Lecture 15: Krylov subspace methods for eigenvalue problems

School of Mathematical Sciences, Xiamen University

1. The Rayleigh–Ritz method for Hermitian eigenproblems

- The Rayleigh–Ritz (RR) method.

  Given $\mathbf{Q}_k \in \mathbb{C}^{n\times k}$ with k orthonormal columns, find approximate eigenpairs $(\theta, \mathbf{Q}_k\mathbf{v})$ satisfying the Galerkin condition:

$$\mathbf{A}(\mathbf{Q}_k\mathbf{v}) - \theta(\mathbf{Q}_k\mathbf{v}) \perp \operatorname{span}\{\mathbf{Q}_k\}.$$

- Assume that $\mathbf{A} \in \mathbb{C}^{n\times n}$ is Hermitian. Let $\mathbf{Q} = \begin{bmatrix}\mathbf{Q}_k & \mathbf{Q}_\mathrm{c}\end{bmatrix}$ be unitary. We will use the following notation:

$$\mathbf{T} := \mathbf{Q}^*\mathbf{A}\mathbf{Q} = \begin{bmatrix}\mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_k & \mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_\mathrm{c} \\ \mathbf{Q}_\mathrm{c}^*\mathbf{A}\mathbf{Q}_k & \mathbf{Q}_\mathrm{c}^*\mathbf{A}\mathbf{Q}_\mathrm{c}\end{bmatrix} =: \begin{bmatrix}\mathbf{T}_k & \mathbf{T}_{k\mathrm{c}}^* \\ \mathbf{T}_{k\mathrm{c}} & \mathbf{T}_\mathrm{c}\end{bmatrix}.$$

  The RR method for Hermitian $\mathbf{A}$ reduces to compute the eigendecomposition $\mathbf{T}_k = \mathbf{V}\mathbf{\Theta}_k\mathbf{V}^*$. The eigenvalues of $\mathbf{T}_k = \mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_k$ and the columns of $\mathbf{Q}_k\mathbf{V}$ are called *Ritz values* and *Ritz vectors* of $\mathbf{A}$ with respect to $\operatorname{span}\{\mathbf{Q}_k\}$, respectively.

Theorem 1

Let $\mathbf{A}$, $\mathbf{Q}_k$, *and* $\mathbf{T}_k$ *be given as above. We have the following optimality property*

$$\mathbf{T}_k \in \operatorname*{argmin}_{\mathbf{S}\in\mathbb{C}^{k\times k},\ \mathbf{S}=\mathbf{S}^*} \|\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S}\|_2^2.$$

Proof. $\|\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S}\|_2^2$

$$\begin{aligned}
&= \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S})^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S})] \quad (\text{assume that } \mathbf{S} = \mathbf{T}_k + \mathbf{Z})\\
&= \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k - \mathbf{Q}_k\mathbf{Z})^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k - \mathbf{Q}_k\mathbf{Z})]\\
&= \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k) - (\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)^*\mathbf{Q}_k\mathbf{Z}\\
&\qquad - (\mathbf{Q}_k\mathbf{Z})^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k) + (\mathbf{Q}_k\mathbf{Z})^*(\mathbf{Q}_k\mathbf{Z})]\\
&= \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k) - (\mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_k - \mathbf{T}_k)\mathbf{Z}\\
&\qquad - \mathbf{Z}^*(\mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_k - \mathbf{T}_k) + \mathbf{Z}^*\mathbf{Z}]\\
&= \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k) + \mathbf{Z}^*\mathbf{Z}]\\
&\geq \lambda_{\max}[(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)^*(\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k)]\\
&= \|\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{T}_k\|_2^2 = \|\mathbf{Q}_c\mathbf{T}_{kc}\|_2^2 = \|\mathbf{T}_{kc}\|_2^2. \quad \square
\end{aligned}$$

- The diagonal entries of $\mathbf{\Theta}_k$ (the Ritz values) are the "best" approximate eigenvalues and the columns of $\mathbf{Q}_k\mathbf{V}$ (the Ritz vectors) are the "best" approximate eigenvectors in the sense of minimizing the residual

$$\|\mathbf{A}\mathbf{P}_k - \mathbf{P}_k\mathbf{D}\|_2^2,$$

over $\text{range}(\mathbf{P}_k) = \text{range}(\mathbf{Q}_k)$, $\mathbf{P}_k^*\mathbf{P}_k = \mathbf{I}_k$, and real and diagonal $\mathbf{D}$.

Theorem 2

Let $\mathbf{T}_k = \mathbf{V}\mathbf{\Theta}_k\mathbf{V}^*$ be the eigendecomposition of $\mathbf{T}_k = \mathbf{Q}_k^*\mathbf{A}\mathbf{Q}_k$. We have

$$\min_{\text{range}(\mathbf{P}_k)=\text{range}(\mathbf{Q}_k),\ \mathbf{P}_k^*\mathbf{P}_k=\mathbf{I}_k,\ \text{real and diagonal } \mathbf{D}} \|\mathbf{A}\mathbf{P}_k - \mathbf{P}_k\mathbf{D}\|_2^2 = \|\mathbf{T}_{kc}\|_2^2.$$

The minimum is attained by $\mathbf{P}_k = \mathbf{Q}_k\mathbf{V}$ and $\mathbf{D} = \mathbf{\Theta}_k$.

- Exercise: Prove Theorem 2.

Theorem 3

Let $\mathbf{T}_k = \mathbf{V}\boldsymbol{\Theta}_k\mathbf{V}^*$ *be the eigendecomposition. Let* $\mathbf{V} = \begin{bmatrix}\mathbf{v}_1 & \cdots & \mathbf{v}_k\end{bmatrix}$ *and* $\boldsymbol{\Theta}_k = \operatorname{diag}\{\theta_1, \ldots, \theta_k\}$. *We have the following results.*

(i) *There are* k *eigenvalues* $\lambda_1, \ldots, \lambda_k$ *of* $\mathbf{A}$ (*not necessarily the largest* k *ones*) *such that*

$$|\theta_i - \lambda_i| \leq \|\mathbf{T}_{k\mathrm{c}}\|_2, \quad i = 1, \ldots, k.$$

(ii) *The Ritz pairs satisfy*

$$\|\mathbf{A}(\mathbf{Q}_k\mathbf{v}_i) - \theta_i(\mathbf{Q}_k\mathbf{v}_i)\|_2 = \|\mathbf{T}_{k\mathrm{c}}\mathbf{v}_i\|_2, \quad i = 1, \ldots, k.$$

Proof. (i) The eigenvalues of

$$\widehat{\mathbf{T}} = \begin{bmatrix} \mathbf{T}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{T}_\mathrm{c} \end{bmatrix}$$

include θ_i.

It follows from Weyl's theorem (see Lecture 7) and

$$\|\widehat{\mathbf{T}} - \mathbf{T}\|_2 = \left\| \begin{bmatrix} \mathbf{0} & \mathbf{T}_{k\mathrm{c}}^* \\ \mathbf{T}_{k\mathrm{c}} & \mathbf{0} \end{bmatrix} \right\|_2 = \|\mathbf{T}_{k\mathrm{c}}\|_2$$

that the eigenvalues of $\widehat{\mathbf{T}}$ and $\mathbf{T}$ differ by at most $\|\mathbf{T}_{k\mathrm{c}}\|_2$. The eigenvalues of $\mathbf{T}$ and $\mathbf{A}$ are identical, proving the result.

(ii) By straightforward calculations, we have

$$\begin{aligned} \|\mathbf{A}(\mathbf{Q}_k\mathbf{v}_i) - \theta_i(\mathbf{Q}_k\mathbf{v}_i)\|_2 &= \|\mathbf{Q}^*\mathbf{A}(\mathbf{Q}_k\mathbf{v}_i) - \theta_i\mathbf{Q}^*(\mathbf{Q}_k\mathbf{v}_i)\|_2 \\ &= \left\| \begin{bmatrix} \mathbf{T}_k \\ \mathbf{T}_{k\mathrm{c}} \end{bmatrix} \mathbf{v}_i - \theta_i \begin{bmatrix} \mathbf{v}_i \\ \mathbf{0} \end{bmatrix} \right\|_2 \\ &= \left\| \begin{bmatrix} \mathbf{0} \\ \mathbf{T}_{k\mathrm{c}}\mathbf{v}_i \end{bmatrix} \right\|_2 = \|\mathbf{T}_{k\mathrm{c}}\mathbf{v}_i\|_2. \quad \square \end{aligned}$$

2. Lanczos algorithm for Hermitian eigenproblems

- If $\mathbf{T}_k$ and $\mathbf{Q}_k$ are computed by the Lanczos process, then

$$
\mathbf{T} = \left[\begin{array}{cccc|cccc}
\alpha_1 & \beta_1 & & & & & & \\
\beta_1 & \ddots & \ddots & & & & & \\
 & \ddots & \ddots & \beta_{k-1} & & & & \\
 & & \beta_{k-1} & \alpha_k & \beta_k & & & \\
\hline
 & & & \beta_k & \alpha_{k+1} & \beta_{k+1} & & \\
 & & & & \beta_{k+1} & \ddots & \ddots & \\
 & & & & & \ddots & \ddots & \beta_{n-1} \\
 & & & & & & \beta_{n-1} & \alpha_n
\end{array}\right].
$$

- All the quantities in Theorem 3 can be computed easily. This is because there are good algorithms for finding eigenvalues and eigenvectors of the symmetric tridiagonal matrix $\mathbf{T}_k$.

Remark 4

Extreme eigenvalues, i.e., the largest and smallest ones, converge first, and the interior eigenvalues converge last. Furthermore, convergence is monotonic, with the ith largest (smallest) eigenvalue of $\mathbf{T}_k$ *increasing (decreasing) to the ith largest (smallest) eigenvalue of* $\mathbf{A}$*, provided that the Lanczos algorithm does not stop prematurely with some* $\beta_k = 0$*.*

Remark 5

Full reorthogonalization and selective orthogoalization techniques in floating point arithmetic. See Demmel's book.

3. Arnoldi algorithm for non-Hermitian eigenproblems

- The Arnoldi process for $\mathbf{A}$ and $\mathbf{b}$ gives the Arnoldi relation

$$\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_{j+1}\widetilde{\mathbf{H}}_j, \qquad \mathbf{H}_j = \mathbf{Q}_j^*\mathbf{A}\mathbf{Q}_j.$$

- The eigenvalues of the Hessenberg matrix $\mathbf{H}_j$ are called "Ritz values". Some of these numbers are typically observed to converge rapidly, often geometrically (i.e., linearly), and when they do, one may assume with reasonable confidence that the converged values are eigenvalues of $\mathbf{A}$.
- Which eigenvalues, then, does the Arnoldi algorithm find? Typically, it finds *extreme* eigenvalues, that is, eigenvalues near the edge of the spectrum of $\mathbf{A}$. Fortunately, these are precisely the eigenvalues of main interest in most applications.

4. Some existing techniques for eigenvalue problems

- Polynomial acceleration.
- Shift-and-invert Arnoldi.
- Restart.
- Davidson and Jacobi–Davidson.
- Rational Krylov. [LAA, 1984; SISC, 1998]

5. Implicitly restarted Arnoldi (IRA) process

- The storage and computational cost of enlarging the Krylov subspace in Arnoldi algorithm for $(\mathbf{A}, \mathbf{b})$ grow with the subspace dimension, j. A simple solution is to restart the iteration.
- Implicitly restarted Arnoldi algorithm uses information from the Arnoldi relation

$$\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_{j+1}\widetilde{\mathbf{H}}_j = \mathbf{Q}_j\mathbf{H}_j + \mathbf{f}_j\mathbf{e}_j^\top$$

  to refine the starting vector $\mathbf{b}$ in a manner that enriches components in the direction of desired eigenvalues while damping unwanted eigenvalues.
- Perform $j-k$ steps of QR algorithm with the shifts $\{\mu_i\}_{i=1}^{j-k}$ to $\mathbf{H}_j$, giving $\mathbf{H}_j\mathbf{V} = \mathbf{V}\mathbf{H}_j^+$, and

$$(\mathbf{H}_j - \mu_1\mathbf{I})(\mathbf{H}_j - \mu_2\mathbf{I})\cdots(\mathbf{H}_j - \mu_{j-k}\mathbf{I}) = \mathbf{V}\mathbf{R},$$

  with $\mathbf{V}$ being unitary and $\mathbf{R}$ being upper triangular.

- Let $\mathbf{H}_k^+$ be the $k \times k$ leading principal submatrix of $\mathbf{H}_j^+ = \mathbf{V}^*\mathbf{H}_j\mathbf{V}$, and
$$\mathbf{Q}_j^+ = \mathbf{Q}_j\mathbf{V} = \begin{bmatrix} \mathbf{Q}_k^+ & \mathbf{Q}_{j-k}^+ \end{bmatrix}.$$
Then it holds the k-step Arnoldi relation
$$\mathbf{A}\mathbf{Q}_k^+ = \mathbf{Q}_k^+\mathbf{H}_k^+ + \mathbf{f}_k^+\mathbf{e}_k^\top,$$
and it is extended to the j-step Arnoldi relation in a standard way.
- The starting vector for the new Arnoldi process takes the form
$$\mathbf{b}^+ = \psi(\mathbf{A})\mathbf{b}$$
with
$$\psi(z) = \prod_{i=1}^{j-k}(z - \mu_i).$$
This polynomial is the so called filter polynomial.

5.1. Implicitly restarted Arnoldi algorithm with exact shifts

- Start: Build a length j Arnoldi relation $\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_j\mathbf{H}_j + \mathbf{f}_j\mathbf{e}_j^\top$
- Iteration: Until convergence
  1. Compute the eigenvalues $\{\theta_i : i = 1, 2, \ldots, j\}$ of $\mathbf{H}_j$. Sort these eigenvalues according to the user selection criterion into a wanted set $\{\theta_i\}_{i=1}^k$ and an unwanted set $\{\theta_i\}_{i=k+1}^j$.
  2. Perform $j - k$ steps of QR algorithm with the shifts $\{\theta_i\}_{i=k+1}^j$ to obtain $\mathbf{H}_j\mathbf{V} = \mathbf{V}\mathbf{H}_j^+$.
  3. Restart: Postmultiply the length j Arnoldi relation with the matrix $\mathbf{V}_k$ consisting of the leading k columns of $\mathbf{V}$ to obtain the length k Arnoldi relation
  $$\mathbf{A}\mathbf{Q}_k^+ = \mathbf{Q}_k^+\mathbf{H}_k^+ + \mathbf{f}_k^+\mathbf{e}_k^\top,$$
  where $\mathbf{Q}_k^+ = \mathbf{Q}_j\mathbf{V}_k$, and $\mathbf{H}_k^+$ is the leading principal submatrix of order k for $\mathbf{H}_j^+$.
  4. Extend the length k Arnoldi relation to a length j Arnoldi relation.

More on IRA

- IRA with exact shifts can fail. See SIMAX, 2009.

5.2. Implicitly restarted harmonic Arnoldi (IRHA) algorithm

- Start: Build a length j Arnoldi relation $\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_j\mathbf{H}_j + \mathbf{f}_j\mathbf{e}_j^\top$
- Iteration: Until convergence
  1. Compute the harmonic Ritz values $\{\theta_i\}_{i=1}^j$ of $\widetilde{\mathbf{H}}_j^*\widetilde{\mathbf{H}}_j\mathbf{y} = \theta\mathbf{H}_j^*\mathbf{y}$. Sort them according to the user selection criterion into a wanted set $\{\theta_i\}_{i=1}^k$ and an unwanted set $\{\theta_i\}_{i=k+1}^j$.
  2. Perform $j-k$ steps of QR algorithm with the shifts $\{\theta_i\}_{i=k+1}^j$ to obtain $\mathbf{H}_j\mathbf{V} = \mathbf{V}\mathbf{H}_j^+$.
  3. Restart: Postmultiply the length j Arnoldi relation with the matrix $\mathbf{V}_k$ consisting of the leading k columns of $\mathbf{V}$ to obtain the length k Arnoldi relation
  $$\mathbf{A}\mathbf{Q}_k^+ = \mathbf{Q}_k^+\mathbf{H}_k^+ + \mathbf{f}_k^+\mathbf{e}_k^\top,$$
  where $\mathbf{Q}_k^+ = \mathbf{Q}_j\mathbf{V}_k$, and $\mathbf{H}_k^+$ is the leading principal submatrix of order k for $\mathbf{H}_j^+$.
  4. Extend the length k Arnoldi relation to a length j Arnoldi relation.

A small research project

- Can IRHA fail? Yes.

6. Davidson [SISC, 1994]

- Suppose we have a k-dimensional subspace $\mathcal{K} = \text{span}\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}$, over which the projected matrix $\mathbf{A}$ has a Ritz pair $(\theta_k, \mathbf{u}_k)$.
- Compute the residual $\mathbf{r}_k = \mathbf{A}\mathbf{u}_k - \theta_k \mathbf{u}_k$, and compute $\mathbf{p}$ from

$$(\mathbf{D_A} - \theta_k \mathbf{I})\mathbf{p} = \mathbf{r}_k$$

  where $\mathbf{D_A}$ is the diagonal of the matrix $\mathbf{A}$.
- Then $\mathbf{p}$ is made orthogonal to the basis vectors $\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}$, and the resulting vector is chosen as $\mathbf{v}_{k+1}$, by which $\mathcal{K}$ is expanded.

7. Jacobi–Davidson [SIMAX, 1996; SIREV, 2000]

1. Start: Choose $\mathbf{v} \neq \mathbf{0}$.
   Compute $\mathbf{v}_1 = \mathbf{v}/\|\mathbf{v}\|_2$, $\mathbf{w}_1 = \mathbf{A}\mathbf{v}_1$, $h_{11} = \mathbf{v}_1^* \mathbf{w}_1$;
   Set $\mathbf{V}_1 = \left[\mathbf{v}_1\right]$, $\mathbf{W}_1 = \left[\mathbf{w}_1\right]$, $\mathbf{H}_1 = \left[h_{11}\right]$, $\mathbf{u} = \mathbf{v}_1$, $\theta = h_{11}$;
   Compute $\mathbf{r} = \mathbf{w}_1 - \theta \mathbf{u}$.
2. Iteration: Until convergence

3. Inner Loop. For $k = 1, \dots, m-1$, do
   - Solve (approximately) $\mathbf{p} \perp \mathbf{u}$,

$$(\mathbf{I} - \mathbf{u}\mathbf{u}^*)(\mathbf{A} - \theta\mathbf{I})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\mathbf{p} = -\mathbf{r}.$$

   - Orthogonalize $\mathbf{p}$ against $\mathbf{V}_k$ via modified Gram–Schmidt and expand $\mathbf{V}_k$ with this vector to $\mathbf{V}_{k+1}$.
   - Compute $\mathbf{w}_{k+1} := \mathbf{A}\mathbf{v}_{k+1}$ and expand $\mathbf{W}_k$ with this vector to $\mathbf{W}_{k+1}$.
   - Compute $\mathbf{V}_{k+1}^* \mathbf{w}_{k+1}$, the last column of

$$\mathbf{H}_{k+1} := \mathbf{V}_{k+1}^* \mathbf{A} \mathbf{V}_{k+1}$$

     and $\mathbf{v}_{k+1}^* \mathbf{W}_k$, the last row of $\mathbf{H}_{k+1}$ (only if $\mathbf{A} \neq \mathbf{A}^*$).
   - Compute the largest eigenpair $(\theta, \mathbf{q})$ of $\mathbf{H}_{k+1}$ (with $\|\mathbf{q}\|_2 = 1$).
   - Compute the Ritz vector $\mathbf{u} := \mathbf{V}_{k+1}\mathbf{q}$, compute

$$\widehat{\mathbf{u}} := \mathbf{A}\mathbf{u} (= \mathbf{W}_{k+1}\mathbf{q}),$$

     and the associated residual vector $\mathbf{r} := \widehat{\mathbf{u}} - \theta\mathbf{u}$.
   - Test for convergence. Stop if satisfied.

4 Restart: Set $\mathbf{V}_1 = [\mathbf{u}]$, $\mathbf{W}_1 = [\widehat{\mathbf{u}}]$, $\mathbf{H}_1 = [\theta]$, and goto 3.

8. Bi-Lanczos algorithm for non-Hermitian eigenproblems

- Bi-Lanczos relations for the biorthogonalization methods:

$$\mathbf{A}\mathbf{V}_j = \mathbf{V}_{j+1}\widetilde{\mathbf{T}}_j, \qquad \mathbf{A}^*\mathbf{W}_j = \mathbf{W}_{j+1}\widetilde{\mathbf{S}}_j,$$

  with

$$\widetilde{\mathbf{T}}_j := \begin{bmatrix} \alpha_1 & \gamma_1 & & & \\ \beta_1 & \alpha_2 & \gamma_2 & & \\ & \beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \gamma_{j-1} \\ & & & \beta_{j-1} & \alpha_j \\ & & & & \beta_j \end{bmatrix}.$$

- $\mathbf{T}_j$ is tridiagonal and is obtained by deleting the last row of $\widetilde{\mathbf{T}}_j$. The eigenvalues of $\mathbf{T}_j$ are the approximate eigenvalues of $\mathbf{A}$.

9. A reference book

- Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst

  Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide

  SIAM, 2000

10. Arnoldi/Lanczos approximation problem

- Let $j \in \mathbb{N}$. Define

$$\mathbb{P}^j = \{\text{monic polynomial of degree } j\}.$$

  The word "monic" means that the coefficient of the term of degree j is 1.

- The jth Arnoldi/Lanczos approximation problem:

  Let $\mathbf{A} \in \mathbb{C}^{m\times m}$ and $\mathbf{b} \in \mathbb{C}^m$ be given. Find $p^j \in \mathbb{P}^j$ such that

$$\|p^j(\mathbf{A})\mathbf{b}\|_2 = \min_{p\in\mathbb{P}^j} \|p(\mathbf{A})\mathbf{b}\|_2.$$

Theorem 6

Assume that $\dim\mathcal{K}_j(\mathbf{A},\mathbf{b}) = j$. *Let* $\mathbf{Q}_j$ *be the matrix in the Arnoldi process for* $\mathbf{A}$ *and* $\mathbf{b}$. *The* j*th Arnoldi/Lanczos approximation problem has a unique solution* p^j*, namely, the characteristic polynomial of* $\mathbf{H}_j = \mathbf{Q}_j^*\mathbf{A}\mathbf{Q}_j$.

Proof. Note that $\mathbf{Q}_j^*\mathbf{Q}_j = \mathbf{I}$ and $\text{range}(\mathbf{Q}_j) = \mathcal{K}_j(\mathbf{A},\mathbf{b})$. If $p \in \mathbb{P}^j$, then the vector $p(\mathbf{A})\mathbf{b}$ can be written

$$p(\mathbf{A})\mathbf{b} = \mathbf{A}^j\mathbf{b} - \mathbf{Q}_j\mathbf{y}$$

for some $\mathbf{y} \in \mathbb{C}^j$. In other words, the jth Arnoldi/Lanczos approximation problem is equivalent to a linear least squares problem: find $\mathbf{y}_j$ such that

$$\mathbf{y}_j = \arg\min_{\mathbf{y}\in\mathbb{C}^j} \|\mathbf{A}^j\mathbf{b} - \mathbf{Q}_j\mathbf{y}\|_2.$$

The solution is characterized by the orthogonality condition

$$p^j(\mathbf{A})\mathbf{b} = \mathbf{A}^j\mathbf{b} - \mathbf{Q}_j\mathbf{y}_j \perp \text{range}(\mathbf{Q}_j).$$

The equivalent condition is

$$\mathbf{Q}_j^* p^j(\mathbf{A})\mathbf{b} = \mathbf{0}.$$

Let

$$\mathbf{V} = \begin{bmatrix} \mathbf{Q}_j & \mathbf{U} \end{bmatrix} \in \mathbb{C}^{m \times m}$$

be a unitary matrix. If the Arnoldi process does not break down at step j, we further assume that the first column of $\mathbf{U}$ is $\mathbf{q}_{j+1}$, i.e.,

$$\mathbf{U}\mathbf{e}_1 = \mathbf{q}_{j+1}.$$

Then, we have

$$\mathbf{H} := \mathbf{V}^*\mathbf{A}\mathbf{V} = \begin{bmatrix} \mathbf{H}_j & \mathbf{X}_1 \\ \mathbf{X}_2 & \mathbf{X}_3 \end{bmatrix},$$

where

$$\mathbf{X}_1 = \mathbf{Q}_j^*\mathbf{A}\mathbf{U}, \quad \mathbf{X}_2 = h_{j+1,j}\mathbf{e}_1\mathbf{e}_j^\top, \quad \mathbf{X}_3 = \mathbf{U}^*\mathbf{A}\mathbf{U}.$$

Note that if the Arnoldi process breaks down at step j, then $h_{j+1,j} = 0$.

The orthogonality condition becomes

$$\mathbf{Q}_j^*\mathbf{V}p^j(\mathbf{H})\mathbf{V}^*\mathbf{b} = \begin{bmatrix}\mathbf{I}_j & \mathbf{0}\end{bmatrix} p^j(\mathbf{H})\|\mathbf{b}\|_2\mathbf{e}_1 = \mathbf{0},$$

which amounts to the condition that the first j entries of the first column of $p^j(\mathbf{H})$ are zero. Because the structure of $\mathbf{H}$, we have

$$\begin{bmatrix}\mathbf{I}_j & \mathbf{0}\end{bmatrix} \mathbf{H}^i\mathbf{e}_1 = \mathbf{H}_j^i\mathbf{e}_1, \qquad \forall\ i = 0, 1, \ldots, j.$$

Then the orthogonality condition further becomes

$$p^j(\mathbf{H}_j)\mathbf{e}_1 = \mathbf{0}.$$

By the Cayley–Hamilton theorem, the condition is satisfied if p^j is the characteristic polynomial of $\mathbf{H}_j$. Now suppose there were another polynomial $\widetilde{p}^j \in \mathbb{P}^j$ with

$$\widetilde{p}^j(\mathbf{A})\mathbf{b} \perp \operatorname{range}(\mathbf{Q}_j).$$

Taking the difference would give a nonzero polynomial $q = p^j - \widetilde{p}^j$ of degree $\leq j-1$ with $q(\mathbf{A})\mathbf{b} = \mathbf{0}$, violating $\dim\mathcal{K}_j(\mathbf{A}, \mathbf{b}) = j$. $\square$