A tuned preconditioner for Hermitian eigenproblems

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Introduction
Consider the computation of a simple eigenvalue and corresponding eigenvector of a large sparse Hermitian positive definite matrix using either inexact inverse iteration with a fixed or Rayleigh quotient shift.

- large sparse linear systems solved approximately by means of symmetrically preconditioned MINRES,
- preconditioners (incomplete Cholesky factorisation)
- derivation of a new tuned Cholesky preconditioner,
- analysis using the convergence theory for MINRES,
- comparison of spectral properties of the tuned with those of the standard preconditioned matrix,
- perturbation and interlacing results.

Inexact inverse iteration (III) with fixed shift

Given \( \sigma \) and \( x_0 \) with \( \| x_0 \| = 1 \). For \( i = 0, 1, 2, \ldots \)

- Choose \( \xi_i \).
- Solve \( (A - \sigma I)x_i = x_{i-1} \) inexact, that is,

\[
\| (A - \sigma I)x_i - x_{i-1} \| \leq \varepsilon_i.
\]

- Compute \( x_i = (A - \sigma I)^{-1}x_{i-1} \).
- Evaluate \( r_i = (A - \sigma I)r_{i-1} \).
- Test for convergence.

Convergence rates

For a decreasing tolerance \( \varepsilon_i \) with \( \varepsilon_i = O(\sin(\theta_i)) \) and close enough starting guesses the inexact method recovers the rate of convergence achieved by exact solves.

- Fixed shift: linear convergence \([4], [11]\).
- Rayleigh quotient shift: cubic convergence \([11], [5]\).

Convergence theory of MINRES

- symmetric B has eigenvalues \( \mu_1, \ldots, \mu_n \), and eigenvectors \( w_1, \ldots, w_n \), \( k = \frac{1}{\mu_1} \leq \ldots \leq k = \frac{1}{\mu_n} \) reduced condition number,

\[
P = \sum_{i=1}^{n} w_i w_i^*.
\]

- \( P^* \) orthogonal projection along \( w_i \) onto span\( \{w_1, \ldots, w_n\} \).

If \( z_0 \) is the result of applying MINRES to \( Bz = b \) with starting value \( z_0 = 0 \) then

\[
\| b - Bz_0 \| \leq 2 \max_{j=2,n} \left| \frac{\mu_j - \mu_1}{\mu_1 \mu_j} \right| \frac{1}{\sqrt{\kappa^2 + 1}} \| P^n b \|.
\]

If, using \( \| P^n b \| = \| \sin(\theta_i) \| \), the number of inner iterations satisfies

\[
k_i \geq \frac{1}{\sqrt{2}} \left( \log \left( \frac{\kappa}{\kappa + 1} \right) + \log \| \sin(\theta_i) \| \right),
\]

then \( \| b - Bz_i \| \leq \kappa_i \). The number of inner iterations does not increase with \( i \), if \( \kappa_1 \) is fixed and \( \kappa_i = O(\sin(\theta_i)) \).

Preconditioned inexact inverse iteration

Let \( A \) be Hermitian positive definite and consider the incomplete Cholesky factorisation \( LL^* \), that is,

\[
A = LL^* + E.
\]

Solve

\[
L^{-1}(A - \sigma LL^*) \tilde{x}_i^{(j)} = L^{-1} x_0^{(j)}, \quad y_i^{(j)} = L^{-1} y_0^{(j)},
\]

to a tolerance \( \gamma_i \| L^{-1} \|_2 \) so that \( \| x_0^{(j)} - (A - \sigma I)y_0^{(j)} \| \leq \gamma_i \)

- does not change the outer iteration of convergence,

\[
k_i^{(j)} \geq \frac{1}{\sqrt{2}} \left( \log \left( \frac{\kappa_i}{\kappa_i + 1} \right) + \log \frac{1}{\gamma_i} \right),
\]

increases for \( \gamma_i \), \( i = 0 \).

The tuned preconditioner

Solve the preconditioned Hermitian system

\[
L^{-1}(A - \sigma LL^*) x_i^{(j)} = L^{-1} x_0^{(j)}, \quad y_i^{(j)} = L^{-1} y_0^{(j)},
\]

 inexactly, where \( L \) is chosen such that the right hand side of (6) is close to the eigenvector of \( L^{-1}(A - \sigma I) L^{-1} \) corresponding to the eigenvalue closest to \( \sigma \).

- reproduces the inner iteration behaviour observed for unpreconditioned solves,

- requires the preconditioner \( LL^* \) to satisfy

\[
\| LL^* x_0^{(j)} - Ax_0^{(j)} \| \leq C \| r_0^{(j)} \|,
\]

Then

\[
\| (P^n LL^*) x_0^{(j)} \| \leq C \| r_0^{(j)} \|
\]

and with \( \tau^{(j)} = C \| r_0^{(j)} \| \), we obtain

\[
k_i^{(j)} \geq 1 + \frac{\sqrt{2}}{\kappa_i} \left( \log \left( \frac{\kappa_i}{\kappa_i + 1} \right) + \log \frac{1}{\gamma_i} \right),
\]

that is no increase with \( i \).

Implementation

Let \( A \) be Hermitian positive definite and consider its incomplete Cholesky factorisation \( LL^* \), \( A = LL^* + E \).

- \( \mu_0 \) approximate eigenvector from the \( i \)th iteration,

\[
x_i^{(0)} = \mu_0 \}

- compute \( x_i^{(0)} \) using \( \left( A - \sigma I \right)^{-1} \).

Evaluate \( r_i^{(0)} = \left( A - \sigma I \right)r_i^{(0)} \).

Test for convergence.

Spectral analysis - Perturbation

Comparison of the spectral properties of

\[
L^{-1}(A - \sigma I) LL^{-1} \quad \text{and} \quad L^{-1}(A - \sigma I) L^{-1}.
\]

Define \( S = L^{-1}(A - \sigma I) LL^{-1} \) and consider the two eigenvalue problems

\[
Sw = \omega w
\]

and

\[
Sw = (1 + \gamma w) v
\]

Then \( \mu \) and \( \xi \) are nonzero and

\[
\min_{\mu \neq \xi} \frac{|\mu - \xi|}{|\xi|} \leq |\gamma w|.
\]

Spectral analysis - Interlacing

Consider the two eigenvalue problems

\[
L^{-1}(A - \sigma I) LL^{-1} w = \mu w
\]

and

\[
L^{-1}(A - \sigma I) L^{-1} w = \xi w,
\]

and assume condition (10) holds. Suppose \( D = diag(\mu_1 < \ldots < \mu_n) \in \mathbb{R}^{n \times n} \). Transform the problem to a generalised eigenproblem

\[
D \tilde{y} = \xi \tilde{y}.
\]

Conclusions

For III the tuning of the preconditioner reduces the number of inner iterations for the iterative solves in each step.

References