# Shift-invert Arnoldi method with preconditioned iterative solves

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joint work with Alastair Spence (Bath)

# Outline

Introduction

Shift-invert Arnoldi method and Implicit Restarts

Inexact Arnoldi/IRA

Preconditioning for the inner iteration

Conclusions

# Problem and iterative methods

Find a small number of eigenvalues and corresponding eigenvectors of:

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

- $A$ is large, sparse, nonsymmetric $\Rightarrow$ iterative solves
  - Power method
  - Simultaneous iteration
  - Arnoldi method
  - Jacobi-Davidson method

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  - Jacobi-Davidson method
- Usually involves repeated application of the matrix $A$ to a vector
- Generally convergence to largest/outlying eigenvector

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- 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 or Galerkin-Krylov method for linear systems.
- leading to inner-outer iterative method.

# Outline

# The algorithm

## Arnoldi's method

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

$$\mathcal{K}_k(\mathcal{A}, q_1) = \text{span}\{q_1, \mathcal{A}q_1, \mathcal{A}^2 q_1, \ldots, \mathcal{A}^{k-1} q_1\},$$

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

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$$\mathcal{A}q_k = \tilde{q}_{k+1}$$

# Enhancement 1: Shift-Invert Arnoldi



## Shift-Invert Arnoldi's method $\mathcal{A} := A^{-1}$ $(\sigma = 0)$

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$$\mathcal{K}_k(A^{-1}, q_1) = \text{span}\{q_1, A^{-1}q_1, {A^{-1}}^2 q_1, \ldots, {A^{-1}}^{k-1} q_1\},$$

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# Enhancement 2: Implicitly restarted Arnoldi (Sorensen (1992))

## Exact shifts

- take an $k + p$ step Arnoldi factorisation

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

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## Aim of IRA

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

# This talk

Extend the results by Simoncini (2005) for Arnoldi to IRA

Apply a "tailor-made" preconditioner for eigenproblems to Arnoldi and IRA

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- Wish to solve

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$$\begin{aligned} A^{-1}Q_m &= Q_{m+1}\begin{bmatrix} H_m \\ h_{m+1,m}e_k^H \end{bmatrix} + D_m \\ &= Q_{m+1}\begin{bmatrix} H_m \\ h_{m+1,m}e_m^H \end{bmatrix} + [d_1|\ldots|d_m] \end{aligned}$$

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- $u$ eigenvector of $H_m$:

$$\|r_m\| = \|(A^{-1}Q_m - Q_m H_m)u\| = |h_{m+1,m}||e_m^H u| + D_m u,$$

$$D_m u = \sum_{k=1}^{m} d_k u_k, \text{ if } \quad |u_k| \quad \text{small, then} \quad \|d_k\| \quad \text{allowed to be large!}$$

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$$D_m u = \sum_{k=1}^{m} d_k u_k, \text{ if } \quad |u_k| \quad \text{small, then} \quad \|d_k\| \quad \text{allowed to be large!}$$
- Simoncini (2005) has shown
$$|u_k| \leq C(k,m)\|r_{k-1}\|$$
which leads to
$$\|\tilde{d}_k\| = C(k,m)\frac{1}{\|r_{k-1}\|}\varepsilon$$
for $\|D_m u\| < \varepsilon$.

# Numerical Examples



`sherman5.mtx` nonsymmetric matrix from the Matrix Market library ($3312 \times 3312$).

- 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).

# Fixed tolerance

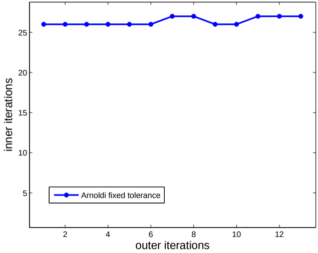



Figure: Inner iterations vs outer iterations

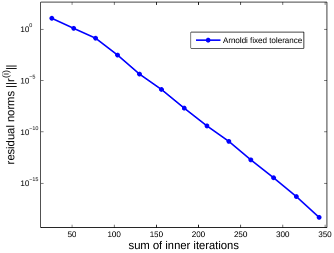
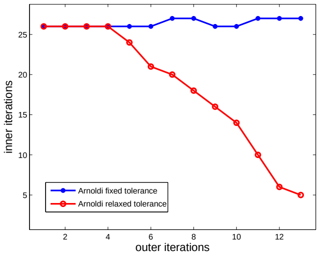



Figure: Eigenvalue residual norms vs total number of inner iterations

# Relaxation (Simoncini 2005)

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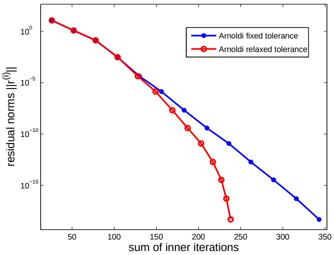


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# Relaxation strategy for invariant subspaces (F./Spence 2008)

- $m = k + p$ steps of the Arnoldi factorisation

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

- let $H_m$ have Schur decomposition

$$H_m = H_{k+p} = \begin{bmatrix} U & W_2 \end{bmatrix} \begin{bmatrix} \Theta & \star \\ 0 & T_{22} \end{bmatrix} \begin{bmatrix} U & W_2 \end{bmatrix}^H$$

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- let $H_k$ be decomposed as $\Theta_k = {U_k}^H H_k U_k$
- let $R_k = q_{k+1}h_{k+1,k}e_k^H U_k$ be the residual after $k$ Arnoldi steps.

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- Then $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$ with $U^H U = I$, such that

$$\|U_2\| \leq \frac{\|R_k\|}{\mathrm{sep}(T_{22}, \Theta_k)}$$

where $\mathrm{sep}(T_{22}, \Theta_k) := \min\limits_{\|V\|=1} \|T_{22}V - V\Theta_k\|$.

# Relaxation strategy for IRA (F./Spence 2008)

**Theorem**

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

$$\|d_l\| \leq \begin{cases} \dfrac{\varepsilon}{2(m-k)} \dfrac{sep(T_{22}, \Theta_k)}{\|R_k\|} & \text{if} \quad l > k, \\ \dfrac{\varepsilon}{2k} & \text{otherwise.} \end{cases}$$

*Then*

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

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

- In practice: perform $m = k + p$ initial steps and then relax the tolerance from the first restart.

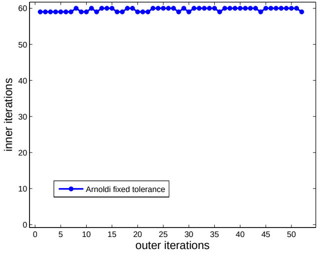
# Numerical Example



**sherman5.mtx** nonsymmetric matrix from the Matrix Market library ($3312 \times 3312$).

- $k = 8$ 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).

# Fixed tolerance

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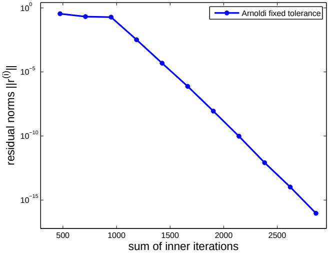


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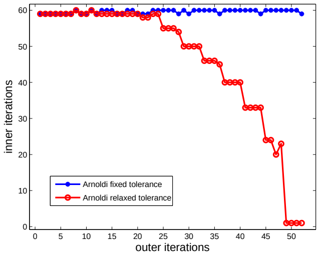


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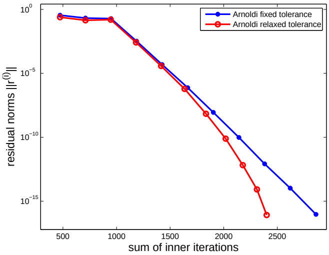


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# Tuning the preconditioner $AP^{-1}\tilde{q}_{k+1} = q_k$

- 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 (assuming $AP^{-1}$ diagonalisable):

$$\|d_l\| = \kappa \min_{p \in \Pi_l} \max_{i=1,\dots,n} |p(\mu_i)| \|d_0\|$$

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  - the condition number $\kappa$
  - the right hand side (initial guess)
- use a tuned preconditioner for Arnoldi's method

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

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

**Theorem (Properties of the tuned preconditioner $\mathbb{P}_k Q_k = AQ_k$)**

*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 equivalent to eigenvalues of $L \in \mathbb{C}^{n-k \times n-k}$ with*

$$\|L - I\| \leq C\|E\|.$$

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## Implementation

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

# Tuning

## Why does tuning help?

- Arnoldi decomposition

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

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- let $A^{-1}$ be transformed into 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

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

# Tuning

## Why does tuning help?

- Assume we have found an approximate invariant subspace, that is
$$A^{-1}Q_k = Q_k H_k + \underbrace{q_{k+1} h_{k+1,k} e_k^H}_{\approx 0}$$
- let $A^{-1}$ have the upper Hessenberg form
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## If $h_{k+1,k} = 0$ then

$$\begin{bmatrix} Q_k & Q_k{}^{\perp} \end{bmatrix}^H A\mathbb{P}_k^{-1} \begin{bmatrix} Q_k & Q_k{}^{\perp} \end{bmatrix} = \begin{bmatrix} I & Q_k^H A\mathbb{P}_k^{-1} Q_k^{\perp} \\ 0 & T_{22}^{-1}(Q_k^{\perp}{}^H P Q_k^{\perp})^{-1} \end{bmatrix}$$

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## Another advantage of tuning

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

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

# Numerical Example (Arnoldi)



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- standard and tuned preconditioner (incomplete LU).

# Relaxation

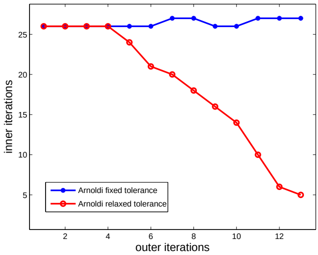


Figure: Inner iterations vs outer iterations

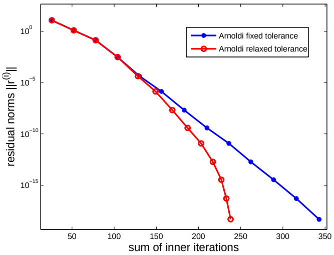


Figure: Eigenvalue residual norms vs total number of inner iterations

# Tuning the preconditioner

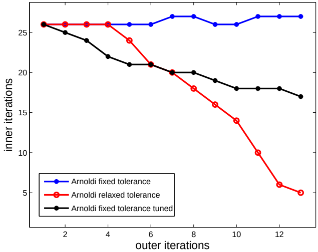


Figure: Inner iterations vs outer iterations

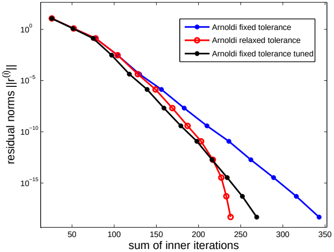


Figure: Eigenvalue residual norms vs total number of inner iterations

# Tuning and relaxation strategy

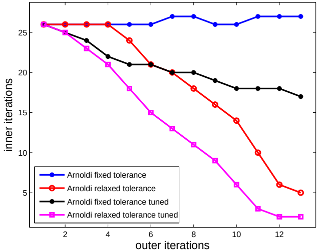


Figure: Inner iterations vs outer iterations

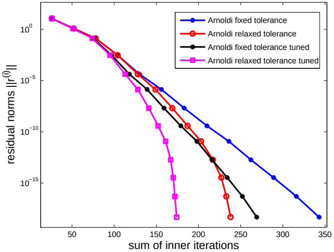


Figure: Eigenvalue residual norms vs total number of inner iterations

# Ritz values of exact and inexact Arnoldi

| Exact eigenvalues | Ritz values (exact Arnoldi) | Ritz values (inexact Arnoldi, tuning) |
|---|---|---|
| +4.69249563e-02 | +4.69249563e-02 | +4.69249563e-02 |
| +1.25445378e-01 | +1.25445378e-01 | +1.25445378e-01 |
| +4.02658363e-01 | +4.02658347e-01 | +4.02658244e-01 |
| +5.79574381e-01 | +5.79625498e-01 | +5.79817301e-01 |
| +6.18836405e-01 | +6.18798666e-01 | +6.18650849e-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.

# Numerical Example (IRA)

`sherman5.mtx` nonsymmetric matrix from the Matrix Market library ($3312 \times 3312$).

- $k = 8$ 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).

# Relaxation

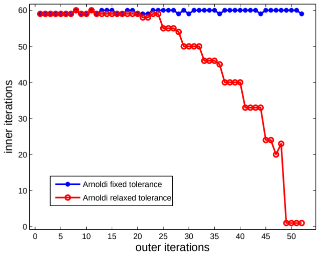


Figure: Inner iterations vs outer iterations

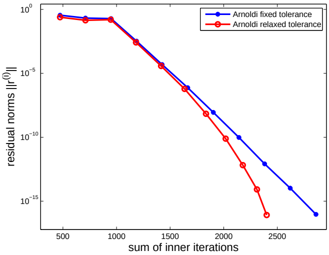


Figure: Eigenvalue residual norms vs total number of inner iterations

# Tuning

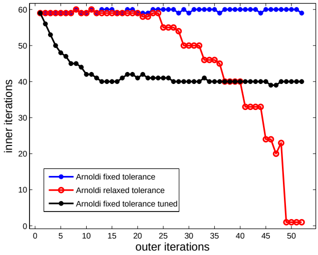


Figure: Inner iterations vs outer iterations

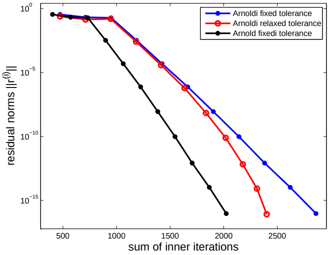


Figure: Eigenvalue residual norms vs total number of inner iterations

# Tuning and relaxation strategy

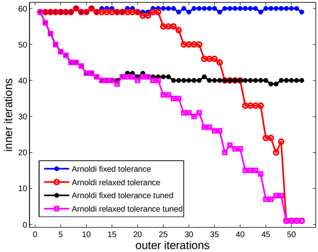


Figure: Inner iterations vs outer iterations

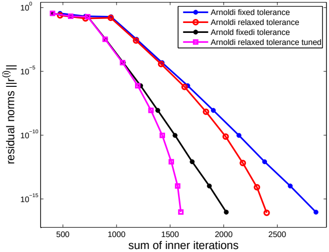


Figure: Eigenvalue residual norms vs total number of inner iterations

# 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

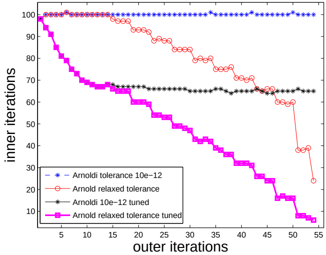


Figure: Inner iterations vs outer iterations

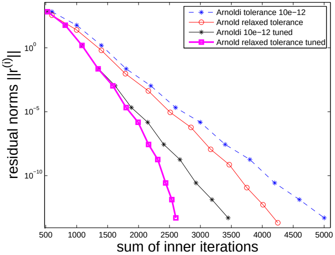


Figure: Eigenvalue residual norms vs total number of inner iterations

# Outline

# Conclusions

- Use modified preconditioners for eigencomputations (works for any preconditioner)
- Extension of the relaxation strategy to IRA
- Upto 50 per cent savings are obtained when relaxation and tuning are combined
- Link to Jacobi-Davidson method (for inexact inverse iteration, see talk A Spence later this week)