Inexact Preconditioned Shift-and-Invert Arnoldi's method and Implicit Restarts for Eigencomputations

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Introduction

Find a small number of eigenvalues and eigenvectors of a nonsymmetric matrix $\mathbf{A}$:

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

since A is large and sparse, iterative solves are used.

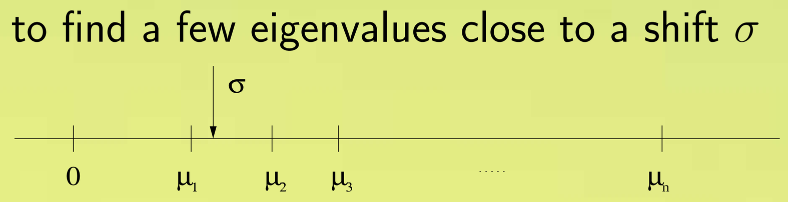
- Power method
- Simultaneous iteration
- Arnoldi method

These methods involve

- repeated application of the matrix A to a vector and
- they generally convergence to largest/outlying eigenvector.

Shift-invert strategy

If we wish to find a few eigenvalues close to a shift σ



then the problem becomes

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

and each step of the iterative method involves repeated application of $(A - \sigma I)^{-1}$ to a vector and hence an Inner iterative solve becomes necessary:

$$(A - \sigma I) y = x$$

This is usually done using Krylov subspace methods and hence this approach leads to inner-outer iterative method.

Shift-Invert Arnoldi's method with $\sigma = 0$

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

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

such that

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

where $Q_k^H Q_k = I$. Eigenvalues of H_k are eigenvalue approximations of (outlying) eigenvalues of A^{-1}

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

At each step, application of A^{-1} to q_k is necessary.

Inexact solves

At each step of Arnoldi's method we wish to solve

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

which leads to an inexact Arnoldi relation

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

For an eigenvector of H_k we have:

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

and the linear combination of the columns of D_k

$$D_k u = \sum_{l=1}^{k} d_l u_l,$$

and if $|u_l|$ is small then $\|d_l\|$ is allowed to be large! (Simoncini 2005, Bouras and Frayssé 2000). One can show that

$$|u_l| \le C(l,k) \|r_{l-1}\|$$

which leads to

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

and hence

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

Preconditioning for the inner iteration

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 convergence bound for GMRES is

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

depending on

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

We propose to use a tuned preconditioner for Arnoldi's method, that is a rank-k update of the standard preconditoner:

$$\mathbf{P}_k Q_k = A Q_k$$

given by

$$\mathbf{P}_k = P + (A - P) Q_k Q_k^H.$$

Properties of the tuned preconditioner

Theorem: 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 $A\mathbf{P}_k^{-1}$ are equal to one:

$$[A\mathbf{P}_k^{-1}] A Q_k = A Q_k$$

and $n - k$ eigenvalues are close to the corresponding eigenvalues of AP^{-1}. They are eigenvalues of $L \in \mathbb{C}^{n-k \times n-k}$ with

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

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
- Use both fixed tolerance and relaxation strategy,
- Use both standard and tuned preconditioner (incomplete LU factorisation).

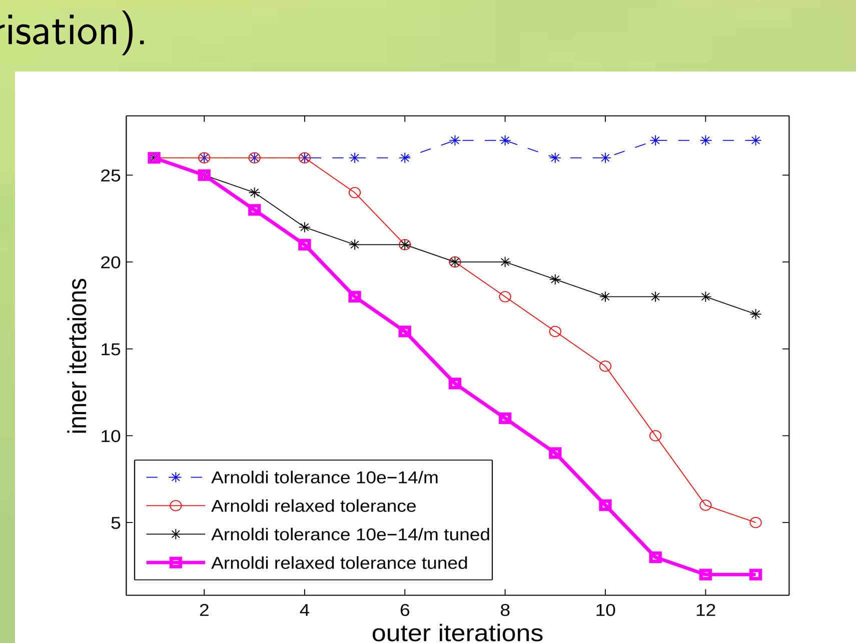


Figure 2: Inner iterations vs outer iterations

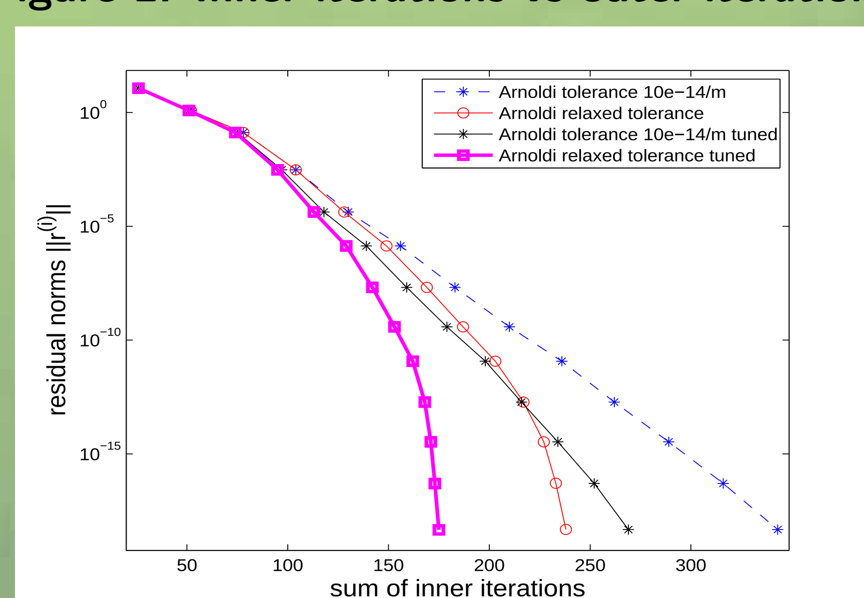


Figure 3: Eigenvalue residual norms vs total number of inner iterations

Implicit restarts with exact shifts

We take an $k + p$ step Arnoldi factorisation

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

Then we compute $\Lambda(H_{k+p})$ and select p shifts for an implicit QR iteration and restart implicitly with new starting vector $\hat{q}^{(1)} = \frac{p(A^{-1})q^{(1)}}{\|p(A^{-1})q^{(1)}\|}$ (Sorensen 1992). The aim of IRA is

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

We can generalise the relaxation strategy to approximate invariant subspaces.

Preconditioning for the inner iteration

Assume we have found an invariant subspace, that is

$$A^{-1} Q_k = Q_k H_k.$$

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

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

where $\left[Q_k \; Q_k^{\perp} \right]$ 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

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

Also, if convergence to an invariant subspace has occured, the right hand side of the system matrix is an eigenvector of the system, and GMRES converges in one iteration.

Numerical Example

- sherman5.mtx, $k = 8$ eigenvalues closest to zero
- IRA with exact shifts $p = 4$
- Preconditioned GMRES as inner solver

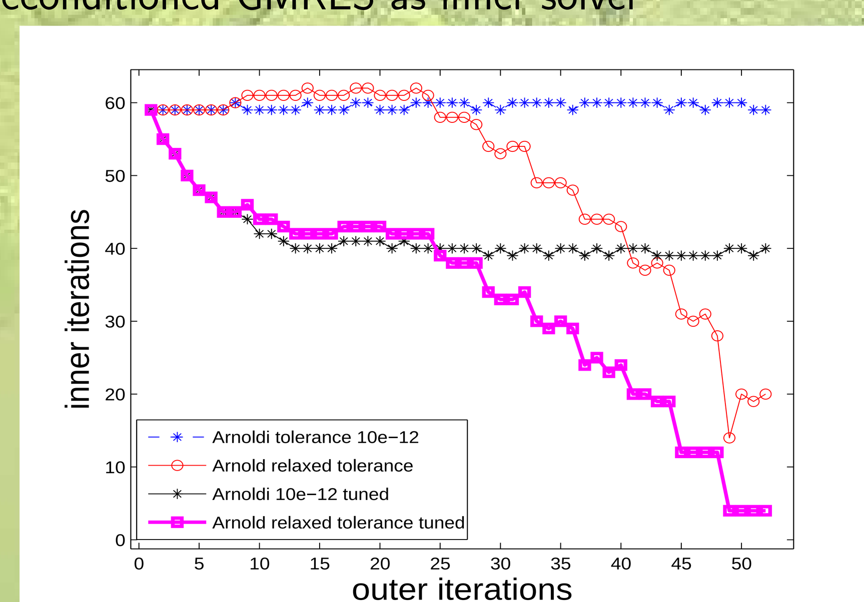


Figure 4: Inner iterations vs outer iterations

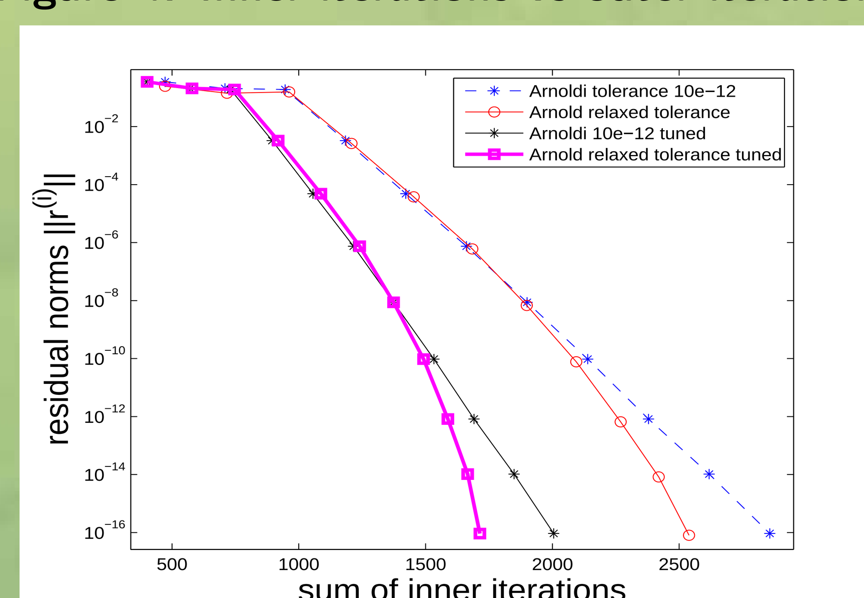


Figure 5: Eigenvalue residual norms vs total number of inner iterations

Conclusions

For eigencomputations it is advantageous to consider small rank changes to the standard preconditioners. Best results are obtained when relaxation and tuning are combined.

References

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