# CME302 class notes

Erich Trieschman

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# 1 Linear algebra review

## 1.1 Vector products

The inner product, also known as the dot product, results in a scalar

•  $x^T y = \sum x_i * y_i$ ;  $x^T y = \|x\|_2 \|y\|_2 \cos \theta$ ;  $x^T y = 0 \Leftrightarrow x \perp y$ 

The outer product results in a matrix. It is the outer sum of the two vectors, which can be of different lengths.

#### 1.2 Norms

All norms, matrix or vector, satisfy

- Only zero vector has zero norm:  $||x||_x = 0 \Leftrightarrow x = 0$
- $\bullet \ \|\alpha x\|_x = |\alpha| \, \|x\|_x$
- $\bullet \ \|x+y\|_x \leq \|x\|_x + \|y\|_x \ (\text{Triangle inequality I}), \ \|x-y\|_x \geq \|x\|_x \|y\|_x \ (\text{Triangle inequality II})$

## 1.2.1 Vector norms

Types of **vector norms**,  $x \in \mathbb{R}^n$  (norm selection can give you solutions with different properties)

•  $||x||_1 = \sum_{i=1}^n |x_i|$ ;  $||x||_2 = \sqrt{\sum_{i=1}^n (x_i)^2}$ ;  $||x||_\infty = \max_{i \in i, ..., n} |x_i|$ ;  $||x||_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$ 

Cauchy-Schwarts Inequality:  $|x^Ty| \leq ||x||_2 ||y||_2$  (note equality when  $x^Ty = 0$ )

Holder's Inequality:  $|x^Ty| \leq \|x\|_p \, \|y\|_q,$  for p,q , s.t.  $\frac{1}{p} + \frac{1}{q} = 1$ 

#### 1.2.2 Matrix norms

Types of **matrix norms**,  $A \in \mathbb{R}^{n \times m}$ 

- $\bullet \ \|A\|_{\infty} = \sup_{x \neq 0} \frac{\|Ax\|_{\infty}}{\|x\|_{\infty}} = \max_{\|x\|_{\infty} = 1} \|Ax\|_{\infty} = \max_{i} \left\|a_{i}^{T}\right\|_{1}$
- $\bullet \ \left\|A\right\|_p = \sup_{x \neq 0} \frac{\left\|Ax\right\|_p}{\left\|x\right\|_p} = \max_{\left\|x\right\|_p = 1} \left\|Ax\right\|_p$
- $\bullet \ \|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2} = \sqrt{tr(AA^T)} = \sqrt{tr(A^TA)} = \sqrt{\sum_{k=1}^{min(m,n)} \sigma_k^2}$

Submultiplicative inverse:  $\|AB\|_p \le \|A\|_p \|B\|_p$ . Note: this is not always true for Frobenius norms.

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 $\textbf{Induced p-norm:} \quad \|Ay\|_p \leq \|A\|_p \, \|y\|_p$ 

Orthogonally invariant: Orthogonal matrices do not change the norms of vectors or matrices:

•  $\|Qx\|_x = \|x\|_x$ ;  $\|QA\|_x = \|A\|_x$ ,  $x \in \{p, F\}$ 

Other norm properties:

 $\bullet \ \left\|x\right\|_{\infty} \leq \left\|x\right\|_{2} \leq \sqrt{n} \left\|x\right\|_{\infty}; \ \left\|A\right\|_{2} \leq \sqrt{m} \left\|A\right\|_{\infty}; \ \left\|A\right\|_{\infty} \leq \sqrt{n} \left\|A\right\|_{2}$ 

## 1.3 Matrix properties

#### 1.3.1 Determinant

The **determinant** represents how the volume of a hypercube is transformed by the matrix.

- For square matrix,  $det(\alpha A) = \alpha^n det(A)$ ; det(AB) = det(A) det(B)
- $det(A) = det(A^T)$ ;  $det(A^{-1}) = \frac{1}{det(A)}$
- For square matrix, A singular  $\Leftrightarrow det(A) = 0 \Leftrightarrow$  columns of A are not linearly independent

#### 1.3.2 Trace

The trace of a matrix  $A \in \mathbb{R}^{mxn}$ , tr(A), is equal to the sum of the entries in its diagonal,  $tr(A) = \sum_{i=1}^{n} a_{ii}$ . And a few properties of the trace:

- $tr(A) = tr(A^T)$ ;  $tr(A + \alpha B) = tr(A) + \alpha tr(B)$ ; For two vectors,  $u, v \in \mathbb{R}$ ,  $tr(uv^T) = v^T u$
- Trace is invariant under cyclic permutations, that is tr(ABCD) = tr(BCDA) = tr(CDAB) = tr(DABC)

### 1.3.3 Inverses and transposes

The inverse of the transpose is the transpose of the inverse:

- $A^T(A^{-1})^T = (A^{-1}A)^T = I^T = I$
- $(A^{-1})^T A^T = (AA^{-1})^T = I^T = I$

#### 1.3.4 Sherman-Morrison-Woodbury formula

for  $A \in \mathbb{R}^{n \times n}$ ,  $U, V \in \mathbb{R}^{n \times k}$ 

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^TA^{-1}U)^{-1}V^TA^{-1}$$

**Proof:** begin with the inverse of the *LHS* multiplied by the *RHS*:  $(A+UV^T)(A^{-1}-A^{-1}U(I+V^TA^{-1}U)^{-1}V^TA^{-1})$ . Next perform matrix multiplication. The end result will be *I*, implying that the *RHS* is an inverse of  $(A+UV^T)$ 

## 1.4 Orthogonal matrices

An orthogonal matrix, Q is a matrix whose columns are orthonormal. That is,  $q_i^T q_j = 1$  for i = j, and  $q_i^T q_j = 0$  for  $i \neq j$ . Equivalently,  $Q^T Q = I$ . For square matrices,  $Q^T Q = QQ^T = I$ 

#### 1.5 Projections, reflections, and rotations

#### 1.5.1 Projections

A projection, v, of vector x onto vector y can be written in the form  $v = \frac{y^T x}{y^T y} y$ . **Projection matrices** are square matrices, P, s.t.,  $P^2 = P$ .

## 1.5.2 Reflection

- P is a reflection matrix  $\Leftrightarrow P^2 = I$
- P can be written in the form  $P = I \beta v v^T$ , with  $\beta = \frac{2}{v^T v}$ , and v the vector orthogonal to the line/plane of reflection
- It can be shown that  $Px = x \Leftrightarrow v^T x = 0$ . These x are called the "fixed points" of P

## 1.6 Symmetric Positive Definite (SPD) Matrices

For A, SPD, i)  $A = A^T$ , ii)  $x^T Ax > 0 \ \forall x \neq 0$ , iii)  $a_{ii} > 0$ , iv)  $\lambda(A) \geq 0$ , v) for B nonsingular,  $B^T AB$  is also SPD.

When proving properties of SPDs, use the **following tricks:** i) Multiply by  $e_i$  since  $e_i \neq 0$ , ii) Use matrix transpose property,  $x^T A^T = (Ax)^T$  to rearrange formulas

## 1.6.1 $B^TAB$ is also SPD

If  $A \text{ SPD} \Rightarrow B^T A B \text{ SPD for } B \text{ nonsingular}$ :

$$x^T B^T A B x = (Bx)^T A (Bx) > 0$$
, (since B nonsingular  $\Rightarrow Bx \neq 0$ )

## 1.7 Eigenvalues

Observe by definition  $Ax = \lambda x \longleftrightarrow Ax - \lambda x = 0 \longleftrightarrow (A - \lambda I)x = 0$ . To find lambda, we solve for the system of equations to satisfy  $(A - \lambda I)x = 0$ 

The algebraic multiplicity of an eigenvalue,  $\lambda_i$ , is the number of times that  $\lambda_1$  appears in  $\lambda(A)$ 

The **geometric multiplicity** of an eigenvalue,  $\lambda_i$ , is the dimension of the space spanned by the eigenvectors of  $\lambda_i$ 

Other eigenvalue properties:  $\lambda(A) = \lambda(A^T)$ ; Courant-Fischer minmax theorem:  $\lambda_1 = \max_{x \neq 0} \frac{x^T A x}{\|x\|_2^2}$ 

#### 1.7.1 Determinants and trace

$$det(A) = \prod_{i=1}^{n} \lambda_i \qquad tr(A) = \sum_{i=1}^{n} \lambda_i$$

#### 1.7.2 Triangular matrices

For T triangular, the eigenvalues appear on the diagonal:  $t_{ii} = \lambda_i, \forall i \in \{1, \dots, n\}$ Corollary: T nonsingular  $\Leftrightarrow$  all  $t_{ii} \neq 0$ 

#### 1.7.3 Gershgorin disc theorem

Gershgorin disc,  $\mathbb{D}_i$ , defined

$$\mathbb{D}_i = \{ z \in \mathbb{C} \mid |z - a_{ii}| \le \sum_{i \ne i} |a_{ij}| \}$$

All eigenvalues of  $A, \lambda(A) \in \mathbb{C}$  are located in one of its Gershgorin discs. **Proof:** 

$$\begin{split} Ax &= \lambda x \longleftrightarrow (A - \lambda I)x = 0 \longleftrightarrow \sum_{j \neq i} a_{ij}x_j + (a_{ii} - \lambda)x_i = 0, \ \forall i \in \{1, \dots, n\} \\ \text{Choose } i \ s.t. |x_i| &= \max_i |x_i| \\ &|(a_{ii} - \lambda)| = |\sum_{j \neq i} \frac{a_{ij}x_j}{x_i}| \leq \sum_{j \neq i} |\frac{a_{ij}x_j}{x_i}| \ , \ \text{by triangle inequality} \\ &|(\lambda - a_{ii})| \leq \sum_{j \neq i} |a_{ij}|, \ \text{since} \ |\frac{x_j}{x_i}| \leq 1 \end{split}$$

# 2 Matrix Decompositions

## 2.1 Schur Decomposition

For any  $A \in \mathbb{C}^{n \times n}$ ,  $A = QTQ^H$ , where Q unitary  $(Q^HQ = I), Q \in \mathbb{C}^{n \times n}$ , T upper triangular

When  $A \in \mathbb{R}^{n \times n}$ ,  $A = QTQ^T$ , where Q orthogonal  $(Q^TQ = I)$ ,  $Q \in \mathbb{R}^{n \times n}$ , T upper triangular

Note: If T is relaxed from strict upper triangular to block upper triangular (blocks of  $2 \times 2$  or  $1 \times 1$  on the diagonal), then Q can be selected to be in  $\mathbb{R}^{n \times n}$ .

#### 2.2 Eigenvalue Decomposition

For A diagonalizable  $(A \in \mathbb{R}^{n \times n})$  with n linearly independent eigenvectors), it can be decomposed as

 $A = X\Lambda X^{-1}$ , where  $\Lambda$  a diagonal matrix of the eigenvalues of A

For A real symmetric, A can be decomposed as  $A = Q\Lambda Q^T$ , Q orthogonal

For A unitarily diagonalizable ( $\Leftrightarrow$  normal:  $A^HA = AA^H$ ),  $A = Q\Lambda Q^H$ , Q unitary. When A complex Hermitian  $(A = A^H)$ ,  $\Lambda \in \mathbb{R}$ 

## 2.3 Singular Value Decomposition

**Definition:** For any  $A \in \mathbb{C}^{m \times n}$  there exist two unitary matrices,  $U \in \mathbb{C}^{m \times m}$  and  $V \in \mathbb{C}^{n \times n}$ , and a diagonal matrix  $\Sigma \in \mathbb{R}^{m \times n}$  such that  $A = U\Sigma V^H$ . When  $A \in \mathbb{R}^{m \times n}$ ,  $A = U\Sigma V^T$  with  $U, V, \Sigma \in \mathbb{R}$ 

The singular values,  $\sigma_i$  of  $\Sigma$  are always  $\geq 0$ . And by convention, they're ordered in decreasing order, so  $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ 

**Derivation:** Observe  $A^T A$  symmetric:  $(A^T A)^T = A^T A$ 

 $A^TA$  symmetric  $\Rightarrow \exists \ Q$  orthogonal and  $\Lambda$  diagonal matrix of  $\lambda_i$  s.t.,  $A^TA = Q\Lambda Q^T$   $Q^TA^TAQ = Q^TQ\Lambda Q^TQ$   $(AQ)^T(AQ) = \Lambda, \text{ note } AQ \text{ is orthogonal, but not scaled to 1. Instead, each row is scaled to the eigenvalue in that row: <math>\lambda_i = \|Aq_i\|_2^2$ 

When A is full rank,

$$A = AQQ^{T}$$

$$= (AQ)Q^{T}$$

$$= AQD^{-1}DQ^{T}, \text{ where } D = \begin{bmatrix} \sqrt{\lambda_{1}} & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & \sqrt{\lambda_{n}} \end{bmatrix} \text{ and } D^{-1} = \begin{bmatrix} \frac{1}{\sqrt{\lambda_{1}}} & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & \frac{1}{\sqrt{\lambda_{n}}} \end{bmatrix}$$

$$A = U\Sigma V^{T}, \text{ where } U = AQD^{-1}, \Sigma = D, V^{T} = Q^{T}$$

When A is not full rank, make the tall/thin SVD

And a few properties and remarks of  $A \in \mathbb{R}^{n \times m}$  SVD

- $\|A\|_2 = \sigma_1$ ;  $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$  when A nonsingular;  $\|A\|_F = \sqrt{\sum_i^{\min\{n,m\}} \sigma_i^2}$ ; Condition number,  $\kappa(A) = \|A\|_2 \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}$
- When A symmetric,  $\sigma_i = |\lambda_i|$ ; When A orthogonal,  $\sigma_1 = \cdots = \sigma_n = 1$
- The eigenvalues of  $A^TA$  and  $AA^T$  are the squares of the singular values of A,  $\sigma_1^2, \ldots, \sigma_n^2$
- By construction, V contains the eigenvectors of  $A^TA$  and U contains the eigenvectors of  $AA^T$ , so  $A^TAv_i = \sigma_i^2 v_i$  and  $AA^Tu_i = \sigma_i^2 u_i$

# 3 Error analysis

## 3.1 Floating point arithmetic

$$\pm (\sum_{i=1}^{t-1} d_i \beta^{-i}) \beta^e$$

Where  $\beta$  is the base (in floating point computation,  $\beta = 2$ ),  $d_0 \ge 1$ , and  $d_i \le \beta - 1$ , e is called the **exponent**, this is the location of the decimal place, t - 1 in the summand is called the **precision** and indicates the number of digits (in base  $\beta$ ) that can be stored with the number.

## 3.2 Unit roundoff

The unit roundoff for a floating-point number is

$$u = \frac{1}{2} \times \beta^{-(t-1)}$$
 (distance between the smallest digits stored in a floating-point number)

For double precision floating point numbers (64 bits),  $u \approx 10^{-16}$ . The relative sensitivity of a problem is often called the **conditioning** of the problem

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• Sensitivity: 
$$\frac{\left\|\tilde{f}(x) - f(x)\right\|_p}{\left\|\tilde{x} - x\right\|_p}; \text{ Relative sensitivity: } \frac{\left\|\tilde{f}(x) - f(x)\right\|_p \|x\|_p}{\left\|\tilde{x} - x\right\|_p \|f(x)\|_p}$$

## 4 LU Factorization

The LU factorization makes it computationally easier to solve linear equations If we can decompose a matrix, A, into a product of a lower triangular matrix, L, and an upper triangular matrix, U, then to solve Ax = b, we can start by solving Lz = b, and then Ux = z. x, here, is the solution!

## 4.1 Basic algorithm

- Construct  $u_1^T$  equal to the first row of  $A, a_1^T$
- Construct  $l_1$  equal to each of the elements in the first column of  $A, a_1$ , divided by  $a_{11}$ , the "pivot"
- Calculate  $A' \leftarrow A l_1 u_1^T$ . In practice (and somewhat confusingly), A' is now referred to as A
- Repeat the algorithm with the updated A, and the next row/column. Observe each  $l_i, u_i^T$  constructed are the rows/columns of the lower and upper triangular matrices of L, U respectively.

#### 4.1.1 Gauss transforms

To compute A = LU, consider  $L^{-1}A = U$ , with  $L^{-1}$  that "zeros-out" the columns of A to get U. Call  $L^{-1}$ , G. As with the iterative algorithm above, we can multiply A by iterative  $G_i$ 's to get U:

$$L^{-1}A = G_n G_{n-1} \dots G_2 G_1 A = U \longrightarrow A = G_1^{-1} \dots G_n^{-1} U = LU$$

## 4.2 Pivoting

#### 4.2.1 When pivoting is needed

Notice that this algorithm relies on the pivots,  $a_{kk}$ , being nonzero. It turns out this will occur if none of the  $k \times k$  blocks of A, A[1:k,1:k], have a determinant of 0. **Proof by induction**: Case k=1:

 $A_1 = L_1U_1 \longleftrightarrow det(A_1) = det(L_1U_1) \longleftrightarrow det(A_1) = det(L_1)det(U_1)$ , by property of determinants  $det(A_1) = det(U_1)$ , since determinant of a triangular matrix is a product of the diagonals and the diagonal of  $L_1$  are 1's  $det(A_1) = a_{11} = u_{11} \to so$  when determinant is not zero, we have a nonzero pivot

#### 4.3 Cholesky factorization

The Cholesky factorization is an LU factorization for Symmetric Positive Definite (SPD) matrices, where SPD matrix,  $A = GG^T$ , with G lower triangular.

## 4.4 Schur complement

A useful way to think about the LU factorization is with the **Schur complement** matrix structure. First observe A can be written in the following form

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

If we run the LU factorization algorithm for k steps, the resulting A' = A is equal to

$$A = \begin{bmatrix} I & 0 \\ A_{21}A_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{21}A_{11}^{-1} A_{12} \end{bmatrix} \begin{bmatrix} I & A_{21}A_{11}^{-1} \\ 0 & I \end{bmatrix}$$

The bottom-right block of A' = A,  $A'_{22} = A_{22}$  is equal to  $A_{22} - A_{21}A_{11}^{-1}A_{12}$  from the original matrix. This is called the **Schur complement** of A

#### 4.4.1 Schur complement derivation

At any step in the LU factorization, A can be written in the form

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

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From this equality, we can create a system of equations and derive the Schur complement

# 5 QR factorization

The QR factorization decomposes a matrix,  $A \in \mathbb{R}^{m \times n}$ ,  $m \ge n$  into an orthogonal (orthonormal) matrix, Q, and an upper triangular matrix, R. When  $A \in \mathbb{C}^{m \times n}$ , Q is unitary.

Recall for  $Q \in \mathbb{R}$ , orthogonal,  $Q^TQ = I$ ; for  $Q \in \mathbb{C}$ , unitary,  $Q^HQ = I$ ;  $||Qx||_2 = ||x||_2$ 

If A is skinny (i.e.,  $n \ll m$ ), QR can take two different forms.  $Q \in \mathbb{R}^{m \times m}$  can be square and  $R \in \mathbb{R}^{m \times n}$  can be skinny. Or  $Q \in \mathbb{R}^{m \times n}$  can be skinny and  $R \in \mathbb{R}^{n \times n}$  can be square.

## 5.1 The QR factorization is unique

**Proof** that the QR factorization is unique for full rank matrix, A:

$$A = QR \longleftrightarrow Q^TA = R \longleftrightarrow^T Q^TA = R^TR \longleftrightarrow (QR)^TA = R^TR \longleftrightarrow A^TA = R^TR$$

We now have a matrix,  $A^TA$  that can be written of the form  $R^TR$ , which is the structure of the Cholesky factorization. Suffice to show that  $A^TA$  is Symmetric and Positive Definite (SPD) to prove the uniqueness of R.

## 5.2 Householder reflection

- Construct  $Q^T$  for each column in A that projects it onto a corresponding column of an upper right triangular matrix, R.
- E.g., for first column  $a_1$ : Want  $Q_1^T$  such that  $Q_1^T a_1 = r_1$ , where  $r_1 = \pm \|a_1\|_2 e_1$  (since  $Q^T$  is orthogonal). This equates to finding  $Q_1^T$  that reflects  $a_1$  onto  $e_1$
- The key to the iterative part of the algorithm is to construct  $Q_i^T$ , i > 1 with an identity matrix in the upper-left  $i 1 \times i 1$  quadrant, and a smaller  $Q_i^{*T}$  in the lower right  $n i \times n i$  quadrant, filling the remaining sections of the matrix with 0's.

The **Householder reflection** maps  $a \to ||a||_2 e_1$  with

$$P = I - \beta v v^T$$
, where  $v = a - ||a||_2 e_1$ , and  $\beta = 2/v^T v$ 

**Aside:** The fixed points of a reflection, P, remain unchanged when multiplied by the reflection, Px = x. Geometrically, these are the points that are *orthogonal* to the vector v defining the reflection (i.e.,  $v^Tx = 0$ )

## 5.3 Givens transformation

#### 5.3.1 Givens transformation algorithm

A Givens rotation rotates  $u = (u_1, u_2)^T$  to  $||u||_2 e_1$ . The matrix that does this,  $G^T$ , is defined by

$$G^T = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}, c = \frac{u_1}{\|u\|_2}, s = -\frac{u_2}{\|u\|_2}$$

Sequentially, the  $P_i$ 's can multiply A to arrive at R

## 5.4 Gram-Schmidt transformation

Construction of  $r_{kk}, q_k, r_{kj}$ 

$$a_k = \sum_{i=1}^k r_{ik} q_i = r_{kk} q_k + \sum_{i=1}^{k-1} r_{ik} q_i$$

1.  $r_{ik} = q_i^T a_k$  for each  $r_{ik}, i < k$ , since Q orthonormal and  $q_{k-1}$  known

2. 
$$z = r_{kk}q_k = q_k - \sum_{i=1}^{k-1} r_{ik}q_i$$

3. 
$$r_{kk} = ||z||_2$$
,  $q_k = \frac{z}{r_{kk}}$ 

## 5.5 QR factorization to solve least-squares problems

When A is tall and thin, it is unlikely that we get a solution to Ax = b. Instead, we choose to solve the least-squares problem,  $argmin_x \|Ax - b\|_2$ .

#### Method of normal equations

Want: 
$$(b - Ax) \perp \{z | z = Ay\} \longleftrightarrow (b - Ax) \perp range(A) \longleftrightarrow (b - Ax) \perp a_i, \forall i \in A$$
  
 $a_1^T(b - Ax) = 0, \forall i \in A \longleftrightarrow A^T(b - Ax) = 0 \longleftrightarrow x = (A^TA)^{-1}A^Tb$ 

#### QR method for least squares 5.5.2

$$A^T(Ax-b)=0\longleftrightarrow R^TQ^T(Ax-b)=0$$
 
$$Q^T(Ax-b)=0, \text{ since we assume } A,R \text{ full rank (multiply both sides by } R^{-T})$$
 
$$Q^TQRx-Q^Tb=0\longleftrightarrow Rx=Q^Tb\longleftrightarrow x=R^{-1}Q^Tb$$

#### SVD for rank-deficient A

When A not full rank, we add constraint  $\min_x ||x||_2$ . We can use the "thin" version of the Singular Value Decomposition to solve this

$$(Ax-b)\perp range(A)\longleftrightarrow (Ax-b)\perp range(U), \text{ since } R(A)=R(U) \text{ for } A=U\Sigma V^T$$
 
$$U^T(Ax-b)=0\longleftrightarrow U^T(U\Sigma V^Tx-b)=0\longleftrightarrow \Sigma V^Tx=U^Tb$$
 
$$x=V\Sigma^{-1}U^Tb \text{ (the "thin" SVD here provides a nonsingular } \Sigma\in\mathbb{R}^{r\times r}, \text{ so we can take the inverse}$$

Observe for  $\min_x \|x\|_2$  that the  $x \perp N(A)$  is the shortest vector between N(A) and the vector/plane of solutions to  $argmin_x \|Ax - b\|_2$ . This value must be in R(V) since  $R(V) = N(A)^{\perp}$ 

#### 6 Iterative methods to find eigenvalues

#### 6.1 Power iteration

Given  $\lambda_1 > \lambda_2 \ge \cdots \ge \lambda_n \in \lambda(A)$ , the **Power iteration** finds  $\lambda_1$ . This process assumes A is diagonalizable

$$\begin{split} A^k &= \sum_{i=1}^n \lambda_i^k x_i y_i^T \text{ where } Y = X^{-1} \\ A^k &\approx \lambda_1^k x_1 y_1^T \text{ since } \lambda_1 > \lambda_2 \\ A^k q &\approx \lambda_1^k x_1 y_1^T q = \lambda_1^k (y_1^T q) x_1 \text{, since } y_1^T q \text{ is a scalar. Observe } A^k q \parallel x_1 \end{split}$$

This theory is implemented in practice with the following formula

1.  $q_0$ , vector chosen at random

2. 
$$z_k = Aq_k = A^kq_0$$
, evaluating for convergence if  $z_k \parallel q_k \to z_k^T x_k = \|z\|_2 \|x\|_2$ 

3. 
$$q_{k+1} = \frac{z_k}{\|z_k\|_2} = \frac{A^k q_0}{\|A^k q_0\|_2} \approx (\frac{\lambda_2}{|\lambda_1|})^k x_1$$

Since  $A^k q_0 = Aq_k \approx \lambda_1 x_1$ , where  $||x_1||_2 = 1$  (WLOG) and  $q_k ||x_1|$ , we can solve for  $\lambda$ :

$$Aq_k \approx \lambda_1 x_1 \Longrightarrow Ax_1 \approx \lambda_1 x_1 \Rightarrow x_1^H Ax_1 \approx \lambda_1$$
Convergence:  $O(|\frac{\lambda_1}{\lambda_2}|)^K$ ), since
$$A^k q_0 = \sum_i \alpha_i A^k x_i = \sum_1 \alpha_i \lambda_i^k x_i = \alpha_1 \lambda_1^k (x_i + \frac{\alpha_2}{\alpha_1} (\frac{\lambda_2}{\lambda_1})^k + \dots + \frac{\alpha_n}{\alpha_1} (\frac{\lambda_n}{\lambda_1})^k) \Longrightarrow ||A^k q_0||_2 = |\alpha_1 \lambda_1^k| (1 + O(\frac{\lambda_2}{\lambda_1})^k)$$

#### Inverse iteration

Get the eigenvector for the eigenvalue closest to  $\mu$ . Observe  $(A - \mu I)^{-1}$  has the same eigenvectors of A:

$$(A - \mu I)^{-1}x = \lambda x \longleftrightarrow x = (A - \mu I)x = \lambda Ax - \lambda \mu x \longleftrightarrow \lambda Ax = x + \lambda \mu x \longleftrightarrow Ax = \frac{(1 + \lambda \mu)}{\lambda}x$$

Performing the power iteration on  $(A - \mu I)^{-1}$ , the largest eigenvalue to emerge will be of the form  $\frac{1}{\lambda_i - \mu}$ , and we get

$$(A - \mu I)^{-1k}q_0 = (A - \mu I)^{-1}q_k \approx \lambda_i x_i$$
, where  $\|x_i\|_2 = 1$  (WLOG) and  $q_k \| x_i$ 

Since  $x_i$  is also an eigenvalue of A, we can solve  $x_i^H A x_i = \lambda_i$  for the  $\lambda_i$  closest in magnitude to  $\mu$ . Convergence:  $O(|\frac{\lambda_i - \mu}{\lambda_j - \mu}|)^k)$ , where  $\lambda_j$  is the next closest eigenvalue to  $\mu$ 

## 6.3 Eigenvalues of similar matrices

**Theorem:** For S nonsingular and  $A = S^{-1}BS$ , then i)  $\lambda(A) = \lambda(B)$  and ii) x eigenvector of  $A \Leftrightarrow S^{-1}x$  eigenvector of B.

## 6.4 Eigenvalues from invariant subspaces

**Theorem:**  $X \in \mathbb{R}^{n \times m}$  is an invariant subspace of  $A \in \mathbb{R}^{n \times n} \Leftrightarrow$  there is a  $B \in \mathbb{R}^{n \times m}$  such that AX = XB. **Proof:** 

$$\Rightarrow$$
: X invariant  $\longrightarrow Ax_i \in X \longrightarrow Ax_i = \sum_{j=1}^m x_j b_{ji} \longrightarrow AX = XB$ 

Furthermore, when AX = XB, the m eigenvalues of B are also eigenvalues of A:  $By = \lambda y \longrightarrow XBy = \lambda Xy \longrightarrow AXy = \lambda Xy$ 

## 6.5 Orthogonal iteration

First, consider how to construct orthogonal columns to reveal subsequent eigenvalues. Assume we use power iteration to compute  $q_1$ 

$$A^k = \lambda_1 x_1 y_1^T + \lambda_2 x_2 y_2^T + \dots$$

$$PA^k = \lambda_1 P x_1 y_1^T + \lambda_2 P x_2 y_2^T + \dots, \text{ where } P = I - x_1 x_1^T$$

$$PA^k = 0 + \lambda_2 P x_2 y_2^T + \dots, \text{ since } Px_1 = Ix_1 - x_1 x_1^T x_1 = x_1 - x_1 = 0$$

$$PA \text{ can now be used to apply the power iteration to to reveal } \lambda_2 \text{ and } (I - x_1^T x_1) x_2$$

The general process is: build  $P_r$ , orthogonal projector onto  $\{q_1, \ldots, q_{r-1}\}^{\perp}$ , use power iteration to reveal  $(\lambda_r, q_r)$ Now consider the QR decomposition of X, observing its connection to the Schur Decomposition:

$$A = X\Lambda X^{-1} = QR\Lambda R^{-1}Q^H = QTQ^H$$
, where upper triangular  $T = R\Lambda R^{-1}$ 

- $\bullet$  The eigenvalues of A are on the diagonal of T
- ullet By construction, each column of Q is projecting the corresponding column of X onto a vector orthogonal to the preceding ones
- The span of the columns of Q,  $span\{q_1, \ldots, q_n\}$  will be equal to the span of the columns of X,  $span\{x_1, \ldots, x_n\}$ .

The process for the **orthogonal iteration** is:

- 1.  $AQ_k \to Z$ , where k is the iteration and  $Q_0 = I$
- 2.  $Z \to Q_{k+1}R_{k+1}$ , the QR factorization of Z
- 3. Repeat  $AQ_{k+1} \to Z$  and eventually  $Q_k \to Q$

Note in each iteration we are calculating  $Q_{k+1}^H A Q_k = R_{k+1}$ 

## **6.5.1** Reveal eigenvectors of A from T

Motivation:  $A = X\Lambda X^{-1}$  can be hard to calculate.

$$A=X\Lambda X^{-1}=QR\Lambda R^{-1}Q^H=QTQ^H, \text{ where } T=R\Lambda R^{-1}$$
 
$$A=QY\Lambda Y^{-1}Q^H, \text{ where } T=Y\Lambda Y^{-1} \text{ is easier to compute}$$

Focusing on  $T = Y\Lambda Y^{-1}$ , choose some  $\lambda_i$  (we could get from power or QR iteration).

$$Tx = \lambda_i x \longleftrightarrow (T - \lambda_i I)x = 0 \longleftrightarrow (T - \lambda_i I)x = \begin{bmatrix} T_{11} - \lambda_i I & T_{12} & T_{13} \\ 0 & 0 & T_{23} \\ 0 & 0 & T_{33} - \lambda_i I \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \text{ where one diagonal element is } 0$$

And solve with back substitution:

$$X_3 = 0: (T_{33} - \lambda_i I)X_3 = 0$$

 $X_2$  is a free parameter  $\in \mathbb{R}: 0X_2 + T_{33}X_3 = 0 \Longrightarrow 0X_2 = 0$ 

$$X_1 = -(T_{11} - \lambda_i I)^{-1} T_{12} X_2 : (T_{11} - \lambda_i I) X_1 + T_{12} X_2 + T_{13} X_3 = 0$$

It follows the eigenvectors of A are  $Qy_i$ . Note,  $(T_{11} - \lambda_i I)$  nonsingular as long as the algebraic multiplicity of  $\lambda_i$  is 1.

#### 6.5.2 Rate of convergence in orthogonal (and QR) iteration

**Property:** the angle between two subspaces, U and V, is defined as  $\|UU^T - VV^T\|_2$ In orthogonal interation,  $span\{q_1, \cdots, q_i\} \longrightarrow X, span\{x_1, \cdots, x_i\}$ . Convergence is dictated by how quickly these spans converge. The rate of convergence is  $O(|\frac{\lambda_{i+1}}{\lambda_i}|^k)$ .

## 6.6 QR iteration

In the QR iteration, we ask if we can go from  $T_k$  to  $T_{k+1}$  directly. Observe

$$A = Q_k T_k Q_k^H \Longrightarrow T_k = Q_k^H A Q_k$$

$$AQ_k = Q_{k+1} R_{k+1} \Longrightarrow Q_{k+1}^H A = R_{k+1} Q_k^H$$

$$T_k = Q_k^H (Q_{k+1} R_{k+1}) \longrightarrow T_k = U_{k+1} R_{k+1} \text{ for } U_{k+1} = Q_k^H Q_{k+1}$$

$$T_{k+1} = (R_{k+1} Q_k^H) Q_{k+1} \longrightarrow T_{k+1} = R_{k+1} U_{k+1} \text{ for } U_{k+1} = Q_k^H Q_{k+1}$$

So we have an algorithm for  $T_k \to T_{k+1}$ , this process is the **QR iteration**:

- 1.  $T_k \longrightarrow U_{k+1}R_{k+1}$ , the QR factorization of  $T_k$
- $2. R_{k+1}U_{k+1} \longrightarrow T_{k+1}$
- 3. Repeat with  $T_{k+1}$

**Proof by induction:**  $R_{k+1}$  is the same in both QR factorization of  $A = Q_{k+1}R_{k+1}$  and  $T_k = U_{k+1}R_{k+1}$ 

case 1: 
$$A = AQ_0 = Q_1R_1$$
,  $A = T_0 = U_1R_1^*$ , and  $T_1 = Q_k^H A Q_1$   
 $U_1R_1^* = Q_0^T Q_1 R_1 = Q_1R_1 \implies R_1^* = R_1$  and  $U_1 = Q_0^T Q_1$   
case  $k$ : Assume  $R_k^* = R_k$ ,  $U_k = Q_{k-1}^T Q_k$ , and  $T_k = Q_k^H A Q_k$ 

## 6.7 QR iteration on upper Hessenberg

Each QR iteration step of a dense matrix is  $O(n^3)$ . If we run for O(k) iterations, then this algorithm is  $O(kn^3)$ . To reduce flops, we can first convert A to upper Hessenberg ( $H = Q^H AQ$ ) with  $O(n^3)$ , and proceed with QR iteration on H using Givens rotations with complexity  $O(n^2)$  (so overall complexity is reduced to  $O(n^3 + kn^2)$ ):

Choose  $Q_1^T = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_1 \end{bmatrix}$  to perform a Householder rotation onto the first two entries of  $a_1 \in A$ 

Observe 
$$Q_1^T A Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P_1} \end{bmatrix} A \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P_1}^T \end{bmatrix} = \begin{bmatrix} x & x & \cdots \\ x & x & \cdots \\ 0 & x & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$
 where  $a_{11}$  is never changed, the rest of  $a_1$ 

is only operated on by  $\tilde{P_1}$ , and the rest of  $a_1^T$  is only operated on by  $\tilde{P_1^T}$ 

Continuing on, 
$$Q_n^T \dots Q_2^T Q_1^T A Q_1 Q_2 \dots Q_n = H = Q^H A Q$$
 where  $Q_k^T = \begin{bmatrix} I_k & 0 \\ 0 & \tilde{P}_k \end{bmatrix}$ 

H remains upper Hessenberg in QR iteration: This follows since in the first step of QR iteration,  $H_k$  is transformed to  $R_k$  with givens rotations,  $U_k^H H_k = R_k$ . And in the second step of QR iteration,  $H_{k+1}$  is created as  $R_k U_k = H_{k+1} = U_k^H H_k U_k$ . Since  $U_k$  is a series of givens rotations, these rotations can be constructed/ordered so that  $H_{k+1}$  preserves upper Hessenberg.

## 6.8 QR iteration with shift

**QR** iteration with shift accelerates convergence. First observe for  $\lambda_i \in \lambda(A) \to (\lambda_i - \mu) \in \lambda(A - \mu I)$ . The resulting converence is  $|[(\lambda_{i+1} - \mu)/(\lambda_i - \mu)]|^k$ . Shift does not require that  $|\lambda_1| > |\lambda_2| \ge \cdots \ge |\lambda_n|$ .

QR iteration with shift process:

1. 
$$\mu_k = T_k[n, n]$$

2.  $(T_k - \mu_k I) \longrightarrow U_{k+1} R_{k+1}$ , QR factorization of the shifted  $T_k$ 

3. 
$$R_k U_k + \mu_k I \longrightarrow T_{k+1}$$
, and repeat!

Observe, this shift preserves the original QR iteration:

$$(T_k - \mu_I) = U_{k+1} R_{k+1} \Longrightarrow U_{k+1}^H T_k - \mu_k U_{k+1}^H = R_{k+1}$$

$$T_{k+1} = R_{k+1} U_{k+1} + \mu_k I \Longrightarrow T_{k+1} = (U_{k+1}^H T_k - \mu_k U_{k+1}^H) U_{k+1} + \mu_k I$$

$$T_{k+1} = U_{k+1}^H T_k U_{k+1} - \mu_k I + \mu_k I = U_{k+1}^H T_k U_{k+1}$$

#### 6.8.1 Implicit Q theorem

The **implicit Q theorem** tells us that if i) we get any upper Hessneberg,  $H_{k+1}$  from a transformation of  $H_k \to H_{k+1}$  of the form  $U^T H_k U$  ii)  $W e_1 = Q e_1$  for two such transformations, then the columns of W and Q are equal, up to a sign.

**Proof:** We show for  $A = QHQ^T$ , Q orthogonal and H upper Hessenberg, that Q, H are determined by A and  $Qe_1$ :

$$AQ = QH, \text{ assume we know } q_1, \dots, q_k \text{ of } Q$$
 
$$A\left[Q_k \quad X\right] = \begin{bmatrix}Q_k \quad X\end{bmatrix} \begin{bmatrix}H_k \quad X\\0 \quad X\end{bmatrix}, X \text{ unknown and } H_k \in \mathbb{R}^{k \times k}$$
 
$$Aq_k = \sum_{i=1}^k h_{i,k}q_i + k_{k+1,k}q_{k+1}, \text{ the kth column of } AQ, \text{ where } q_j^T A q_k = h_{j,k}$$
 
$$k_{k+1,k}q_{k+1} = Aq_k - \sum_{i=1}^k h_{i,k}q_i, \text{ the RHS of which is known}$$
 
$$\Rightarrow |h_{k+1,k}| = \left\|Aq_k - \sum_{i=1}^k h_{i,k}q_i\right\|_2 \text{ and } q_{k+1} = \frac{Aq_k - \sum_{i=1}^k h_{i,k}q_i}{h_{k+1,k}}$$

#### 6.8.2 Fracis shift

The **Francis** shift is a way of selecting shifts based on the bottom-right  $2 \times 2$  block in a way that maintains a real-valued matrix. In effect, we double-shift using complex conjugates,  $\mu, \overline{\mu}$ :

$$\begin{split} H_{k-1} - \mu I &= U_k R_k \\ H_k &= R_k U_k + \mu I \\ H_k - \overline{\mu} I &= U_{k+1} R_{k+1} \\ H_{k+1} &= R_{k+1} U_{k+1} + \overline{\mu} I \\ H_{k+1} &= U_{k+1}^H H_k U_{k+1} = U_{k+1}^H U_k^H H_{k-1} U_k 1 U_{k+1} = (U_k U_{k+1})^H H_{k-1} (U_k U_{k+1}) \end{split}$$

**Proof** Consider QR factorization to show  $(U_1U_2)$  is real

$$(U_k U_{k+1})(R_{k+1} R_k) = H_{k-1}^2 - (\mu + \overline{\mu})H_{k-1} + |\mu|^2 I$$
, where each component of the polynomial is  $\in \mathbb{R}$ 

From uniqueness of QR factorization,  $(U_1U_2)$  must be real as well. So at any step of the Francis shift, we want  $H_{k+1} = Q^T H_{k-1}Q$ 

## 6.9 QR iteration with deflation

If any sub-diagonal element of an upper Hessenberg matrix, H, is 0, it can be written as  $H = \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix}$  with  $H_{11}$  and  $H_{22}$  upper Hessenberg and  $\lambda(H) = \lambda(H_{11}) \cup \lambda(H_{22})$ 

**Theorem:**  $\lambda(H) = \lambda(H_{11}) \cup \lambda(H_{22})$  for H block upper triangular. **Proof:** 

$$\Longrightarrow Hx = \lambda x \longrightarrow \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} H_{11}x_1 + H_{12}x_2 \\ H_{22}x_2 \end{bmatrix} = \begin{bmatrix} \lambda x_1 \\ \lambda x_2 \end{bmatrix}$$
and either  $x_2 = 0$  and  $\lambda \in \lambda(H_{11})$  or not and  $\lambda \in \lambda(H_{22})$ 

$$\iff H_{11}p_1 = \lambda p_1 \longrightarrow \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} \begin{bmatrix} p_1 \\ 0 \end{bmatrix} = \begin{bmatrix} H_{11}p_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \lambda p_1 \\ 0 \end{bmatrix}$$

$$\iff H_{22}p_2 = \lambda p_2 \longrightarrow \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} \begin{bmatrix} x \\ p_2 \end{bmatrix} = \begin{bmatrix} H_{11}x + H_{12}p_2 \\ H_{22}p_2 \end{bmatrix} = \begin{bmatrix} \lambda x_1 \\ 0 \end{bmatrix}$$
where  $H_{11}x + H_{12}p_2 = \lambda x$  for  $x = -(H_{11} - \lambda I)^{-1}H_{12}p_2$ , making  $\lambda \in \lambda(H)$ 

**Theorem:** If H is singular unreduced upper Hessenberg, then in QR factorization, H = QR, the last row of R is zero. **Explanation:** When constructing QR iteration, each column of R can be linearly independent from the previous ones (since we're adding a dimension) except for the last one (since H and R must be singluar):

$$h_1 = h_{11}e_1 + h_{21}e_2$$
  $h_2 = h_{12}e_1 + h_{22}e_2 + h_{32}e_3$   $h_{n-1} = \sum_{i=1}^n h_{n-1,i}e_i$ 

## 6.10 QR iteration on symmetric matrices

Upper Hessenberg symmetric matrices are tri-diagonal matrices

- Unsymmetric case complexity: Transform to upper Hessenberg:  $O(n^3)$ ; QR iteration step:  $O(n^2)$ ; overall QR iteration:  $O(pn^3)$ , where p is the number of iterations per eval (assume quadratic convergence)
- Symmetric case complexity: Transform to upper Hessenberg:  $O(n^3)$ ; QR iteration step: O(n); overall QR iteration:  $O(pn^2)$ , where p is the number of iterations per eval (assume cubic convergence)

# 7 Finding eigenvalues of sparse matrices

## 7.1 Arnoldi process

The **Arnoldi process** reveals first k eigenvalues of a sparse matrix as follows:

1. Begin with random  $q_1 \in Q$ , such that  $||q_1||_2 = 1$ 

Iterate through each of the first k columns of Q with

2. 
$$Aq_j = \sum_{k=1}^{j+1} h_{kj} q_k$$
, observing we can recover all  $h_{ij}$  for  $i \leq j$  since  $q_i^T A q_j = h_{ij}$   
3.  $Aq_j = \sum_{k=1}^{j} h_{kj} q_k + h_{j+1,j} q_{j+1}$ 

3. 
$$Aq_j = \sum_{k=1}^{j} h_{kj} q_k + h_{j+1,j} q_{j+1}$$

4. 
$$r = Aq_j - \sum_{k=1}^{j} h_{kj}q_k = h_{j+1,j}q_{j+1}$$
, where only  $r$  is unknown

5. 
$$\|q_{j+1}\|_2 = 1 \Longrightarrow h_{j+1,j} = \|r\|_2$$
 and  $q_{j+1} = \frac{r}{h_{j+1,j}}$ 

**Output:** k columns of Q and the upper  $k \times k$  block of H, which can be used in the QR iteration to reveal k eigenvalues close to  $\lambda(A)$ :

$$AQ = QH \Longrightarrow AQ_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^T, \text{ where } Q_k = Q[:, 1:k], H_k = [1:k, 1:k]$$

$$AQ_k = Q_k X_k \Lambda_k X_k^{-1} + h_{k+1,k} q_{k+1} e_k^T, \text{ where } H_k = X_k \Lambda_k X_k^{-1} \text{ through QR iteration}$$

$$A(Q_k X_k) = (Q_k X_k) \Lambda_k + h_{k+1,k} q_{k+1} x_k^T, \text{ where } x_k^T \text{ is the } k^{th} \text{ column of } X$$

And we get an equation where i)  $AQ_k \approx Q_k H_k$ , ii)  $\Lambda_k$  contains k eigenvalues close to  $\lambda_i \in \lambda(A)$ , iii)  $(Q_k X_k)$  serve as eigenvectors for those eigenvalues, and iv)  $h_{k+1,k} q_{k+1} x_k^T$  represents something like an error term.

#### 7.2 Krylov spaces

A space of sparse Matrix-vector products:  $K(A, q, k) = span\{q_1, Aq_1, A^2q_1, \dots, A^kq_1\}$ 

## 7.2.1 QR factorization of Krylov subspace contains $Q_k$ from Arnoldi

**Proof:** We show for  $K_k = Q_k R_k$ , that  $R_k$  is upper triangular.

Start with 
$$Q^T K_k = R$$
 upper triangular for  $K_k = \begin{bmatrix} | & | & | \\ q_1 & Aq_1 & \dots & A^k q_1 \\ | & | & | & \end{bmatrix}$ 

$$Q^T k_j = Q^T A^{j-1} q_1 = Q^T Q H^{j-1} Q^T q_1, \text{ since } A^k = Q^T H^k Q$$

$$= H^{j-1} Q^T q_1 = H^{j-1} e_1, \text{ since } Q \text{ orthogonal}$$

$$\Rightarrow r_j \in R = h_1 \in H^{j-1}, \text{ which has top } j \text{ rows nonzero}$$

The last statement can be checked by iteratively checking the first column of  $H^i$ . This result indicates that  $Q_kK_k$ , produces an upper right triangular matrix since  $Q_k$  is the first k columns of Q. This also means  $Q_k$  forms a basis for  $K(A, q_1, k)$ .

## 7.2.2 Arnoldi process generates a minimal polynomial

#### Polynomial properties

- If A is diagonalizable, i.e.,  $A = X\Lambda X^{-1}$ , then polynomial  $f(A) = Xf(\Lambda)X^{-1}$
- Characteristic polynomial of A is  $p_A(z) = det(zI A) = \prod (z \lambda_i)$  and  $p_A(\lambda_i) = 0$  for  $\lambda_i \in \lambda(A)$
- $f(A) = 0 \Longrightarrow \lambda_i \in \lambda(A)$  are the roots of the polynomial (e.g.,  $p_A(A) = Xp_A(\Lambda)X^{-1} = 0$

Our hope is that for  $p_k(H_k) = 0$ ,  $p_k(A)$  is minimally small. We show  $||p_K(A)q_1||_2$  is minimized:

$$f(x) = x^k + f_{k-1}x^{k-1} + \dots + f_0, \text{ for } f \text{ that minimizes } \|f(A)q_1\|_2$$

$$f(A) = (A^k + f_{k-1}A^{k-1} + \dots + f_0)q_1 = A^kq_1 + K_kf, \text{ where } f \text{ is a vector of coefficients}$$

$$= A^kq_1 + Q_ky, \text{ for some } y, \text{ since } Q_k \text{ forms a basis for Krylov space}$$

$$\text{Minimal } \|f(A)q_1\|_2 \Longrightarrow \text{minimal } \|A^kq_1 + Q_ky\|_2, \text{ so we need to choose } y \text{ to minimize polynomial}$$

$$\text{minimal } \|A^kq_1 + Q_ky\|_2 \Longrightarrow Q_k^Tf(A)q_1 = 0$$

$$Q_k^Tf(A)q_1 = Q_k^TQf(A)Q^Tq_1 = \begin{bmatrix} I_k & 0 \end{bmatrix} f(H)e_1 = I_kf(H_k)e_1$$

This proof shows that  $||f(A)q_1||_2$  is minimal  $\Leftrightarrow I_k f(H_k)e_1 = 0$ , which  $p_k(H_k)$  achieves since  $p_k(H_k) = 0$ 

## 7.3 Lanczos process

The Lanczos process is a parallel process to the Arnoldi process, but for symmetric matrices. Reminder: A symmetric upper Hessenberg matrix, T is tri-diagonal. The process follows

1. 
$$\alpha_k = q_k^T A q_k \Longrightarrow \alpha_k q_k = A q_k$$
  
2.  $r_k = A q_k - \beta_{k-1} q_{k-1} - \alpha_k q_k \Longrightarrow r_k = \beta_{k-1} q_{k-1}, r_k$  becomes the orthogonal part of  $A q_k$   
3.  $\beta_k = \|r_k\|_2$   
4.  $q_{k+1} = \frac{r_k}{\beta_k}$ 

The orthogonalization in step 2 is reduced from O(k) in Arnoldi to O(1) in Lanczos because of the symmetry of A

#### 7.3.1 Process for revealing the max eigenvalue of A

$$\lambda(T_k) \approx \lambda(A)$$

$$\lambda_1 \in \lambda(T_k) = \max_{x \neq 0} \frac{y^T Q_k^T A Q y}{\|y\|_2^2}, \text{ by property that } \lambda_1 \in \lambda(A) = \max_{x \neq 0} \frac{x^T A x}{\|x\|_2^2}$$

$$\implies \text{ want max } x \text{ of the form } Q_k y$$

$$\implies \text{ want max } x \text{ in Krylov space, a subspace of } \mathbb{R}^k$$

$$\implies \lambda_1 \in \lambda(T_k) \leq \lambda_1 \in \lambda(A), \text{ since it is the max in a smaller space}$$

$$\lambda_1 \in \lambda(T_k) = \max_{x \neq 0} \frac{q_1^T p(A) A p(A) q_1}{q_1^T p(A)^2 q_1}, \text{ and see textbook for step from here to next step}$$

$$\Longrightarrow \lambda_1 \in \lambda(T_k) \leq \lambda_1 - (\lambda_1 - \lambda_n) \left(\frac{\tan(\theta)}{T_{k-1}^{Cheb}(1 + 2p_1)}\right), \text{ where } p_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

Observe that the RHS approaches  $\lambda_1$  when  $\lambda_1$  is well separated from the other eigenvalues.