Graduate School
Numerical Linear Algebra

Lecture on

Arnoldi and Lanczos method

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1 Intro and revision

Find a few eigenvalues and eigenvectors of $A \in \mathbb{C}^{n,n}$:

$$Ax = \lambda x.$$

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|, \quad (\lambda_i, x_i), i = 1, \ldots, n$$

Many matrices in applications are sparse, i.e

- Hessenberg reduction and QR algorithm introduce fill-in (similarity transfrom, change A)
- we only want to use algorithms that don't change A (matrix-vector multiplications)
- examples (see previous lectures):
  - Power method (RQI, Inverse Iteration): pick a vector q and form the sequence
    $$q, Aq, A^2q, A^3q, ...$$
    Then $\text{span}\{A^m q\} \to \text{span}\{v_1\}$, v_1 dominant eigenvector

– Simultaneous iteration: choose subspace $\mathcal{S}$ with $\mathcal{S} = \text{span}\{q_1^{(0)}, \ldots, q_k^{(0)}\}$ and form the sequence

$$\mathcal{S}, A\mathcal{S}, A^2\mathcal{S}, A^3\mathcal{S}, ...$$

Then $\text{span}\{A^m\mathcal{S}\} \to \text{span}\{v_1, \ldots, v_k\}$ dominant invariant subspace

– Arnoldi's method, Lanczos method

2 Arnoldi's method

2.1 Idea

- keep iterates of the power method: after k steps we have $k+1$ vectors $q, Aq, \ldots, A^k q$
- look for good eigenvector approximations in the $k+1$-dimensional subspace spanned by these vectors
- $q, Aq, \ldots, A^k q$ ill-conditioned
- orthogonalise $q_1, \ldots, q_{k+1}$
- Gram-Schmidt: orthogonalise Aq_k against $q_1, \ldots, q_k$ (is the same as Gram-Schmidt applied to $q, Aq, \ldots, A^k q$ (see Theorem)

2.2 The Arnoldi process

Choose a starting vector q. Normalisation

$$q_1 = \frac{q}{\|q\|_2}$$

On subsequent steps $k = 1, 2, \ldots$ take

$$\tilde{q}_{k+1} = Aq_k - \sum_{j=1}^{k} q_j h_{jk}$$

where h_{jk} is the Gram-Schmidt coefficient $h_{jk} =< Aq_k, q_j >$.
Normalisation

$$q_{k+1} = \frac{\tilde{q}_{k+1}}{h_{k+1,k}} \quad \text{where} \quad h_{k+1,k} = \|\tilde{q}_{k+1}\|_2$$

Classical Gram-Schmidt

for $j = 1$ to k **do**
  $h_{jk} = (Aq_k)^* q_j$
end for
$q_{k+1} = Aq_k - \sum_{j=1}^{k} q_j h_{jk}$

Modified Gram-Schmidt

$q_{k+1} = Aq_k$
for $j = 1$ to k **do**
  $q_{k+1} = q_{k+1} - (q_{k+1}^T q_j) q_j$
end for

The following implementation uses modified Gram-Schmidt.

$q_1 = \dfrac{q}{\|q\|_2}$
for $k = 1$ to $m - 1$ **do**
  $q_{k+1} \leftarrow Aq_k$
  for $j = 1$ to k **do**
    $h_{jk} \leftarrow q_j^* q_{k+1}$
    $q_{k+1} \leftarrow q_{k+1} - q_j h_{jk}$
  end for
  reorthogonalise
  $h_{k+1,k} \leftarrow \|q_{k+1}\|_2$
  if $h_{k+1,k} = 0$ **then**
    span$\{q_1, \ldots, q_k\}$ is invariant under A
  end if
  $q_{k+1} = \dfrac{q_{k+1}}{h_{k+1,k}}$
end for

Definition 2.1. *For any m the space span$\{q, Aq, \ldots, A^{m-1}q\}$ is called the mth Krylov subspace associated with A and q and is denoted by $\mathcal{K}_m(A, q)$.*

Theorem 2.1. *Suppose $q, Aq, \ldots, A^{m-1}q$ are linearly independent and $q_1, \ldots, q_m$ are generated by the Arnoldi process. Then*

1. *span$\{q_1, \ldots, q_k\} = \mathcal{K}_k(A, q)$ for $k = 1, \ldots, m$.*
2. *For $k = 1, \ldots, m - 1$, $h_{k+1,k} > 0$.*
3. *$h_{m+1,m} = 0$ iff $q, Aq, \ldots, A^m q$ are linearly dependent which holds in turn iff the Krylov subspace $\mathcal{K}_m(A, q)$ is invariant under A.*

Proof. Exercise. ☐

Matrix representations of the Arnoldi process Arnoldi process:

$$Aq_k = \sum_{j=1}^{k+1} q_j h_{jk}$$

$$\Rightarrow AQ_m = Q_{m+1} H_{m+1,m}$$

where

$$Q_m = [q_1, \dots, q_m] \in \mathbb{C}^{n,m} \quad \text{and}$$

$$H_{m+1,m} = \begin{bmatrix} h_{11} & h_{22} & \cdots & h_{1,m-1} & h_{1m} \\ h_{21} & h_{22} & \cdots & h_{2,m-1} & h_{2m} \\ 0 & h_{32} & \cdots & h_{3,m-1} & h_{3m} \\ \vdots & & \ddots & & \vdots \\ 0 & & & h_{m,m-1} & h_{mm} \\ 0 & 0 & & 0 & h_{m+1,m} \end{bmatrix} \in \mathbb{C}^{m+1,m}$$

The Arnoldi process can be written in the form

$$AQ_m = Q_m H_m + q_{m+1} h_{m+1,m} e_m^T \tag{1}$$

where H_m is square upper Hessenberg.

2.3 Arnoldi and eigenvalues

Theorem 2.2. *If $h_{m+1,m} = 0$ then $q, Aq, \dots, A^m q$ are linearly dependent, i.e. span$\{Q_m\}$ is invariant under A and*

$$AQ_m = Q_m H_m$$

and the eigenvalues of H_m are the eigenvalues of A.

Proof. Using (1) the result is obvious. □

Remark 2.1. *Note that*

1. *for n steps we get $q_1, \dots, q_n$ is an orthonormal basis of $\mathbb{C}^n$ and $Q_n^{-1} A Q_n = H_n$ is a unitary similarity transform*

2. *want to stop after m steps $m << n$*

3. *$h_{m+1,m} = 0$ only if we are lucky*

Theorem 2.3 ((Error estimates (Ritz values and Ritz vectors)). *Let Q_m, H_m and $h_{m+1,m}$ be generated by the Arnoldi process. Let μ be an eigenvalue of H_m with associated eigenvector x normalised so that $\|x\|_2$=1. Let $y = Q_m x \in \mathbb{C}^n$ (also with $\|y\|_2$=1). Then*

$$\|Ay - \mu y\|_2 = |h_{m+1,m}||x_m|,$$

where x_m denotes the mth (and last) component of x.

Proof. Multiplying (1) by x and using $H_m x = \mu x$ we get

$$\begin{aligned} AQ_m x &= Q_m H_m x + q_{m+1} h_{m+1,m} e_m^T x \\ AQ_m x &= Q_m \mu x + q_{m+1} h_{m+1,m} e_m^T x \\ Ay &= \mu y + q_{m+1} h_{m+1,m} x_m \\ \|Ay - \mu y\| &= \|q_{m+1} h_{m+1,m} x_m\| \\ &= |h_{m+1,m}||x_m| \end{aligned}$$

□

Definition 2.2. *The vector y is called Ritz-vector of A associated with the subspace $\mathcal{K}_m(A, q)$ and the μ is called Ritz value.*

Remark 2.2. *Note that*

- *outer eigenvalues approximated first (see convergence theory for Lanczos)*
- *Shift-Invert technique*

3 Implicitly Restarted Arnoldi (IRA)

Idea of IRA

- convergence depends very much on starting vector q
- find a better starting vector $\hat{q}$ (less storage)
- we want $h_{m+1,m} \approx 0$ for small m, i.e. a low dimensional invariant subspace containing the desired eigenvectors
- assume A is semisimple with linearly independent eigenvectors $v_1, \dots, v_n$ and eigenvalues $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$ and $|\lambda_k| > |\lambda_{k+1}|$.
- Write $q = \sum_{i=1}^n c_i v_i$ and find $\hat{q}$, s.t. $\hat{q} = \sum_{i=1}^n \hat{c}_i v_i$ where $\hat{c}_1, \dots, \hat{c}_k$ have been augmented and $\hat{c}_{k+1}, \dots, \hat{c}_n$ have been diminished.

- Suppose $\hat{q} = p(A)q$ where p is some polynomial, then

$$\hat{q} = \sum_{i=1}^{n} c_i p(\lambda_i) v_i$$

and choose p s.t. $p(\lambda_1), \ldots, p(\lambda_k)$ are large in comparison with $p(\lambda_{k+1}), \ldots, p(\lambda_n)$

Iteration of the IRA

- make Arnoldi runs of length $m = k + j$ (to find k eigenvalues)

$$AQ_m = Q_m H_m + q_{m+1} h_{m+1,m} e_m^T$$

- find m eigenvalues $|\mu_1| \geq |\mu_2| \geq \ldots \geq |\mu_m|$ of H_m
- largest ones $|\mu_1| \geq |\mu_2| \geq \ldots \geq |\mu_k|$ are estimates for the *largest eigenvalues* of A, the smallest ones $|\mu_{k+1}| \geq | \ldots \geq |\mu_m|$ approximate the *undesired* part of the spectrum
- perform j iterations of the QR algorithm on H_m using j shifts $\nu_1, \ldots, \nu_j$ in the region of the spectrum we want to suppress (most popular choice is $\nu_1 = \mu_{k+1}, \ldots, \nu_j = \mu_m$)
- QR algorithm with shifts is given by

$$p(H_m) = V_m R_m, \quad \text{where} \quad p(z) = (z - \nu_1) \cdots (z - \nu_j)$$

- combined effect is a similarity transform

$$\hat{H}_m = V_m^{-1} H_m V_m$$

- Let $\hat{Q}_m = Q_m V_m$ and $\hat{q}_1$ be the first column of $\hat{Q}_m$.
- Carry out another m Arnoldi steps with $\hat{q}_1$ as starting vector
- don't need to start Arnoldi from scratch, since

$$A\hat{Q}_m = \hat{Q}_m \hat{H}_m + q_{m+1} h_{m+1,m} e_m^T V_m,$$

where $e_m^T V_m$ has exactly $m - j - 1$ leading zeros.

- drop last j columns to get

$$A\hat{Q}_k = \hat{Q}_k \hat{H}_k + (\underbrace{\hat{q}_{k+1} \hat{h}_{k+1,k} + q_{m+1} h_{m+1,m} V_{m,k}}_{\|\cdot\| = h_{k+1,k}^{\text{new}}}) e_k^T,$$

- do another j steps of Arnoldi

take k Arnoldi steps to produce H_k, Q_k
for $ii = 1$ to $imax$ **do**
  take another j Arnoldi steps to produce H_m, Q_m, $m = k + j$
  find j shifts $\nu_1, \ldots, \nu_j$
  take j steps of the QR algorithm on H_m with shifts $\nu_1, \ldots, \nu_j$ to obtain the transformation matrix V_m
  $H_m \leftarrow V_m^{-1} H_m V_m$
  $Q_m = Q_m V_m$
  if $|h_{k+1,k}| \leq \text{tol}$ **then**
    $\text{span}\{q_1, \ldots, q_k\}$ is invariant under A
  end if
end for

Why does IRA work?

- want new starting vector $\hat{q} = p(A)q$, where p is choosen to suppress unwanted eigenvectors and enhance wanted ones

- Recall

$$AQ_m = Q_m H_m + q_{m+1} h_{m+1,m} e_m^T$$

and insert shift

$$(A - \nu_1 I)Q_m = Q_m(H_m - \nu_1 I) + E_1$$

where E_1 is zero except for the last column,

$$(A - \nu_2 I)(A - \nu_1 I)Q_m = Q_m(H_m - \nu_1 I)(H_m - \nu_1 I) + E_2$$

where E_2 is zero except for the last two columns.

Theorem 3.1. *Suppose $AQ_m = Q_m H_m + q_{m+1} h_{m+1,m} e_m^T$ and let p be a polynomial of degree $j \leq m$. Then*

$$p(A)Q_m = Q_m p(H_m) + E_j,$$

where $E_j \in \mathbb{C}^{n,m}$ is identically zero except in the last j columns.

Remark 3.1. *The new starting vector satisfies*

- $p(A)Q_m = Q_m V_m R_m + E_j$

- $p(A)Q_m e_1 = \hat{Q}_m R_m$

- $\hat{q}_1 = \frac{1}{r_{11}} p(A) q_1$

4 Lanczos' method

The Lanczos process can be written in the form

$$AQ_m = Q_m T_m + q_{m+1}\beta_m e_m^T$$

where T_m is square tridiagonal matrix:

$$T_m = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_{m-1} \\ & & \beta_{m-1} & \alpha_m \end{bmatrix}$$

Thus we obtain only a three-term recurrence and therefore need to store only three vectors at each step.

$q_1 = \dfrac{q}{\|q\|_2}$
for $k = 1$ to $m-1$ **do**
  $q_{k+1} \leftarrow Aq_k$
  $\alpha_k = q_k^* q_{k+1}$
  $q_{k+1} \leftarrow q_{k+1} - \alpha_k q_k$
  if $k > 1$ **then**
    $q_{k+1} \leftarrow q_{k+1} - q_{k-1}\beta_{k-1}$
  end if
  $\beta_k \leftarrow \|q_{k+1}\|_2$
  if $\beta_k = 0$ **then**
    span$\{q_1, \ldots, q_k\}$ is invariant under A
  end if
  $q_{k+1} = \dfrac{q_{k+1}}{\beta_k}$
end for

Remark 4.1. *Not that*

- *all the results for Arnoldi's method hold*
- *Kaniel-Paige convergence theory*
- *outer eigenvalues approximated first*

Reorthogonalisation

- store only three vectors q_{j-1}, q_j, q_{j+1} at each step

- roundoff errors will lead to loss of orthogonality!
- after m Lanczos steps we get the computed vectors $\hat{Q}_m = [\hat{q}_1, \ldots, \hat{q}_m]$ and the associated tridiagonal matrix

$$\hat{T}_m = \begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_1 & & \\ \hat{\beta}_1 & \hat{\alpha}_2 & \ddots & \\ & \ddots & \ddots & \hat{\beta}_{m-1} \\ & & \hat{\beta}_{m-1} & \hat{\alpha}_m \end{bmatrix}$$

- Lanczos in exact arithmetic

$$AQ_m = Q_m T_m + \underbrace{q_{m+1}\beta_m}_{r_m} e_m^T$$

- computed Lanczos with roundoff errors gives

$$A\hat{Q}_m = \hat{Q}_m \hat{T}_m + \hat{r}_m e_m^T + E_m$$

where $\|E_m\|_2 = \epsilon \|A\|_2$.

- Orthogonality: If $\hat{\beta}_m = fl(\|\hat{r}_m\|_2)$ and we compute

$$\hat{q}_{m+1} = fl\left(\frac{\hat{r}_m}{\hat{\beta}_m}\right)$$

then (using floating point arithmetic)

$$\hat{\beta}_m \hat{q}_{m+1} \approx \hat{r}_m + w_m$$

where $\|w_m\|_2 \approx \epsilon \|\hat{r}_m\|_2 \approx \epsilon \|A\|_2$.

- Hence

$$\hat{q}_{m+1} = \frac{\hat{r}_m + w_m}{\hat{\beta}_m},$$

where $w_m \approx \epsilon \|A\|_2$ is the roundoff error.

- check orthogonality

$$|\hat{q}_{m+1}^T \hat{q}_i| = \frac{|\hat{r}_m^T \hat{q}_i| + \epsilon \|A\|_2}{|\hat{\beta}_m|} \, i = 1, \ldots, m$$

- orthogonality is lost (even in ideal situation $\hat{r}_m^T \hat{q}_i = 0$, especially for converged eigenvectors (i.e. when $\hat{\beta}_m$ is small)
- this problem is solved by either complete or selective reorthogonalisation

Ghost eigenvalues

- Ghost (or spurious) eigenvalues are multiple eigenvalues of $\hat{T}_m$ that belong to single eigenvalues of A.
- They arise due to loss of orthogonality
- the iteration essentially restarts itself, when the orthogonality to a converged Ritz vector is lost
- this is the same as if we would use Orthogonal iteration (see previous lectures 4.4) without orthogonalising:
- Example: Let $Q_0 = [q_1|q_2]$. Then

$$
\begin{aligned}
Z_1 &= AQ_0 \\
Z_2 &= AZ_1 = A^2 Q_0 \\
&\vdots \\
Z_k &= A^k Q_0 \\
&= A^k [q_1|q_2] \\
&= [A^k q_1 | A^k q_2]
\end{aligned}
$$

  This is like "Power method" applied to q_1 and q_2 separately, converging to the eivenvector belonging to the eigenvalue of largest modulus.