x - \theta x\| = \|(\mathcal{A}Q_k - Q_k H_k)u\| = |h_{k+1,k}||e_k^H u|,$$

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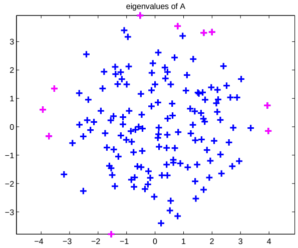
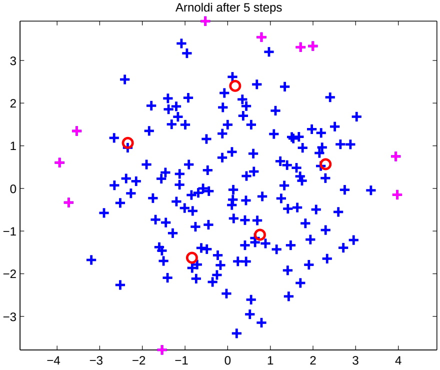
- at each step, application of $\mathcal{A}$ to q_k: $\mathcal{A}q_k = \tilde{q}_{k+1}$

Example

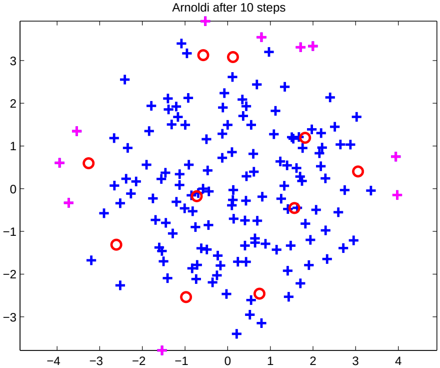
random complex matrix of dimension $n = 144$ generated in MATLAB:
`G=numgrid('N',14);B=delsq(G);A=sprandn(B)+i*sprandn(B)`



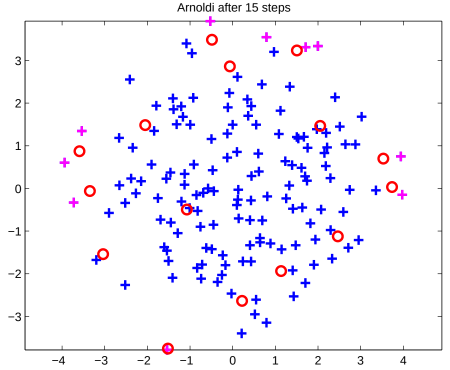
after 5 Arnoldi steps



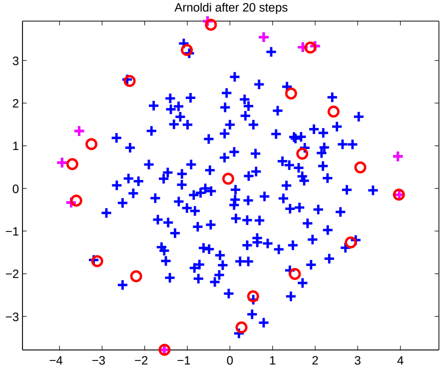
after 10 Arnoldi steps



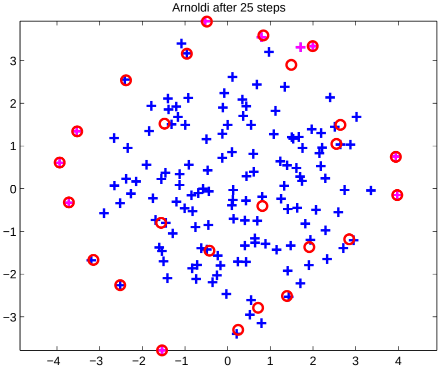
after 15 Arnoldi steps



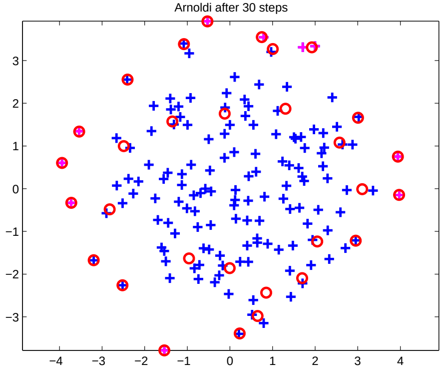
after 20 Arnoldi steps



after 25 Arnoldi steps



after 30 Arnoldi steps



The algorithm: take $\sigma = 0$

Shift-Invert Arnoldi's method $\mathcal{A} := A^{-1}$

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

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- at each step, application of A^{-1} to q_k: $A^{-1}q_k = \tilde{q}_{k+1}$

Inexact solves

Inexact solves (Simoncini 2005), Bouras and Frayssé (2000)

- Wish to solve

$$\|q_k - A\tilde{q}_{k+1}\| = \|\tilde{d}_k\| \leq \tau_k$$

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- leads to inexact Arnoldi relation

$$A^{-1}Q_k = Q_{k+1}\begin{bmatrix} H_k \\ h_{k+1,k}e_k^H \end{bmatrix} + D_k = Q_{k+1}\begin{bmatrix} H_k \\ h_{k+1,k}e_k^H \end{bmatrix} + [d_1|\dots|d_k]$$

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- u eigenvector of H_k:
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- Linear combination of the columns of D_k

$$D_k u = \sum_{l=1}^{k} d_l u_l, \quad \text{if} \quad u_l \quad \text{small, then} \quad \|d_l\| \quad \text{allowed to be large!}$$

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$$\|d_l u_l\| \leq \frac{1}{k}\varepsilon \Rightarrow \|D_k u\| < \varepsilon$$

and

$$|u_l| \leq C(l,k)\|r_{l-1}\| \qquad \star$$

leads to

$$\|q_k - A\tilde{q}_{k+1}\| = \|\tilde{d}_k\|$$

$$\|\tilde{d}_k\| = C\frac{1}{\|r_{k-1}\|} \qquad \diamond$$

Solve tolerance can be relaxed.

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

GMRES convergence bound

$$\|q_k - AP^{-1}\tilde{q}^l_{k+1}\| = \kappa \min_{p\in\Pi_l} \max_{i=1,\dots,n} |p(\mu_i)| \|q_k\|$$

depending on

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depending on

- the eigenvalue clustering of AP^{-1}
- the condition number
- the right hand side (initial guess)

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

- Introduce preconditioner P and solve

$$AP^{-1}\tilde{q}_{k+1} = q_k, \quad P^{-1}\tilde{q}_{k+1} = q_{k+1}$$

using GMRES

The inner iteration for $AP^{-1}\tilde{q}_{k+1} = q_k$

Preconditioning

- Introduce preconditioner P and solve

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using GMRES

Tuned Preconditioner

using a tuned preconditioner for Arnoldi's method

$$\mathbb{P}_k Q_k = AQ_k; \quad \text{given by} \quad \mathbb{P}_k = P + (A - P)Q_k Q_k^H$$

The inner iteration for $A\tilde{q} = q$

Theorem (Properties of the tuned preconditioner)

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

$$[A\mathbb{P}_k^{-1}]AQ_k = AQ_k$$

and $n - k$ eigenvalues are close to the corresponding eigenvalues of AP^{-1}.

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Implementation

- Sherman-Morrison-Woodbury.
- Only minor extra costs (one back substitution per outer iteration)

Numerical Example

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

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

No tuning and standard preconditioner

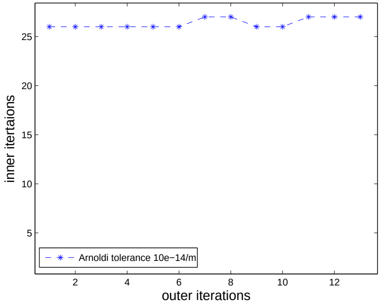


Figure: Inner iterations vs outer iterations

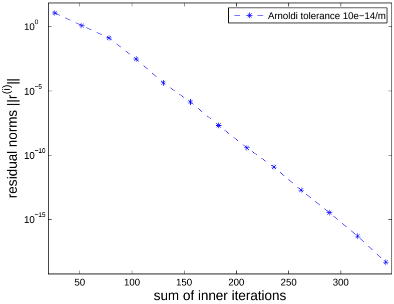
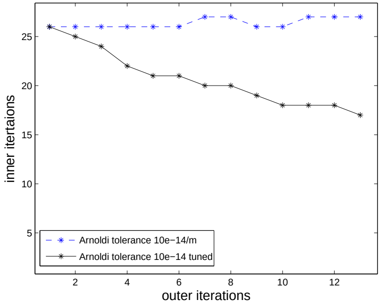


Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning the preconditioner



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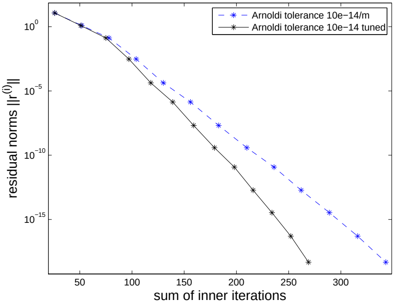

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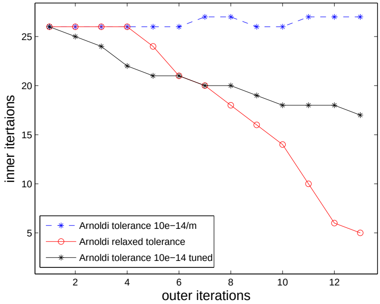
Relaxation



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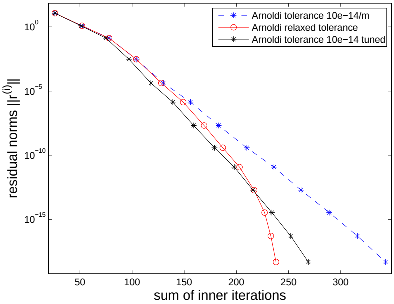

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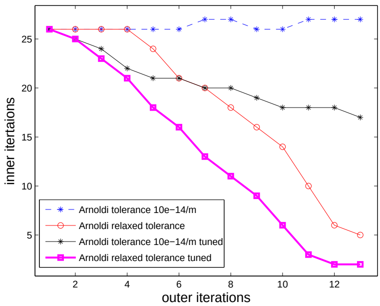
Tuning and relaxation strategy



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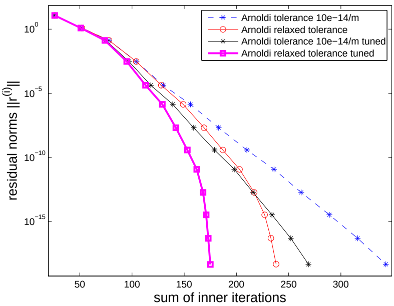

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Ritz values of exact and inexact Arnoldi

Exact eigenvalues	Ritz values (exact Arnoldi)	Ritz values (inexact Arnoldi, tuning)
+4.69249563e-02	+$\underline{4.69249563}$e-02	+$\underline{4.69249563}$e-02
+1.25445378e-01	+$\underline{1.25445378}$e-01	+$\underline{1.25445378}$e-01
+4.02658363e-01	+$\underline{4.02658}$347e-01	+$\underline{4.02658}$244e-01
+5.79574381e-01	+$\underline{5.79}$625498e-01	+$\underline{5.79}$817301e-01
+6.18836405e-01	+$\underline{6.18}$798666e-01	+$\underline{6.18}$650849e-01

Table: Ritz values of exact Arnoldi's method and inexact Arnoldi's method with the tuning strategy compared to exact eigenvalues closest to zero after 14 shift-invert Arnoldi steps.

Outline

Implicitly restarted Arnoldi (Sorensen (1992))

Exact shifts

- take an $k+p$ step Arnoldi factorisation

$$\mathcal{A}Q_{k+p} = Q_{k+p}H_{k+p} + q_{k+p+1}h_{k+p+1,k+p}e_{k+p}^{H}$$

- Compute $\Lambda(H_{k+p})$ and select p shifts for an implicit QR iteration
- implicit restart with new starting vector $\hat{q}^{(1)} = \dfrac{p(\mathcal{A})q^{(1)}}{\|p(\mathcal{A})q^{(1)}\|}$

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Aim of IRA

$$\mathcal{A}Q_k = Q_kH_k + q_{k+1}\underbrace{h_{k+1,k}}_{\to 0}e_k^H$$

Relaxation strategy for IRA

Theorem

For any given $\varepsilon \in \mathbb{R}$ *with* $\varepsilon > 0$ *assume that*

$$\|d_l\| \leq \begin{cases} \varepsilon \dfrac{C}{\|R_k\|} & \text{if} \quad l > k, \\ \varepsilon & \text{otherwise}. \end{cases} \qquad \diamond$$

Then

$$\|\mathcal{A}Q_m U - Q_m U \Theta - R_m\| \leq \varepsilon.$$

- Very technical
- Relaxation strategy also works for IRA!

Tuning

Tuning for implicitly restarted Arnoldi's method

- Introduce preconditioner P and solve

$$A\mathbb{P}_k^{-1}\tilde{q}_{k+1} = q_k, \quad \mathbb{P}_k^{-1}\tilde{q}_{k+1} = q_{k+1}$$

using GMRES and a tuned preconditioner

$$\mathbb{P}_k Q_k = AQ_k; \quad \text{given by} \quad \mathbb{P}_k = P + (A-P)Q_kQ_k^H$$

Tuning

Why does tuning help?

- Assume we have found an approximate invariant subspace, that is

$$A^{-1}Q_k = Q_k H_k + \underbrace{q_{k+1} h_{k+1,k} e_k^H}_{\approx 0}$$

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- let A^{-1} have the upper Hessenberg form

$$\begin{bmatrix} Q_k & {Q_k}^{\perp} \end{bmatrix}^H A^{-1} \begin{bmatrix} Q_k & {Q_k}^{\perp} \end{bmatrix} = \begin{bmatrix} H_k & T_{12} \\ h_{k+1,k}e_1{e_k}^H & T_{22} \end{bmatrix},$$

where $\begin{bmatrix} Q_k & {Q_k}^{\perp} \end{bmatrix}$ is unitary and $H_k \in \mathbb{C}^{k,k}$ and $T_{22} \in \mathbb{C}^{n-k,n-k}$ are upper Hessenberg.

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If $h_{k+1,k} \neq 0$ then

$$\begin{bmatrix} Q_k & Q_k{}^{\perp} \end{bmatrix}^H A\mathbb{P}_k^{-1} \begin{bmatrix} Q_k & Q_k{}^{\perp} \end{bmatrix} = \begin{bmatrix} I + \star & Q_k^H A\mathbb{P}_k^{-1} Q_k^{\perp} \\ \star & T_{22}^{-1}(Q_k^{\perp H} P Q_k^{\perp})^{-1} + \star \end{bmatrix}$$

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$$\left[\begin{array}{cc} Q_k & Q_k{}^{\perp} \end{array}\right]^H A^{-1} \left[\begin{array}{cc} Q_k & Q_k{}^{\perp} \end{array}\right] = \left[\begin{array}{cc} H_k & T_{12} \\ h_{k+1,k}e_1 e_k{}^H & T_{22} \end{array}\right],$$

where $\left[\begin{array}{cc} Q_k & Q_k{}^{\perp} \end{array}\right]$ is unitary and $H_k \in \mathbb{C}^{k,k}$ and $T_{22} \in \mathbb{C}^{n-k,n-k}$ are upper Hessenberg.

If $h_{k+1,k} = 0$ then

$$\left[\begin{array}{cc} Q_k & Q_k{}^{\perp} \end{array}\right]^H A\mathbb{P}_k^{-1} \left[\begin{array}{cc} Q_k & Q_k{}^{\perp} \end{array}\right] = \left[\begin{array}{cc} I & Q_k^H A\mathbb{P}_k^{-1} Q_k^{\perp} \\ 0 & T_{22}^{-1}(Q_k^{\perp}{}^H P Q_k^{\perp})^{-1} \end{array}\right]$$

Another advantage of tuning

- System to be solved at each step of Arnoldi's method is

$$A\mathbb{P}_k^{-1}\tilde{q}_{k+1} = q_k, \quad \mathbb{P}_k^{-1}\tilde{q}_{k+1} = \tilde{q}_k$$

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- Assuming invariant subspace found then ($A^{-1}Q_k = Q_k H_k$):

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- the right hand side of the system matrix is an eigenvector of the system!

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- Assuming invariant subspace found then $(A^{-1}Q_k = Q_k H_k)$:

$$A\mathbb{P}_k^{-1}q_k = q_k$$

- the right hand side of the system matrix is an eigenvector of the system!
- Krylov methods converge in one iteration

Tuning

Another advantage of tuning

- In practice:

$$A^{-1}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H$$

  and

$$\| A\mathbb{P}_k^{-1} q_k - q_k \| = \mathcal{O}(|h_{k+1,k}|)$$

Tuning

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- In practice:
$$A^{-1}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H$$
and
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- number of iterations decreases as the outer iteration proceeds

Tuning

Another advantage of tuning

- In practice:

$$A^{-1}Q_k = Q_k H_k + q_{k+1} h_{k+1,k} e_k^H$$

  and

$$\|A\mathbb{P}_k^{-1} q_k - q_k\| = \mathcal{O}(|h_{k+1,k}|)$$

- number of iterations decreases as the outer iteration proceeds
- Rigorous analysis quite technical.

Numerical Example

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

- $k = 8$ eigenvalues closest to zero
- IRA with exact shifts $p = 4$
- Preconditioned GMRES as inner solver (fixed tolerance and relaxation strategy),
- standard and tuned preconditioner (incomplete LU).

No tuning and standard preconditioner

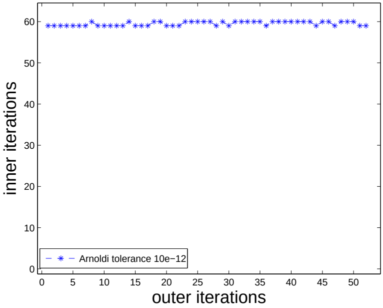

Figure: Inner iterations vs outer iterations

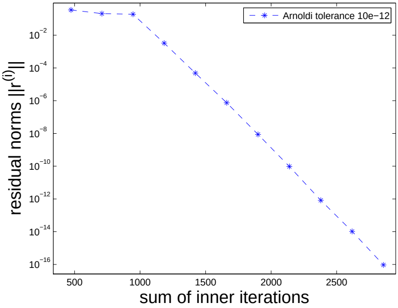

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning

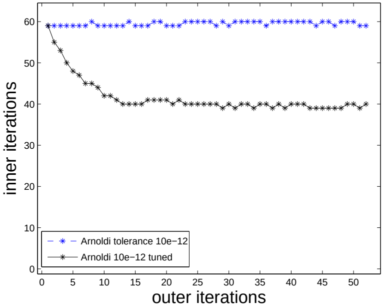

Figure: Inner iterations vs outer iterations

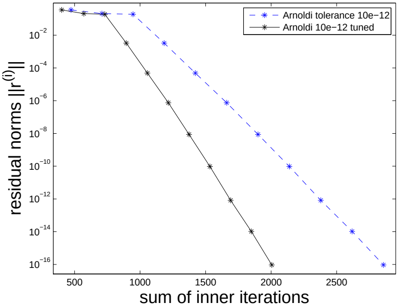

Figure: Eigenvalue residual norms vs total number of inner iterations

Relaxation

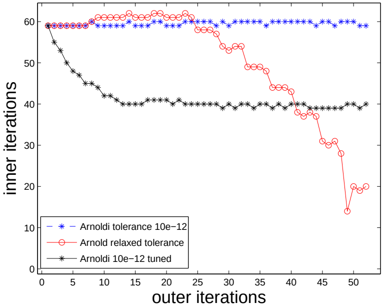

Figure: Inner iterations vs outer iterations

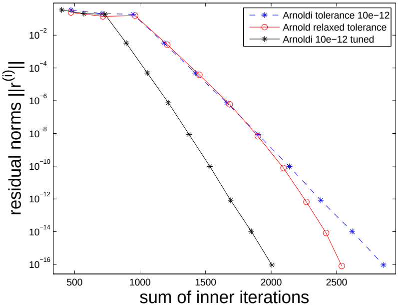

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning and relaxation strategy

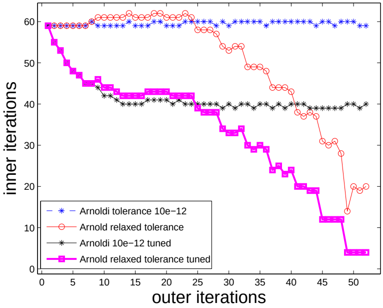

Figure: Inner iterations vs outer iterations

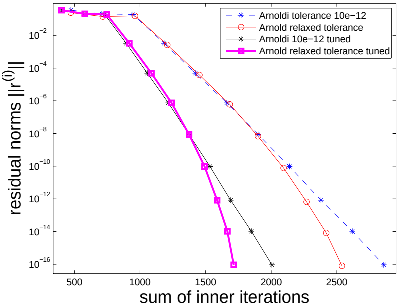

Figure: Eigenvalue residual norms vs total number of inner iterations

Numerical Example

`qc2534.mtx` matrix from the Matrix Market library.

- $k = 6$ eigenvalues closest to zero
- IRA with exact shifts $p = 4$
- Preconditioned GMRES as inner solver (fixed tolerance and relaxation strategy),
- standard and tuned preconditioner (incomplete LU).

Tuning and relaxation strategy

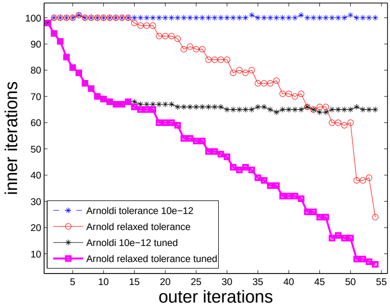

Figure: Inner iterations vs outer iterations

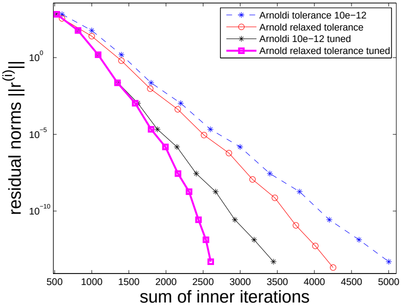

Figure: Eigenvalue residual norms vs total number of inner iterations

Outline

Conclusions

- For eigenvalue computations it is advantageous to consider small rank changes to the standard preconditioners
- Works for any preconditioner
- Works for SI versions of Power method, Simultaneous iteration, Arnoldi method
- Inexact inverse iteration with a special tuned preconditioner is equivalent to the Jacobi-Davidson method (without subspace expansion)
- For Arnoldi method best results are obtained when relaxation and tuning are combined

M. A. Freitag and A. Spence, *Rayleigh quotient iteration and simplified Jacobi-Davidson method with preconditioned iterative solves.*

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

———, *A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems*, IMA journal of numerical analysis, 28 (2008), p. 522.

———, *Shift-invert Arnoldi's method with preconditioned iterative solves*, SIAM Journal on Matrix Analysis and Applications, 31 (2009), pp. 942–969.

F. Xue and H. C. Elman, *Convergence analysis of iterative solvers in inexact rayleigh quotient iteration*, SIAM J. Matrix Anal. Appl., 31 (2009), pp. 877–899.

———, *Fast inexact subspace iteration for generalized eigenvalue problems with spectral transformation*, Linear Algebra and its Applications, (2010).