Numerical Linear Algebra for Computational Science and Information Engineering

Lecture 11
Arnoldi and Lanczos Procedures

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Outline I

Krylov subspace methods for few eigenpairs

- So far we've seen:
  - **Power iterations**, **inverse iterations** and **Rayleigh quotient iterations** to compute a single eigenpair
  - **QR iterations**, the **divide-and-conquer method** and the **method of bissection** to compute all the eigenpairs of a small-to-medium size and dense matrix
  - **LOBPCG** to compute a few extremal generalized eigenpairs of a large, possibly sparse matrix pencil (A, B).
- **Krylov subspace methods** are another set of iterative methods to compute a few eigenpairs of a large matrix A
  - We assume that the mapping $x \mapsto Ax$ can be operated efficiently, possibly because A is sparse
  - We denote two methods in particular:
    - The **Arnoldi** process is meant for non-symmetric matrices, and
    - The **Lanczos** process, which was introduced later for symmetric matrices.

Arnoldi process

Section 6.1 in Darve & Wootters (2021)

Arnoldi process as a Krylov subspace method

- Given a vector $v \in \mathbb{R}^n$, the k-th Krylov subspace of $A \in \mathbb{R}^{n \times n}$ is

$$\mathcal{K}_k(A, v) := \operatorname{span}\{v, Av, \ldots, A^{k-1}v\}.$$

- The Arnoldi process which we present in this section is a procedure to generate an orthogonal $Q_k := [q_1, \ldots, q_k]$, i.e., $Q_k^T Q_k = I_k$ such that

$$\operatorname{span}\{q_1, \ldots, q_k\} = \mathcal{K}_k(A, v).$$

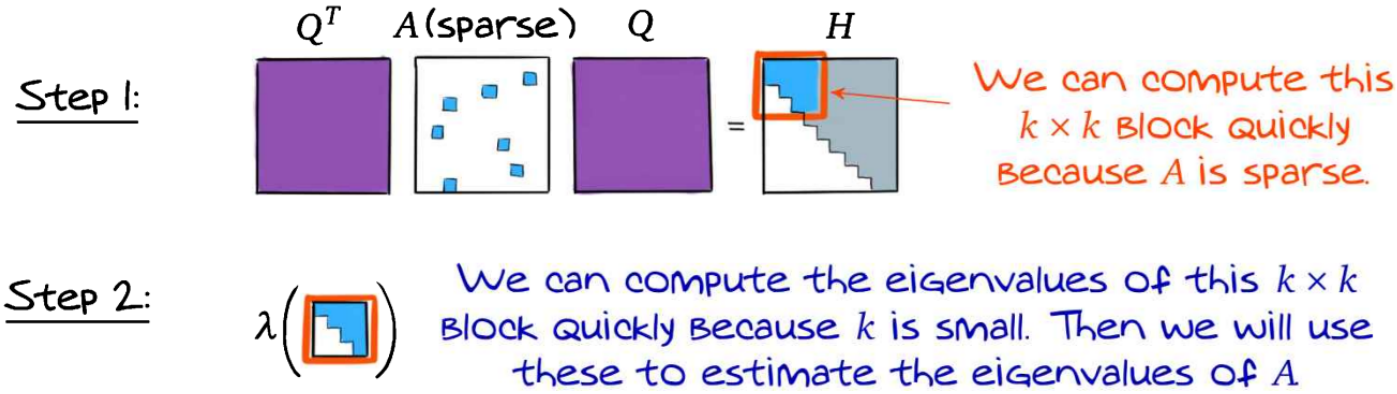
  The orthonormal basis in the columns of Q_k is such that $H_k := Q_k^T A Q_k$ is an upper Hessenberg matrix.
- We present two different ways to derive Arnoldi procedures:
  1. Deduction of Arnoldi iteration from the $AQ = QH$ relation where $Q \in \mathbb{R}^{n \times n}$ is orthogonal and $H \in \mathbb{R}^{n \times n}$ is Hessenberg.
  2. Orthogonalization of Aq_k against $q_1, \ldots, q_k$.
- Later, we see that approximate eigenpairs of A can be sought within the Kylov subspace $\mathcal{K}_k(A, v)$.

Reduction to Hessenberg form

- Householder transformations can be used to transform a matrix into Hessenberg form. That is, there exists an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ s.t.

$$Q^T A Q = H$$

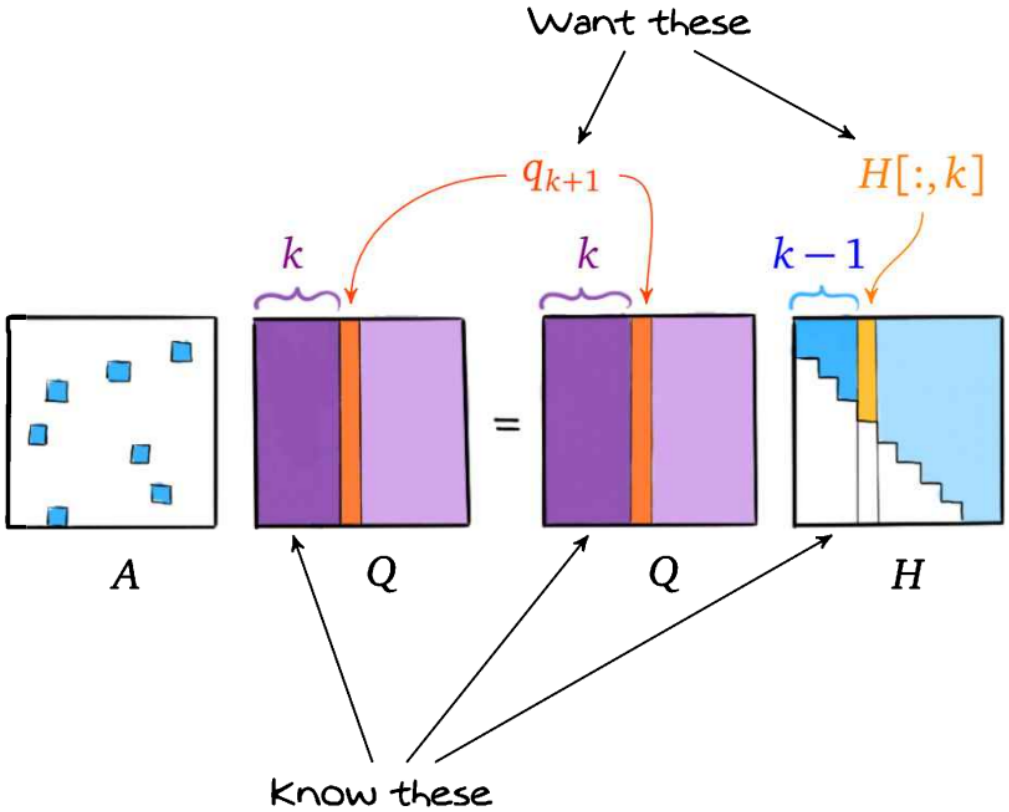
  is upper Hessenberg.
- As with any similarity transformation, the eigenvalues of H are the same as those of A, which can be exploited to find eigenvalues of A.
- Instead of considering the full Hessenberg matrix H, we approximate eigenpairs of A with eigenpairs of a leading block H_k of H with $k \ll n$.



- As it turns out, the eigenpairs of the leading block H_k of H are good approximations of some eigenpairs of A.

Deducting the Arnoldi process from $AQ = QH$

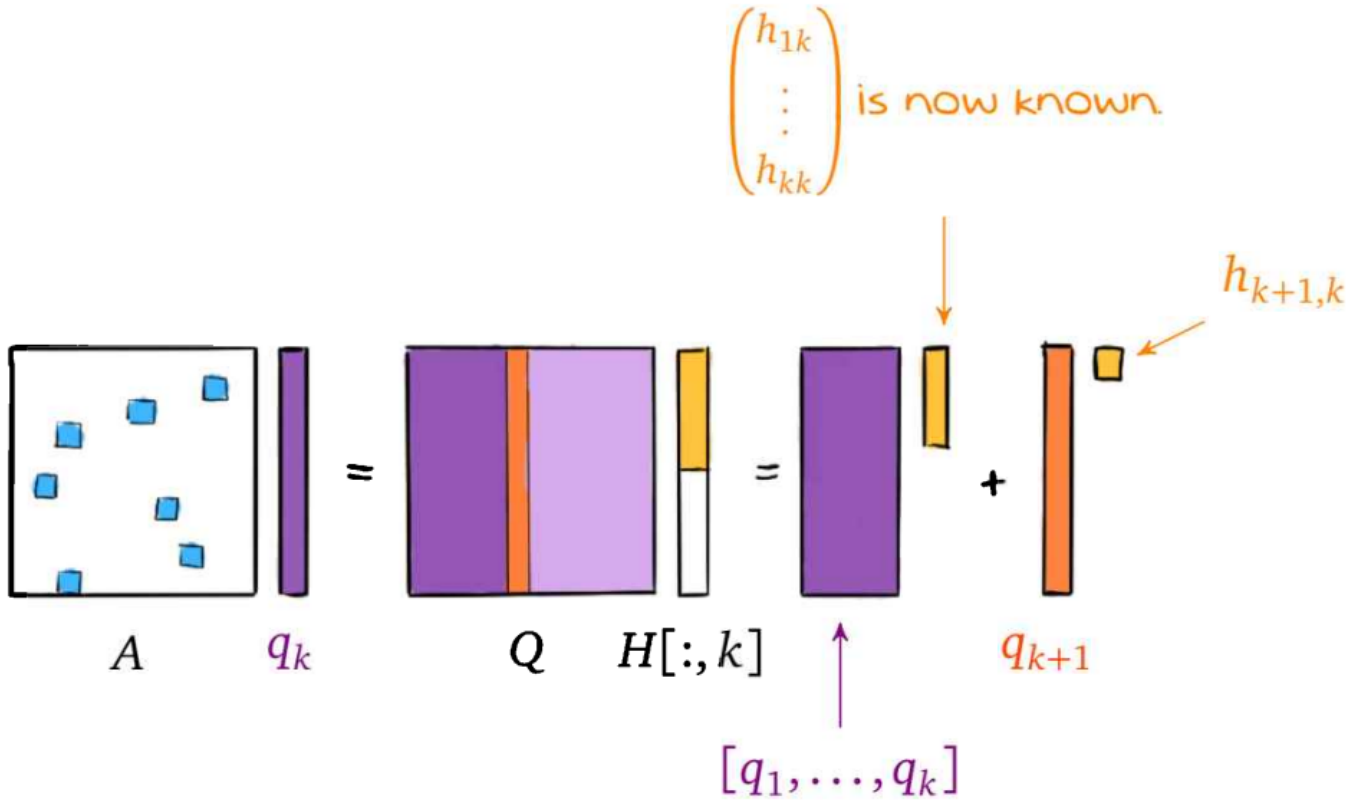
- Computing the leading block H_k of H is called the **Arnoldi process**. One possible form of this process is similar to the Gram-Schmidt procedure.
- Because Q is orthogonal, we can rewrite $Q^T AQ = H$ as $AQ = QH$.
- We'd like to design an iterative procedure to recover Q and H.
  - Suppose that we already have the k first columns of Q, and the first $k-1$ columns of H. How can we recover the next columns of Q and H?



Deducting the Arnoldi process from $AQ = QH$, cont'd$_1$

- The first thing we observe is that we can recover the entries h_{ik} for $i \leq k$ using what we know, because $q_i^T A q_k = h_{ik}$.
  Now that we know h_{ik} for $i \leq k$, we focus on recovering $h_{k+1,k}$ and q_{k+1}.
  To do this, from the k-th column of $AQ = QH$, we write

$$Aq_k = h_{1k}q_1 + \cdots + h_{kk}q_k + h_{k+1,k}q_{k+1}.$$



Deducting the Arnoldi process from $AQ = QH$, cont'd$_2$

of which we can compute the left-hand side Aq_k, and the only part of the right-hand side that we don't know is the vector $h_{k+1,k}q_{k+1}$. So we can solve for it. Denote

$$r_k := Aq_k - h_{1k}q_1 - \cdots - h_{kk}q_k = h_{k+1,k}q_{k+1}$$

where q_{k+1} has unit norm, so that

$$h_{k+1,k} = \|r_k\|_2, \; q_{k+1} = r_k/h_{k+1,k}.$$

(Note that we could also choose $h_{k+1,k} = -\|r_k\|_2$, which would lead to a different sign choice for q_{k+1}. This choice is arbitrary.)

Thus we have figured out q_{k+1} and h_{ik} for $i \leq k+1$. This is what we wanted to know, and we can now proceed to the step to obtain q_{k+2} and $h_{i,k+1}$ for $i \leq k+2$.

Deducting the Arnoldi process from $AQ = QH$, cont'd$_3$

- Consequently, we have the following iteration:

Arnoldi recurrence relation:

Suppose we have $q_1, \ldots, q_k$ and $h_{:,j}$ for $j < k$. Then we can find q_{k+1} and $h_{:,k}$ as follows:

for $i \leq k$:

$h_{ik} := q_i^T A q_k$

$r_k := Aq_k - \sum_{i=1}^{k} h_{ik} q_i$

$h_{k+1,k} := \|r_k\|_2$

$q_{k+1} := \frac{r_k}{h_{k+1,k}}$

- Performing this iteration starting from a given vector q_1, we get a method to calculate the columns of the matrices H and Q that satisfy $Q^T AQ = H$. This is, in a nuttshell, the Arnoldi process.

Alternative way to define Arnoldi procedures

- Given a vector $X_{:,1}$, the Arnoldi procedure is defined by

$$\text{Arnoldi} : (X_{:,1}, k) \in \mathbb{R}^n \times \mathbb{N} \mapsto Q = [q_1, \ldots, q_k] \in \mathbb{R}^{n \times k}$$

  s.t. $Q^T Q = I_k$ and $\text{span}\{q_1, \ldots, q_k\} = \text{span}\{q_1, Aq_1, \ldots, A^{k-1}q_1\}$ where $q_1 := X_{:,1}/\|X_{:,1}\|_2$.

- We are interested by the QR decomposition $X = QR$ such that $X_{:,j} := Aq_{j-1}$ for $j = 2, \ldots, k$. X is defined column-by-column with respect to Q, so that the Gram-Schmidt procedure is particularly well adapted.
- Let $\Pi^{(j)}$ be a projector onto $\text{Span}\{q_1, \ldots, q_j\}^\perp$, then Arnoldi$(X_{:,1}, k)$ is given by the following GS procedure:

Algorithm 1 $\text{Arnoldi} : (X_{:,1}, k) \mapsto Q$

1: $q_1 := X_{:,1}/\|X_{:,1}\|_2$
2: **for** $j = 2, \ldots, k$ **do**
3: $\quad X_{:,j} := Aq_{j-1}$
4: $\quad q_j := \Pi^{(j-1)} X_{:,j}$
5: $\quad q_j := q_j/\|q_j\|_2$

Matrices of interest and notation

- From the orthogonality of Q, the QR decomposition of X is such that $Q^T X = R$. Given that $X_{:,j} = Aq_{j-1}$ for $j = 2, \dots, k$, we have $R_{ij} = Q_{:,i}^T X_{:,j} = q_i^T A q_{j-1}$ for $(i, j) \in [1, k] \times [2, k]$.
- In the Arnoldi procedure, we are interested in some of the components of R. In particular, we wish to compute the matrix defined by $H := Q^T AQ$. The components of H are given by $h_{ij} = q_i^T A q_j$.
- So as to explicitly state the dimension of Q during intermediate states $j < k$ of the Arnoldi algorithm, we write $Q_j := [q_1, \dots, q_j]$. Similarly, we denote the corresponding matrix by $H_j := Q_j^T AQ_j$.
- Some properties of the Arnoldi procedure rely on the matrix defined by $\underline{H}_j := Q_{j+1}^T AQ_j$.

CGS-based Arnoldi procedure

- For the CGS-based Arnoldi procedure, we let $\Pi^{(j)} := I_n - Q_j Q_j^T$.
- We obtain the following algorithm:

Algorithm 2 CGS-based Arnoldi: $(X_{:,1}, k) \mapsto Q_k$

1: $q_1 := X_{:,1}/\|X_{:,1}\|_2$
2: **for** $j = 2, \ldots, k$ **do**
3: $\quad X_{:,j} := Aq_{j-1}$
4: $\quad H_{1:j-1,j-1} := Q_{j-1}^T X_{:,j}$
5: $\quad q_j := X_{:,j} - Q_{j-1} H_{1:j-1,j-1}$
6: $\quad q_j := q_j/\|q_j\|_2$

- Let $\|q_j\|_2$ be computed after line 5, then, after line 6, we have

$$\begin{aligned}
\|q_j\|_2 q_j &= (I_n - Q_{j-1}Q_{j-1}^T)Aq_{j-1} \\
\|q_j\|_2 q_j^T q_j &= q_j^T(I_n - Q_{j-1}Q_{j-1}^T)Aq_{j-1} \\
\|q_j\|_2 &= q_j^T Aq_{j-1} \\
\|q_j\|_2 &= h_{j,j-1}.
\end{aligned}$$

CGS-based Arnoldi procedure

- For the CGS-based Arnoldi procedure, we let $\Pi^{(j)} := I_n - Q_j Q_j^T$.
- We obtain the following algorithm:

Algorithm 3 CGS-based Arnoldi: $(X_{:,1}, k) \mapsto Q_k$

$q_1 := X_{:,1} / \|X_{:,1}\|_2$
for $j = 2, \ldots, k$ **do**
  $X_{:,j} := A q_{j-1}$
  $H_{1:j-1,j-1} := Q_{j-1}^T X_{:,j}$
  $q_j := X_{:,j} - Q_{j-1} H_{1:j-1,j-1}$
  $h_{j,j-1} := \|q_j\|_2$ ▷ $H_{j+1:k,j-1} := 0$
  $q_j := q_j / H_{j,j-1}$

Hessenberg matrices and property of the Arnoldi algorithm

- From lines 4-7 of the algorithm, we have

$$h_{j,j-1}q_j = (I_n - Q_{j-1}Q_{j-1}^T)Aq_{j-1},$$
$$h_{j,j-1}q_i^T q_j = q_i^T(I_n - Q_{j-1}Q_{j-1}^T)Aq_{j-1}.$$

  Let $i > j$, then we have $q_i^T Aq_{j-1} = 0$ so that $h_{ij} = 0$ for $i > j+1$, i.e., H_j is upper Hessenberg.

- We have $Aq_j = \sum_{i=1}^{j+1} h_{ij}q_i$.

  Proof: From lines 4-7 of the algorithm, we have

$$h_{j,j-1}q_j = Aq_{j-1} - Q_{j-1}Q_{j-1}^T Aq_{j-1}$$
$$h_{j+1,j}q_{j+1} = Aq_j - Q_j Q_j^T Aq_j$$
$$h_{j+1,j}q_{j+1} = Aq_j - Q_j H_{1:j,j}$$

  so that we can write

$$Aq_j = \begin{bmatrix} q_1 & \dots & q_j \end{bmatrix} \begin{bmatrix} h_{1j} \\ \vdots \\ h_{jj} \end{bmatrix} + h_{j+1,j}q_{j+1}. \quad \square$$

The Arnoldi relation

- Writing down the components of $Q_j H_j$ and AQ_j leads us to

$$\begin{bmatrix} \sum_{i=1}^{j} h_{i1} q_i & \dots & \sum_{i=1}^{j} h_{ij} q_i \end{bmatrix} = Q_j H_j,$$

$$\begin{bmatrix} Aq_1 & \dots & Aq_j \end{bmatrix} = AQ_j.$$

- Then, using the fact that $Aq_j = \sum_{i=1}^{j+1} h_{ij} q_i$ and that H_j is upper Hessenberg, we have $h_{j+1,i} = 0$ for $i = 1, \dots, j-1$ so that

$$\begin{bmatrix} Aq_1 & \dots & Aq_j \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{j} h_{i1} q_i & \dots & \sum_{i=1}^{j} h_{ij} q_i \end{bmatrix} + \begin{bmatrix} 0 & \dots & 0 & h_{j+1,j} q_{j+1} \end{bmatrix}$$

which can be written as $\boxed{AQ_j = Q_j H_j + h_{j+1,j} q_{j+1} e_j^T}$ where e_j is the j-th column of the j-dimensional identity matrix. Note the difference with the relation $AQ = QH$ obtained only when $j = n$.

- Similarly, we have

$$\begin{bmatrix} Aq_1 & \dots & Aq_j \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{j+1} h_{i1} q_i & \dots & \sum_{i=1}^{j+1} h_{ij} q_i \end{bmatrix}$$

which can be written as $\boxed{AQ_j = Q_{j+1} \underline{H}_j}$.

CGS-based Arnoldi procedure

- Approximate solutions in $\mathcal{K}_k(A, r_0)$ for linear systems and eigenvalue problems have residuals which depend on the product AQ_k.
- Exploit the Arnoldi relation $AQ_k = Q_{k+1}\underline{H}_k$ for faster computation.
- The Arnoldi algorithm is reformulated as follows so as to compute $\underline{H}_k$ at the k-th iteration:

Algorithm 4 CGS-based Arnoldi

$q_1 := X_{:,1}/\|X_{:,1}\|_2$
for $j = 1, \ldots, k$ **do**
  $X_{:,j+1} := Aq_j$
  $H_{1:j,j} := Q_j^T X_{:,j+1}$
  $q_{j+1} := X_{:,j+1} - Q_j H_{1:j,j}$
  $H_{j+1,j} := \|q_{j+1}\|_2$ ▷ $H_{j+2:k+1,j} := 0$
  $q_{j+1} := q_{j+1}/H_{j+1,j}$

- The approach of the book of Darve and Wootters (2021) we presented is equivalent to CGS-based Arnoldi.

MGS-based Arnoldi procedure

- MGS-based Arnoldi $\implies$ $\Pi^{(i)} := (I_n - q_i q_i^T) \dots (I_n - q_1 q_1^T)$.
- We obtain the following algorithm:

Algorithm 5 MGS-based Arnoldi: $(X_{:,1}, k) \mapsto Q_k$

1: $q_1 := X_{:,1} / \|X_{:,1}\|_2$
2: **for** $j = 2, \dots, k$ **do**
3: $\quad q_j := A q_{j-1}$
4: $\quad$ **for** $i = 1, \dots, j-1$ **do**
5: $\quad\quad q_j := q_j - q_i q_i^T q_j$
6: $\quad q_j := q_j / \|q_j\|_2$

- For all $(i, j) \in [1, j-1] \times [2, k]$, prior to executing line 5, we have

$$q_j = (I_n - q_{i-1} q_{i-1}^T) \dots (I_n - q_1 q_1^T) A q_{j-1}$$

so that, assuming perfect orthogonality of Q_j, we have

$$q_i^T q_j = q_i^T (I_n - q_{i-1} q_{i-1}^T) \dots (I_n - q_1 q_1^T) A q_{j-1} = q_i^T A q_{j-1} = h_{i,j-1}.$$

MGS-based Arnoldi procedure

- Also, when computing $\|q_j\|_2$ prior to line 7, we have $\|q_j\|_2 = h_{j,j-1}$.
- We obtain the following algorithm:

Algorithm 6 MGS-based Arnoldi: $(X_{:,1}, k) \mapsto Q_k$

1: $q_1 := X_{:,1}/\|X_{:,1}\|_2$
2: **for** $j = 2, \ldots, k$ **do**
3: $\quad q_j := Aq_{j-1}$
4: $\quad$ **for** $i = 1, \ldots, j-1$ **do**
5: $\quad\quad H_{i,j-1} := q_i^T q_j$
6: $\quad\quad q_j := q_j - H_{i,j-1} q_i$
7: $\quad H_{j,j-1} := \|q_j\|_2$ $\quad \triangleright\ H_{j+1:k,j-1} := 0$
8: $\quad q_j := q_j / h_{j,j-1}$

- All the properties we showed for the CGS-based Arnoldi procedure remain valid for MGS-based Arnoldi.

MGS-based Arnoldi procedure

- Similarly as before, we want the upper Hessenberg matrix $\underline{H}_k$ to be computed at the end of the k-th iteration.
- Consequently, the Arnoldi algorithm is reformulated as follows:

Algorithm 7 MGS-based Arnoldi

$q_1 := X_{:,1}/\|X_{:,1}\|_2$
for $j = 1, \ldots, k$ **do**
  $q_{j+1} := Aq_j$
  for $i = 1, \ldots, j$ **do**
    $H_{ij} := q_i^T q_{j+1}$
    $q_{j+1} := q_{j+1} - H_{ij} q_i$
  $H_{j+1,j} := \|q_{j+1}\|_2$ ▷ $H_{j+2:k+1,j} := 0$
  $q_{j+1} := q_{j+1}/h_{j+1,j}$

- MGS-based Arnoldi is the most commonly used implementation of Arnoldi process.
- Other variants include CGS2 and Householder-based Arnoldi.

Arnoldi Rayleigh-Ritz for dominant eigenpairs

Arnoldi procedure with Rayleigh-Ritz vectors

- **Eigenvectors with eigenvalues whose norms are the largest** among the spectrum of A tend to be **well approximated by Rayleigh-Ritz** projections, as explained by Parlett (1998) and Saad (2011).
- Rayleigh-Ritz projections are **commonly defined with respect to Krylov subspaces** whose bases Q_k are obtained by a Arnoldi procedure:
  - Then, a **Rayleigh-Ritz vector** $y \in \text{range}(Q_k)$ approximates an eigenvector of A with the **Ritz value** λ such that $Ay - \lambda y \perp \text{range}(Q_k)$. That is, we **search for** $(\lambda, \hat{y}) \in \mathbb{C} \times \mathbb{C}^k \setminus \{0\}$ s.t. $z^H (Ay - \lambda y) = 0$ $\forall\, z \in \text{range}(Q_k)$ with $y = Q_k \hat{y}$. This **simplifies to**

$$Q_k^T (AQ_k\hat{y} - \lambda Q_k \hat{y}) = 0$$

$$H_k\hat{y} - \lambda\hat{y} = 0 \quad \Longrightarrow \quad \boxed{H_k\hat{y} = \lambda\hat{y}}$$

    where use was made of the Arnoldi relation and $Q_k^T Q_k = I_k$.
  - $nev < k$ **dominant eigenpairs** $\{(\lambda_\ell, \hat{y}_\ell)\}_{\ell=1}^{nev}$ **of** H_k are **used to approximate dominant eigenpairs of** A **with** $\{(\lambda_\ell, y_\ell)\}_{\ell=1}^{nev}$ where $y_\ell := Q_k \hat{y}_\ell$.

B. N. Parlett, The symmetric eigenvalue problem. Society for Industrial and Applied Mathematics (1998).

Y. Saad, Numerical methods for large eigenvalue problems: revised edition. Society for Industrial and Applied Mathematics (2011).

Arnoldi procedure with Rayleigh-Ritz vectors, cont'd$_1$

- A desirable property of the Rayleigh-Ritz approximation y_ℓ is that **the Ritz value θ_ℓ equates the corresponding Rayleigh quotient**:

$$y_\ell^H A y_\ell = (Q_k \hat{y}_\ell)^H A Q_k \hat{y}_\ell = \hat{y}_\ell^H Q_k^T A Q_k \hat{y}_\ell = \hat{y}_\ell^H H_k \hat{y}_\ell = \lambda_\ell \hat{y}_\ell^H \hat{y}_\ell = \lambda_\ell$$

  where $\hat{y}_\ell$ is assumed to have unit length.
- The **eigen-residual** $\tilde{r}_\ell := A y_\ell - \lambda_\ell y_\ell$ of the Rayleigh-Ritz vector y_ℓ is s.t.

$$\begin{aligned}
\tilde{r}_\ell &= A Q_k \hat{y}_\ell - \lambda_\ell Q_k \hat{y}_\ell \\
&= Q_k H_m \hat{y}_\ell + h_{k+1,k} q_{k+1} e_k^T \hat{y}_\ell - \lambda_\ell Q_k \hat{y}_\ell \\
&= \lambda_\ell Q_k \hat{y}_\ell + h_{k+1,k} q_{k+1} e_k^T \hat{y}_\ell - \lambda_\ell Q_k \hat{y}_\ell \\
&= h_{k+1,k} q_{k+1} e_k^T \hat{y}_\ell
\end{aligned}$$

$$\boxed{\tilde{r}_\ell = \beta_{k,\ell} q_{k+1}} \quad \text{where} \quad \boxed{\beta_{k,\ell} := h_{k+1,k} e_k^T \hat{y}_\ell}.$$

  - Essentially, **the eigen-residuals $\tilde{r}_1, \ldots, \tilde{r}_k$ of the Rayleigh-Ritz vectors $y_1, \ldots, y_k$** defined with respect to the **Krylov subspace** $\mathcal{K}_k(A, q_1)$ are **all parallel, along the Arnoldi vector q_{k+1}**.

Arnoldi procedure with Rayleigh-Ritz vectors, cont'd$_2$

- From the fact that $\tilde{r}_\ell = \beta_{k,\ell} q_{k+1}$, the norm of the eigen-residual is such that $\|\tilde{r}_\ell\|_2^2 = |\beta_{k,\ell}|^2 q_{k+1}^T q_{k+1} = |\beta_{k,\ell}|^2$ where $|\beta_{k,\ell}| = |h_{k+1,k}|\,|e_k^T \hat{y}_\ell|$.
  - Consequently, **a stopping criterion of the form** $\|\tilde{r}_\ell\|_2 < \epsilon|\lambda_\ell|$ **can be checked efficiently** at every iteration **without** having to compute the **matrix-vector product** Ay_ℓ or even to assemble the vector $y_\ell := Q_k \hat{y}_\ell$.
- As explained earlier,
  - the **orthogonalization** which is at the root of the Arnoldi procedure has time complexity $\mathcal{O}(k^2 n)$,
  - the **reduced eigensolve** of H_m has time complexity $\mathcal{O}(k^3)$,
  - the **storage of the Arnoldi basis** in Q_k has space complexity $\mathcal{O}(kn)$ so that, **if convergence is not achieved** for some number k of iterations, it is **necessary to start the Arnoldi procedure over** with a new initial vector q_1.
- A **naive restart** of the Arnoldi procedure **can be highly detrimental to** the **convergence** of approximate eigenvectors. Some **care needs to be taken** so as **to reduce convergence slowdown**.

Shift-and-invert Arnoldi Rayleigh-Ritz for interior eigenpairs

Shift-and-invert spectral transformation

- Rayleigh-Ritz pairs (λ, y) converge first towards eigenpairs (θ, z) of A with the largest value of $|\theta|$.
  - In practice, we may want to approximate an eigenpair with eigenvalue θ close to some σ, i.e., with small value of $|\sigma - \theta|$. E.g., $\sigma = 0$.
  - Rayleigh-Ritz approximations (λ, y) of such eigenpairs (θ, z) in Krylov subspaces converge very slowly when $|\sigma|$ is small compared to the spectral radius of A.
- The shift-and-invert spectral transformation was introduced by Ericsson and Ruhe (1980) as a means to circumvent this issue:
  - Consider the eigenvalue problem given by

$$(A - \sigma I_n)^{-1} w = \vartheta w$$

where it is assumed that σ is not an eigenvalue of A. Then, we have

$$w = \vartheta (A - \sigma I_n) w$$
$$w = \vartheta A w - \vartheta \sigma w.$$

Ericsson, T., & Ruhe, A. (1980). The spectral transformation Lanczos method for the numerical solution of large sparse generalized symmetric eigenvalue problems. Mathematics of Computation, 35(152), 1251-1268.

Shift-and-invert spectral transformation, cont'd

Since σ is not an eigenvalue of the non-singular matrix A, the shift-and-invert operator $(A - \sigma I_n)^{-1}$ is not singular and $\vartheta \neq 0$ so that

$$Aw = \left(\sigma + \frac{1}{\vartheta}\right) w.$$

Essentially, $(\sigma + 1/\vartheta, w)$ is an eigenpair of A.

- Now, if an Arnoldi procedure is applied to $(A - \sigma I_n)^{-1}$, the corresponding Rayleigh-Ritz pairs will first converge to the eigenpairs (ϑ, w) of the shift-and-invert operator with largest $|\vartheta|$.
- However, when $|\vartheta|$ is maximized, the magnitude of $\sigma - (\sigma + 1/\vartheta)$ is minimized. Therefore, the Rayleigh-Ritz pairs of a shift-and-invert Arnoldi procedure will first converge to the eigenpairs of A with eigenvalues closest to σ.

- Shift-and-invert operators are implemented in ARPACK to compute interior eigenpairs.
- Shift-and-invert Arnoldi procedures rely on repetitive applications of the $(A - \sigma I_n)^{-1}$ operator.

Arnoldi harmonic Ritz for interior eigenpairs

Harmonic Ritz approximation of interior eigenpairs

- While shift-and-invert Arnoldi procedures allow fast convergence of Rayleigh-Ritz pairs towards interior eigenpairs, it comes at the cost of repeated applications of $(A - \sigma I_n)^{-1}$. However:
  1. Factorizing the shifted operator $A - \sigma I_n$ is not always possible.
  2. One may actually need to generate a basis for a Krylov subspace of A, and have little use for a basis of Krylov subspace of the shift-and-invert operator $(A - \sigma I_n)^{-1}$:
     - E.g., if interior eigenvectors of A are needed to restart GMRES when solving $Ax = b$.
- As a means to bypass the need to apply shift-and-invert operators, Morgan (1991) introduces a new projection method in which the shift-and-invert operator is applied implicitly:
  - Consider the case in which we are equipped with a basis for the search space range(P) stored in the columns of P.
  - Let $Q := (A - \sigma I_n)P$, and consider the Rayleigh-Ritz pairs of the shift-and-invert operator $(A - \sigma I_n)^{-1}$ with respect to range(Q).

Morgan, R. B. (1991). Computing interior eigenvalues of large matrices. Linear Algebra and its Applications, 154, 289-309.

Harmonic Ritz approximation of interior eigenpairs, cont'd$_1$

That is, consider the pair $(\vartheta, Q\hat{y})$ such that

$$Q^H(A - \sigma I_n)^{-1} Q\hat{y} = \vartheta Q^H Q\hat{y},$$

which develops into the reduced generalized eigenvalue problem

$$P^T(A - \sigma I_n)^H P\hat{y} = \vartheta P^T(A - \sigma I_n)^H (A - \sigma I_n) P\hat{y}$$

which does not require any application of the shift-and-invert operator.

- Resulting from a Rayleigh-Ritz projection of the shift-and-invert operator $(A - \sigma I_n)^{-1}$, the pair $(\sigma + 1/\vartheta, Q\hat{y})$ should be a good approximation with respect to range(Q) of the eigenpair closest to σ.
- As good of an approximation $Q\hat{y}$ might be, $P\hat{y} = (A - \sigma I_n)^{-1} Q\hat{y}$ is the first power iterate of the shift-and-invert operator initiated with $Q\hat{y}$, so that $P\hat{y}$ should be an even slightly better approximation of the eigenvector with eigenvalue closest to σ.
- Stewart (2001) showed that solutions $(\theta, Q\hat{y})$ for which $Q\hat{y}$ has unit norm are such that$\|Ay_i\| \leq |\theta_i|$, so that it is guaranteed that $\|\tilde{r}_i\|_2$ is small if θ_i is near zero.

Morgan, R.B. (1991). Computing interior eigenvalues of large matrices. Linear Algebra and its Applications, 154, 289-309.
G. W. Stewart, Matrix Algorithms II: Eigensystems, SIAM, Philadelphia, (2001).

Harmonic Ritz approximation of interior eigenpairs, cont'd$_2$

- Consequently, Morgan (1991) proposes a Petrov-Galerkin projection and seeks for pairs $(\sigma + \lambda, y)$ to approximate eigenpairs of A near σ with respect to range(P), leading to the following procedure:

  Find λ and $y \in \text{range}(P)$ s.t. $(A - \sigma I_n)y - \lambda y \perp (A - \sigma I_n)\text{range}(P)$,

  which first converges to eigenpairs of A near σ, thus motivating the selection of reduced generalized eigenpairs $(\lambda, \hat{y})$ with smallest values of $|\lambda|$ such that

$$P^T(A - \sigma I_n)^H(A - \sigma I_n)P\hat{y} = \lambda P^T(A - \sigma I_n)^H P\hat{y}.$$

- The projection proposed by Morgan (1991) is first studied for symmetric matrices, then further analyzed and first referred to as harmonic Ritz by Paige et al. (1995) before being considered in the context of non-symmetric eigenvalue problems by Sleijpen and Van der Vorst (1996).

Morgan, R. B. (1991). Computing interior eigenvalues of large matrices. Linear Algebra and its Applications, 154, 289-309.

Paige, C. C., Parlett, B. N., & Van der Vorst, H. A. (1995). Approximate solutions and eigenvalue bounds from Krylov subspaces. Numerical linear algebra with applications, 2(2), 115-133.

Sleijpen, G. L., & Van der Vorst, H. A. (1996). A Jacobi–Davidson Iteration Method for Linear Eigenvalue Problems. Matrix, 17(2), 401-425.

Harmonic Ritz approximation of interior eigenpairs, cont'd$_3$

- To simplify what follows, let us define

$$G_1 := P^T(A-\sigma I_n)^H(A-\sigma I_n)P \text{ and } G_2 := P^T(A-\sigma I_n)P$$

  so that, assuming σ is not an eigenvalue of A, the reduced eigenpair $(\lambda, \hat{y})$ is such that $G_2^{-H}G_1\hat{y} = \lambda\hat{y}$.
- It is well established that the Rayleigh quotient ρ of y with respect to A is a better approximation of the eigenvalue of A near σ than $\sigma + \lambda$. The Rayleigh quotient can be efficiently computed as

$$\rho = \frac{y^HAy}{y^Hy} = \frac{\hat{y}^HP^TAP\hat{y}}{\hat{y}P^TP\hat{y}} = \sigma + \frac{\hat{y}^HP^T(A-\sigma I_n)P\hat{y}}{\hat{y}P^TP\hat{y}} = \sigma + \frac{\hat{y}^HG_2\hat{y}}{\hat{y}P^TP\hat{y}}$$

  so that, if $P^TP = I_k$ and $\hat{y}^H\hat{y} = 1$, then we have $\boxed{\rho = \sigma + \hat{y}^HG_2\hat{y}}$.
- It is also common to monitor convergence through stopping criteria defined with respect to the residual

$$\hat{r} := Ay - \rho y$$

Harmonic Ritz approximation of interior eigenpairs, cont'd$_4$

whose norm can also be efficiently computed as we have

$$\begin{aligned}
\hat{r}^H\hat{r} &= (Ay-\rho y)^H(Ay-\rho y)\\
&= ((A-\sigma I_n)y+(\sigma-\rho)y)^H((A-\sigma I_n)y+(\sigma-\rho)y)\\
&= y^H(A-\sigma I_n)^H(A-\sigma I_n)y+(\sigma-\rho)y^H(A-\sigma I_n)^Hy\\
&\quad+\overline{(\sigma-\rho)}y^H(A-\sigma I_n)y+\overline{(\sigma-\rho)}(\sigma-\rho)y^Hy\\
&= \hat{y}^HG_1\hat{y}+(\sigma-\rho)\hat{y}^HG_2^H\hat{y}+\overline{(\sigma-\rho)}\hat{y}^HG_2\hat{y}+\overline{(\sigma-\rho)}(\sigma-\rho)y^Hy
\end{aligned}$$

where, once again, we assume $P^TP=I_k$ and $\hat{y}^H\hat{y}=1$ so that

$$\begin{aligned}
\hat{r}^H\hat{r} &= \hat{y}^HG_1\hat{y}+(\sigma-\rho)\hat{y}^HG_2^H\hat{y}+\overline{(\sigma-\rho)}\hat{y}^HG_2\hat{y}+\overline{(\sigma-\rho)}(\sigma-\rho)\\
&= \lambda\hat{y}^HG_2^H\hat{y}+(\sigma-\rho)\hat{y}^HG_2^H\hat{y}+\overline{(\sigma-\rho)}(\rho-\sigma)+\overline{(\sigma-\rho)}(\sigma-\rho)\\
&= (\sigma+\lambda-\rho)\hat{y}^HG_2^H\hat{y}\\
&= (\sigma+\lambda-\rho)\overline{\hat{y}^HG_2\hat{y}}
\end{aligned}$$

which leads to $\boxed{\hat{r}^H\hat{r}=(\sigma+\lambda-\rho)\overline{(\rho-\sigma)}}$.

Harmonic Ritz approximation of interior eigenpairs, cont'd$_5$

- The norm of the harmonic residual $\tilde{r} := Ay - (\sigma + \lambda)y$ can also be used to monitor convergence. Still assuming $P^T P = I_k$ and $\hat{y}^H \hat{y} = 1$, we then have

$$\begin{aligned}
\tilde{r}^H \tilde{r} &= (Ay - (\sigma + \lambda)y)^H (Ay - (\sigma + \lambda)y) \\
&= ((A - \sigma I_n)y - \lambda y)^H ((A - \sigma I_n)y - \lambda y) \\
&= \hat{y}^H P^T (A - \sigma I_n)^H (A - \sigma I_n) P\hat{y} - \lambda \hat{y}^H P^T (A - \sigma I_n)^H P\hat{y} \\
&\quad - \overline{\lambda} \hat{y}^H P^T (A - \sigma I_n) P\hat{y} + \lambda\overline{\lambda} \\
&= \hat{y}^H G_1 \hat{y} - \lambda \hat{y}^H G_2^H \hat{y} - \overline{\lambda} \hat{y}^H G_2 \hat{y} + \lambda\overline{\lambda} \\
&= \lambda \hat{y}^H G_2^H \hat{y} - \lambda \hat{y}^H G_2^H \hat{y} - \overline{\lambda} \hat{y}^H G_2 \hat{y} + \lambda\overline{\lambda} \\
&= \overline{\lambda}(\lambda - \hat{y}^H G_2 \hat{y})
\end{aligned}$$

where $\hat{y}^H G_2 \hat{y} = \rho - \sigma$ so that

$$\boxed{\tilde{r}^H \tilde{r} = (\sigma + \lambda - \rho)\overline{\lambda}}.$$

Harmonic Ritz approximation of interior eigenpairs, cont'd$_6$

- Alternatively, the harmonic Ritz pairs may be formed from non-shifted procedures. That is, let

$$G_1 := (AP)^H AP \quad \text{and} \quad G_2 := P^T AP,$$

then, the reduced eigenvalue problem of the shifted approximation

$$y \in \text{range}(P) \quad \text{such that} \quad (A - \sigma I_n)y - \lambda y \perp (A - \sigma I_n)\text{range}(P)$$

is obtained as follows:

$$\begin{aligned}
((A - \sigma I_n)P)^H AP\hat{y} &= (\sigma + \lambda)((A - \sigma I_n)P)^H P\hat{y} \\
[(AP)^H AP - \overline{\sigma} P^T AP]\hat{y} &= (\sigma + \lambda)(P^T A^H P - \overline{\sigma} I_k)\hat{y} \\
(G_1 - \overline{\sigma} G_2)\hat{y} &= (\sigma + \lambda)(G_2^H - \overline{\sigma} I_k)\hat{y} \\
(G_1 - \overline{\sigma} G_2)\hat{y} &= (\sigma + \lambda)(G_2 - \sigma I_k)^H \hat{y} \\
(G_2 - \sigma I_k)^{-H}(G_1 - \overline{\sigma} G_2)\hat{y} &= (\sigma + \lambda)\hat{y}
\end{aligned}$$

in which case we have $\rho = \hat{y}^H G_2 \hat{y}$.

Arnoldi procedure with harmonic Ritz vectors

- More can be said for the case in which the search space is Krylov and generated by an Arnoldi procedure, see Morgan and Zheng (1998).
- Consider the shifted procedure $\texttt{Arnoldi}(A - \sigma I_n,\, q_1,\, k) \mapsto (Q_{k+1}, \underline{H}_k)$ which returns an orthonormal basis $Q_k := [q_1 \,\ldots\, q_k]$ of $\mathcal{K}_k(A - \sigma I_n, q_1)$ such that $(A - \sigma I_n)Q_k = Q_{k+1}\underline{H}_k$ where $Q_{k+1} := [Q_k\, q_{k+1}]$ as well as $\underline{H}_k = Q_{k+1}^T(A - \sigma I_n)Q_k$ and $H_k = Q_k^T(A - \sigma I_n)Q_k$.
- Then, harmonic Ritz vectors $y \in \text{range}(Q_k)$ are such that

$$(A - \sigma I_n)y - \lambda y \perp (A - \sigma I_n)\text{range}(Q_k)$$

yields the following reduced generalized eigenvalue problem in which we search for non-trivial pairs $(\lambda, \hat{y}) \in \mathbb{C} \times \mathbb{C}^k$ such that $y = Q_k\hat{y}$ and

$$\begin{aligned} Q_k^T(A - \sigma I_n)^H(A - \sigma I_n)Q_k\hat{y} &= \lambda Q_k^T(A - \sigma I_n)^H Q_k\hat{y} \\ \underline{H}_k^H Q_{k+1}^T Q_{k+1}\underline{H}_k\hat{y} &= \lambda H_k^H\hat{y} \\ \underline{H}_k^H\underline{H}_k\hat{y} &= \lambda H_k^H\hat{y} \end{aligned}$$

Morgan, R. B., & Zeng, M. (1998). Harmonic projection methods for large non-symmetric eigenvalue problems. Numerical linear algebra with applications, 5(1), 33-55.

Arnoldi procedure with harmonic Ritz vectors, cont'd$_1$

- Reformulating the Arnoldi relation into

$$(A - \sigma I_n)Q_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^T$$

allows to rewrite the reduced eigenvalue problem of the harmonic Ritz projection as follows:

$$(H_k^H H_k + |h_{k+1,k}|^2 e_k e_k^T)\hat{y} = \lambda H_k^H \hat{y}$$

$$\boxed{(H_k + |h_{k+1,k}|^2 f e_k^T)\hat{y} = \lambda \hat{y}}$$

where $f := H_k^{-H} e_k \in \mathbb{C}^k$ and $e_k := I_k[:, k]$.

- Then, the harmonic eigen-residual $\tilde{r} := Ay - (\sigma + \lambda)y$ of a given harmonic Ritz approximate eigenpair $(\sigma + \lambda, y)$ with $y := Q_k \hat{y}$ is such that

$$\begin{aligned}
\tilde{r} &= AQ_m\hat{y} - (\sigma + \lambda)Q_m\hat{y} \\
&= (A - \sigma I_n)Q_k\hat{y} - \lambda Q_k\hat{y} = (Q_k H_k + h_{k+1,k} q_{k+1} e_k^T)\hat{y} - \lambda Q_k\hat{y} \\
&= Q_k(\lambda I_n - |h_{k+1,k}|^2 f e_k^T)\hat{y} + h_{k+1,k} q_{k+1} e_k^T \hat{y} - \lambda Q_k\hat{y} \\
&= h_{k+1,k}(e_k^T\hat{y})q_{k+1} - |h_{k+1,k}|^2 (e_k^T\hat{y})Q_k f
\end{aligned}$$

Arnoldi procedure with harmonic Ritz vectors, cont'd$_2$

which can be written

$$\begin{aligned}
\tilde{r} &= h_{k+1,k}(e_k^T \hat{y}) Q_{k+1} \begin{bmatrix} 0_{k\times 1} \\ 1 \end{bmatrix} - |h_{k+1,k}|^2 (e_k^T \hat{y}) Q_{k+1} \begin{bmatrix} f \\ 0 \end{bmatrix} \\
&= h_{k+1,k}(e_k^T \hat{y}) Q_{k+1} \begin{bmatrix} 0_{k\times 1} \\ 1 \end{bmatrix} + h_{k+1,k}(e_k^T \hat{y}) Q_{k+1} \begin{bmatrix} -\overline{h_{k+1,k}} f \\ 0 \end{bmatrix} \\
&= h_{k+1,k}(e_k^T \hat{y}) Q_{k+1} \begin{bmatrix} -\overline{h_{k+1,k}} f \\ 1 \end{bmatrix} \\
&= \beta_k Q_{k+1} s
\end{aligned}$$

so that

$$\boxed{\tilde{r} = \beta_k Q_{k+1} s} \text{ where } \boxed{\beta_k := h_{k+1,k} e_k^T \hat{y}} \text{ and } \boxed{s := \begin{bmatrix} -\overline{h_{k+1,k}} f \\ 1 \end{bmatrix}}.$$

- The norm of $\tilde{r}$ is then given by $\boxed{\|\tilde{r}\|_2 = |\beta_k|(|h_{k+1,k}|^2 f^H f + 1)^{1/2}}$.

Arnoldi procedure with harmonic Ritz vectors, cont'd$_3$

- When precise eigenvalues are wanted, it is preferred to use the Rayleigh quotient rather than $\sigma + \lambda$. Assuming $\hat{y}$ has unit norm, so does $y := Q_k \hat{y}$, and the Rayleigh quotient of y is given by

$$\rho = \sigma + \hat{y}^H H_k \hat{y} = \sigma + \lambda - |h_{k+1,k}|^2 (\hat{y}^H f)(e_k^T \hat{y}).$$

- Moreover, the norm of the eigen-residual $\hat{r} := Ay - \rho y$ is still such that

$$\|\hat{r}\|_2^2 = (\sigma + \lambda - \rho)\overline{(\rho - \sigma)}$$

and that of the harmonic residual $\tilde{r} := Ay - (\sigma + \lambda)y$ is still such that

$$\|\tilde{r}\|_2^2 = (\sigma + \lambda - \rho)\overline{\lambda}.$$

Arnoldi procedure with harmonic Ritz vectors, cont'd$_4$

- As mentioned before, we are interested by the case in which harmonic Ritz approximations are considered in the context of the non-shifted procedure $\texttt{Arnoldi}(A, q_1, k) \mapsto (Q_{k+1}, \underline{H}_k)$ which returns an orthonormal basis $Q_k := [q_1 \dots q_k]$ of $\mathcal{K}_k(A, q_1)$ such that $AQ_k = Q_{k+1}\underline{H}_k$ where $Q_{k+1} := [Q_k\, q_{k+1}]$, $\underline{H}_k = Q_{k+1}^T A Q_k$ and $H_k = Q_k^T A Q_k$.
  - Then, the harmonic Ritz vector $y \in \text{range}(Q_k)$ is still such that

$$(A - \sigma I_n)y - \lambda y \perp (A - \sigma I_n)\text{range}(Q_k)$$

but now yields the following reduced generalized eigenvalue problem:

$$((A - \sigma I_n)Q_k)^H (A - \sigma I_n)Q_k \hat{y} = \lambda((A - \sigma I_n)Q_k)^H Q_k \hat{y}$$
$$((A - \sigma I_n)Q_k)^H AQ_k \hat{y} - \sigma((A - \sigma I_n)Q_k)^H Q_k \hat{y} = \lambda((A - \sigma I_n)Q_k)^H Q_k \hat{y}$$

so that

$$((A - \sigma I_n)Q_k)^H AQ_k \hat{y} = (\sigma + \lambda)((A - \sigma I_n)Q_k)^H Q_k \hat{y}$$

Arnoldi procedure with harmonic Ritz vectors, cont'd$_5$

which develops as follows:

$$\begin{aligned}
((AQ_k)^T AQ_k - \overline{\sigma} Q_k^T AQ_k)\hat{y} &= (\sigma + \lambda)(Q_k^T A^T Q_k - \overline{\sigma} I_k)\hat{y} \\
(H_k^T H_k + |h_{k+1,k}|^2 e_k e_k^T - \overline{\sigma} H_k)\hat{y} &= (\sigma + \lambda)(H_k^T - \overline{\sigma} I_k)\hat{y} \\
((H_k^T - \overline{\sigma} I_k) H_k + |h_{k+1,k}|^2 e_k e_k^T)\hat{y} &= (\sigma + \lambda)(H_k - \sigma I_k)^H \hat{y} \\
((H_k - \sigma I_k)^H H_k + |h_{k+1,k}|^2 e_k e_k^T)\hat{y} &= (\sigma + \lambda)(H_k - \sigma I_k)^H \hat{y}
\end{aligned}$$

to finally yield

$$\boxed{(H_k + |h_{k+1,k}|^2 f e_k^T)\hat{y} = (\sigma + \lambda)\hat{y}} \text{ where } \boxed{f := (H_k - \sigma I_k)^{-H} e_k},$$

so that the expression for f differs from the shifted procedure. Still, the harmonic Ritz pairs should converge first to the eigenpairs of A closest to σ so that, now, we should not retain the least dominant reduced eigenpairs, but rather those with eigenvalues closest to σ.

Arnoldi procedure with harmonic Ritz vectors, cont'd$_6$

- Now, still assuming $\hat{y}^H \hat{y} = 1$, the Rayleigh quotient is given by

$$\rho = y^H A y = \hat{y}^H Q_k^T A Q_k \hat{y} = \hat{y}^H H_k \hat{y} = \sigma + \lambda - |h_{k+1,k}|^2 (\hat{y}^H f)(e_k^T \hat{y}).$$

- Irrespective of the basis generated, as long as it's orthonormal, we already saw the residual given by $\hat{r} := Ay - \rho y$ is such that

$$\hat{r}^H \hat{r} = (\sigma + \lambda - \rho)\overline{(\rho - \sigma)}.$$

- And the harmonic eigen-residual $\tilde{r} := Ay - (\sigma + \lambda)y$ is such that

$$\begin{aligned}
\tilde{r} &= A Q_k \hat{y} - (\sigma + \lambda) Q_k \hat{y} \\
&= Q_k H_k \hat{y} + h_{k+1,k} q_{k+1} e_k^T \hat{y} - (\sigma + \lambda) Q_k \hat{y} \\
&= (\sigma + \lambda) Q_k \hat{y} - |h_{k+1,k}|^2 Q_k f e_k^T \hat{y} + h_{k+1,m} q_{k+1} e_k^T \hat{y} - (\sigma + \lambda) Q_k \hat{y} \\
&= -|h_{k+1,k}|^2 (e_k^T \hat{y}) Q_k f + h_{k+1,k} q_{k+1} e_m^T \hat{y}
\end{aligned}$$

  which, similarly as before, can be recast into

$$\tilde{r} = \beta_k Q_{k+1} s \quad \text{where} \quad \beta_k := h_{k+1,k} e_k^T \hat{y} \quad \text{and} \quad s = \begin{bmatrix} -\overline{h_{k+1,k}} f \\ 1 \end{bmatrix},$$

  where the difference with shifted Arnoldi is the expression for f.

Lanczos process

Section 6.2 in Darve & Wootters (2021)

Lanczos process for symmetric matrices

- The Lanczos process is a specialized form of the Arnoldi process for **symmetric matrices**.
- When A is symmetric (i.e., $A = A^T$), the Hessenberg matrix $H_k = Q_k^T A Q_k$ is symmetric too. Consequently, it is **tridiagonal**:

$$T_k = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \cdots & 0 \\ 0 & \beta_2 & \alpha_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha_k \end{bmatrix}$$

  where $\alpha_i = q_i^T A q_i$ are the diagonal elements and $\beta_i = q_i^T A q_{i+1} = q_{i+1}^T A q_i$ are the off-diagonal elements.
- This tridiagonal structure means that in the Arnoldi recurrence relation, most terms vanish:

$$A q_j = \beta_{j-1} q_{j-1} + \alpha_j q_j + \beta_j q_{j+1}$$

- This three-term recurrence relation is the foundation of the Lanczos process.

Derivation of the Lanczos process

- From the three-term recurrence relation, we can derive the Lanczos algorithm:

$$\beta_j q_{j+1} = Aq_j - \alpha_j q_j - \beta_{j-1} q_{j-1}$$

- Rearranging to compute q_{j+1}:

$$q_{j+1} = \frac{1}{\beta_j}(Aq_j - \alpha_j q_j - \beta_{j-1} q_{j-1})$$

- The coefficients are determined as:

$$\alpha_j = q_j^T A q_j \quad \text{and} \quad \beta_j = \|Aq_j - \alpha_j q_j - \beta_{j-1} q_{j-1}\|_2$$

- This leads to a much simpler algorithm compared to the full Arnoldi process:
  - we only need to maintain three vectors in memory at any time: q_{j-1}, q_j, and q_{j+1}.
  - the work done remains constant as the iteration count increases.

Lanczos algorithm

- The Lanczos algorithm can be formulated as follows:

Algorithm 8 Lanczos

1: Choose a starting vector q_1 with $\|q_1\|_2 = 1$
2: Set $\beta_0 = 0$ and $q_0 = 0$
3: **for** $j = 1, 2, \ldots, k$ **do**
4: $\quad v = Aq_j$
5: $\quad \alpha_j = q_j^T v$
6: $\quad v = v - \alpha_j q_j - \beta_{j-1} q_{j-1}$
7: $\quad \beta_j = \|v\|_2$
8: $\quad q_{j+1} = v/\beta_j$

- After k steps, we have:
  - An orthonormal basis $Q_k = [q_1, q_2, \ldots, q_k]$ for the Krylov subspace $\mathcal{K}_k(A, q_1)$
  - A tridiagonal matrix $T_k = Q_k^T A Q_k$ with diagonal elements α_i and off-diagonal elements β_i

The Lanczos relation

- Similar to the Arnoldi relation, we have the Lanczos relation:

$$AQ_k = Q_k T_k + \beta_k q_{k+1} e_k^T$$

where T_k is the tridiagonal matrix.

- We can also write:

$$AQ_k = Q_{k+1} \underline{T}_k$$

where $\underline{T}_k$ is the $(k+1) \times k$ tridiagonal matrix:

$$\underline{T}_k = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \cdots & 0 \\ 0 & \beta_2 & \alpha_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha_k \\ 0 & 0 & 0 & \cdots & \beta_k \end{bmatrix}.$$

Lanczos Rayleigh-Ritz for dominant eigenpairs

- **Eigenvectors with eigenvalues whose norms are the largest** among the spectrum of A are **well approximated by Rayleigh-Ritz** projections.
- A **Rayleigh-Ritz vector** $y \in \text{range}(Q_k)$ approximates an eigenvector of A with the **Ritz value** λ such that $Ay - \lambda y \perp \text{range}(Q_k)$. That is, we **search for** $(\lambda, \hat{y}) \in \mathbb{R} \times \mathbb{R}^k \setminus \{0\}$ s.t. $z^T (Ay - \lambda y) = 0 \; \forall \; z \in \text{range}(Q_k)$ with $y = Q_k \hat{y}$. This **simplifies to**

$$Q_k^T (AQ_k\hat{y} - \lambda Q_k \hat{y}) = 0$$

$$T_k\hat{y} - \lambda\hat{y} = 0 \quad \Longrightarrow \quad \boxed{T_k\hat{y} = \lambda\hat{y}}$$

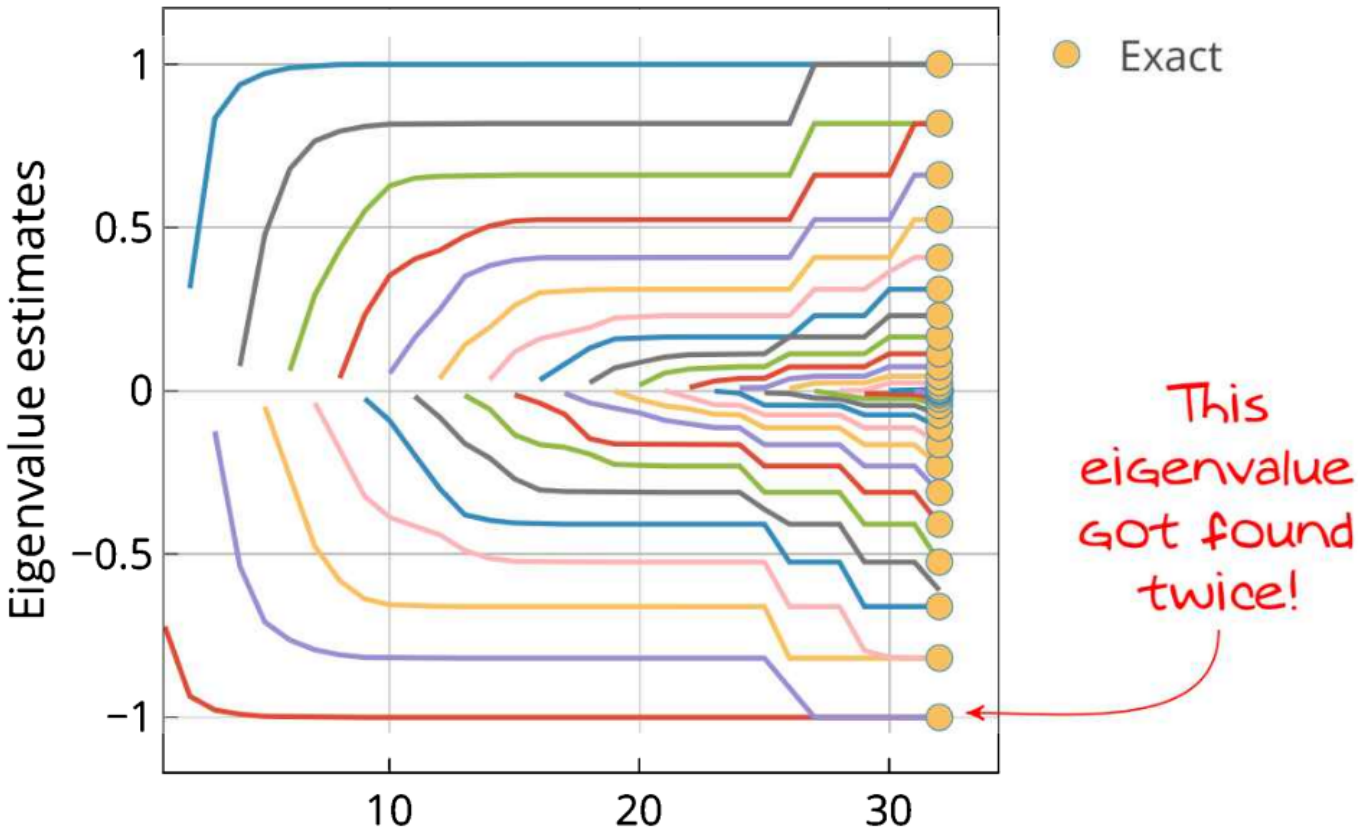
  where use is made of the Lanczos relation and $Q_k^T Q_k = I_k$.
- The eigen-residual $\tilde{r} := Ay - \lambda y$ can be computed as:

$$\tilde{r} = AQ_k\hat{y} - \lambda Q_k\hat{y} = \beta_k(e_k^T\hat{y})q_{k+1}$$

- This means $\|\tilde{r}\|_2 = \beta_k |e_k^T \hat{y}|$, providing a simple way to assess convergence without explicitly computing Ay.

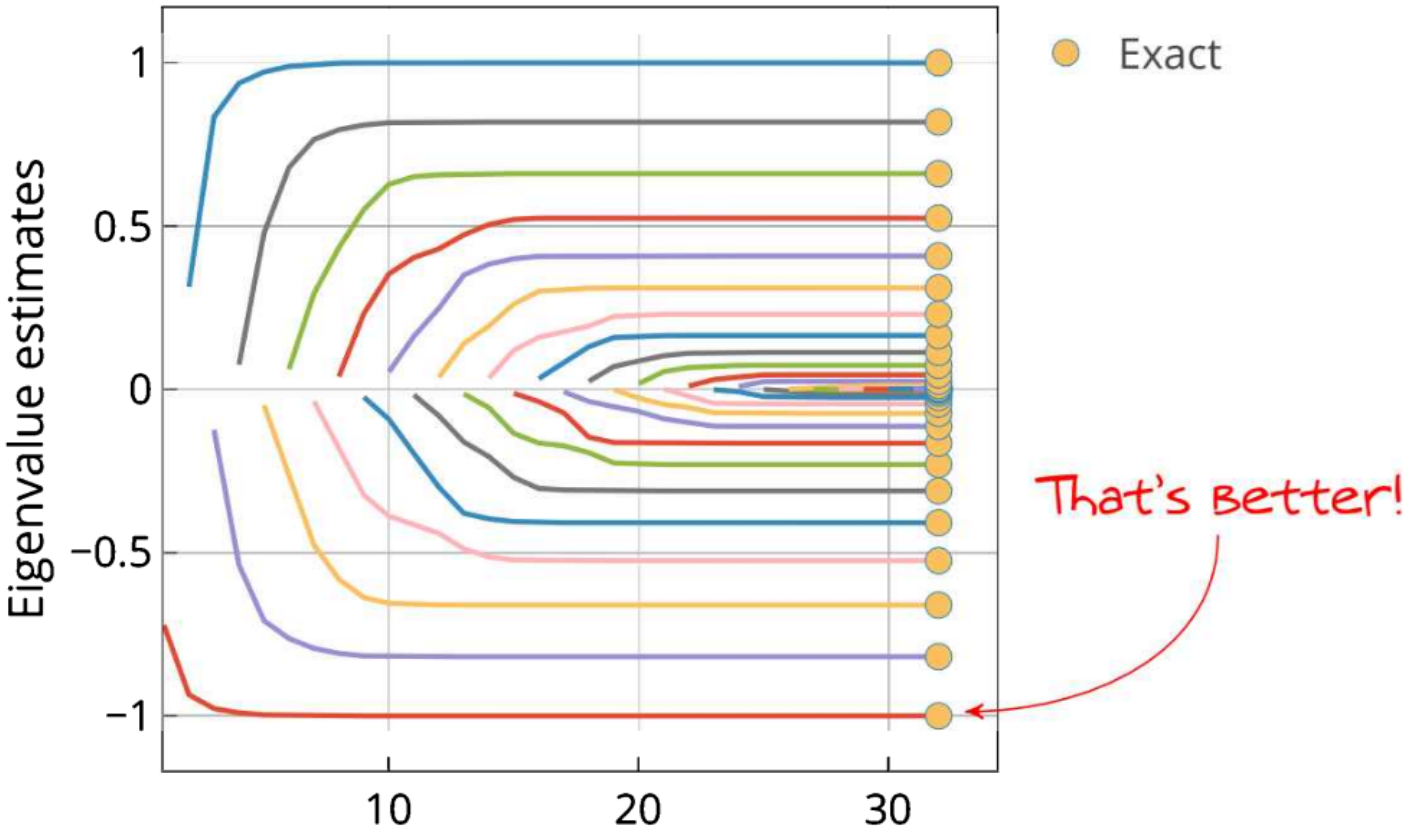
Lanczos Rayleigh-Ritz in finite precision

- **Loss of orthogonality:** In finite precision arithmetic, the Lanczos vectors quickly lose orthogonality, which can lead to:
  - Multiple copies of the same eigenvalue appearing (ghost eigenvalues)
  - Inaccurate eigenvalue approximations



Reorthogonalization strategies

- Different strategies exist to circumvent the issue of loss of orthogonality in finite precision.
  - **Full reorthogonalization**: Explicitly orthogonalize each new vector against all previous vectors.



Reorthogonalization strategies, cont'd

Algorithm 9 Lanczos with full reorthogonalization

1: Choose a starting vector q_1 with $\|q_1\|_2 = 1$
2: Set $\beta_0 = 0$ and $q_0 = 0$
3: **for** $j = 1, 2, \ldots, k$ **do**
4: $\quad v = Aq_j$
5: $\quad \alpha_j = q_j^T v$
6: $\quad v = v - \alpha_j q_j - \beta_{j-1} q_{j-1}$
7: $\quad$ **for** $i = 1, 2, \ldots, j$ **do**
8: $\quad\quad v = v - (q_i^T v) q_i$ ▷ Reorthogonalization step
9: $\quad \beta_j = \|v\|_2$
10: $\quad q_{j+1} = v/\beta_j$

Full reorthogonalization turns Lanczos back into Arnoldi. Alternatives:

- **Selective reorthogonalization:** Only reorthogonalize when necessary, based on loss of orthogonality measures
- **Partial reorthogonalization:** Reorthogonalize against a subset of previous vectors

Lanczos harmonic Ritz for interior eigenpairs

- **Eigenvectors with interior eigenvalues** are **better approximated by harmonic Ritz** projections.
- A **harmonic Ritz vector** $y \in \text{range}(Q_k)$ approximates an eigenvector of A with the **harmonic Ritz value** $\sigma + \lambda$ in the vicinity of σ such that

$$(A - \sigma I_n)y - \lambda y \perp (A - \sigma I_n)\text{range}(Q_k).$$

Let the columns of Q_k form an orthonormal basis of $\mathcal{K}_k(A, q_1)$. Then, the **search for** for the pair $(\sigma + \lambda, \hat{y})$ is such that

$$\begin{aligned}
Q_k^T(A - \sigma I_n)^T(A - \sigma I_n)Q_k\hat{y} &= \lambda Q_k^T(A - \sigma I_n)^T Q_k\hat{y} \\
((AQ_k)^T AQ_k - \sigma Q_k^T AQ_k)\hat{y} &= (\sigma + \lambda)(Q_k^T AQ_k - \sigma I_k)\hat{y} \\
(T_k T_k + \beta_k^2 e_k e_k^T - \sigma T_k)\hat{y} &= (\sigma + \lambda)(T_k - \sigma I_k)\hat{y} \\
((T_k - \sigma I_k)T_k + \beta_k^2 e_k e_k^T)\hat{y} &= (\sigma + \lambda)(T_k - \sigma I_k)\hat{y} \\
(T_k + \beta_k^2 f e_k^T)\hat{y} &= (\sigma + \lambda)\hat{y}
\end{aligned}$$

where $f := (T_k - \sigma I_k)^{-1} e_k$.

Lanczos harmonic Ritz for interior eigenpairs

- Note that fe_k^T is not symmetric so that the **reduced eigenpairs of** the **harmonic Ritz procedure** are **generally complex**.

  However, they do **converge towards** the **real eigenpairs**.
- Similarly as with Arnoldi, the Rayleigh quotient is given by

$$\rho = \sigma + \lambda - \beta_k^2 (\hat{y}^H f)(e_k^T \hat{y})$$

whereas the residual $\hat{r} := Ay - \rho y$ is such that

$$\hat{r}^H \hat{r} = (\sigma + \lambda - \rho)\overline{(\rho - \sigma)}.$$

Summary of Krylov subspace methods

- We studied two main Krylov subspace methods for eigenvalue problems:
  - **Arnoldi process:** For general matrices, produces a Hessenberg matrix H_k, requires orthogonalization against all previously formed vectors
  - **Lanczos process:** For symmetric matrices, produces a tridiagonal matrix T_k, relies on a three terms recurence formula
- Both methods:
  - Construct an orthonormal basis for the Krylov subspace $\mathcal{K}_k(A, v)$
  - Can be used with either Rayleigh Ritz or harmonic Ritz projections
- Key advantages of Krylov subspace methods:
  - Only require matrix-vector products, ideal for large sparse matrices
  - Can find several eigenvalues simultaneously
- Modern implementations use:
  - Restarting techniques to limit memory requirements and increasing computational cost of Arnoldi (will be covered in Lecture 15)
  - Reorthogonalization strategies for numerical stability of Lanczos

Homework problems

Homework problem

Turn in **your own** solution to **Pb. 23**:

Pb. 23 For the matrices

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix},$$

(a) Find the Rayleigh Ritz pairs of A with respect to range(V).

(b) Assemble the reduced eigenvalue problem to solve in order to find the harmonic Ritz values of A with respect to range(V) for $\sigma = 0$.

Pb. 24 For the matrix $A = \begin{bmatrix} 2 & 3 & 0 \\ 1 & 2 & 3 \\ 0 & 1 & 2 \end{bmatrix}$ and $q_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, use the Arnoldi process to build an orthonormal basis $Q_2 = [q_1, q_2]$ of the Krylov subspace $\mathcal{K}_2(A, q_1)$, and compute the projected matrix $H_2 = Q_2^T A Q_2$.

Practice session

Practice session

1. Implement MGS and CGS2-based Arnoldi procedures.
2. For both methods, check how close $Q_{k+1}^T A Q_k$ is to your Hessenberg matrix, and with what accuracy does your Arnoldi relation $AQ_k = Q_{k+1}\underline{H}_k$ hold. Quantify also the loss of orthgonality of the basis, and compare runtimes. For all this, use the matrix `G3_circuit` from the SuiteSparse collection.
3. Implement a Rayleigh-Ritz procedure on top of your CGS2-based Arnoldi process. For the matrix `nxp1` from the SuiteSparse collection, solve for the 5 largest eigenpairs using the reduced expressions derived in class to monitor convergence of residuals. Verify your residual estimates and compare your converged eigenpairs with those obtained using `ArnoldiMethod.jl`.
4. Implement a haronic Ritz procedure on top of your CGS2-based Arnoldi process. Still using the `nxp1` matrix, solve for the 2 eigenpairs closest to $\sigma = 150$ using the reduced expressions derived in class to monitor convergence of residuals. Verify your residual estimates.

Practice session, cont'd

5. Implement the Lanczos algorithm. Check how close $Q_{k+1}^T A Q_k$ is to your tridiagonal matrix, and with what accuracy does your Lanczos relation $AQ_k = Q_{k+1}\underline{T}_k$ hold. Quantify also the loss of orthogonality of the basis. For all this, use the matrix `Kuu` from the SuiteSparse collection.
6. Implement a Rayleigh-Ritz procedure on top of your Lanczos process. For the matrix `Kuu` from the SuiteSparse collection, solve for the 5 largest eigenpairs using the reduced expressions derived in class to monitor convergence of residuals. Verify your residual estimates.
7. Implement a harmonic Ritz procedure on top of your Lanczos process. For the matrix `Kuu` from the SuiteSparse collection, solve for the 2 eigenpairs closest to $\sigma = 25$ using the reduced expressions derived in class to monitor convergence of residuals. Verify your residual estimates.