NUMERICAL LINEAR ALGEBRA

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P3: Solving large scale eigenvalue problems

Eigenvalue problems

The algebraic eigenvalue problem reads as follows:

Given a matrix $A \in \mathbb{C}^{n\times n}$, find $(\lambda, \mathbf{v}) \in \mathbb{C} \times \mathbb{C}^n \backslash \{\mathbf{0}\}$ such that

$$A\mathbf{v} = \lambda\mathbf{v}$$

where

λ is an eigenvalue of A

$\mathbf{v}$ (non- zero) is the corresponding eigenvector

- The set of all the eigenvalues of a matrix A is called the spectrum of A ($\sigma(A)$)
- The maximum modulus of all the eigenvalues is called the spectral radius of A:

$$\rho(A) = \max\{\,|\lambda| : \lambda \in \lambda(A)\}$$

Exercise. Take $A = \begin{pmatrix} 1 & 2 \\ 8 & 1 \end{pmatrix}$ and show that $\lambda = 5$ is an eigenvalue and $\mathbf{v} = (1,2)^T$ is the corresponding eigenvector.

Some applications

Eigenvalue problems occur in many areas of science and engineering.

1. Communication systems: Eigenvalues were used by C. Shannon to determine the theoretical limit to how much information can be transmitted through a communication medium like your telephone line or through the air.
2. Designing of bridges:The natural frequency of the bridge is the eigenvalue of smallest magnitude of a system that models the bridge. The engineers exploit this knowledge to ensure the stability of their constructions.
3. Designing car stereo system: Eigenvalue analysis is also used in the design of the car stereo systems, where it helps to reproduce the vibration of the car due to the music.
4. Geophysics: Oil companies use eigenvalue analysis for oil extraction. Oil other substances all give rise to linear systems which have different eigenvalues, so eigenvalue analysis can give a good indication of where oil reserves are located.

Geometric interpretation

Eigenvalues and eigenvectors provide a means of understanding the complicated behavior of a general linear transformation by decomposing it into simpler actions

An eigenvector (corresponding to a real nonzero eigenvalue) points in a direction in which it is stretched by the linear transformation; the associated eigenvalue is the factor by which it is “stretched/contracted”.

Mathematical background

1. The problem $A\mathbf{v} = \lambda\mathbf{v}$ is equivalent to $(A - \lambda I)\mathbf{v} = 0$.
2. This homogeneous equation has a nonzero solution $\mathbf{v}$ if and only if its matrix is singular , that is the eigenvalues of A are the values λ such that $\det(A - \lambda I) = 0$
3. $\det(A - \lambda I) = 0$ is a polynomial of degree n in λ: it is called the characteristic polynomial of A and its roots are the eigenvalues of A

Some useful remarks

- From the Fundamental Theorem of Algebra, an $n \times n$ matrix A always has n eigenvalues $\lambda_i, i = 1, \ldots, n$
- Each λ_i may be real but in general is a complex number
- The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ may not all have distinct values
- Rayleigh quotient: Let (λ_i, $\mathbf{v}_i$) be an eigenpair of A, then

$$\lambda_i = \frac{\mathbf{v}_i^H A \mathbf{v}_i}{\mathbf{v}_i^H \mathbf{v}_i}$$

Similarity transformations

We first need to identify:
- what types of transformations preserve eigenvalues
- for what types of matrices the eigenvalues are easily determined

Definition. The matrix B is similar to the matrix A if there exists a nonsingular matrix T such that $B = T^{-1}AT$.

With the above definition, it is trivial to show that

$$B\mathbf{y} = \lambda\mathbf{y} \rightarrow T^{-1}1ATy = \lambda\mathbf{y} \rightarrow A(T\mathbf{y}) = \lambda(T\mathbf{y})$$

so that A and B have the same eigenvalues, and if $\mathbf{y}$ is an eigenvector of B, then $\mathbf{v} = T\mathbf{y}$ is an eigenvector of A

Similarity transformations

Similarity transformations:
- Preserve eigenvalues
- Do not preserve eigenvectors (but the eigenvectors can be easily recovered)

Note that the converse is not true: two matrices that have the same eigenvalues are not necessarily similar!

Similarity transformations

- The eigenvalues of a diagonal matrix are its diagonal entries
- The eigenvalues of a triangular matrix are also the diagonal entries

Note that:

- Diagonal form simplifies eigenvalue problems for general matrices by similarity transformations
- Some matrices cannot be transformed into diagonal form by a similarity transformation

A square matrix A is called diagonalisable (or non-defective) if it is similar to a diagonal matrix

The general idea from the numerical viewpoint

Some of numerical methods for computing eigenvalues and eigenvectors are based on reducing the original matrix to a simpler form, whose eigenvalues and eigenvectors are can be easily determined.

Ideally we would like to transform the underlying system of equations into a special set of coordinate axes in which the matrix is diagonal. The eigenvalues are therefore entries of the diagonal matrix and the eigenvectors are the new set of coordinate axes

Computing eigenvalues and eigenvectors

There are several methods designed to compute all of the eigenvalues of a matrix (and some of them require a great deal of work)

In practice, one may need only one or a few eigenvalues and corresponding eigenvectors (take advantage of this in designing the numerical scheme)

The simplest method for computing a single eigenvalue and eigenvector of a matrix is the so called power method.

Power method

The power method

Assume that the matrix A has a unique eigenvalue λ_1 of maximum modulus, i.e.

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \ldots |\lambda_n|$$

with corresponding eigenvector $\mathbf{v}_1$

Starting from a given nonzero vector $\mathbf{x}^{(0)}$, such that $\|\mathbf{x}^{(0)}\| = 1$, let us consider the following iteration scheme, for $k \geq 0$:

$$\mathbf{y}^{(k+1)} \leftarrow A\mathbf{x}^{(k)}$$

$$\mathbf{x}^{(k+1)} \leftarrow \frac{\mathbf{y}^{(k+1)}}{\|\mathbf{y}^{(k+1)}\|}$$

$$\nu^{(k+1)} \leftarrow [\mathbf{x}^{(k+1)}]^H A\mathbf{x}^{(k+1)}$$

It can be shown that the above iteration scheme converges to a multiple of $\mathbf{v}_1$, the eigenvector corresponding to the dominant eigenvalue λ_1

Proof (hints)

- Observe that since A is diagonalisable, its eigenvector $\mathbf{v}_i$ forms a basis for $\mathbb{C}^n$
- Express the starting vector $\mathbf{x}^{(0)}$ as a linear combination of the eigenvectors
- Do some calculations to obtain

$$Ax^{(k)} = \alpha_1 \lambda_1^k \left(\mathbf{v_1} + \sum_{i=2}^{n} \frac{\alpha_i}{\alpha_1} \left[\frac{\lambda_i}{\lambda_1} \right]^k \mathbf{v_i} \right)$$

- Use that λ_1 is a dominant eigenvalue

Convergence rate of the power method

The convergence rate of the power method depends on the ratio $|\lambda_2|/|\lambda_1|$, where λ_2 is the eigenvalue having the second - largest modulus

The smaller $|\lambda_2|/|\lambda_1|$ is, the faster the convergence is

Hence the power method will converge

- Quickly if $|\lambda_2|/|\lambda_1|$ is small
- Slowly if $|\lambda_2|/|\lambda_1|$ is close to 1

Deflation methods

Suppose that an eigenvalue λ_1 and corresponding eigenvector $\mathbf{v}_1$ for a matrix A have been computed

We can compute additional eigenvalues $\lambda_2, \ldots, \lambda_n$ of A, by a process called deflation, which removes the known eigenvalue

Idea: constructs a new matrix B with eigenvalues $\lambda_2, \ldots, \lambda_n$, that is deflate the matrix A, removing λ_1

Then λ_2 can be obtained by the power method.

Deflation methods

Let S be any nonsingular matrix such that $S\mathbf{v}_1 = \alpha\mathbf{e}_1$, that is S is a scalar multiple of the first column $\mathbf{e}_1$ of the identity matrix I

Then the similarity transformation determined by S transforms A into the form

$$SAS^{-1} = \begin{pmatrix} \lambda_1 & b^T \\ 0 & B \end{pmatrix}$$

For example, good choice for S can be an appropriate Householder transformation (linear transformation that describes a reflection about a plane or hyperplane containing the origin)

We use B to compute next eigenvalue λ_2 and eigenvector $\mathbf{z_2}$.

Given $\mathbf{z}_2$ eigenvector of B, we want to compute the second eigenvector $\mathbf{v}_2$ of the matrix A

Deflation methods

We need to add an element to vector $\mathbf{z}_2$ (that consist of $n-1$ elements), that is $\mathbf{v}_2 = S^{-1}\begin{pmatrix}\alpha \\ \mathbf{z}_2\end{pmatrix}$ $\qquad \alpha = \dfrac{\mathbf{b}^H \mathbf{z}_2}{\lambda_1 - \lambda_2}$

Hence, $\mathbf{v}_2$ is an eigenvector corresponding to λ_2 for the original matrix A

The process can be repeated to find additional eigenvalues and eigenvectors

Inverse power method

For some applications, the smallest eigenvalue of a matrix is required rather than the largest

We use the fact that the eigenvalues of A^{-1} are the reciprocals of those of A

Hence the smallest eigenvalue of A is the reciprocal of the largest eigenvalue of A^{-1}

Starting from a given nonzero vector $\mathbf{q}^{(0)}$, such that $\|\mathbf{q}^{(0)}\| = 1$, let us consider the following iteration scheme, for $k \geq 0$:

$$\text{Solve } A\mathbf{z}^{(k+1)} = \mathbf{q}^{(k)}$$

$$\mathbf{q}^{(k+1)} \leftarrow \frac{\mathbf{z}^{(k+1)}}{\|\mathbf{z}^{(k+1)}\|}$$

$$\sigma^{(k+1)} \leftarrow [\mathbf{q}^{(k+1)}]^H A\mathbf{q}^{(k+1)}$$

Inverse power method with shift

If we want to approximate the eigenvalue λ of A which is the closest to a given number $\mu \notin \sigma(A)$.

We denim $M_\mu = A - \mu I$ and observe that the eigenvalue λ of A which is the closes to μ is the minimum eigenvalue of M_μ

Starting from a given nonzero vector $\mathbf{q}^{(0)}$, such that $\|\mathbf{q}^{(0)}\| = 1$, let us consider the following iteration scheme, for $k \geq 0$:

$$\text{Solve } M_\mu \mathbf{z}^{(k+1)} = \mathbf{q}^{(k)}$$

$$\mathbf{q}^{(k+1)} \leftarrow \frac{\mathbf{z}^{(k+1)}}{\|\mathbf{z}^{(k+1)}\|}$$

$$\nu^{(k+1)} \leftarrow [\mathbf{q}^{(k+1)}]^H A \mathbf{q}^{(k+1)}$$

QR Factorization

Projectors and complementary projectors

- A *projector* is a square matrix $P \in \mathbb{R}^{n \times n}$ that satisfies $P^2 = P$

- If $\mathbf{w} \in \text{range}(P)$, then $P\mathbf{w} = \mathbf{w}$. Indeed, since $\mathbf{w} \in \text{range}(P)$, then $\mathbf{w} = P\mathbf{z}$, for some $\mathbf{z}$. Therefore:

$$P\mathbf{w} = P(P\mathbf{z}) = P^2\mathbf{z} = P\mathbf{z} = \mathbf{w}$$

- The matrix $I - P$ is the complementary projector to P
- $I - P$ projects on the nullspace of P: if $P\mathbf{w} = 0$, then $(I - P)\mathbf{w} = \mathbf{w}$, so $\text{null}(P) \subseteq \text{range}(I - P)$
- But for any $\mathbf{w}$, $(I - P)\mathbf{w} = \mathbf{w} - P\mathbf{w} \in \text{null}(P)$, so $\text{range}(I - P) \subseteq \text{null}(P)$
- Therefore

$$\text{range}(I - P) = \text{null}(P)$$

and

$$\text{null}(I - P) = \text{range}(P)$$

Orthogonal Projectors

- A projector P is orthogonal i f $P = P^2 = P^T$

The QR factorisation - Main idea

- Find orthonormal vectors $[\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n]$ that span the successive spaces spanned by the columns of $A = [\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n]$:

$$< \mathbf{a}_1 > \subseteq < \mathbf{a}_1, \mathbf{a}_2 > \ldots \subseteq < \mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n >$$

- This means that (for full rank A)

$$< \mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_j > = < \mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_j > \qquad \forall j = 1, \ldots, n$$

The QR Factorization - matrix form

In matrix form $< \mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_j > = < \mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_j > \qquad \forall j = 1, \ldots, n$

becomes

$$\left[\mathbf{a}_1 \,\middle|\, \mathbf{a}_2 \,|\cdots|\, \mathbf{a}_n\right] = \left[\mathbf{q}_1 \,\middle|\, \mathbf{q}_2 \,|\cdots|\, \mathbf{q}_n\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & \vdots \\ 0 & 0 & \ddots & r_{nn} \end{bmatrix}$$

that is

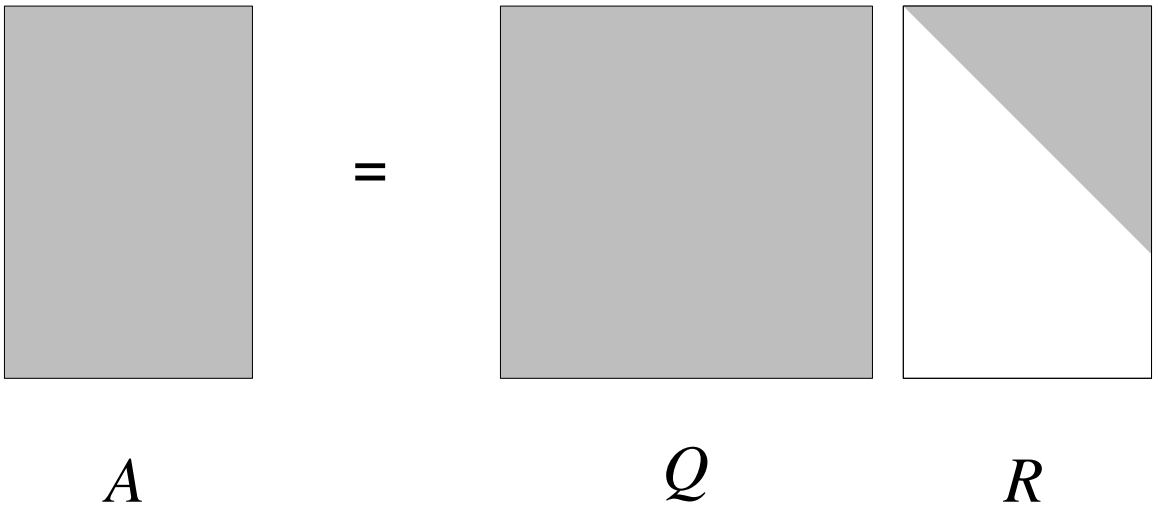
$$A = \hat{Q}\hat{R}$$

This is called the reduced QR factorization

The Full QR Factorization

Let A be an $m \times n$ matrix. The full QR factorization of A is the factorization $A = QR$, where

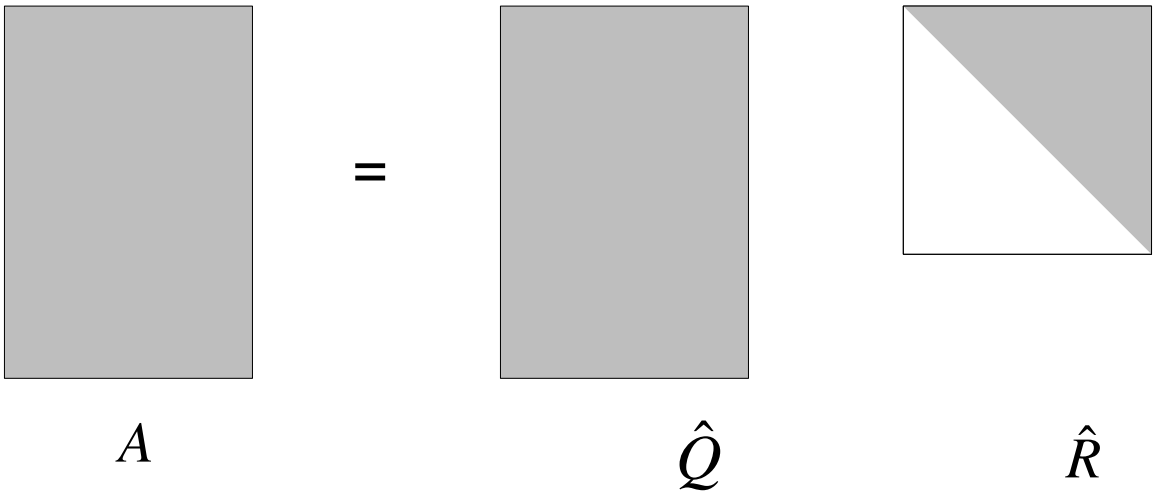
Q is $m \times m$ orthogonal ($QQ^T = I$)
R is $m \times n$ upper-trapeziodal



The reduced QR factorization

Let A be an $m \times n$ matrix. The reduced QR factorization of A is the factorization $A = \hat{Q}\hat{R}$, where

Q is $m \times n$
R is $n \times n$ upper-triangular



Gram-Schmidt orthogonalisation

- Given $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n$ (the columns of A)

- Find new $\mathbf{q}_j$ (the j-th column of $\hat{Q}$) orthogonal to $\mathbf{q}_1, \ldots, \mathbf{q}_{j-1}$ by subtracting components along previous vectors

$$\mathbf{w}_j = \mathbf{a}_j - \sum_{k=1}^{j-1} (\overline{\mathbf{q}}_k^T \mathbf{a}_j)\mathbf{q}_k$$

- Normalize to get $\mathbf{q}_j = \dfrac{\mathbf{w}_j}{\|\mathbf{w}_j\|}$

- We then obtain a reduced QR factorization $A = \hat{Q}\hat{R}$, with

$$r_{ij} = \overline{\mathbf{q}}_i^T \mathbf{a}_j \qquad (i \neq j)$$

and

$$r_{jj} = \|\mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij}\mathbf{q}_i\|$$

- *Numerically unstable (see later Modified Gram-Schmidt)*

Existence and uniqueness

- Every $A \in \mathbb{C}^{m \times n} (m \geq n)$ has a full QR factorization and a reduced QR factorisation
- Proof. For full rank A, Gram-Schmidt proves existence of $A = \hat{Q}\hat{R}$. Otherwise, when $\mathbf{w}_j = 0$ choose arbitrary vector orthogonal to previous $\mathbf{q}_i$. For full QR, add orthogonal extension to Q and zero rows to R.
- Each $A \in \mathbb{C}^{m \times n} (m \geq n)$ of full rank has *unique* $A = \hat{Q}\hat{R}$ with $r_{jj} > 0$, $j = 1, \ldots, n$. Proof. Again Gram-Schmidt (r_{jj} determines the sign).

Classical vs. Modified Gram-Schmidt

- Small modification of classical G-S gives modified G-S (but see next slide)
- Modified G-S is numerically stable (less sensitive to rounding errors)

for $j = 1, \ldots, n$

$\mathbf{w}_j = \mathbf{a}_j$

for $i = 1, \ldots, j-1$

$$\begin{cases} r_{ij} = \overline{\mathbf{q}}_i^T \mathbf{a}_j & \text{(GS)} \\ r_{ij} = \overline{\mathbf{q}}_i^T \mathbf{w}_j & \text{(MGS)} \end{cases}$$

$\mathbf{w}_j = \mathbf{w}_j - r_{ij}\mathbf{q}_i$

$r_{jj} = \|\mathbf{w}_j\|$

$$\mathbf{q}_j = \frac{\mathbf{w}_j}{\|\mathbf{w}_j\|}$$

end

end

FLOP Counts - MGS

- No distinction between real and complex
- No consideration of memory accesses or other performance aspects
- Flops count $\sim 2mn^2$

The QR algorithm

- Basic QR algorithm
- Hessenberg QR algorithm
- QR algorithm with shifts
- Double step QR algorithm for real matrices

Schur decomposition

If $A \in \mathbb{C}^{n\times n}$ then there is a unitary matrix $U \in \mathbb{C}^{n\times n}$ such that

$$U^H A U = T$$

is upper triangular. The diagonal elements of T are the eigenvalues of A.

$U = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n]$ are called Schur vectors. They are in general **not** eigenvectors.

Schur vectors

The k-th column of $U^H A U = T$ read

$$A\mathbf{u}_k = \lambda_k \mathbf{u}_k + \sum_{i=1}^{k-1} t_{ik}\mathbf{u}_i$$

that is

$$A\mathbf{u}_k \in \text{span}\left\{\mathbf{u}_1, \ldots, \mathbf{u}_k\right\} \qquad \forall k$$

- The first Schur vector $\mathbf{u}_1$ is an eigenvector of A.
- The first k Schur vectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ form an invariant subspace for A.
- The Schur decomposition is not unique.

Basic QR algorithm

Let $A \in \mathbb{C}^{n \times n}$. The QR algorithm computes an upper triangular matrix T and a unitary matrix Usuch that $A = UTU^H$ is the Schur decomposition of A.

1. Set $A^{(0)} = A, U^{(0)} = I$
2. while(STOPPING CRITERIA)
3. $A^{(k-1)} = Q^{(k)}R^{(k)}$ (QR factorisation of $A^{(k-1)}$)
4. $A^{(k)} = R^{(k)}Q^{(k)}$
5. $U^{(k)} = U^{(k-1)}Q^{(k)}$ (Update transformation matrix)
6. end for
7. Return $T = A^{(k)}, U = U^{(k)}$.

Basic QR algorithm: some remarks

1. Notice that $A^{(k)} = R^{(k)}Q^{(k)} = [Q^{(k)}]^H A^{(k-1)}Q^{(k)}$, and therefore $A^{(k)}$ and $A^{(k-1)}$ are similar
2. Moreover, from the above observation, we have

$$\begin{aligned} A^{(k)} &= [Q^{(k)}]^H A^{(k-1)}Q^{(k)} \\ &= [Q^{(k)}]^H [Q^{(k-1)}]^H A^{(k-2)}Q^{(k-1)}Q^{(k)} \\ &= \dots \\ &= [Q^{(k)}]^H \dots [Q^{(1)}]^H A^{(0)}Q^{(1)} \dots Q^{(k)} \end{aligned}$$

Basic QR algorithm: convergence

Let us assume that all the eigenvalues are isolated, i.e.,

$$|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n|.$$

Then the elements of $A^{(k)}$ below the diagonal converge to zero, i.e.

$$\lim_{k\to\infty} a_{ij}^{(k)} = 0 \quad \forall i > j$$

Moreover, it can be shown that

$$a_{ij}^{(k)} = O\left(\left|\frac{\lambda_i}{\lambda_j}\right|^k\right) \qquad i > j$$

Remarks:

Convergence is low if the eigenvalues are close.

Computational costs: $O(n^3)$

Stopping criteria:

Basic QR algorithm: convergence

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QR algorithm - remarks

The basic QR algorithm can be used to compute eigenvalues, but

1. it is computationally expensive (requiring $O(n^3)$ operations per iteration)
2. it can have a very slow convergence depending on the eigenvalues of A

There are approaches to improve the situation:

- Reduce the matrix A to a similar matrix that is upper Hessenberg. Notice that Hessenberg structure is preserved by the QR algorithm (see later). This reduces the cost per iteration to $O(n^2)$ operations.
- Once an eigenvalue has been computed deflate away this matrix. This greatly speeds up later eigenvalue computations.
- Use "shifts" in the QR algorithm.

QR iteration on Hessenberg matrices

A matrix $H \in \mathbb{C}^{n\times n}$ is called a Hessenberg matrix if its elements below the lower off-diagonal are zero

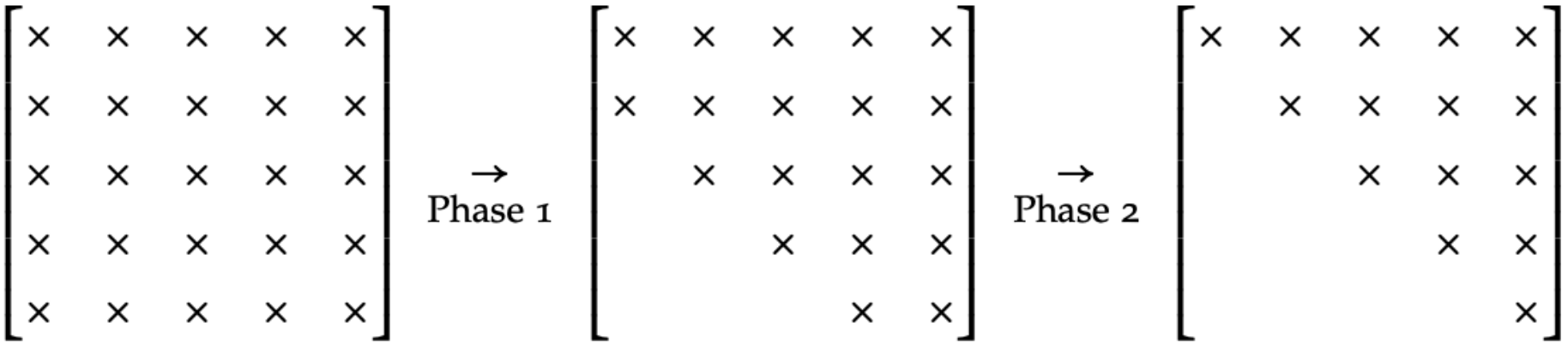
$$h_{ij} = 0, \quad i > j + 1.$$

$$H = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & 0 & * & * \end{bmatrix}$$

A QR iteration on a Hessenberg matrix H costs only $O(n^2)$ flops and the resulting matrix is again a Hessenberg matrix.

Hessenberg QR-method

To improve the QR-method we make use of an algorithm consisting of two phases:



- **Phase 1**. Compute a Hessenberg matrix H (and an orthogonal matrix U) such that $A = UHU^H$. Such a reduction can be done with a finite number of operations.
- **Phase 2**. Apply the basic QR-method to the matrix H. It turns out when applying the basic QR-method to a Hessenberg matrix such that the complexity of one step is$O(n^2)$, instead of $O(n^3)$ in the basic version.

The Lanzos algorithm

The Lanzos algorithm

The Lanczos algorithm can be used to efficiently find the extremal eigenvalues (maximum and minimum) of a symmetric matrix A of size $n \times n$.

It is based on computing the following decomposition of A:

$$A = QTQ^T$$

where Q is an orthonormal basis of vectors $\mathbf{q}_1, \ldots, \mathbf{q}_n$ and T is tri-diagonal:

$$Q = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n] \qquad T = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \ldots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \ldots & 0 \\ 0 & \ddots & \ddots & \vdots & 0 \\ 0 & \ddots & \ddots & \vdots & \beta_{n-1} \\ 0 & \ldots & 0 & \beta_{n-1} & \alpha_n \end{bmatrix}$$

The decomposition always exists and is unique given that $\mathbf{q}_1$ has been specified.

Lanczos Iterations

We know that $T = Q^T A Q$ which gives

$$\alpha_k = \mathbf{q}_k^T A \mathbf{q}_k \qquad \beta_k = \mathbf{q}_{k+1}^T A \mathbf{q}_k$$

The full decomposition is obtained by imposing $AQ = QT$:

$$[A\mathbf{q}_1, A\mathbf{q}_2, \ldots, A\mathbf{q}_n] = \left[\alpha_1\mathbf{q}_1 + \beta_1\mathbf{q}_2, \beta_1\mathbf{q}_1 + \alpha_2\mathbf{q}_2 + \beta_2\mathbf{q}_3, \ldots, \ldots, \beta_{n-1}\mathbf{q}_{n-1} + \alpha_n\mathbf{q}_n\right]$$

Lanczos algorithm

At iteration k the algorithm generates intermediate matrices Q_k and T_k that satisfy $T_k = Q_k^T A Q_k$

$$\mathbf{Q}_k = [\ \mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_k\ ],$$

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

Lanczos algorithm

$\mathbf{r}_0 = \mathbf{q}_1$; $\mathbf{q}_0 = \mathbf{0}$; $\beta_0 = 1$;

for $(k = 1, \ldots, n)$

- if $(\beta_{k-1} = 0)$
  - break;
- end
- $\mathbf{q}_k = \mathbf{r}_{k-1}/\beta_{k-1}$;
- $\alpha_k = \mathbf{q}_k^T \mathbf{A} \mathbf{q}_k$;
- $\mathbf{r}_k = (\mathbf{A} - \alpha_k)\mathbf{q}_k - \beta_{k-1}\mathbf{q}_{k-1}$;
- $\beta_k = |\mathbf{r}_k|$;

end

Remark 1: $\mathbf{q}_1$ is set randomly.

Remark 2: the (orthonormal) vectors $\mathbf{q}_k$ are called the Lanczos vectors.

Properties of $\mathbf{q}_k$ and T_k

At iteration k, the $k-$th Lanczos vector $\mathbf{q}_k$ is proven to maximise the l.h.s. of

$$\max_{\mathbf{y}\neq\mathbf{0}} \frac{\mathbf{y}^T(Q_k^T A Q_k)\mathbf{y}}{\mathbf{y}^T\mathbf{y}} = \lambda_1(T_k) \leq \lambda_1(A) = \lambda_1(T)$$

and to simultaneously minimize the l.h.s. of

$$\min_{\mathbf{y}\neq\mathbf{0}} \frac{\mathbf{y}^T(Q_k^T A Q_k)\mathbf{y}}{\mathbf{y}^T\mathbf{y}} = \lambda_n(T_k) \geq \lambda_n(A) = \lambda_n(T)$$

where $\lambda_1(A)$ and $\lambda_n(A)$ are the maximum and the minimum eigenvalue of A, respectively.

The extremal eigenvalues of T_k progressively become more similar to the ones of A.

Summary

- The Lanczos algorithm can be used to compute the extremal eigenvalues of a symmetric matrix A.
- The Lanczos algorithm only requires matrix-vector multiplications with respect to A (matrix free, very useful if A has a sparse form).
- The algorithm is very sensitive to round-off problems. The Lanczos vectors $\mathbf{q}_k$ loose orthogonality.
- The Lanczos algorithm can be used to efficiently find a low-rank approximation of A.