Lecture 15: Krylov subspace methods for eigenvalue problems

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1. The Rayleigh–Ritz method for Hermitian eigenproblems

- Let $\mathbf{Q} = \begin{bmatrix} \mathbf{Q}_k & \mathbf{Q}_c \end{bmatrix}$ be any $n \times n$ unitary matrix, where $\mathbf{Q}_k \in \mathbb{C}^{n \times k}$ and $\mathbf{Q}_c \in \mathbb{C}^{n \times (n-k)}$. Assume that $\mathbf{A} \in \mathbb{C}^{n \times n}$ is Hermitian. We will use the following notation:

$$\mathbf{T} = \mathbf{Q}^* \mathbf{A} \mathbf{Q} = \begin{bmatrix} \mathbf{Q}_k & \mathbf{Q}_c \end{bmatrix}^* \mathbf{A} \begin{bmatrix} \mathbf{Q}_k & \mathbf{Q}_c \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_k^* \mathbf{A} \mathbf{Q}_k & \mathbf{Q}_k^* \mathbf{A} \mathbf{Q}_c \\ \mathbf{Q}_c^* \mathbf{A} \mathbf{Q}_k & \mathbf{Q}_c^* \mathbf{A} \mathbf{Q}_c \end{bmatrix}$$
$$= \begin{bmatrix} \mathbf{T}_k & \mathbf{T}_{ck} \\ \mathbf{T}_{kc} & \mathbf{T}_c \end{bmatrix} = \begin{bmatrix} \mathbf{T}_k & \mathbf{T}_{kc}^* \\ \mathbf{T}_{kc} & \mathbf{T}_c \end{bmatrix}.$$

- The Rayleigh–Ritz procedure is to approximate the eigenvalues of $\mathbf{A}$ by the eigenvalues of $\mathbf{T}_k = \mathbf{Q}_k^* \mathbf{A} \mathbf{Q}_k$. These approximations are called *Ritz values*.
- Let $\mathbf{T}_k = \mathbf{V} \mathbf{\Lambda}_k \mathbf{V}^*$ be the eigendecomposition. The columns of $\mathbf{Q}_k \mathbf{V}$, called *Ritz vectors*, are the corresponding eigenvector approximations.

Theorem 1

We have the following optimality property

$$\mathbf{T}_k = \arg \min_{\mathbf{S}\in\mathbb{C}^{k\times k}, \mathbf{S}=\mathbf{S}^*} \|\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S}\|_2.$$

Proof.

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

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

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

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 $\mathbf{T}_k = \mathbf{V}\mathbf{\Lambda}_k\mathbf{V}^*$ be the eigendecomposition of $\mathbf{T}_k$. We have

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

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

Proof. The proof is left as an exercise. □

Theorem 3

Let $\mathbf{T}_k = \mathbf{V}\mathbf{\Lambda}_k\mathbf{V}^*$ *be the eigendecomposition. Let* $\mathbf{V} = \begin{bmatrix}\mathbf{v}_1 & \cdots & \mathbf{v}_k\end{bmatrix}$ *and* $\mathbf{\Lambda}_k = \mathrm{diag}\{\theta_1, \cdots, \theta_k\}$. *Then*

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

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

(ii) *We have*

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

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

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

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

(ii) We compute

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

2. Lanczos algorithm for Hermitian eigenproblems

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

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

All the quantities in the above theorem can be computed easily. This is because there are good algorithms for finding eigenvalues and eigenvectors of the Hermitian 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. Acceleration 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 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 orthogonal and $\mathbf{R}$ being upper triangular.

- Let $\mathbf{H}_j^+ = \mathbf{V}^*\mathbf{H}_j\mathbf{V}$, $\mathbf{H}_k^+$ be the $k \times k$ leading principal submatrix of $\mathbf{H}_j^+$, 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

$$(\mathbf{D}_\mathbf{A} - \theta_k \mathbf{I})\mathbf{p} = \mathbf{r}_k$$

  where $\mathbf{D}_\mathbf{A}$ 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 $\mathbf{V}_1 = \begin{bmatrix}\mathbf{v}_1\end{bmatrix}$, $\mathbf{W}_1 = \begin{bmatrix}\mathbf{w}_1\end{bmatrix}$, $\mathbf{H}_1 = \begin{bmatrix}h_{11}\end{bmatrix}$, $\mathbf{u} = \mathbf{v}_1$, $\theta = h_{11}$;

   Compute $\mathbf{r} = \mathbf{w}_1 - \theta \mathbf{u}$.
2. Iteration: Until convergence

3. Inner Loop. For $k = 1, \ldots, m-1$, 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 Ritz values (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.

- 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

$$\|p^j(\mathbf{A})\mathbf{b}\|_2 = \text{minimum}.$$

- The Arnoldi process for $\mathbf{A}$ and $\mathbf{b}$ has the remarkable property that it solve the approximation problem exactly.

Theorem 6

As long as the Arnoldi process does not break down (i.e., $\mathbf{K}_j$ is of full column rank j), the approximation problem has a unique solution p^j, namely, the characteristic polynomial of $\mathbf{H}_j$.

Proof. 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 $\mathbf{y} \in \mathbb{C}^j$, where $\mathbf{Q}_j$ is the matrix in the Arnoldi process for $\mathbf{A}$ and $\mathbf{b}$. In other words, the approximation problem is equivalent to a linear least squares problem: find the vector in $\mathcal{K}_j(\mathbf{A}, \mathbf{b})$ closest to $\mathbf{A}^j\mathbf{b}$, or in matrix terms, 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

$$p^j(\mathbf{A})\mathbf{b} \perp \mathcal{K}_j(\mathbf{A}, \mathbf{b}).$$

The equivalent condition is

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

Since the Arnoldi process does not break down at step j, we have

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

Let

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

where $\mathbf{U}$ satisfies

$$\mathbf{U}\mathbf{e}_1 = \mathbf{q}_{j+1}, \quad \mathbf{U}^*\mathbf{U} = \mathbf{I}, \quad \mathbf{U}^*\mathbf{Q}_j = \mathbf{0}.$$

Then, we have $\mathbf{V}^*\mathbf{V} = \mathbf{I}$ and

$$\mathbf{H} = \mathbf{V}^*\mathbf{A}\mathbf{V} = \begin{bmatrix}\mathbf{H}_j & \mathbf{X}_1 \\ \mathbf{X}_2 & \mathbf{X}_3\end{bmatrix}, \quad \mathbf{X}_2 = h_{j+1,j}\mathbf{e}_1\mathbf{e}_j^\top.$$

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 $p^j \in \mathbb{P}^j$ with $p^j(\mathbf{A})\mathbf{b} \perp \mathcal{K}_j(\mathbf{A}, \mathbf{b})$. Taking the difference would give a nonzero polynomial q of degree $\leq j - 1$ with $q(\mathbf{A})\mathbf{b} = \mathbf{0}$, violating the assumption that $\mathbf{K}_j$ is of full column rank. □