Inexact shift-and-invert Arnoldi's method and implicit restarts with preconditioning for eigencomputations

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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

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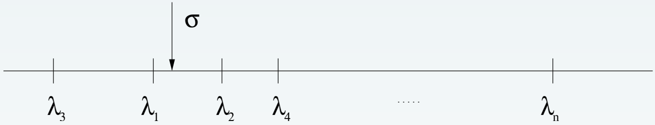
- A is large, sparse, nonsymmetric
- Iterative solves
  - Power method
  - Simultaneous iteration
  - Arnoldi method
  - Jacobi-Davidson method
- The first three of these involve repeated application of the matrix A to a vector
- Generally convergence to largest/outlying eigenvector

Shift-invert strategy

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



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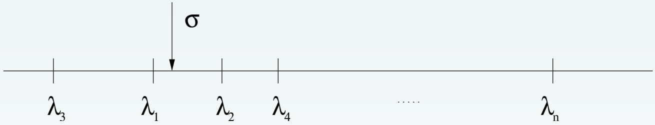

- Problem becomes

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

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

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

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

Outline

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The algorithm

Arnoldi's method

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

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

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

$$Q_k^H Q_k = I.$$

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

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

The algorithm: take $\sigma = 0$ then $\mathcal{A} := A^{-1}$

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

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

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

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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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- 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

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

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

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

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

  depending on

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- 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}. They are eigenvalues of $L \in \mathbb{C}^{n-k\times n-k}$ with

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

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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

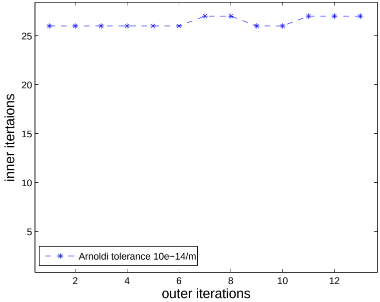


Figure: Inner iterations vs outer iterations

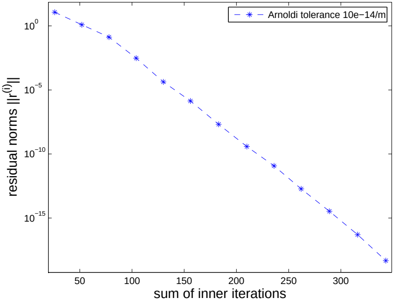
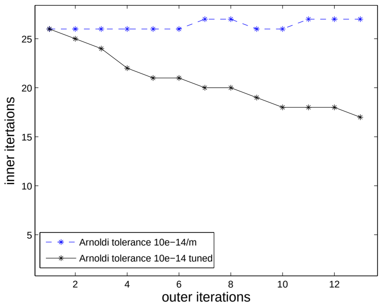


Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning the preconditioner



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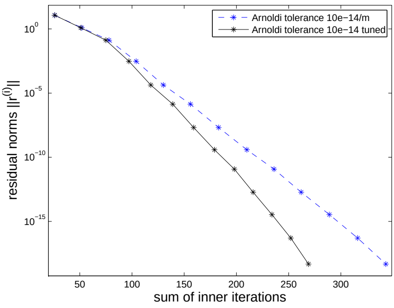

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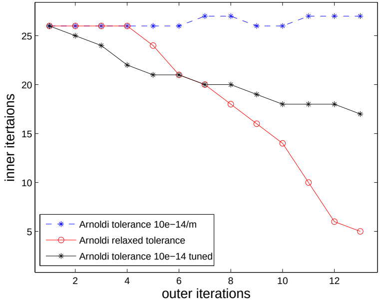
Relaxation



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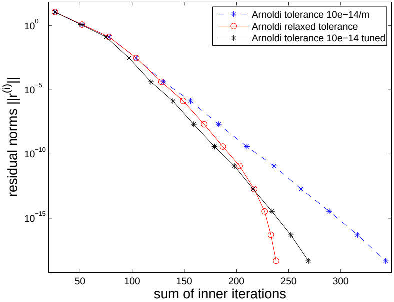

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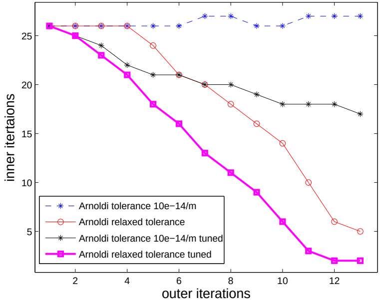
Tuning and relaxation strategy



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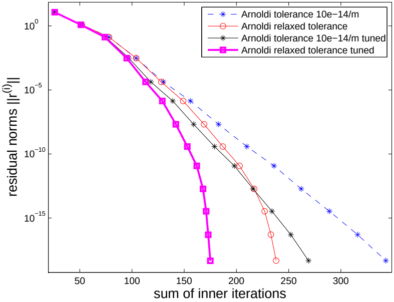

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Ritz values of exact and inexact Arnoldi

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

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

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- 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

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

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

- let H_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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- let $R_k = q_{k+1}h_{k+1,k}e_k^H U_k$ be the residual after k Arnoldi steps.
- Then $U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}$ with $U^H U = I$, whose columns span a k-dimensional invariant subspace of H_m, such that

$$\|U_2\| \leq C(k)\|R_k\| \qquad \star$$

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

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

Relaxation strategy for IRA

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Then

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

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

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

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

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

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

Tuning

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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- 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

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

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

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

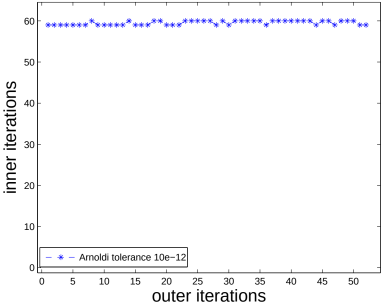

Figure: Inner iterations vs outer iterations

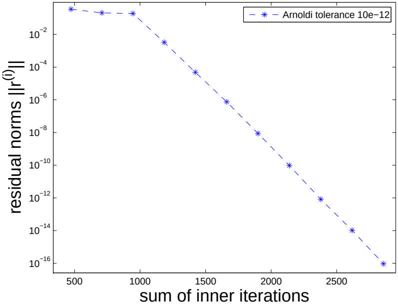

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning

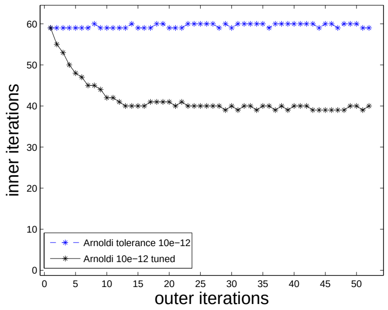

Figure: Inner iterations vs outer iterations

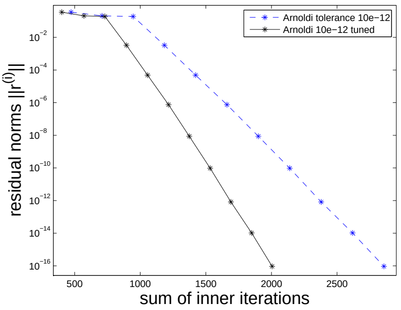

Figure: Eigenvalue residual norms vs total number of inner iterations

Relaxation

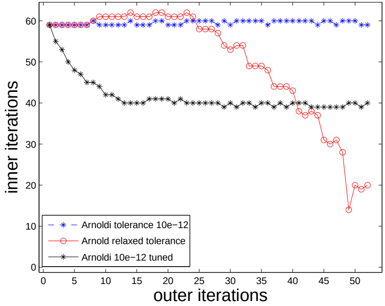

Figure: Inner iterations vs outer iterations

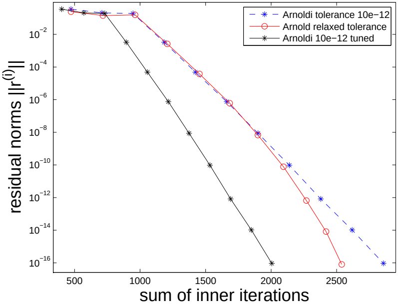

Figure: Eigenvalue residual norms vs total number of inner iterations

Tuning and relaxation strategy

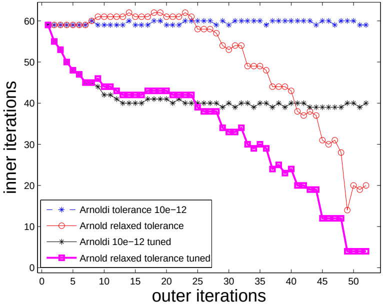

Figure: Inner iterations vs outer iterations

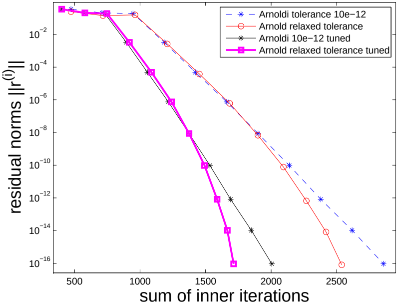

Figure: Eigenvalue residual norms vs total number of inner iterations

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

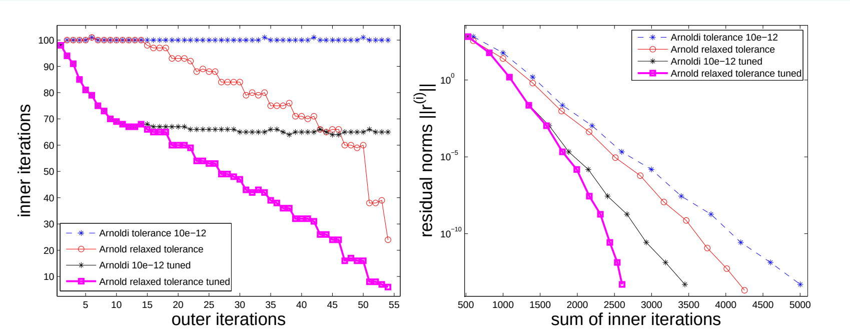

Figure: Inner iterations vs outer iterations

Figure: Eigenvalue residual norms vs total number of inner iterations

Outline

Conclusions

- For eigencomputations it is advantageous to consider small rank changes to the standard preconditioners (works for any preconditioner)
- Extension of the relaxation strategy to IRA
- Best results are obtained when relaxation and tuning are combined
- Current work: Link to Jacobi-Davidson

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