I.1.(a) Krylov subspace projection methods

Orthogonal projection technique : *framework*

Let A be an $n \times n$ complex matrix and $\mathcal{K}$ be an m-dimensional subspace of $\mathcal{C}^n$. An **orthogonal projection technique** seeks an approximate eigenpair

$$(\tilde{\lambda}, \widetilde{u}) \text{ with } \widetilde{\lambda} \in \mathcal{C} \text{ and } \widetilde{u} \in \mathcal{K}.$$

This approximate eigenpair is obtained by imposing the following ***Galerkin condition***:

$$A\widetilde{u} - \tilde{\lambda}\widetilde{u} \perp \mathcal{K} \ , \tag{1}$$

or, equivalently,

$$v^H(A\widetilde{u} - \tilde{\lambda}\widetilde{u}) = 0, \ \ \forall \, v \in \mathcal{K}. \tag{2}$$

In matrix form, assume that an orthonormal basis $\{v_1, v_2, \ldots, v_k\}$ of $\mathcal{K}$ is available. Denote $V = (v_1, v_2, \ldots, v_k)$, and let $\widetilde{u} = Vy$. Then, the condition (2) becomes

$$v_j^H(AVy - \tilde{\lambda}Vy) = 0, \quad j = 1, \ldots, k.$$

Therefore, y and $\tilde{\lambda}$ must satisfy

$$B_k y \;=\; \tilde{\lambda} y, \tag{3}$$

where

$$B_k \;=\; V^H A V.$$

Each eigenvalue $\widetilde{\lambda}_i$ of B_k is called a ***Ritz value***, and $V y_i$ is called ***Ritz vector***, where y_i is the eigenvector of B_k associated with $\widetilde{\lambda}_i$.

Rayleigh-Ritz procedure - orthogonal projection

1. Compute an orthonormal basis $\{v_i\}_{i=1,\ldots,k}$ of the subspace $\mathcal{K}$. Let $V = (v_1, v_2, \ldots, v_k)$.
2. Compute $B_k = V^H A V$.
3. Compute the eigenvalues of B_k and select k_0 desired ones: $\tilde{\lambda}_i, i = 1, 2, \ldots, k_0$, where $k_0 \leq k$.
4. Compute the eigenvectors $y_i, i = 1, \ldots, k_0$, of B_k associated with $\tilde{\lambda}_i, i = 1, \ldots, k_0$, and the corresponding approximate eigenvectors of A, $\widetilde{u}_i = V y_i, i = 1, \ldots, k_0$.

Oblique projection technique : *framework*

Select two subspaces $\mathcal{L}$ and $\mathcal{K}$ and then seek an approximate eigenpair

$$(\tilde{\lambda}, \widetilde{u}) \text{ with } \lambda \in \mathcal{C} \text{ and } \widetilde{u} \in \mathcal{K}$$

that satisfies the ***Petrov-Galerkin condition***:

$$v^H(A\widetilde{u} - \tilde{\lambda}\widetilde{u}) = 0, \quad \forall\, v \in \mathcal{L}\,. \tag{4}$$

In matrix form, let V denote the basis for the subspace $\mathcal{K}$ and W for $\mathcal{L}$. Then, writing $\widetilde{u} = Vy$, the Petrov-Galerkin condition (4) yields the reduced eigenvalue problem

$$B_k y \;=\; \tilde{\lambda} C_k y,$$

where

$$B_k \;=\; W^H A V \quad \text{and} \quad C_k = W^H V.$$

If $C_k = V^H V = I$, then the two bases are called ***biorthonormal***.

In order for a biorthonormal pair V and W to exist the following additional assumption for $\mathcal{L}$ and $\mathcal{K}$ must hold. *For any two bases V and W of $\mathcal{K}$ and $\mathcal{L}$, respectively,*

$$\det(W^H V) \neq 0 \quad . \tag{5}$$

Rayleigh-Ritz procedure - oblique projection

1. Compute an orthonormal bases $\{v_i\}_{i=1,\ldots,k}$ of the subspace $\mathcal{K}$. and $\{w_i\}_{i=1,\ldots,k}$ of the subspace $\mathcal{L}$.

   Let $V = (v_1, v_2, \ldots, v_k)$ and $W = (w_1, w_2, \ldots, w_k)$.

2. Compute $B_k = W^H A V$ and $C_k = W^H V$.

3. Compute the eigenvalues of $B_k - \lambda C_k$ and select k_0 desired ones: $\tilde{\lambda}_i, i = 1, 2, \ldots, k_0$, where $k_0 \leq k$.

4. Compute the right and left eigenvectors y_i and z_i, $i = 1, \ldots, k_0$, of $B_k - \lambda C_k$ associated with $\tilde{\lambda}_i, i = 1, \ldots, k_0$, and the corresponding approximate right and left eigenvectors of A, $\widetilde{u}_i = V y_i$, and $\tilde{v}_i = W z_i$, $i = 1, \ldots, k_0$.

Optimality

Let $Q = (Q_k, Q_u)$ be an n-by-n orthogonal matrix, where Q_k is n-by-k, and Q_u is n-by-$(n-k)$, and span$(Q_k) = \mathcal{K}$. Then

$$T = Q^T A Q = \begin{bmatrix} Q_k^T A Q_k & Q_k^T A Q_u \\ Q_u^T A Q_k & Q_u^T A Q_u \end{bmatrix} \equiv \begin{bmatrix} T_k & T_{uk} \\ T_{ku} & T_u \end{bmatrix}$$

The Ritz values and Ritz vectors are considered *optimal* approximations to the eigenvalues and eigenvectors of A from the selected subsapce $\mathcal{K} =$ span(Q_k) as justified by the follows.

Theorem.

$$\min_{S, k\times k} \|AQ_k - Q_k S\|_2 = \|AQ_k - Q_k T_k\|_2$$

Krylov subspace

$$\begin{aligned}\mathcal{K}_{k+1}(A, u_0) &= \text{span}\{u_0, Au_0, A^2u_0, \ldots, A^k u_0\} \\ &= \{q(A)u_0 \mid q \in \mathcal{P}_k\},\end{aligned}$$

where $\mathcal{P}_k$ is the set of all polynomial of degree less than $k+1$.

Properties of $\mathcal{K}_{k+1}(A, u_0)$:

1. $\mathcal{K}_k(A, u_0) \subset \mathcal{K}_{k+1}(A, u_0)$.
   $A\mathcal{K}_k(A, u_0) \subset \mathcal{K}_{k+1}(A, u_0)$.
2. If $\sigma \neq 0$, $\mathcal{K}_k(A, u_0) = \mathcal{K}_k(\sigma A, u_0) = \mathcal{K}_k(A, \sigma u_0)$.
3. For any scalar κ, $\mathcal{K}_k(A, u_0) = \mathcal{K}_k(A - \kappa I, u_0)$.
4. If W is nonsingular, $\mathcal{K}_k(W^{-1}AW, W^{-1}u_0) = W^{-1}\mathcal{K}_k(A, u_0)$.

Arnoldi decomposition

An explicit Krylov basis $\{u_0, Au_0, A^2u_0, \ldots, A^ku_0\}$ is not suitable for numerical computing. It is extremely ill-conditioned. Therefore, our first task is to replace a Krylov basis with a better conditioned basis, say an orthonormal basis.

Theorem. Let the columns of $K_{j+1} = \begin{pmatrix} u_0 & Au_0 & \ldots & A^ju_0 \end{pmatrix}$ be linearly independent. Let

$$K_{j+1} = U_{j+1}R_{j+1} \tag{6}$$

be the QR factorization of K_{j+1}. Then there is a $(j+1) \times j$ unreduced upper Hessenberg matrix $\widehat{H}_j$ such that

$$AU_j = U_{j+1}\widehat{H}_j. \tag{7}$$

Conversely, if U_{j+1} is orthonormal and satisfies (7), then

$$\text{span}(U_{j+1}) = \text{span}\{u_0, Au_0, \ldots, A^ju_0\}. \tag{8}$$

Proof: Partitioning the QR decomposition (6), we have

$$\begin{pmatrix} K_j & A^j u_0 \end{pmatrix} = \begin{pmatrix} U_j & u_{j+1} \end{pmatrix} \begin{pmatrix} R_j & r_{j+1} \\ 0 & r_{j+1,j+1} \end{pmatrix},$$

where $K_j = U_j R_j$ is the QR decomposition of K_j. Then

$$AK_j = AU_j R_j$$

or

$$AU_j = AK_j R_j^{-1} = K_{j+1} \begin{pmatrix} 0 \\ R_j^{-1} \end{pmatrix} = U_{j+1} R_{j+1} \begin{pmatrix} 0 \\ R_j^{-1} \end{pmatrix}.$$

It is easy to verify that

$$\widehat{H}_j = R_{j+1} \begin{pmatrix} 0 \\ R_j^{-1} \end{pmatrix}$$

is a $(j+1) \times j$ unreduced upper Hessenberg matrix. Therefore we complete the proof of (7).
Conversely, suppose that U_{j+1} satisfies (7), then by induction, we can prove the identity (8).

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Arnoldi decomposition: by partitioning,

$$\widehat{H}_j = \begin{pmatrix} H_j \\ h_{j+1,j} e_j^T \end{pmatrix},$$

the decomposition (7) can be written as follows:

$$AU_j = U_j H_j + h_{j+1,j} u_{j+1} e_j^T. \tag{9}$$

We call (9) an ***Arnoldi decomposition*** of order j. The decomposition (7) is a compact form.

Arnoldi procedure

By the Arnoldi decomposition (9), we deduce the following process to generate an orthogonormal basis $\{v_1, v_2, \ldots, v_m\}$ of the Krylov subspace $\mathcal{K}_m(A, v)$:

Arnoldi Process:

1. $v_1 = v/\|v\|_2$
2. for $j = 1, 2, \ldots, k$
3. compute $w = Av_j$
4. for $i = 1, 2, \ldots, j$
5. $h_{ij} = v_i^T w$
6. $w = w - h_{ij} v_i$
7. end for
8. $h_{j+1,j} = \|w\|_2$
9. If $h_{j+1,j} = 0$, *stop*
10. $v_{j+1} = w_j / h_{j+1,j}$
11. endfor

Remarks:

1. The matrix A is only referenced via the matrix-vector multiplication Av_j. Therefore, it is ideal for large scale matrices. Any sparsity or structure of a matrix can be exploited.
2. The main storage requirement is $(m+1)n$ for storing Arnoldi vectors $\{v_i\}$
3. the cost of arithmetic is m matrix-vector products plus $2m^2n$ for the rest. It is common that the matrix-vector multiplication is the dominant cost.
4. The Arnoldi procedure breaks down when $h_{j+1,j} = 0$ for some j. It is easy to see that if the Arnoldi procedure breaks down at step j (i.e. $h_{j+1,j} = 0$), then $\mathcal{K}_j = \text{span}(V_j)$ is **invariant subspace** of A.
5. Some care must be taken to insure that the vectors v_j remain orthogonal to working accuracy in the presence of rounding error. The usual technique is ***reorthogonalization***.

Arnoldi decomposition

- Denote

$$V_k = \begin{pmatrix} v_1 & v_2 & \dots & v_k \end{pmatrix}$$

and

$$H_k = \begin{pmatrix} h_{11} & h_{12} & \cdots & h_{1,k-1} & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2,k-1} & h_{2k} \\ & h_{32} & \ddots & h_{3,k-1} & h_{3k} \\ & & \ddots & \vdots & \vdots \\ & & & h_{k,k-1} & h_{kk} \end{pmatrix}.$$

- The Arnoldi process can be expressed in the following governing relations:

$$AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^T \tag{10}$$

and

$$V_k^H V_k = I \quad \text{and} \quad V_k^H v_{k+1} = 0.$$

- The decomposition is uniquely determined by the starting vector v (the implicit Q-Theorem).
- Since $V_k^H v_{k+1} = 0$, we have

$$H_k = V_k^T A V_k.$$

- Let μ be an eigenvalue of H_k and y be a corresponding eigenvector y, i.e.,

$$H_k y = \mu y, \quad \|y\|_2 = 1.$$

Then the corresponding Ritz pair is $(\mu, V_k y)$. Applying y to the right hand side of (10), the residual vector for $(\mu, V_k y)$ is given by

$$A(V_k y) - \mu(V_k y) = h_{k+1,k} v_{k+1}(e_k^T y).$$

- Using the backward error interpretation, we know that $(\mu, V_k y)$ is an exact eigenpair of $A + E$:

$$(A + E)(V_k y) = \mu(V_k y),$$

where

$$\|E\|_2 = |h_{k+1,k}| \cdot |e_k^T y|.$$

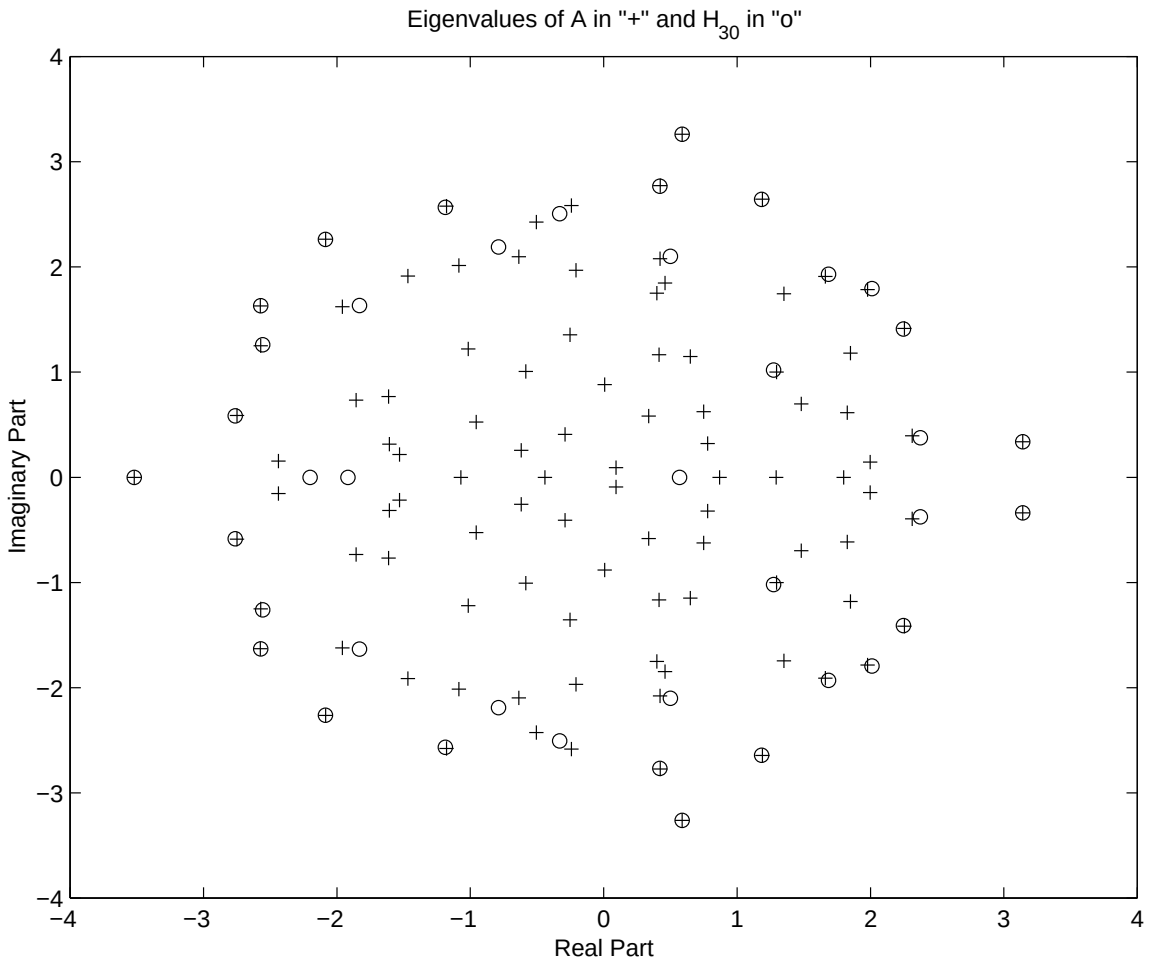
This gives us a criterion of whether to accept the Ritz pair $(\mu, V_k y)$ as an accurate approximate eigenpair of A.

Arnoldi method = RR + Arnoldi

1. Choose a starting vector v;
2. Generate the Arnoldi decomposition of length k by the Arnoldi process;
3. Compute the Ritz pairs and decide which ones are acceptable;
4. If necessary, increase k and repeat.

An example

A = `sprandn(100,100,0.1)` and $v = (1, 1, \ldots, 1)^T$.
"+" are the eigenvalues of matrix A
"$\circ$" are the eigenvalues of the upper Hessenberg matrix H_{30}



Observation: *exterior eigenvalues converge first*, a typical convergence phenomenon.

The need of restarting

The algorithm has two nice aspects:

1. H_k is already in the Hessenberg form, so we can immediately apply the QR algorithm to find its eigenvalues.
2. After we increase k to, say $k+p$, we only have to orthogonalize p vectors to compute the $(k+p)$th Arnoldi decomposition. The work already completed previously is not thrown away.

Unfortunately, the algorithm has its drawbacks, too:

1. If A is large, we cannot increase k indefinitely, since V_k requires nk memory locations to store.
2. We have little control over which eigenpairs the algorithm finds.

Implicit restarting

Goal: purge the unwanted eigenvalues μ from H_k.

1. Exact arithmetic case:

   By one step of the QR algorithm with shift μ, we have

   $$R = U^H(H - \mu I) = \text{upper triangular}$$

   Note that $H - \mu I$ is singular, hence R must have a zero on its diagonal. Because H is unreduced, then $r_{nn} = 0$.

   Furthermore, note that $U = P_{12}P_{23}\cdots P_{n-1,n}$, where $P_{i,i+1}$ is a rotation in the $(i, i+1)$-plane. Consequently, U is Hessenberg:

   $$U = \begin{pmatrix} U_* & u \\ u_{k,k-1}e_{k-1}^T & u_{k,k} \end{pmatrix}.$$

   Hence

   $$H' = RU + \mu I = \begin{pmatrix} \hat{H}_* & \hat{h} \\ 0 & \mu \end{pmatrix} = U^H H U.$$

In other words, one step of the shifted QR has found the eigenvalue μ exactly and has deflated the problem.

2. Finite precision arithmetic case:

   - In the presence of rounding error, after one step of the shifted QR, we have

$$\widehat{H}' = \widehat{U}^H H \widehat{U} = \begin{pmatrix} \widehat{H}_* & \widehat{h} \\ \widehat{h}_{k,k-1} e_{k-1}^T & \widehat{\mu} \end{pmatrix}.$$

   - From the Arnoldi decomposition, we have

$$AV_k\widehat{U} = V_k\widehat{U}(\widehat{U}^T H_k \widehat{U}) + h_{k+1,k} v_{k+1} e_k^T \widehat{U}.$$

   - Partition

$$\widehat{V}_k = V_k\widehat{U} = \begin{pmatrix} \widehat{V}_{k-1} & \widehat{v}_k \end{pmatrix}$$

     Then

$$A \begin{pmatrix} \widehat{V}_{k-1} & \widehat{v}_k \end{pmatrix} = \begin{pmatrix} \widehat{V}_{k-1} & \widehat{v}_k \end{pmatrix} \begin{pmatrix} \widehat{H}_* & \widehat{h} \\ \widehat{h}_{k,k-1} e_{k-1}^T & \widehat{\mu} \end{pmatrix} + h_{k+1,k} v_{k+1} \begin{pmatrix} \widehat{u}_{k,k-1} e_{k-1}^T & \widehat{u}$$

- From the first $k-1$ columns of this partition, we get

$$A\widehat{V}_{k-1} = \widehat{V}_{k-1}\widehat{H}_* + fe_{k-1}^T, \tag{11}$$

  where $f = \widehat{h}_{k,k-1}\widehat{v}_k + h_{k+1,k}\widehat{u}_{k,k-1}v_{k+1}$.
- Note that $\widehat{H}_*$ is Hessenberg. f is orthogonal to $\widehat{V}_{k-1}$. Hence (11) is an Arnoldi decomposition of length $k-1$.
- The process may be repeated to remove other unwanted values from H.

The symmetric Lanczos procedure

- Observation: in the Arnoldi decomposition, if A is symmetric, then the upper Hessenberg matrix H_j is symmetric tridiagonal.
- The following is a simplified process to compute an orthonormal basis of a Krylov subspace:

  Lanczos process:

  1 $q_1 = v/\|v\|_2$, $\beta_0 = 0$; $q_0 = 0$;
  2 for $j = 1$ to k, do
  3 $w = Aq_j$;
  4 $\alpha_j = q_j^T w$;
  5 $w = w - \alpha_j q_j - \beta_{j-1} q_{j-1}$;
  6 $\beta_j = \|w\|_2$;
  7 if $\beta_j = 0$, quit;
  8 $q_{j+1} = w/\beta_j$;
  9 endfor

The symmetric Lanczos algorithm : governing equation

Denote

$$Q_k = \begin{pmatrix} q_1 & q_2 & \dots & q_k \end{pmatrix}$$

and

$$T_k = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \alpha_{k-1} & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_k \end{pmatrix} = \text{tridiag}(\beta_j, \alpha_j, \beta_{j+1}),$$

the k-step Lanczos process yields

$$AQ_k = Q_k T_k + f_k e_k^T, \quad f_k = \beta_k q_{k+1} \tag{12}$$

and $Q_k^T Q_k = I$ and $Q_k^T q_{k+1} = 0$.

Let

$$T_k y = \mu y, \quad \|y\|_2 = 1.$$

Then

$$A(Q_k y) = Q_k T_k y + f_k(e_k^T y) = \mu(Q_k y) + f_k(e_k^T y).$$

Here μ is a *Ritz value*, and $Q_k y$ is the corresponding *Ritz vector*.

Error bound

Lemma. Let H be symmetric, and $Hz - \mu z = r$ and $z \neq 0$. Then

$$\min_{\lambda \in \lambda(H)} |\lambda - \mu| \leq \frac{\|r\|_2}{\|z\|_2}.$$

Proof: Let $H = U \Lambda U^T$ be the eigen-decomposition of H. Then

$$(H - \mu I)z = r \quad \Rightarrow \quad U(\Lambda - \mu I)U^T z = r \quad \Rightarrow \quad (\Lambda - \mu I)(U^T z) = U^T r.$$

Notice that $\Lambda - \mu I$ is diagonal. Thus

$$\begin{aligned} \|r\|_2 &= \|U^T r\|_2 = \|(\Lambda - \mu I)(U^T z)\|_2 \\ &\geq \min_{\lambda \in \lambda(H)} |\lambda - \mu| \, \|U^T z\|_2 \\ &= \min_{\lambda \in \lambda(H)} |\lambda - \mu| \|z\|_2, \end{aligned}$$

as expected.

Error bound

- If $f_k(e_k^T y) = 0$ for some k, then the associated Ritz value μ is an eigenvalue of A with the corresponding eigenvector $Q_k y$.
- Let $\|r\|_2 = \|f_k(e_k^T y)\|_2$, then by the lemma, we know that for the Ritz pair $(\mu, Q_k y)$, there is an eigenvalue λ of A, such that

$$|\lambda - \mu| \leq \frac{\|f_k(e_k^T y)\|_2}{\|Q_k y\|_2}$$

Lanczos method = RR + Lanczos

Simple Lanczos Algorithm:

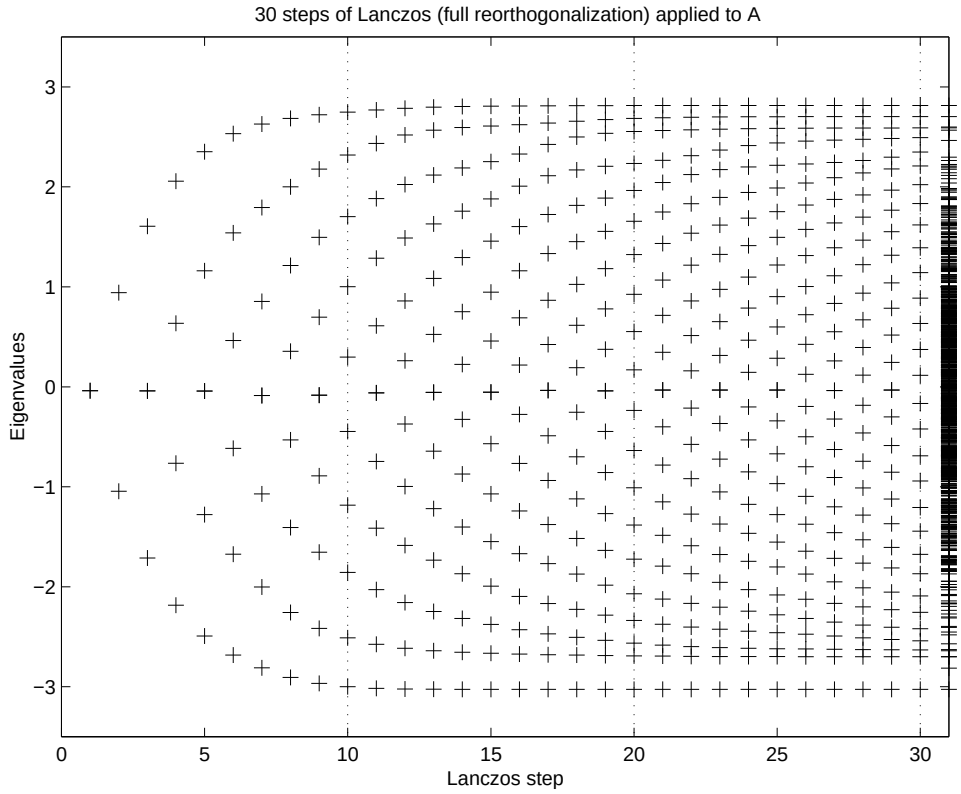
1. $q_1 = v/\|v\|_2$, $\beta_0 = 0$, $q_0 = 0$;
2. for $j = 1$ to k do
3. $w = Aq_j$;
4. $\alpha_j = q_j^T w$;
5. $w = w - \alpha_j q_j - \beta_{j-1} q_{j-1}$;
6. $\beta_j = \|w\|_2$;
7. if $\beta_j = 0$, quit;
8. $q_{j+1} = w/\beta_j$;
9. Compute eigenvalues and eigenvectors of T_j
10. Test for convergence
11. endfor

Example

A = a random diagonal matrix A of order $n = 1000$

$v = (1, 1, \ldots, 1)^T$

Convergence behavior:



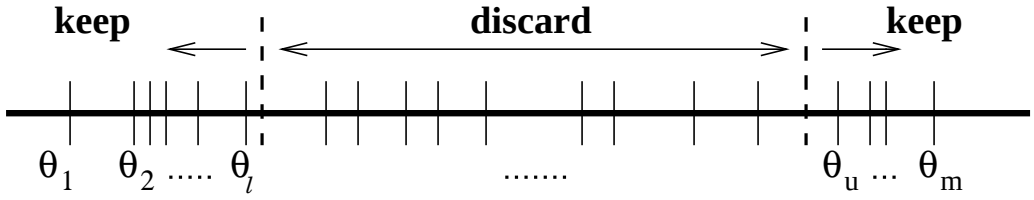
We observe that

1. Extreme eigenvalues, i.e., the largest and smallest ones, converge first, and the interior eigenvalues converge last.
2. Convergence is monotonic, with the ith largest (smallest) eigenvalues of T_k increasing (decreasing) to the ith laregst (smallest) eigenvalue of A.

$\Longrightarrow$ *Convergence analysis*

Thick Restarting

- Selects two indices ℓ and u to indicate those Ritz values to be kept at both ends of spectrum:



- The corresponding kept Ritz vectors are denoted by

$$\widehat{Q}_k = [\widehat{q}_1, \widehat{q}_2, \ldots, \widehat{q}_k] = Q_m Y_k, \tag{13}$$

where

$$k = \ell + (m - u + 1), \tag{14}$$

$$Y_k = [y_1, y_2, \ldots, y_\ell,\ y_u, y_{u+1}, \ldots, y_m], \tag{15}$$

and y_i is the eigenvector of T_m corresponding to θ_i.

- Sets these Ritz vectors $\widehat{Q}_k$ as the first k basis vectors at the restart and $\widehat{q}_{k+1} = q_{m+1}$.
- To compute the $(k+2)$th basis vector $\widehat{q}_{k+2}$, TRLan computes $A\widehat{q}_{k+1}$ and orthonormalizes it against the previous $k+1$ basis vectors. That is,

$$\widehat{\beta}_{k+1}\widehat{q}_{k+2} = A\widehat{q}_{k+1} - \widehat{Q}_k(\widehat{Q}_k^H A\widehat{q}_{k+1}) - \widehat{q}_{k+1}(\widehat{q}_{k+1}^H A\widehat{q}_{k+1}).$$

  Note that $A\widehat{Q}_k$ satisfies the relation:

$$A\widehat{Q}_k = \widehat{Q}_k D_k + \beta_m \widehat{q}_{k+1} s^H,$$

  where D_k is the $k \times k$ diagonal matrix whose diagonal elements are the kept Ritz values, and $s = Y_k^H e_m$.

  Thus, the coefficients $\widehat{Q}_k^H A\widehat{q}_{k+1}$ can be computed efficiently:

$$\begin{aligned} \widehat{Q}_k^H A\widehat{q}_{k+1} &= (A\widehat{Q}_k)^H \widehat{q}_{k+1} = (\widehat{Q}_k D_k + \beta_m \widehat{q}_{k+1} s^H)^H \widehat{q}_{k+1} \\ &= D_k Y_k^H (Q_m^H q_{m+1}) + \beta_m s(\widehat{q}_{k+1}^H \widehat{q}_{k+1}) = \beta_m s. \end{aligned}$$

- Then after the first iteration after the restart, we have

$$A\widehat{Q}_{k+1} = \widehat{Q}_{k+1}\widehat{T}_{k+1} + \widehat{\beta}_{k+1}\widehat{q}_{k+2}e_{k+i}^H,$$

where

$$\widehat{T}_{k+1} = \begin{bmatrix} D_k & \beta_m s \\ \beta_m s^H & \widehat{\alpha}_{k+1} \end{bmatrix}$$

- In general, at the ith iteration after the restart, the new basis vector $\widehat{q}_{k+i+1}$ satisfies the relation:

$$A\widehat{Q}_{k+i} = \widehat{Q}_{k+i}\widehat{T}_{k+i} + \widehat{\beta}_{k+i}\widehat{q}_{k+i+1}e_{k+i}^H,$$

where $\widehat{T}_{k+i} = \widehat{Q}_{k+i}^H A\widehat{Q}_{k+i}$ is of the form

$$\widehat{T}_{k+i} = \begin{pmatrix} D_k & \beta_m s & & & & \\ \beta_m s^H & \widehat{\alpha}_{k+1} & \widehat{\beta}_{k+1} & & & \\ & \widehat{\beta}_{k+1} & \widehat{\alpha}_{k+2} & \widehat{\beta}_{k+2} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \widehat{\beta}_{k+i-2} & \widehat{\alpha}_{k+i-1} & \widehat{\beta}_{k+i-1} \\ & & & & \widehat{\beta}_{k+i-1} & \widehat{\alpha}_{k+i} \end{pmatrix}.$$

- Note that the three-term recurrence is not valid only for computing the $(k+2)$th basis vector and is resumed afterward.