Termination in Arnoldi

$K_n = \operatorname{span}(b, Ab, A^2b, \ldots A^{n-1}b)$

Earlier, we wrote: "Assume for now that $\dim K_n(A, b) = n$, i.e., $b, Ab, \ldots, A^{n-1}b$ are linearly independent."

At some point this assumption must become false. For instance, assume we arrive at step $m = n$: $q_1, q_2, \ldots, q_m$ are a basis of $\mathbb{R}^m$, so

$$Aq_m = \beta_1 q_1 + \cdots + \beta_m q_m + 0$$

(without an additional term $\beta_{m+1} q_{m+1}$.)

$A\left[q_1 \middle| q_2 \middle| \cdots \middle| q_n\right] = \left[q_1 \middle| \cdots \middle| q_{n+1}\right] \begin{bmatrix} H \\ \times \end{bmatrix}$

We get a complete factorization of A:

$$AQ_m = Q_m H_m \Longrightarrow A = Q_m H_m Q_m^T.$$

We can use it to solve linear systems, too, but most of the time we want to stop the iteration much earlier.

$A\left[q_1 \middle| \cdots \middle| q_m\right] = \left[q_1 \middle| \cdots \middle| q_m\right] \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \end{bmatrix}$ $\rightarrow H_m$

$\rightarrow$ Hessenberg matrix

Breakdown in Arnoldi

Note that the 'breakdown' can happen much earlier: for instance, if b is an eigenvector of A, it happens already at $n = 1$.

Suppose that at step n

$$A^n b \in \text{span}(b, Ab, \ldots, A^{n-1} b).$$

Then,

$$Aq_n = \beta_1 q_1 + \cdots + \beta_n q_n + 0$$

and the vector q_{n+1} that continues the orthonormal basis is not uniquely determined.

We take $\beta_{n+1} = 0$, $q_{n+1} =$ any vector orthonormal to $q_1, \ldots, q_n$, and continue.

(At this point $q_1, \ldots, q_n, q_{n+1}$ is not anymore a basis of $K_{n+1}(A, b)$ — but we continue nevertheless.)

b = eigenvector of A $\quad Ab = \lambda b$

$q_1 = \frac{b}{\|b\|}$ $\quad z = A_1 q_1 - \beta_1 q_1 = 0$

$q_2 = \frac{z}{\|z\|}$ no breakdown

$w = Aq_1 = \beta_1 q_1 + \beta_2 q_2$

$\downarrow \qquad \downarrow$

$\lambda \cdot q_1 \quad 0 \cdot q_2$

$Aq_1 = \lambda q_1$

If this happens, we set q_{j+1} = any vector orthogonal to $q_1, q_2, \dots q_j$, $\beta_{j+1} = 0$.

After breakdown,

$[q_1, q_2, \dots q_{n+1}]$ is no longer a basis of

$$K_{n+1}(A, b) = \text{span}\left(b, Ab, A^2b, \dots A^n b\right)$$

$$Aq_n = \beta_1 q_1 + \dots + \beta_n q_n \quad (1)$$

Since $q_1, \dots q_n \in K_n(A, b)$

we can write each of them

as $q_i = \gamma_{1,i}\, b + \gamma_{2,i}\, Ab + \dots + \gamma_{n,i}\, A^{n-1}b$.

Expand everything in (1) as lin. comb. of $A^k b$ to get a

non-trivial linear combination among the $A^k b$:

$$A\left(\gamma_{1n} b + \dots + \gamma_{n-1,n} A^{n-1} b\right) = \beta_1 \left(\gamma_{11} b + \dots + \gamma_{n-1,1} A^{n-1} b\right) + \dots$$

$$\dots + \beta_n \left(\gamma_{1n} b + \dots + \gamma_{n-1,n} A^{n-1} b\right)$$

$\gamma_{n-1,n} A^n b$

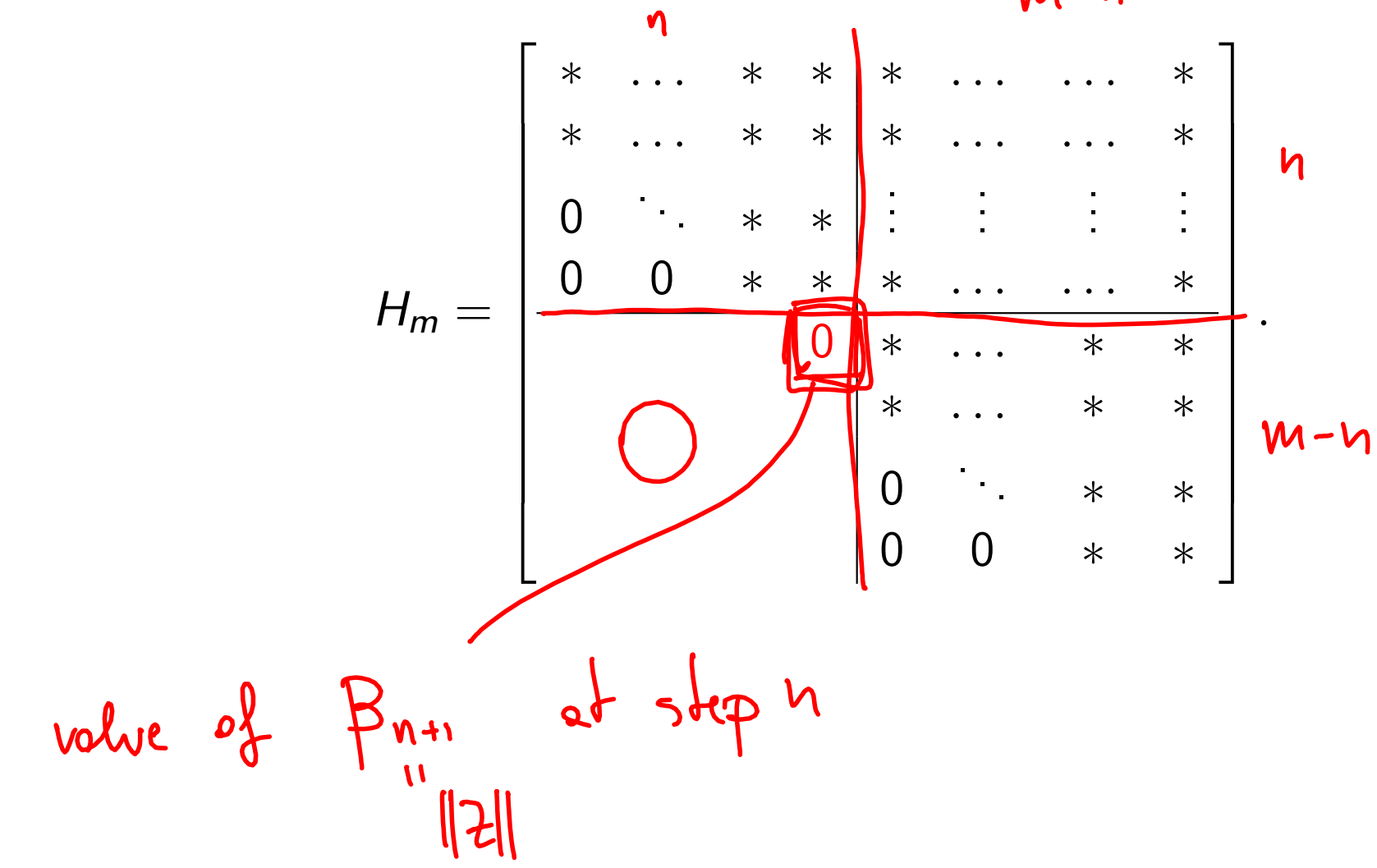
linear comb. of $A^k b$

After the breakdown

In the end, we get a full factorization

$$AQ_m = H_m Q_m,$$

$$H_m = \begin{bmatrix} * & \dots & * & * & * & \dots & \dots & * \\ * & \dots & * & * & * & \dots & \dots & * \\ 0 & \ddots & * & * & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & * & * & * & \dots & \dots & * \\ & & & 0 & * & \dots & * & * \\ & & & & * & \dots & * & * \\ & & & & 0 & \ddots & * & * \\ & & & & 0 & 0 & * & * \end{bmatrix}.$$



Arnoldi completed to a full factorization

$$A = Q_m H_m Q_m^T = \left[\begin{array}{c|c} Q_n & \widehat{Q} \end{array}\right] \left[\begin{array}{cc} H_n & L \\ 0 & M \end{array}\right] \left[\begin{array}{c|c} Q_n & \widehat{Q} \end{array}\right]^T$$

Consequence #1 The eigenvalues of A are the union of those of H_n and those of M.

Consequence #2 We can use this factorization to solve the linear system $Ax = b$:

$$\begin{aligned} x &= \begin{bmatrix} Q_n & \widehat{Q} \end{bmatrix} \begin{bmatrix} H_n & L \\ 0 & M \end{bmatrix}^{-1} \begin{bmatrix} Q_n & \widehat{Q} \end{bmatrix}^T b \\ &= \begin{bmatrix} Q_n & \widehat{Q} \end{bmatrix} \begin{bmatrix} H_n & L \\ 0 & M \end{bmatrix}^{-1} \begin{bmatrix} \|b\| e_1 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} Q_n & \widehat{Q} \end{bmatrix} \begin{bmatrix} \|b\| H_n^{-1} e_1 \\ 0 \end{bmatrix} = Q_n \|b\| H_n^{-1} e_1. \end{aligned}$$

(Check the computations, they are not obvious.)

$$A = \left[\begin{array}{c|c} Q_n & \hat{Q} \end{array}\right] \left[\begin{array}{c|c} H_n & L \\ \hline 0 & M \end{array}\right] \left[\begin{array}{c|c} Q_n & \hat{Q} \end{array}\right]^T$$

$$Ax = b$$

$$q_1 = \frac{1}{\|b\|} \cdot b$$

$$x = A^{-1} b = \left[\begin{array}{c|c} Q_n & \hat{Q} \end{array}\right] \left[\begin{array}{c|c} H_n & L \\ \hline 0 & M \end{array}\right]^{-1} \left[\begin{array}{c|c} Q_n & \hat{Q} \end{array}\right]^T b =$$

$$= \left[\begin{array}{c|c} Q_n & \hat{Q} \end{array}\right] \left[\begin{array}{c|c} H_n^{-1} & -H_n^{-1} L M^{-1} \\ \hline 0 & M^{-1} \end{array}\right]$$

$$\begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_n^T \\ \vdots \\ q_m^T \end{bmatrix} \cdot b = \begin{bmatrix} q_1^T b \\ q_2^T b \\ \vdots \\ q_m^T b \end{bmatrix} = \begin{bmatrix}$$

$$q_1 = \frac{1}{\|b\|} \cdot b$$

$$q_1^T q_1 = 1$$

These results as a theorem

Suppose that there is breakdown at step n in Arnoldi, i.e., $A^n b \in K_n(A, b)$. Then,

- if $H_n v = \lambda v$ is an eigenvalue of H_n, then $w = Q_n v$ satisfies $Aw = \lambda w$, i.e., it is an eigenvector of A with the same eigenvalue. (And, in particular, the eigenvalues of H_n are a subset of those of A.)
- the exact solution of $Ax = b$ is given by $Q_n \|b\| H_n^{-1} e_1$.

We can stop immediately at breakdown: we only need Q_n, H_n.

'Lucky breakdown': if it happens at an early step, we can solve linear systems (or compute eigenvalues) cheaply: costs n matrix-vector products + $O(mn^2)$.

When there is no breakdown

Let (λ, v) be an eigenpair of H_n; then $(\lambda, Q_n v)$ is called a Ritz pair (Ritz value, Ritz vector) of A.

Amazing fact: even without 'lucky breakdown', Ritz values are often good approximations of the eigenvalues of A.

Typically, they approximate the largest (in modulus) eigenvalues of A.

Example

```
% Generates 1000x1000 A with 10 larger eigenvalues
>> A = sprandn(1000,1000,0.01);
>> A(1:20,1:20) = 20*sprandn(20,20,0.2);
>> ev = eig(full(A)); plot(real(ev), imag(ev), 'x');
>> [Q, H] = arnoldi(A, randn(size(A,1),1), 15);
>> rv = eig(H(1:end-1,1:end));
>> plot(real(ev),imag(ev),'x', real(rv),imag(rv),'o');
```

The convergence improves with the dimension n of the Krylov space.

Convergence of Arnoldi

Bad explanation The eigenvalues of H_n are eigenvalues of a 'nearby matrix' obtained by taking H_m (full process) and replacing $H_{n+1,n}$ with zero.

$$H_m = \left[\begin{array}{cccc|cccc} * & \cdots & * & * & * & \cdots & \cdots & * \\ * & \cdots & * & * & * & \cdots & \cdots & * \\ 0 & \ddots & * & * & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & * & * & * & \cdots & \cdots & * \\ \hline & & & 0 & * & \cdots & * & * \\ & & & & * & \cdots & * & * \\ & & & & 0 & \ddots & * & * \\ & & & & 0 & 0 & * & * \end{array}\right].$$

Convergence of Arnoldi

Better explanation The space $K_n(A, b) = \text{span}(b, Ab, \ldots, A^{n-1}b)$ contains the right 'features' to represent the eigenvectors of A with largest eigenvalues: if $A = V\Lambda V^{-1}$ is diagonalizable, then

$$\begin{aligned} A^k b &= (V\Lambda V^{-1})\ldots(V\Lambda V^{-1})b = V\Lambda^k V^{-1} b \\ &= v_1\lambda_1^k c_1 + v_2\lambda_2^k c_2 + \cdots + v_m\lambda_m^k c_m \end{aligned}$$

where $c = V^{-1}b$.
$A^k b$ is a linear combination of the eigenvectors v_i in which those with largest $|\lambda_i|$ are 'more represented'.

Exception: v_i won't appear if the corresponding c_i is very small or zero. Note that the c_i's are the coefficients in the linear combination $b = v_1 c_1 + \cdots + v_m c_m$.

Matlab's eigs

`eigs(A, n)` or `[V, D] = eigs(A, n)` (**eig** **s**parse) computes approximations of the top-n (largest in modulus) eigenvalues.

A can be either a matrix or a function (syntax: `@fname` or `@(x) A*x`).

Uses Arnoldi + some tricks (may use a Krylov space of size larger than n and 'restart' the computation if there are too many iterations).

Convergence not always fast; can return much worse results than `eig`. There is no free lunch: to work on large matrices we have to make approximations / tradeoffs.

Variants

What if I want all eigenvalues?

1. Are you sure you want them all?
2. Convert A to a full matrix and use normal `eig`.

What if I want eigenvalues that are not the largest, e.g., the smallest, or the leftmost, or the closest to 1?

Theorem

Let $(\lambda_1, v_1), \ldots, (\lambda_k, v_k)$ be the eigenvalues/vectors of A.

- $(\lambda_i + \alpha, v_i)$ are eigenvalues/vectors of $A + \alpha I$.
- $(\frac{1}{\lambda_i}, v_i)$ are eigenvalues/vectors of A^{-1}.
- (λ_i^k, v_i) are eigenvalues/vectors of A^k.

Shifted/inverted Arnoldi

Let $(\lambda_1, v_1), \ldots, (\lambda_k, v_k)$ be the eigenvalues/vectors of A. Then, $B = (A - \mu I)^{-1}$ has eigenvalues $\frac{1}{\lambda_i - \mu}$.
The largest eigenvalues of B are those for which $|\lambda_i - \mu|$ is smallest, i.e., the closest ones to μ.

Run Arnoldi on $B = (A - \mu I)^{-1}$ to get the eigenvalues of A closest to a given $\mu \in \mathbb{C}$.

You don't need to compute $B = (A - \mu I)^{-1}$ (and you don't *want* to: it's a full matrix).

Instead, compute a factorization of $A - \mu I$, and then use a function to solve linear systems with it.

Example

```
>> A = bucky();
>> B = inv(A-mu*eye(size(A)));
>> size(A), nnz(A), nnz(B)
ans =
    60 60
ans =
   180
ans =
        3600
% computes 5 eigs of B (bad idea: B is full)
>> fl = eigs(B, 5);
% recover eigs of A
>> lambdas = 1./fl + mu;
```

Example

```
% better idea
>> [L,U] = lu(A - mu*speye(size(A)));
>> f = @(v) U \ (L \ v); % lambda function
>> fl = eigs(f, length(A), 5);
```

Matlab (and scipy) do it automatically for you.

```
% computes 5 eigenvalues closest to mu=2
>> fl = eigs(A, 5, mu);
>> fl = eigs(A, 5, 'SM'); %smallest magnitude
```

Exercises

- Show that if there is breakdown at step n in Arnoldi, i.e., $A^n b \in K_n(A, b)$, then $A^{n+1} b \in K_n(A, b)$, too. Hint: use the relation $A^{n+1} b = A(A^n b)$, and write everything as linear combinations.
- Expand the previous argument (using induction, for instance) to show that $A^k b \in K_n(A, b)$ for all $k \geq n$.
- Take a matrix A, and $b = \sum_{i=1}^{10} v_i$, where v_i are the eigenvectors (in some order). What happens in Arnoldi? At which step do we have breakdown? Why?
- Run Arnoldi on

$$\begin{bmatrix} 0 & & & & 1 \\ 1 & 0 & & & \\ & 1 & \ddots & & \\ & & \ddots & & \\ & & & 1 & 0 \end{bmatrix}$$

(on a computer, by hand, or both). What are the Ritz values at each step? Do they approximate well the eigenvalues?