Spectral Transformation Lanczos Algorithm for the Symmetric Definite Generalized Eigenvalue Problem

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Problem Statement

The Symmetric Definite Generalized Eigenvalue Problem

For $n \times n$ real matrices $A = A^{\mathrm{T}}$ and positive definite (or semidefinite) $B = B^{\mathrm{T}}$, find $\boldsymbol{v} \neq \mathbf{0}$ and λ such that

$$A\boldsymbol{v} = \lambda B\boldsymbol{v}$$

where $\mathcal{N}(A) \cap \mathcal{N}(B) = \{\mathbf{0}\}$. The value λ is a generalized eigenvalue and $\boldsymbol{v}$ is the corresponding generalized eigenvector. If B is invertible, the generalized eigenvalues are eigenvalues for $B^{-1}A\boldsymbol{v} = \lambda\boldsymbol{v}$. Otherwise, for $B\boldsymbol{v} = \mathbf{0}$, we say that $\lambda = \infty$ is an eigenvalue. If B is positive definite, there are n linearly independent eigenvectors.

We assume throughout that $A \neq 0$ and $B \neq 0$.

Applications and Algorithms

- Vibration Analysis in Structural engineering e.g (Boeing). For example, equation of a vibrating system:

$$K\mathbf{x} = \lambda M\mathbf{x}$$

  where M is the mass matrix, K is the stiffness matrix, $\mathbf{x}$ is the displacement vector, and λ is the eigenfrequencies of the system.
- Existing factorization algorithms for the dense problem all have performance and/or stability issues.
- Recent work on direct methods have proven residual bounds for dense problems. [Michael Stewart, 2024].
- This work is about applying an iterative method to the sparse problem, and verifying the residual bounds predicted by direct methods.
- We start with a survey of existing methods.

The Standard Algorithm (J.H. Wilkinson, 1965)

If B is positive definite then it has a Cholesky factor

$$B = C_b C_b^{\mathrm{T}}.$$

Thus

$$\begin{aligned} & A\boldsymbol{v} = \lambda B\boldsymbol{v} \\ \Leftrightarrow\ & A\boldsymbol{v} = \lambda C_b C_b^{\mathrm{T}}\boldsymbol{v} \\ \Leftrightarrow\ & C_b^{-1} A C_b^{-\mathrm{T}} C_b^{\mathrm{T}}\boldsymbol{v} = \lambda C_b^{\mathrm{T}}\boldsymbol{v}. \end{aligned}$$

Standard Reduction to an Ordinary Eigenvalue Problem

Solve the symmetric eigenvalue problem

$$C_b^{-1} A C_b^{-\mathrm{T}}\boldsymbol{u} = \lambda\boldsymbol{u}, \qquad \boldsymbol{u} \neq \mathbf{0}$$

Then solve $C_b^{\mathrm{T}}\boldsymbol{v} = \boldsymbol{u}$.

The Standard Algorithm (cont'd)

- This shows that the symmetric definite generalized eigenvalue problem has real eigenvalues. Eigenvectors are orthogonal with respect to the inner product $(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{y}^{\mathrm{T}} B \boldsymbol{x}$.
- It is fast and it is the approach used by LAPACK.
- It fails if B is semidefinite and is unstable when B is ill-conditioned (i.e. $\kappa_2(B) = \|B\|_2 \|B^{-1}\|_2$ is large.)
- If B is ill-conditioned, it usually delivers small residuals for large eigenvalues and large residuals for small eigenvalues.
- There are alternatives, each with its own set of problems. . .

An Alternate Formulation

The generalized eigenvalue problem can be formulated in another way as follows:

The Generalized Eigenvalue Problem Version II

The eigenvalue problem can be written

$$\beta A\boldsymbol{v} = \alpha B\boldsymbol{v}$$

where $\boldsymbol{v} \neq \mathbf{0}$ and β and α are not both zero. The original formulation eigenvalues are given by $\lambda = \alpha/\beta$. Each eigenvalue is a nonunique pair (α, β) that can be scaled by $c \neq 0$. It can be identified with a subspace of $\mathbb{R}^2$ (or $\mathbb{C}^2$):

$$\mathcal{E} = \{c \cdot (\alpha, \beta) : c \in \mathbb{R}\}$$

The QZ Algorithm I (C. B. Moler and G. W. Stewart, 1972)

Generalized Schur Form

For A and B not necessarily symmetric, there exist unitary Q and Z such that

$$Q^H A Z = T_a, \qquad Q^H B Z = T_b.$$

where T_a and T_b are upper triangular with diagonal elements α_i and β_i. The eigenvalues for $A\boldsymbol{v} = \lambda B\boldsymbol{v}$ are given by $\lambda_i = \alpha_i/\beta_i$. Eigenvectors can be obtained from Z with additional computation.

- With rounding, the QZ algorithm for computing this is backward stable: There exist exactly unitary $\tilde{Q}$ and $\tilde{Z}$ close to the computed Q and Z for which the computed T_a and T_b satisfy

$$\tilde{Q}^H (A + E)\tilde{Z} = T_a, \qquad \tilde{Q}^H (B + F)\tilde{Z} = T_b.$$

More on the QZ Algorithm

- The errors satisfy $\|E\| = O(u)\|A\|$ and $\|F\| = O(u)\|B\|$, where u is the unit roundoff. ($u \approx 10^{-16}$ for double precision.)
- The pairs (α_i, β_i) are exact generalized eigenvalues of matrices close to A and B.
- The algorithm is much slower than the standard algorithm.
- Unfortunately E and F are not guaranteed to be symmetric even when A and B are. The computed eigenvalues can even have imaginary parts that are not small. Simply truncating the imaginary part does not give satisfactory results.

Diagonalization Using Congruences
S. Chandrasekaran 2000

Diagonalization

For the symmetric definite problem there exists nonsingular Z such that

$$A = ZD_aZ^{\mathrm{T}}, \qquad B = ZD_bZ^{\mathrm{T}}.$$

If α_i and β_i are the diagonal elements of D_a and D_b, then the generalized eigenvalues are (α_i, β_i) or $\lambda_i = \alpha_i/\beta_i$. The eigenvectors are the columns of $V = Z^{-\mathrm{T}}$.

- It can be shown that $V = Z^{-\mathrm{T}}$ is a good eigenvector matrix.
- It is as close to ideal numerically as any current algorithm.
- It involves solving multiple ordinary eigenvalue problems and its complexity is not proven to be $O(n^3)$.

Spectral Transformation Lanczos [T. Ericsson and A. Ruhe, 1980]

Lemma

Let $\lambda = \alpha/\beta \neq \infty$ and $\boldsymbol{v} \neq 0$ satisfy $A\boldsymbol{v} = \lambda B\boldsymbol{v}$. Assume that $A - \sigma B$ is nonsingular and $B = C_b C_b^{\mathrm{T}}$, $C_b \in \mathbb{R}^{n\times r}$ with linearly independent columns. Then $\theta = 1/(\lambda - \sigma)$ is an eigenvalue of the shifted and inverted problem

$$C_b^{\mathrm{T}}(A - \sigma B)^{-1} C_b \boldsymbol{u} = \theta \boldsymbol{u}, \qquad \boldsymbol{u} \neq \mathbf{0}.$$

with eigenvector $\boldsymbol{u} = C_b^{\mathrm{T}}\boldsymbol{v} \neq \mathbf{0}$.
Conversely, assume that $\boldsymbol{u} \neq \mathbf{0}$ is an eigenvector for the shifted and inverted problem with eigenvalue θ. Then the vector $\boldsymbol{v} = (A - \sigma B)^{-1} C_b \boldsymbol{u} \neq 0$ is an eigenvector for the eigenvalue $(1 + \sigma\theta, \theta)$ of the original problem.

Spectral Transformation for Dense Problems [Michael Stewart, 2024]

This direct method employs the spectral transformation described by [T. Ericsson and A. Ruhe, 1980], and symmetric decompositions of $A - \sigma B$ and B such that

$$A - \sigma B = C_a D C_a^{\mathrm{T}}, \qquad \text{and} \qquad B = C_b C_b^{\mathrm{T}},$$

to transform the problem into a symmetric standard eigenvalue problem given by

$$C_b^{\mathrm{T}} C_a^{-T} D_a C_a^{-1} C_b \boldsymbol{u} = \theta \boldsymbol{u}, \qquad \boldsymbol{v} = C_a^{-\mathrm{T}} D_a C_a^{-1} C_b \boldsymbol{u}$$

with $(\alpha, \beta) = (1 + \sigma\theta, \theta)$ or $\lambda = (1 + \sigma\theta)/\theta$.

- B can factored using pivoted Cholesky and A using LDL^{T} factorization with rook pivoting, both available in LAPACK.
- We cannot expect a shift to result in well conditioned $A - \sigma B$ or C_a, **but ill conditioning is not what matters!**

Interesting Questions

- Do the residual bounds proven for a direct method applies when an iterative method is used for the spectral transformed problem?
- Does the spectral transformed problem respects symmetry in the decomposition of $A - \sigma B$?

What is our approach?

- Apply the Lanczos algorithm to the spectral problem
- Investigate if the residuals for the computed eigenvalues follows the bounds for the direct methods in terms of the choice of shift?
- Explore the effect of symmetric decomposition of $A - \sigma B$ on residuals

Spectral Transformation Lanczos Algorithm I

1: **function** SPECTRAL_LANCZOS(A, B, m, n, σ, tol)
2: Choose an arbitrary vector $\mathbf{b}$ and set an initial vector $\mathbf{q_1} = \mathbf{b}/\|\mathbf{b}\|_2$
3: Set $\beta_0 = 0$ and $\mathbf{q_0} = \mathbf{0}$
4: Set $Q = \text{zeros}(m, n+1)$
5: Precompute the LU factorization of $A - \sigma B$: $LU = (A - \sigma B)$
6: Factor: $B = CC^T$
7: **for** $j = 1, 2, \ldots, n$ **do**
8: $Q[:, j] = \mathbf{q}_j$
9: $\mathbf{u} = C\mathbf{q}_j$
10: Solve: $(LU)\mathbf{v} = \mathbf{u}$ for $\mathbf{v}$

Spectral Transformation Lanczos Algorithm II

$\mathbf{v} = \mathbf{v} - \beta_{j-1}\mathbf{q}_{j-1} - \alpha_j \mathbf{q}_j$

Full reorthogonalization: $\mathbf{v} = \mathbf{v} - \sum_{i \leq j} (\mathbf{q}_i^T \mathbf{v}) \mathbf{q}_i$

$\beta_j = \|\mathbf{v}\|_2$

if $\beta_j < tol$ **then**

    restart or **exit**

end if

$\mathbf{q}_{j+1} := \mathbf{v}/\beta_j$

end if

end for

$Q = Q[:, : n]$

$\mathbf{q} = Q[:, n]$

return $(Q, T, \mathbf{q})$

end function

Some Definitions from [Michael Stewart, 2024]

$$X = C_a^{-1} C_b, \qquad W = X^{\mathrm{T}} D_a X, \qquad \mu = \frac{\|X\|_2^2}{\|W\|_2} \geq 1.$$

$$\eta = \frac{\|A - \sigma B\|_2^{1/2}}{\|B\|_2^{1/2}}, \qquad \sigma_0 = \sigma \frac{\|B\|_2}{\|A\|_2}, \qquad \text{and} \qquad \gamma = \frac{\|A\|_2}{\|A - \sigma B\|_2}.$$

- The shifted and inverted problem is $W\boldsymbol{u} = \theta \boldsymbol{u}$.
- The only "inversion" is in solving $C_a X = C_b$.
- The values of μ, $\eta\|X\|_2$, σ_0, and γ can potentially impact stability.
- $\eta\|X\|_2$ is the most interesting and important of these.

Bounds for $\eta\|X\|_2$

We have

$$\eta^2\|X\|_2^2 \leq \mu\kappa_2(A - \sigma B)$$

and even better

Lemma

Assume that $\sigma \neq 0$ and $A - \sigma B$ is invertible. Then

$$\begin{aligned}\eta^2\|X\|_2^2 &\leq \left(1 + \frac{1}{|\sigma_0|}\right)\frac{\mu}{\min_i \left|1 - \frac{\lambda_i}{\sigma}\right|} \\ &= (1 + |\sigma_0|)\frac{\mu}{\min_i \left|\frac{\|B\|_2}{\|A\|_2}\lambda_i - \sigma_0\right|}.\end{aligned}$$

Forward Errors

- **The size of $\eta^2\|X\|_2^2$ determines stability and it is usually much smaller than $\kappa_2(A-\sigma B)$.**
- It is surprisingly easy to avoid large $\eta\|X\|_2$. In practice, if $|\sigma_0|$ is not small, $\eta\|X\|_2$ is large only if σ is chosen to match an eigenvalue λ to several digits. A random shift in a reasonable interval almost always works.
- If A and B are both positive definite, all generalized eigenvalues are positive, $\mu = 1$, and simply choosing $\sigma_0 = -1$ gives

$$\eta^2\|X\|_2^2 \leq \left(1+\frac{1}{1}\right)\frac{1}{\min_i\left|1+\frac{|\lambda_i|}{|\sigma|}\right|} \leq 2$$

Error Bounds: Moderate Shifts and Eigenvalue Stability

Eigenvalue Backward Errors

For the computed θ_i, there exist symmetric E and F and a vector $\tilde{\boldsymbol{v}}_i \neq \mathbf{0}$ such that

$$\theta_i(A+E)\tilde{\boldsymbol{v}}_i = (1+\sigma\theta_i)(B+F)\tilde{\boldsymbol{v}}_i$$

and

$$\max\left(\frac{\|E\|_2}{\|A\|_2}, \frac{\|F\|_2}{\|B\|_2}\right) \leq O(u)(1+|\sigma_0|)\eta^2\|X\|_2^2 + O(u^2)$$

If $|\sigma_0|$ is not large and $\eta^2\|X\|_2^2$ is not large, each $(1+\sigma\theta_i, \theta_i)$ is an eigenvalue of a pair close to (A, B).

Error Bounds: Moderate Shifts with Computed Eigenvectors

Computed Eigenvector Bounds

There exist symmetric E and F such that the computed θ_i and the computed eigenvector $\boldsymbol{v}_i$ satisfy

$$\theta_i(A+E)\boldsymbol{v}_i = (1+\sigma\theta_i)(B+F)\boldsymbol{v}_i$$

with

$$\max\left(\frac{\|E\|_2}{\|A\|_2}, \frac{\|F\|_2}{\|B\|_2}\right) \leq$$

$$O(u)|1-\lambda_i/\sigma||\sigma_0|\left(1+\max(\gamma,1)\left(1+|1-\lambda_i/\sigma|\right)\eta^2\|X\|_2^2\right)+O(u^2)$$

If $|\sigma_0|$ and $\eta^2\|X\|_2^2$ are not large, $A-\sigma B$ does not cancel, and $\lambda_i = (1+\sigma\theta_i)/\theta_i$ is not much larger than σ, then each $(1+\sigma\theta_i, \theta_i)$ and $\boldsymbol{v}_i$ is an eigenvalue/eigenvector of a pair close to (A, B).

Error Bounds: Large Shifts with Computed Eigenvectors

Computed Eigenvector Bounds

There exist symmetric E and F such that the computed θ_i and the computed eigenvector $\boldsymbol{v}_i$ satisfy

$$\theta_i(A+E)\boldsymbol{v}_i = (1+\sigma\theta_i)(B+F)\boldsymbol{v}_i$$

with

$$\max\left(\frac{\|E\|_2}{\|A\|_2}, \frac{\|F\|_2}{\|B\|_2}\right) \leq$$
$$O(u)|1-\sigma/\lambda_i|\left(1+\max(\gamma,1)\left(1+|1-\lambda_i/\sigma|\right)\eta^2\|X\|_2^2\right)+O(u^2)$$

If $\eta^2\|X\|_2^2$ is not large, $A-\sigma B$ does not cancel, and $\lambda_i = (1+\sigma\theta_i)/\theta_i$ is not much larger or smaller than σ, then each $(1+\sigma\theta_i, \theta_i)$ and $\boldsymbol{v}_i$ is an eigenvalue/eigenvector of a pair close to (A, B).

Setting up a Generalized Eigenvalue Problem I

Given a diagonal matrix $D \in \mathbb{R}^{m \times m}$ with predefined eigenvalues, and regularization hyperparameter δ, the following algorithm sets up a generalized eigenvalue problem

1: **function** GENERATE_MATRIX(D, δ)
2: Set $m = \texttt{size}(D)$
3: Q, _ = $\texttt{qr}(\text{random.randn}(m, m))$
4: $C = QDQ^T$
5: $L_0 = \texttt{tril}(\texttt{random.randn}(m, m))$
6: $B = (L_0 L_0^T) + \delta I$
7: $L = \texttt{cholesky}(B)$
8: $A = LCL^T$
9: **return** (A, B)
10: **end function**

Setting up a Generalized Eigenvalue Problem II

- Generate a diagonal matrix $D \in \mathbb{R}^{3000\times 3000}$ of eigenvalues in the range $(10^{-3}, 10^{7})$
- Set regularization hyperparameter $\delta = 10^{1}$
- Generate matrices A and B with `GENERATE_MATRIX` function so that

$$\kappa_2(A) = 5.96 \times 10^{11}, \qquad \|A\|_2 = 1.18 \times 10^{11}$$

$$\kappa_2(B) = 8.09 \times 10^{2}, \qquad \text{and} \qquad \|B\|_2 = 1.34 \times 10^{5}.$$

- Both matrices are positive definite with their eigenvalues $\Lambda(A, B)$ equal to the diagonal elements of D.

Relative Residuals I

- Relative Decomposition Residual

$$\frac{\|C_b^T(A-\sigma B)^{-1}C_bQ_n - Q_nT_n - \delta_n\mathbf{q}_{n+1}\mathbf{e}_n^T\|}{\|C_b^T(A-\sigma B)^{-1}C_b\|}$$

- Generalized Relative Residuals

$$\|\tilde{\mathbf{r}}_i\| = \frac{\|(\beta_iA-\alpha_iB)\mathbf{v}_i\|}{(|\beta_i|\|A\|+|\alpha_i|\|B\|)\|\mathbf{v}_i\|}$$

- Spectral Transform Residuals

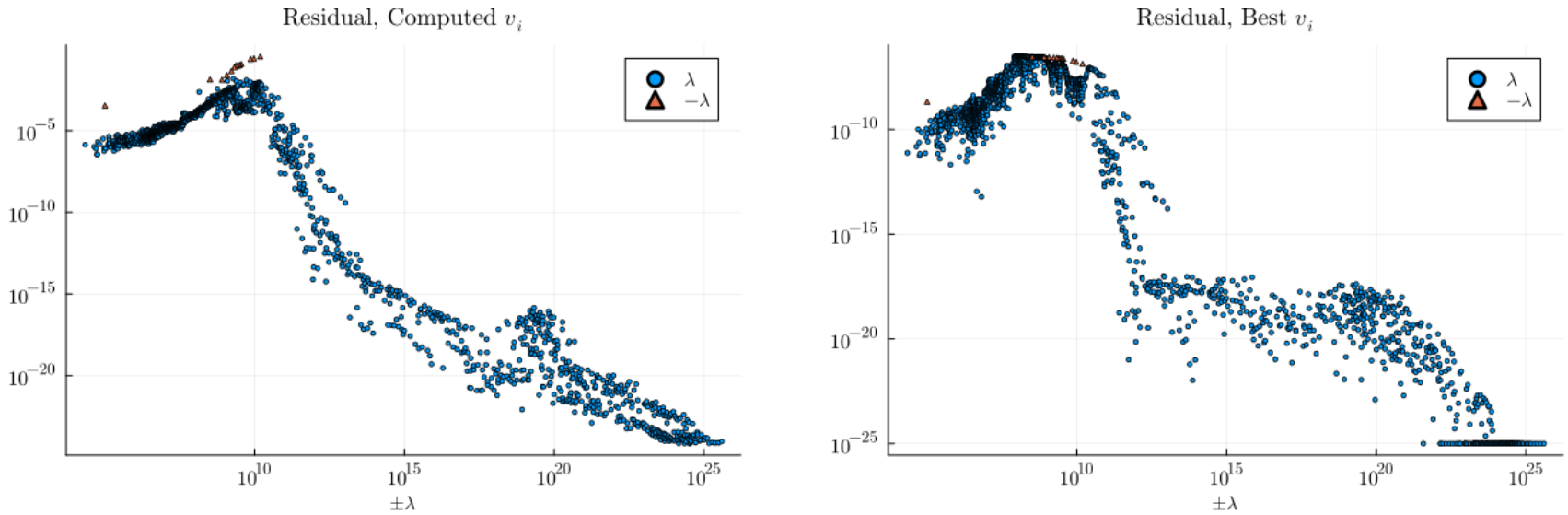
$$\frac{\|C_b^T(A-\sigma B)^{-1}C_b\mathbf{u}_i - \theta_i\mathbf{u}_i\|}{(\|C_b^T(A-\sigma B)^{-1}C_b\|+|\theta_i|)\|\mathbf{u}_i\|}$$

- Best Residuals

$$\frac{\|C_b^T(A-\sigma B)^{-1}C_b\mathbf{u}_i - \theta_i\mathbf{u}_i\|}{(\|C_b^T(A-\sigma B)^{-1}C_b\|+|\theta_i|)\|\mathbf{u}_i\|}$$

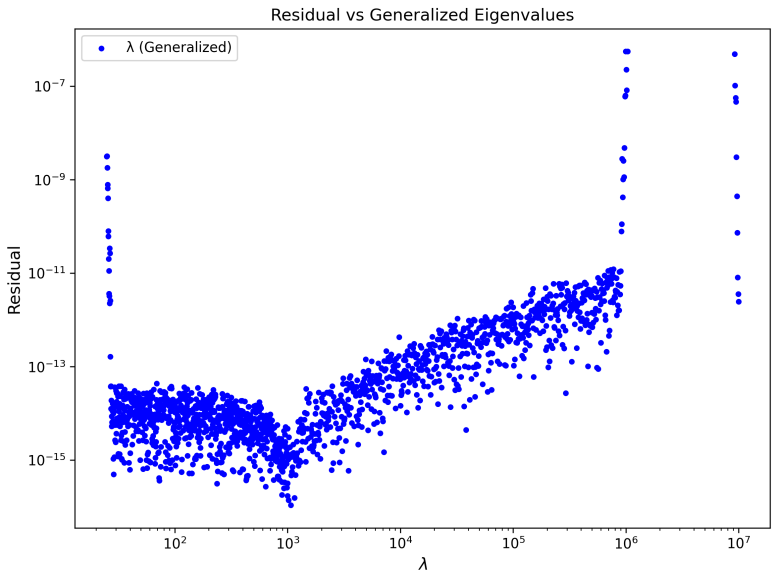
Standard Algorithm

Figure: Relative Residual vs. $\pm\lambda$, Standard Algorithm

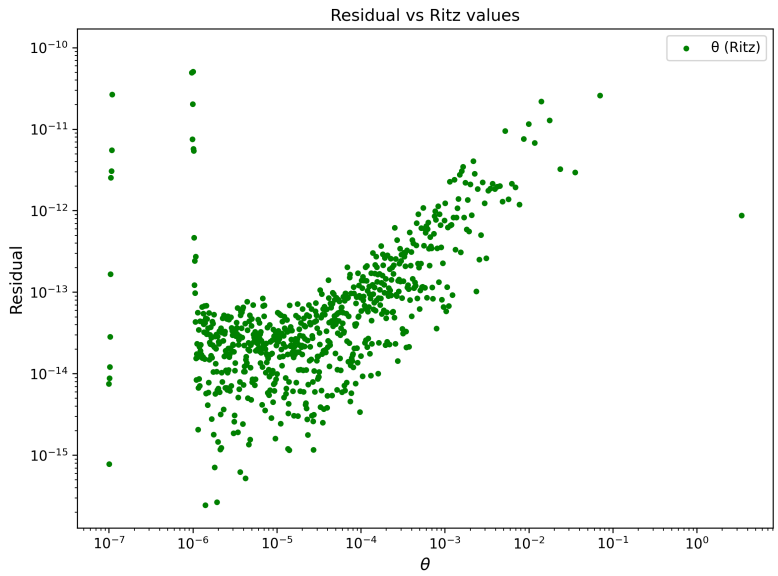


Spectral Transformation Lanczos(LU Decomposition) I

Figure: Residuals plot with moderate shift $\sigma = 1.5 \times 10^3$

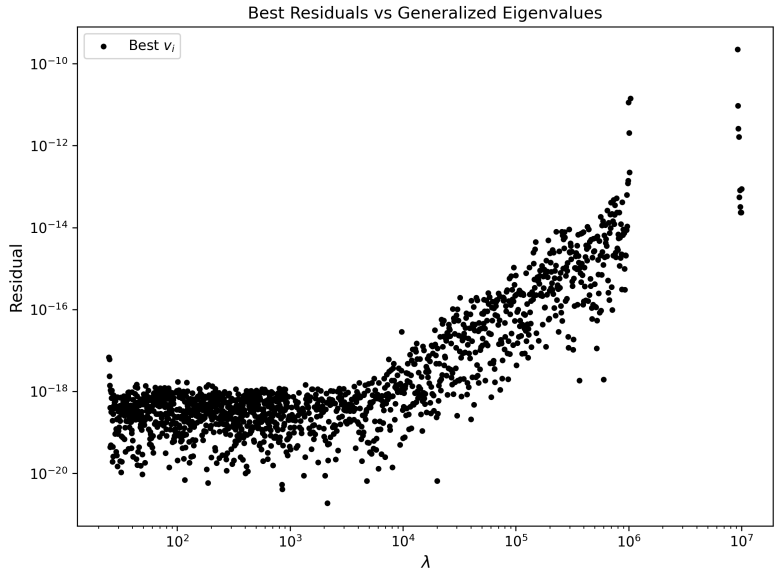


(a)



(b)

Spectral Transformation Lanczos(LU Decomposition) II

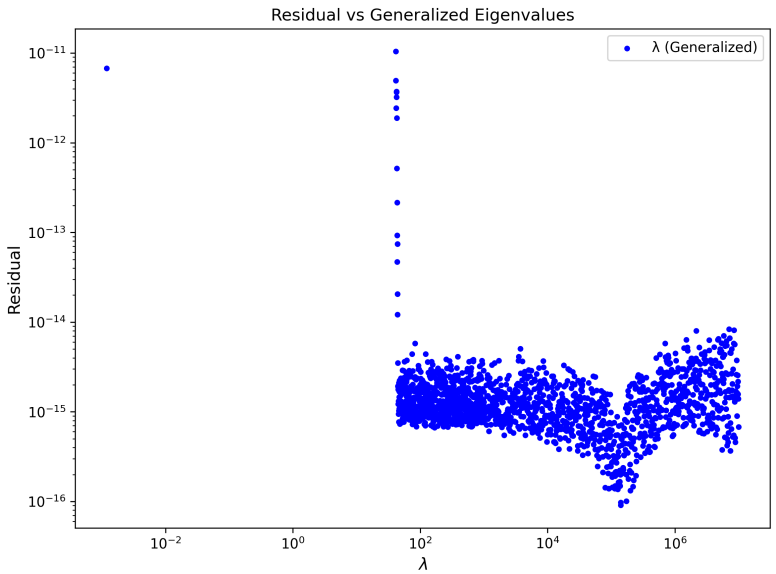


(c)

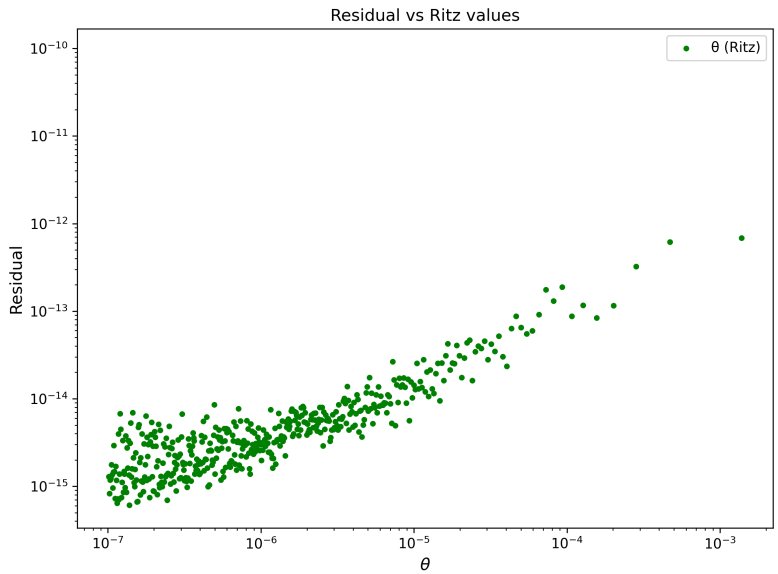
The computation gave the decomposition residual as 6.63×10^{-11}. Plot (a) is the generalized relative residual with the curve given by $10^{-14}|1 - \lambda_i/\sigma|$. Plot (b) is the relative Ritz residuals. Plot (c) is the best achievable residual for an idealized eigenvector.

Spectral Transformation Lanczos(LU Decomposition) I

Figure: Residuals plot with large shift $\sigma = 1.5 \times 10^5$

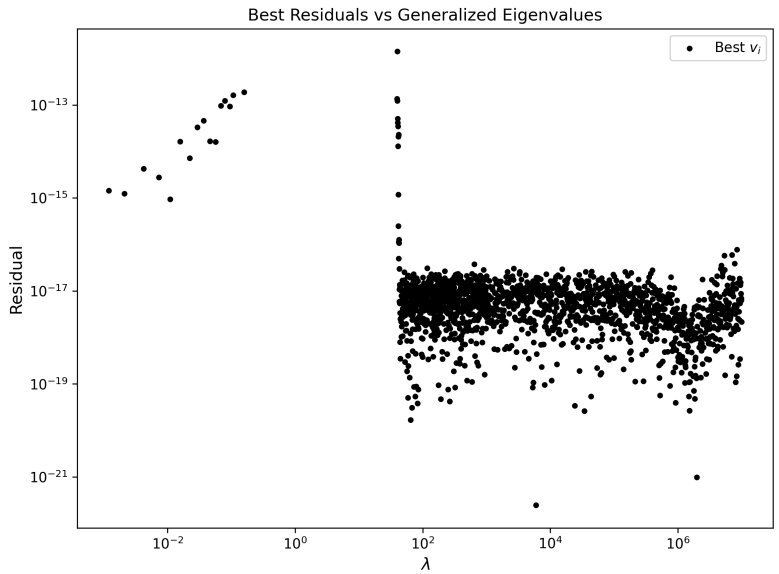


(a)



(b)

Spectral Transformation Lanczos(LU Decomposition) II

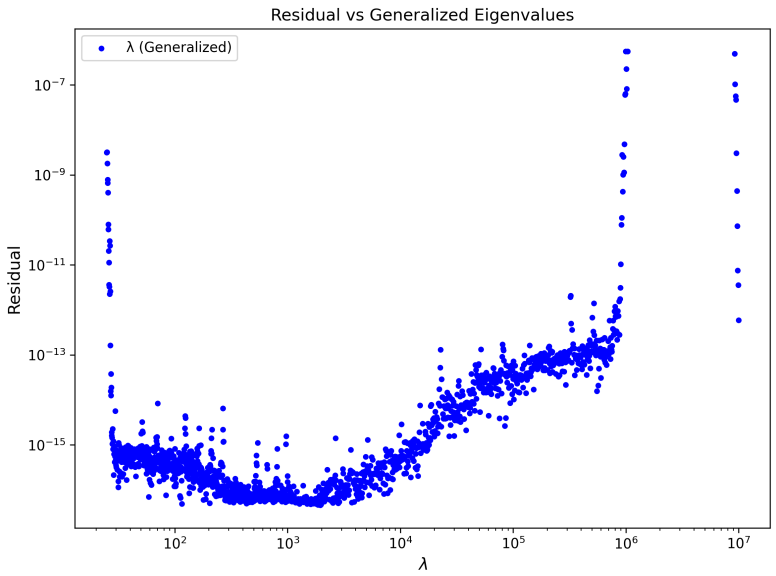


(c)

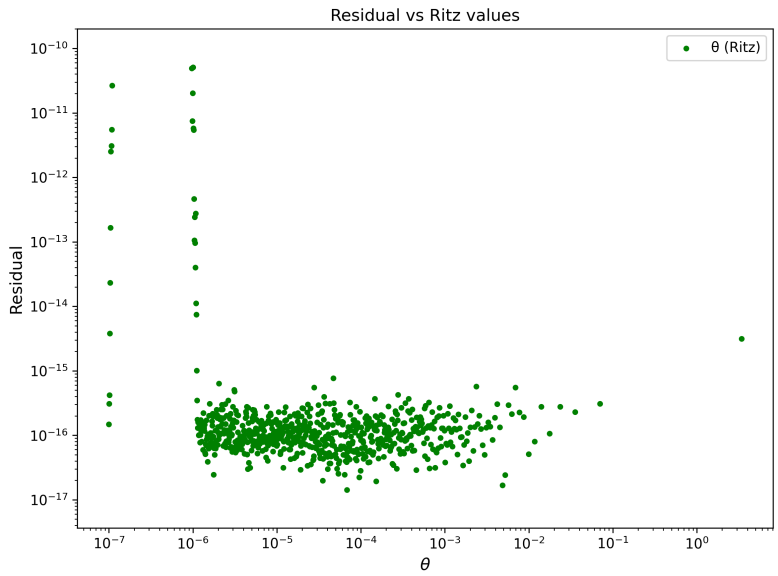
The computation gave the decomposition residual as 5.42×10^{-12}. Plot (a) is the generalized relative residual with the curve given by $10^{-15}|(1-\lambda_i/\sigma)(1-\sigma/\lambda_i)|$. Plot (b) is the relative Ritz residuals. Plot (c) is the best achievable residual for an idealized eigenvector.

ST Lanczos with Eigenvalue Decomposition I

Figure: Residuals plot with small shift $\sigma = 1.5 \times 10^3$

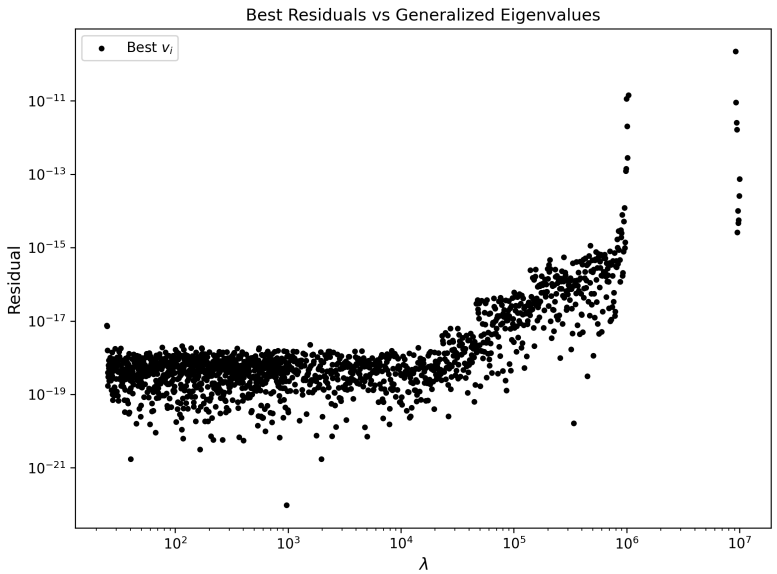


(a)



(b)

ST Lanczos with Eigenvalue Decomposition II



(c)

The computation gave the decomposition residual to the order of 10^{-29}. Plot (a) is the generalized relative residual which shows lower residual to the order of unit round off $u \approx 10^{-16}$ for eigenvalues close the shift as compared to an LU decomposition. Plot (b) is the relative Ritz residuals. Plot (c) is the best achievable residual for an idealized eigenvector.

Pros and Cons

Pros:

- The algorithm is fast for sparse matrices since it uses Lanczos algorithm which is $O(nm^2 + n^2m)$.
- It is efficient in computing a subset of eigenvalues, making it memory efficient.
- Since all the work is done in matrix decompositions that are implemented in LAPACK, the algorithm is almost as fast as the standard method and is easy to implement efficiently, even in a slow language.
- With a little effort, it can be designed to handles the case of semidefinite B effectively.
- Delivers really small residuals for symmetric decompositions.

Cons:

- The eigenvector computation is not unconditionally stable.
- Choosing the shift annoying, even if it is relatively easy to choose, especially if one wants a black box algorithm.