Numerical Linear Algebra for Computational Science and Information Engineering

Lecture 15
Restarted Krylov Subspace Methods

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Outline I

Introduction

Recap of Arnoldi procedures

- For a general non-singular matrix $A \in \mathbb{F}^{n\times n}$ and a unit-length vector $v_1 \in \mathbb{F}^n$, the Arnoldi procedure computes an orthonormal basis of the Krylov subspace given by

$$\mathcal{K}_m(A, v_1) := \mathrm{Span}\{v_1, Av_1, \ldots, A^{m-1}v_1\},$$

typically for some $m \ll n$. That is,

$$\texttt{Arnoldi}(A, v_1, m) \mapsto (V_{m+1}, \underline{H}_m)$$

where the basis in $V_m := [v_1 \ \ldots \ v_m]$ is such that $\mathrm{range}(V_m) = \mathcal{K}_m(A, v_1)$, $V_m^T V_m = I_m$, and the **upper Hessenberg** matrix $\underline{H}_m = V_{m+1}^H A V_m$ is a **by-product** of the procedure.

- The **Arnoldi relation**, given by

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^{(m)} \quad \text{where} \quad H_m = V_m^H A V_m$$
$$AV_m = V_{m+1}\underline{H}_m,$$

is **essential to** the **analysis** of Arnoldi procedures and the **development of Krylov subspace-based methods**, typically, for **non-symmetric matrices**.

Recap of Arnoldi procedures, cont'd

- Most variants of Arnoldi procedures can be recast into:

$$\boxed{\begin{array}{l}\textbf{for } j = 1, \ldots, m \textbf{ do} \\ \quad v_{j+1} := \Pi_{V_j} A v_j;\ v_{j+1} := v_{j+1}/\|v_{j+1}\|_2\end{array}}$$

where Π_{V_j} is a projector onto range$(V_j)^\perp$, plus some book-keeping work to recover the upper-Hessenberg matrix.
The sole specification of the projector Π_{V_j} yields a number of variants of Arnoldi procedures. In particular,

- **Classical Gram-schmidt** (`CGS`) variant with $\Pi_{V_j} := I_n - V_j V_j^H$.
  `CGS` is rarely used for `GMRES` due to stability issues.
- **Modified Gram-Schmidt** (`MGS`) variant with
$$\Pi_{V_j} := (I_n - v_j v_j^H) \ldots (I_n - v_1 v_1^H).$$
  `MGS` is often used in practice due to a better stability than `CGS`.
- **Reorthogonalized CGS** (`CGS2`) with $\Pi_{V_j} := (I_n - V_j V_j^H)(I_n - V_j V_j^H)$.
  `CGS2` used for even lower loss of orthogonality, and low-communication.
- Other variants include **Householder**, **block versions**, ...

Recap of the Lanczos procedure

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

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

where $\alpha_j = v_j^T A v_j$ is a diagonal element and $\beta_j = v_j^T A v_{j+1} = v_{j+1}^T A v_j$ an off-diagonal elements.

- This tridiagonal structure means that **most terms vanish** in the Arnoldi recurrence relation:

$$A v_j = \beta_{j-1} v_{j-1} + \alpha_j v_j + \beta_j v_{j+1}.$$

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

Recap of the Lanzos procedure, cont'd$_1$

- The Lanczos algorithm can be formulated as follows:

Algorithm 1 Lanczos procedure

1: Choose a starting vector v_1 with $\|v_1\|_2 = 1$
2: Set $\beta_0 := 0$ and $v_0 := 0$
3: **for** $j = 1, 2, \ldots, m$ **do**
4: $\quad w := Av_j$
5: $\quad \alpha_j := v_j^T w$
6: $\quad w := w - \alpha_j v_j - \beta_{j-1} v_{j-1}$
7: $\quad \beta_j := \|w\|_2$
8: $\quad v_{j+1} := w/\beta_j$

- After m steps, we have:
  - An orthonormal basis $V_m = [v_1, v_2, \ldots, v_m]$ of $\mathcal{K}_m(A, v_1)$,
  - A tridiagonal matrix $T_m = V_m^T A V_m$ with diagonal elements α_j and off-diagonal elements β_j.
- Variants of the Lanczos procedure are introduced by
  - Reorthogonalization, e.g., full vs selective reorthogonalization,
  - Block versions.

Recap of the Lanzos procedure, cont'd$_2$

- Similar to the Arnoldi relation, there is a **Lanczos relation**:

$$AV_m = V_m T_m + \beta_m v_{m+1} e_m^{(m)T}$$

where T_m is the tridiagonal matrix.

We can also write:

$$AV_m = V_{m+1} \underline{T}_m$$

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

$$\underline{T}_j = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \cdots & 0 \\ 0 & \beta_2 & \alpha_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha_m \\ 0 & 0 & 0 & \cdots & \beta_m \end{bmatrix}.$$

Practical limitations of Krylov subspace-based methods

- Ever since Arnoldi (1951), methods that rely on **Arnoldi procedures** to construct orthonormal bases for, say, some Krylov subspace $\mathcal{K}_m(A, v_1)$ of $A \in \mathbb{R}^{n \times n}$, have been **affected by** the following **limitations**:
  - **Orthogonalization** has time complexity of $\mathcal{O}(m^2 n)$,
  - **Krylov bases** are usually **dense**, and **must be stored**, for both linear and eigen solves, with spatial complexity of $\mathcal{O}(mn)$,
  - In case of eigensolves, **solving the reduced eigenvalue problem** has time complexity of $\mathcal{O}(m^3)$.
- For Lanczos-based approaches, the **orthogonalization** is **not a problem**, **due to** reduction to **short-recurrence** relations. Moreover, **linear solvers need not save the entire basis**. Remaining limitations are
  - **Reorthogonalization**, when necessary, can have up to $\mathcal{O}(m^2 n)$ time complexity,
  - For **eigensolves only**, the **basis**, usually **dense**, needs be **stored**, with spatial complexity of $\mathcal{O}(mn)$.

Arnoldi, W. E. (1951). The principle of minimized iterations in the solution of the matrix eigenvalue problem. Quarterly of applied mathematics, 9(1), 17-29

Motivation for restarting strategies

- When applied to **large**, **challenging problems** with **limited resources**, Krylov subspace-based methods face limitations which need be remedied.

  Restarting a procedure **with** the **best approximation available** is the **most natural**, and **oldest strategy**. However,

  - **When restarting** a Krylov subspace-based method, **information** about the Krylov subspace **is lost**, and this reflects into the quality of subsequent iterates, **slowing down convergence**, sometimes **even leading to stagnation**,
  - For **linear solves**, the best choice of restart vector is unambiguous. But, for **eigensolves**, as we often attempt to calculate several eigenpairs simultaneously, **the best choice for a single restart vector is not as straightforward**.

- Insight remains to be gained on **how to minimize convergence hindering due to restart**, and clever **strategies** are **needed**.

  We'll see that, over the years, a number of works were published on this topic, pushing forward better, **more robust restarting practices**.

Polynomial restart of Arnoldi process

Polynomial restart of Arnoldi

- The first documented attempt to restart an Arnoldi procedure for the **simultaneous computation of several eigenpairs** is by Saad (1980).

  Let $\{\lambda_\ell, y_\ell\}_{\ell=1}^{nev}$ be Ritz vectors in a Krylov subspace $\mathcal{K}_m(A, v_1)$.

  Then, Saad (1980) suggests to restart the Arnoldi procedure with

$$v_1^{(r)} \propto \sum_{\ell=1}^{nev} \|Ay_\ell - \lambda_\ell y_\ell\|_2 \, \Re\{y_\ell\}.$$

  Reasons invoked for this choice are:

  - Using $\Re\{y_\ell\}$ circumvents the need for complex arithmetic.
  - Using the eigen-residual $\|Ay_\ell - \lambda_\ell y_\ell\|_2$ to weigh the ℓ-th Ritz vector in the restart vector $v_1^{(r)}$ favors the contribution of slower converging eigenpairs. Thus, the slow convergence of those approximate eigenpairs is tentatively set off using a starting vector $v_1^{(r)}$ which is richer in the corresponding exact eigenvectors.

Saad, Y. (1980). Variations on Arnoldi's method for computing eigenelements of large unsymmetric matrices. Linear algebra and its applications, 34, 269-295.

Polynomial restart of Arnoldi, cont'd

- Since all vectors in $\mathcal{K}_m(A, v_1)$ can be represented as the product of a matrix polynomial with the starting vector v_1, i.e.,

$$\mathcal{K}_m(A, v) = \{p(A)v_1,\, p \in \mathcal{P}_{m-1}\}\,,$$

the restart vector $v_1^{(r)}$ proposed by Saad (1980) admits a representation

$$v_1^{(r)} = \psi^{(r)}(A)v_1$$

where $\psi^{(r)} \in \mathcal{P}_{m-1}$ may be specified by setting its roots.

- The restart polynomial $\psi^{(r)}$ should be small on the unwanted portion of the spectrum, and amplify the components of the starting vector in the direction of desired eigenvectors.
- Saad (1984) made use of Chebyshev polynomials for when the unwanted portion of the spectrum is contained in an ellipse.
- Heuveline and Sadkane (1996) introduced the use of Faber polynomials for cases where the unwanted part of the spectrum does not fit in an ellipse.

Saad, Y. (1984). Chebyshev acceleration techniques for solving nonsymmetric eigenvalue problems. Mathematics of Computation, 42(166), 567-588.

Heuveline, V., & Sadkane, M. (1996). Arnoldi-Faber method for large non hermitian eigenvalue problems. Inria report no 3007.

Implicitly restarted Arnoldi (IRA) process

Implicitly restarted Arnoldi

- Explicit restarting involves directly applying a restart polynomial or building a linear combination of Ritz vectors to create a restart vector, which is then used to initiate an entirely new Arnoldi procedure.
- As an alternative to explicit restart, Sorensen (1992) interprets the Arnoldi method from the perspective of a **QR eigenvalue iteration**, including implicit shifting and deflation.
  The resulting **implicitly restarted Arnoldi** (**IRA**) method
  - allows for more stable restarts,
  - uses Ritz values of unwanted eigenpairs, referred to as exact shifts, as roots of the restart polynomial,
  - is proven to converge to wanted eigenpairs in case of Hermitian matrices.

  IRA is at the heart of ARPACK (Lehoucq et al., 1998), the current state-of-the-art software for the computation of limited numbers of eigenpairs of large (typically sparse) matrices.

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Lehoucq, R. B., Sorensen, D. C., & Yang, C. (1998). ARPACK users' guide: solution of large-scale eigenvalue problems with implicitly restarted Arnoldi methods. Society for Industrial and Applied Mathematics.

Implicitly restarted Arnoldi, cont'd$_1$

- After $m = k + p$ Arnoldi iterations, we have

$$AV_m = V_m H_m + r_m e_m^{(m)T} \quad \text{where} \quad r_m := h_{m+1,m} v_{m+1}.$$

Then, Sorensen (1992) applies p shifted QR iterations to H_m as follows:

$$\begin{array}{l} H_m^{(0)} := H_m \\ \textbf{for } i = 1, \ldots, p \textbf{ do} \\ \quad \text{Find } Q_i, R_i \text{ s.t. } Q_i R_i = H_m^{(i-1)} - \mu_i I_m \\ \quad H_m^{(i)} := Q_i^T H_m^{(i-1)} Q_i \end{array}$$

We then have:

$$H_m^{(p)} = Q^{(p)T} H_m Q^{(p)} \quad \text{where} \quad Q^{(p)} := Q_1 \cdots Q_p$$

so that $H_m^{(p)}$ is upper-Hessenberg.

The $Q_1, \ldots, Q_p$ matrices are orthonormal and upper-Hessenberg, so that $Q^{(p)}$ is banded with a lower bandwidth of p.

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Implicitly restarted Arnoldi, cont'd$_2$

- Right-multiplying the Arnoldi relation by $Q^{(p)}$, we get:

$$\begin{aligned} AV_m Q^{(p)} &= V_m H_m Q^{(p)} + r_m e_m^{(m)T} Q^{(p)} \\ AV_m Q^{(p)} &= V_m Q^{(p)} Q^{(p)T} H_m Q^{(p)} + r_m e_m^{(m)T} Q^{(p)} \\ AV_m^{(p)} &= V_m^{(p)} H_m^{(p)} + r_m e_m^{(m)T} Q^{(p)} \end{aligned}$$

where $V_m^{(p)} := V_m Q^{(p)}$.

Due to the banded structure of $Q^{(p)}$, $e_m^{(m)T} Q^{(p)}$ has the following structure:

$$e_m^{(m)T} Q^{(p)} = [\underbrace{0 \cdots 0}_{k-1} \underbrace{* \cdots *}_{p+1}].$$

Moreover, since $H_m^{(p)}$ is upper-Hessenberg, we obtain

$$AV_m^{(p)}[:, 1:k] = V_m^{(p)}[:, 1:k] H_m^{(p)}[1:k, 1:k] + \left(h_{k+1,k}^{(k)} v_{k+1}^{(p)} + q_{m,k}^{(p)} r_m \right) e_k^{(k)T}$$

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Implicitly restarted Arnoldi, cont'd$_3$

so that we have a new Arnoldi relation:

$$AV_m^{(p)}[:, 1:k] = V_m^{(p)}[:, 1:k]H_m^{(p)}[1:k, 1:k] + r_k^{(p)} e_k^{(k)T}$$

where $r_k^{(p)} := h_{k+1,k}^{(p)} v_{k+1}^{(p)} + q_{m,k}^{(p)} r_m$.

- There remains to specify the shifts $\mu_1, \ldots, \mu_p$. For that, we compute all the eigenvalues of H_m and set the shifts $\mu_1, \ldots, \mu_p$ to the p eigenvalues which are the furthest from the targeted part of the spectrum.

  By induction, we can show (homework) that

$$v_1^{(r)} := V_m^{(p)} e_1^{(m)} \propto (A - \mu_p I_n) \cdots (A - \mu_1 I_n) v_1. \tag{1}$$

  Essentially, that is, the shifted QR iterations *implicitly* apply polynomial filtering to the starting vector v_1.

  Therefore, upon picking-up an Arnoldi procedure from Eq. (1), we have *implicitly* applied a *restart polynomial* $\psi(A) := \Pi_{i=1}^{p}(A - \mu_i I_n)$ to v_1.

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Implicitly restarted Arnoldi, cont'd$_4$

- If the shifts $\mu_1, \ldots, \mu_p$ are exact eigenvalues of A, then the induced restart polynomial deflates the components of v_1 in the direction of the corresponding eigenvectors. This motivates setting the shifts to the Ritz values which are the most remote from the targeted part of the spectrum.
- In practice, the shifts are not exact eigenvalues of A. But if a shift μ_i is close to an eigenvalue of A, then the corresponding monomial of the restart polynomial removes small components of v_1 in the direction of nearby eigenvectors, thus relatively amplifying v_1's components in the direction of the targeted eigenvectors, thus making the restarted subspace a better candidate for their approximation.
- Morgan (1996) shows that the implicitly restarted subspace of degree $k+i$ is Krylov, and given by

$$\text{span}\{y_1, \ldots, y_k, Ay_j, \ldots, A^i y_j\} \quad \text{for} \quad j = 1, \ldots, k,$$

where $y_1, \ldots, y_k$ are the targeted Ritz vectors.

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Morgan, R. (1996). On restarting the Arnoldi method for large nonsymmetric eigenvalue problems. Mathematics of Computation, 65(215), 1213-1230.

Implicitly restarted Arnoldi, cont'd$_5$

The implicitly restarted Arnorldi (IRA) procedure is given by:

Algorithm 2 IRA

1: Perform $m := k + p$ steps of standard Arnoldi procedure
2: We have $V_m := [v_1, \ldots, v_m]$ and $H_m = V_m^T A V_m$ s.t. $AV_m = V_m H_m + r_m e_m^{(m)T}$
3: Compute m eigenvalues $\lambda_1, \ldots, \lambda_m$ of H_m
4: Set the shifts $\mu_1, \ldots, \mu_p$ to the eigenvalues λ_i which are the furthest from the targeted part of the spectrum
5: $Q := I_m$
6: **for** $i = 1, 2 \ldots, p$ **do**
7: Find Q_i, R_i such that $Q_i R_i = H_m - \mu_i I_m$
8: $H_m := Q_i^T H_m Q_i$
9: $Q := QQ_i$
10: $V_{k+1} := V_m Q[:, 1\!:\!k+1]$
11: $r_k := h_{k+1,k} v_{k+1} + q_{m,k} r_m$
12: $H_k := H_m[1\!:\!k, 1\!:\!k]$
13: Continue Arnoldi iteration from $AV_k = V_k H_k + r_k e_k^{(k)T}$

Sorensen, D. C. (1992). Implicit application of polynomial filters in a k-step Arnoldi method. SIAM journal on matrix analysis and applications, 13(1), 357-385.

Arnoldi process thick-restarted with Rayleigh-Ritz vectors

Origin and adaptation of thick-restarting

- Thick-restart was introduced by Wu and Simon (2000) as a way to explicitly restart Lanczos procedures with several approximate eigenvectors while limiting convergence hindering.
- The concept of thick-restarting was later adapted by Morgan (2000) and Morgan & Zeng (2006) to improve convergence behaviors of restarted GMRES and Arnoldi processes, respectively.

  In this Section, we focus on the thick-restart of Arnoldi processes with Rayleigh-Ritz vectors.

Wu, K., & Simon, H. (2000). Thick-restart Lanczos method for large symmetric eigenvalue problems. SIAM Journal on Matrix Analysis and Applications, 22(2), 602-616.

Morgan, R. B. (2002). GMRES with deflated restarting. SIAM Journal on Scientific Computing, 24(1), 20-37.

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Reminders of Rayleigh-Ritz vectors in an Arnoldi process

- From Lecture 11, we recall that, after performing m iterations of an Arnoldi process, we are equipped with:
  - An orthonormal basis in the columns of $V_m := [v_1, \ldots, v_m]$ such that

$$\text{range}(V_m) = \mathcal{K}_m(A, v_1).$$

  - An upper-Hessenberg matrix $H_m = V_m^H A V_m$ such that

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^{(m)T}.$$

  - $k \leq m$ Rayleigh-Ritz vectors $y_1, \ldots, y_k \in \text{range}(V_m)$ such that

$$y_\ell := V_m \hat{y}_\ell \quad \text{where} \quad \hat{y}_\ell \neq 0 \quad \text{is s.t.} \quad H_m \hat{y}_\ell = \lambda_\ell \hat{y}_\ell,$$

  with eigen-residual

$$\tilde{r}_\ell := A y_\ell - \lambda_\ell \hat{y}_\ell \propto v_{m+1}$$

  for $\ell = 1, \ldots, k$.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors

- From here, we describe the method introduced in Morgan & Zeng (2006) to restart the Arnoldi process with Rayleigh-Ritz vectors.
- Let the restart vector be given by

$$v_{k+1}^{(r)} := v_{m+1}.$$

Then we want to generate a new orthonormal basis

$$\{v_1^{(r)}, \ldots, v_k^{(r)}, v_{k+1}^{(r)}, \ldots, v_m^{(r)}\}$$

for the restarted subspace given by:

$$\text{span}\{y_1, \ldots, y_k, v_{k+1}^{(r)}, Av_{k+1}^{(r)}, \ldots, A^{m-k-1}v_{k+1}^{(r)}\}.$$

This is done in two steps.

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

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

- First, let the k first basis vectors $v_1^{(r)}, \ldots, v_k^{(r)}$ be the columns of the orthogonal factor Q from the thin QR decomposition of the stack of Rayleigh-Ritz vectors $Y_k := [y_1, \ldots, y_k]$:
  - Since $Y_k := V_m \hat{Y}_k$ and V_m is orthonormal, we have

$$V_k^{(r)} := [v_1^{(r)}, \ldots, v_k^{(r)}] = V_m \hat{Q}_k \tag{2}$$

    where $\hat{Q}_k$ is the orthonormal factor of the thin QR decomposition of $\hat{Y}_k$:

$$\hat{Y}_k = \hat{Q}_k R_k.$$

  - So, essentially, we only need to compute the thin QR decomposition of the low-dimensional m-by-k matrix $\hat{Y}_k$, and then evaluate the right-hand-side of Eq. (2).

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

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

- Second, construct $v_{k+1}^{(r)}, \ldots, v_m^{(r)}$ by orthonormalizing $Av_j^{(r)}$ against

$$v_1^{(r)}, \ldots, v_k^{(r)}, v_{k+1}^{(r)}, \ldots, v_j^{(r)}$$

for $j = k+1, \ldots m-1$:

- First, $v_{k+1}^{(r)} = v_{m+1}$ is orthogonal to $v_1^{(r)}, \ldots, v_k^{(r)}$ by construction.
- Then, just as with a standard Arnoldi procedure, we need a projector $\Pi_{V_j^{(r)}}$ onto span$\{v_1^{(r)}, \ldots, v_j^{(r)}\}^\perp$ so that

$$v_{j+1}^{(r)} := \Pi_{V_j^{(r)}} A v_j^{(r)} / \|\Pi_{V_j^{(r)}} A v_j^{(r)}\|_2$$

for $j = k+1, \ldots, m-1$.

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_3$

- Then, the restarted search space is such that

$$\begin{aligned}
\text{range}(V_m^{(r)}) &= \text{span}\{y_1, \ldots, y_k, v_{k+1}^{(r)}, Av_{k+1}^{(r)}, \ldots, A^{m-k-1}v_{k+1}^{(r)}\} \\
&= \text{span}\{y_1, \ldots, y_k, v_{m+1}, Av_{m+1}, \ldots, A^{m-k-1}v_{m+1}\} \\
&= \text{span}\{y_1, \ldots, y_k, \tilde{r}_\ell, A\tilde{r}_\ell, \ldots, A^{m-k-1}\tilde{r}_\ell\} \quad \text{for} \quad \ell = 1, \ldots, k \\
&= \text{span}\{y_1, \ldots, y_k, y_\ell, Ay_\ell, \ldots, A^{m-k-1}y_\ell\} \quad \text{for} \quad \ell = 1, \ldots, k
\end{aligned}$$

so that the restarted search space range$(V_m^{(r)})$ contains

$$\mathcal{K}_{m-k+1}(A, y_\ell) \quad \text{for} \quad \ell = 1, \ldots, k.$$

Moreover, it was proven by Eiermann et al. (2000), Morgan (2000), Morgan (2002) and Stewart (2002) that the restarted search space is also Krylov as a whole.

Morgan, R. B. (2000). Implicitly restarted GMRES and Arnoldi methods for nonsymmetric systems of equations. SIAM Journal on Matrix Analysis and Applications, 21(4), 1112-1135.
Eiermann, M., Ernst, O. G., & Schneider, O. (2000). Analysis of acceleration strategies for restarted minimal residual methods. Journal of Computational and Applied Mathematics, 123(1-2), 261-292.
Stewart, G. W. (2002). A Krylov–Schur algorithm for large eigenproblems. SIAM Journal on Matrix Analysis and Applications, 23(3), 601-614.
Morgan, R. B. (2002). GMRES with deflated restarting. SIAM Journal on Scientific Computing, 24(1), 20-37.
Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_4$

- Let us now look into how we can generate new Rayleigh-Ritz vectors with respect to the restarted search space.
  That is, we want Ritz pairs (λ, y) such that

$$y \in \text{range}(V_m^{(r)}) \quad \text{and} \quad Ay - \lambda y \perp \text{range}(V_m^{(r)})$$

  where $V_m^{(r)}$ is orthonormal so that we search for non-trivial pairs $(\lambda, \hat{y})$ such that

$$H_m^{(r)} \hat{y} = \lambda \hat{y} \quad \text{where} \quad H_m^{(r)} := V_m^{(r)T} A V_m^{(r)},$$

  after what a Rayleigh-Ritz vector is given by $y := V_m^{(r)} \hat{y}$.
  The projected matrix has the following block structure:

$$H_m^{(r)} = \begin{bmatrix} V_k^{(r)T} A V_k^{(r)} & V_k^{(r)T} A V_{k+1:m}^{(r)} \\ V_{k+1:m}^{(r)T} A V_k^{(r)} & V_{k+1:m}^{(r)T} A V_{k+1:m}^{(r)} \end{bmatrix}$$

  There remains to look into how those blocks can be efficiently assembled.

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_4$

- Without loss of generality, we may assume that the orthonormalization is achieved by modified Gram-Schmidt. That is:

$$\Pi_{V_j^{(r)}} := \left(I_n - v_j^{(r)} v_j^{(r)T}\right) \cdots \left(I_n - v_1^{(r)} v_1^{(r)T}\right)$$

so that, for $j = k+1, \ldots, m-1$, we have:

1. $v_{j+1}^{(r)} := A v_j^{(r)}$
2. **for** $i = 1, \ldots, j$
3. $\quad h_{ij}^{(r)} := v_i^{(r)T} v_{j+1}^{(r)}$
4. $\quad v_{j+1}^{(r)} := v_{j+1}^{(r)} - h_{ij}^{(r)} v_i^{(r)}$
5. $h_{j+1,j}^{(r)} := \|v_{j+1}^{(r)}\|_2$
6. $v_{j+1}^{(r)} := v_{j+1}^{(r)} / h_{j+1,j}^{(r)}$

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_5$

- Then, for $j = k+1, \ldots, m-1$, we have:

$$\begin{aligned} h_{ij}^{(r)} &= v_i^{(r)T} \left(I_n - v_{i-1}^{(r)T} v_{i-1}^{(r)} \right) \cdots \left(I_n - v_1^{(r)T} v_1^{(r)} \right) A v_j^{(r)} \\ &= v_i^{(r)H} A v_j^{(r)} \quad \text{for} \quad i = 1, \ldots, j. \end{aligned}$$

We also have:

$$\begin{aligned} h_{j+1,j}^{(r)} v_{j+1}^{(r)} &= \Pi_{V_j^{(r)}} A v_j^{(r)} \\ h_{j+1,j}^{(r)} v_{j+1}^{(r)T} v_{j+1}^{(r)} &= v_{j+1}^{(r)T} \Pi_{V_j^{(r)}} A v_j^{(r)} \\ h_{j+1,j}^{(r)} &= v_{j+1}^{(r)T} A v_j^{(r)}. \end{aligned}$$

Finally, we have:

$$h_{j+1,j}^{(r)} v_i^{(r)T} v_{j+1}^{(r)} = v_i^{(r)T} \Pi_{V_j^{(r)}} A v_j^{(r)} \implies v_i^{(r)T} A v_j^{(r)} = 0 \quad \text{for} \quad i > j+1,$$

so that all the non-zero components of $H_m^{(r)}[:, 1:m]$ are by-products of the orthogonalization procedure.

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Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_6$

- As for the leading k-by-k block of $H_m^{(r)}$, we have:

$$H_m^{(r)}[1:k,1:k] = V_k^{(r)T} A V_k^{(r)} = (V_m \hat{Q}_k)^T A (V_m \hat{Q}_k) = \hat{Q}_k^T H_m \hat{Q}_k,$$

  whose dimensions are independent of n, and can be efficiently evaluated.
- Last, we need to look into the off-diagonal block $H_m^{(r)}[k+1:m,1:k]$. We recall that $\hat{Y}_k = \hat{Q}_k R_k$, so that

$$V_k^{(r)} = V_m \hat{Q}_k = V_m \hat{Y}_k R_k^{-1}.$$

  Using this equation along with the standard Arnoldi relation, we get:

$$\begin{aligned} v_j^{(r)T} A V_k^{(r)} &= v_j^{(r)T} A V_m \hat{Y}_k R_k^{-1} \\ &= v_j^{(r)T} (V_m H_m + h_{m+1,m} v_{m+1} e_m^{(m)T}) \hat{Y}_k R_k^{-1}. \end{aligned}$$

- Then, for $j = k+1$, we obtain:

$$\begin{aligned} v_j^{(r)T} A V_k^{(r)} &= v_{m+1}^T (V_m H_m + h_{m+1,m} v_{m+1} e_m^{(m)T}) \hat{Y}_k R_k^{-1} \\ &= h_{m+1,m} e_m^{(m)T} \hat{Y}_k R_k^{-1} = h_{m+1,m} e_m^{(m)T} \hat{Q}_k. \end{aligned}$$

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Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_7$

- And, for $j = k+2, \ldots, m$, we obtain:

$$v_j^{(r)T} A V_k^{(r)} = v_j^{(r)T} (V_m H_m + h_{m+1,m} v_{m+1} e_m^{(m)T}) \hat{Y}_k R_k^{-1} = v_j^{(r)T} V_m H_m \hat{Y}_k R_k^{-1}$$

in which $H_m \hat{Y}_k = \hat{Y}_k \Lambda_k$, where $\Lambda_k := \text{diag}(\lambda_1, \ldots, \lambda_k)$ contains the Rayleigh-Ritz values, so that

$$v_j^{(r)T} A V_k^{(r)} = v_j^{(r)T} V_m \hat{Y}_k \Lambda_k R_k^{-1} = v_j^{(r)T} Y_k \Lambda_k R_k^{-1}. \tag{3}$$

Remember that, by construction, we have

$$v_j^{(r)T} V_k^{(r)} = 0 \quad \text{for} \quad j = k+1, \ldots, m,$$

so that

$$v_j^{(r)T} V_k^{(r)} = v_j^{(r)T} V_m \hat{Q}_k = v_j^{(r)T} V_m \hat{Y}_k R_k^{-1} = v_j^{(r)T} Y_k R_k^{-1} = 0.$$

Then, Eq. (3) becomes

$$v_j^{(r)T} A V_k^{(r)} = 0 \quad \text{for} \quad j = k+2, \ldots, m.$$

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Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_8$

- Finally, this means that the off-diagonal block $H_m^{(r)}[k+1:m, 1:k]$ is given by:

$$H_m^{(r)}[k+1:m, 1:k] = \begin{bmatrix} h_{m+1,m} e_m^{(m)T} \hat{Q}_k \\ 0_{(m-k-1)\times 1} \end{bmatrix} = h_{m+1,m} e_1^{(m-k)} e_m^{(m)T} \hat{Q}_k.$$

We now know how to efficiently assemble $H_m^{(r)}$ in order to evaluate new Rayleigh-Ritz pairs after a thick-restart. In particular, we have

$$H_m^{(r)} = \begin{bmatrix} \hat{Q}_k^T H_m \hat{Q}_k & V_k^{(r)T} A V_{k+1:m}^{(r)} \\ h_{m+1,m} e_1^{m-k} e_m^{(m)T} \hat{Q}_k & V_{k+1:m}^{(r)T} A V_{k+1:m}^{(r)} \end{bmatrix}$$

where $V_k^{(r)T} A V_{k+1:m}^{(r)}$ and $V_{k+1:m}^{(r)T} A V_{k+1:m}^{(r)}$ are by-products of the orthogonlization procedure.

Morgan, R. B., & Zeng, M. (2006). A harmonic restarted Arnoldi algorithm for calculating eigenvalues and determining multiplicity. Linear algebra and its applications, 415(1), 96-113.

Thick-restarting Arnoldi with Rayleigh-Ritz vectors, cont'd$_8$

- One can also show that the following Arnoldi relation holds:

$$AV_m^{(r)} = V_m^{(r)} H_m^{(r)} + h_{m+1,m}^{(r)} v_{m+1}^{(r)} e_m^{(m)T}$$

so that new Rayleigh-Ritz pairs (λ, y) with respect to range$(V_m^{(r)})$, i.e., so that there exists a non-zero $\hat{y}$ such that

$$H_m^{(r)} \hat{y} = \lambda \hat{y} \quad \text{with} \quad y := V_m^{(r)} \hat{y},$$

have residuals given by:

$$\tilde{r} := Ay - \lambda y = h_{m+1,m}^{(r)} (e_m^{(m)T} \hat{y}) v_{m+1}^{(r)}.$$

One can then monitor the eigen-residual norm of Rayleigh-Ritz iterates after the thick-restart, without having to assemble the approximate eigenvectors, nor to carry additional matrix-vector products.

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Arnoldi process thick-restarted with harmonic Ritz vectors

GMRES with deflated restart

Loose GMRES

Thick-restart of Lanczos process

Homework problems

Homework problems

Turn in **your own** solution to **Pb. 33**:

Pb. 33 Consider the Arnoldi relation achieved after an implicit restart:

$$AV_m^{(p)} = V_m^{(p)} H_m^{(p)} + r_k^{(p)} e_m^{(m)T}$$

where $V_m^{(p)} := V_m Q^{(p)}$ and

$$H_m^{(p)} = Q_{p+1} R_{p+1} + \mu_{p+1} I_m = Q_p^T H_m^{(p-1)} Q_p = Q^{(p)T} H_m Q^{(p)}$$

with $Q^{(p)} := Q_1 \cdots Q_p$. Show that

$$v_1^{(r)} := V_m^{(p)} e_1^{(p)} \propto (A - \mu_p I_n) \cdots (A - \mu_1 I_n) v_1.$$

Pb. 34 *.