MA4230 Matrix Computation

Chapter 6: Eigenvalue Problems

6.1 The eigenvalue problem: the basics

The Eigenvalue Problem

We study the **eigenvalue problem** corresponding to a matrix $A \in \mathbb{C}^{n\times n}$:

Find $x \in \mathbb{C}^n \setminus \{0\}$ and $\lambda \in \mathbb{C}$ such that $Ax = \lambda x$.

Notation: We write $\mathbb{C}^{m\times n}$ for the set of complex $m \times n$ matrices, and $\mathbb{C}^m := \mathbb{C}^{m\times 1}$ for the set of complex column m-vectors.

For $A = (a_{ij}) \in \mathbb{C}^{m\times n}$ write $\bar{A} := (\overline{a_{ij}}) \in \mathbb{C}^{m\times n}$ (complex conjugate each entry), and denote the **adjoint** by $A^* := \overline{A^{\mathrm{T}}} \in \mathbb{C}^{n\times m}$.

We introduce three important classes of square matrices:

- $A \in \mathbb{C}^{n\times n}$ is called **hermitian** iff $A^* = A$,
  (if A real: *hermitian* $\Leftrightarrow$ *symmetric*)
- $A \in \mathbb{C}^{n\times n}$ is called **normal** iff $A^*A = AA^*$,
- $A \in \mathbb{C}^{n\times n}$ is called **unitary** iff $A^*A = AA^* = I_n$.
  (if A real: *unitary* $\Leftrightarrow$ *orthogonal*)

The basics: For $A \in \mathbb{C}^{n\times n}$, ...

- $\lambda \in \mathbb{C}$ is called **eigenvalue** of A iff $Ax = \lambda x$ for some $x \in \mathbb{C}^n \backslash \{0\}$. Then, any $x \in \mathbb{C}^n \backslash \{0\}$ with $Ax = \lambda x$ is called an **eigenvector** of A corresponding to the eigenvalue λ.
- define the **characteristic polynomial**
$$p_A : \mathbb{C} \to \mathbb{C}, \quad z \mapsto \det(zI_n - A).$$
- define the **spectrum**
$$\Lambda(A) := \{\lambda \in \mathbb{C} : \lambda \text{ is an eigenvalue of } A\}$$
and the **spectral radius**
$$\rho(A) := \max\{|\lambda| : \lambda \in \Lambda(A)\}.$$

Some results:

- If A is hermitian, then $\Lambda(A) \subseteq \mathbb{R}$.
- $\Lambda(A) = \{\lambda \in \mathbb{C} : p_A(\lambda) = 0\}$.
- $\exists \lambda_1, \dots, \lambda_n \in \mathbb{C} : p_A(z) = \prod_{i=1}^n (z - \lambda_i)$ ($\Rightarrow \Lambda(A) = \{\lambda_1, \dots, \lambda_n\}$).
- $\det(A) = \prod_{i=1}^n \lambda_i$ and $\mathrm{tr}(A) = \sum_{i=1}^n \lambda_i$.

The basics: For $A \in \mathbb{C}^{n \times n}$, ...

- the **algebraic multiplicity** $\mu_A(\lambda) \in \{1, \ldots, n\}$ of an eigenvalue $\lambda \in \Lambda(A)$ is the multiplicity of λ as a root of p_A.
  We call $\lambda \in \Lambda(A)$ with $\mu_A(\lambda) = 1$ a **simple eigenvalue**.

- the **eigenspace** $E_\lambda \subseteq \mathbb{C}^n$ of an eigenvalue $\lambda \in \Lambda(A)$ is defined to be $E_\lambda := \mathcal{N}(\lambda I_n - A)$. We call $\gamma_A(\lambda) := \dim(E_\lambda) \in \{1, \ldots, n\}$ the **geometric multiplicity** of $\lambda \in \Lambda(A)$.

- an eigenvalue $\lambda \in \Lambda(A)$ is called **defective** iff $\gamma_A(\lambda) < \mu_A(\lambda)$. A matrix $A \in \mathbb{C}^{n \times n}$ is called defective iff it has a defective eigenvalue.

- If $X \in \mathbb{C}^{n \times n}$ invertible, the map $S_X : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n}$, $A \mapsto X^{-1}AX$ is called a **similarity transformation** of A. Further, $B \in \mathbb{C}^{n \times n}$ is called **similar** to $A \in \mathbb{C}^{n \times n}$ iff $\exists\, X \in \mathbb{C}^{n \times n}$ invertible: $B = X^{-1}AX$.

Some results:

- $\gamma_A(\lambda) \leq \mu_A(\lambda)$ for any $\lambda \in \Lambda(A)$.
- If $B \in \mathbb{C}^{n \times n}$ is similar to $A \in \mathbb{C}^{n \times n}$, then $p_A = p_B$, $\Lambda(A) = \Lambda(B)$, and $\mu_A(\lambda) = \mu_B(\lambda)$ and $\gamma_A(\lambda) = \gamma_B(\lambda)$ for all $\lambda \in \Lambda(A) = \Lambda(B)$.

Estimating the location of eigenvalues: Gerschgorin's thm

Notation: We denote the closed disc in the complex plane around a point $a \in \mathbb{C}$ with radius $r > 0$ by $D(a, r) := \{z \in \mathbb{C} : |z - a| \leq r\} \subseteq \mathbb{C}$.

Theorem (Gerschgorin's theorem)

Let $A = (a_{ij})_{1 \leq i,j \leq n} \in \mathbb{C}^{n \times n}$. Define $r_1, \ldots, r_n \geq 0$ given by

$$r_i := \sum_{j \in \{1,\ldots,n\} \setminus \{i\}} |a_{ij}|, \qquad i \in \{1, \ldots, n\}.$$

Then, there holds $\Lambda(A) \subseteq \bigcup_{i=1}^{n} D(a_{ii}, r_i)$, i.e., every eigenvalue of A lies in at least one of the n **Gerschgorin discs** *$D(a_{11}, r_1), \ldots, D(a_{nn}, r_n)$.*

Moreover, if there are $1 \leq k \leq n$ Gerschgorin discs such that their union U is a connected set which is disjoint from the union of the remaining $n - k$ Gerschgorin discs, then U contains exactly k eigenvalues of A.

Note: Since $\Lambda(A) = \Lambda(A^{\mathrm{T}})$ for any $A \in \mathbb{C}^{n \times n}$, we can obtain additional information on $\Lambda(A)$ by applying Gerschgorin's theorem to A^{T} as well.

Proof of Gerschgorin's theorem

Claim: Let $A = (a_{ij})_{1\leq i,j\leq n} \in \mathbb{C}^{n\times n}$. Define $r_1, \ldots, r_n \geq 0$ given by

$$r_i := \sum_{j\in\{1,\ldots,n\}\setminus\{i\}} |a_{ij}|, \qquad i \in \{1, \ldots, n\}.$$

Then, there holds $\Lambda(A) \subseteq \bigcup_{i=1}^n D(a_{ii}, r_i)$.

Proof: Let $\lambda \in \Lambda(A)$. Let $x = (x_1, \ldots, x_n)^{\mathrm{T}} \in \mathbb{C}^n\setminus\{0\}$ with $Ax = \lambda x$ and $\|x\|_\infty = \max_{k\in\{1,\ldots,n\}}|x_k| = 1$. Let $i \in \{1, \ldots, n\}$ with $|x_i| = 1$. Then,

$$\begin{aligned}|\lambda - a_{ii}| &= |(\lambda - a_{ii})x_i| = |(Ax)_i - a_{ii}x_i| \\ &= \left|\sum_{j=1}^n a_{ij}x_j - a_{ii}x_i\right| = \left|\sum_{j\in\{1,\ldots,n\}\setminus\{i\}} a_{ij}x_j\right| \leq r_i\|x\|_\infty = r_i,\end{aligned}$$

i.e., $\lambda \in D(a_{ii}, r_i)$. $\square$

(proof of second part of the theorem omitted)

6.2 Eigenvalue-revealing factorizations

Eigenvalue-revealing factn 1: Eigenvalue decomposition

Definition (Eigenvalue decomposition, diagonalizable matrices)

Let $A \in \mathbb{C}^{n \times n}$. If there exists an invertible matrix $X \in \mathbb{C}^{n \times n}$ and a diagonal matrix $D \in \mathbb{C}^{n \times n}$ such that

$$A = XDX^{-1}, \tag{1}$$

then we call (1) an **eigenvalue decomposition** of A.

(i) We say A is **diagonalizable** iff there exists an eigenvalue decomposition of A.

(ii) We say A is **unitary diagonalizable** iff there exists an eigenvalue decomposition (1) of A with X unitary, i.e., iff $\exists\, X \in \mathbb{C}^{n \times n}$ unitary, $D \in \mathbb{C}^{n \times n}$ diagonal: $A = XDX^*$.

Note that (1) is equivalent to $AX = XD$. Writing $X = (x_1| \dots |x_n)$ and $D = \operatorname{diag}_{n \times n}(\lambda_1, \dots, \lambda_n)$, this yields $Ax_i = \lambda_i x_i$ for $i \in \{1, \dots, n\}$.

$\Longrightarrow$ The eigenvalue decompn is an **eigenvalue-revealing decomposition** as we can directly read off the eigvals from the diagonal of D.

Characterization of diagonalizable matrices

Theorem (Characterization of diagonalizable matrices)

A matrix $A \in \mathbb{C}^{n\times n}$ is diagonalizable iff it is non-defective, i.e., iff $\gamma_A(\lambda) = \mu_A(\lambda)$ for all $\lambda \in \Lambda(A)$.

Proof: "$\Longrightarrow$" Suppose $A \in \mathbb{C}^{n\times n}$ has an eigenvalue decomposition $A = XDX^{-1}$ with $X \in \mathbb{C}^{n\times n}$ invertible and $D \in \mathbb{C}^{n\times n}$ diagonal.
A is similar to D. Hence,

- $\Lambda(A) = \Lambda(D) =: \Lambda$,
- $\forall\lambda \in \Lambda$: $\mu_A(\lambda) = \mu_D(\lambda)$, $\gamma_A(\lambda) = \gamma_D(\lambda)$

D is diagonal $\Longrightarrow \gamma_D(\lambda) = \mu_D(\lambda)\ \forall\lambda \in \Lambda \Longrightarrow \gamma_A(\lambda) = \mu_A(\lambda)\ \forall\lambda \in \Lambda$.

"$\Longleftarrow$" Suppose $A \in \mathbb{C}^{n\times n}$ is non-defective. Denote its distinct eigenvalues by $\lambda_1, \ldots, \lambda_k \in \Lambda(A)$, $k \le n$. To each λ_i can find $\gamma_A(\lambda_i)$ lin.indep. eigenvecs of A. Since eigenvecs to distinct eigenvals are lin.indep., can find a total of $\sum_{i=1}^k \gamma_A(\lambda_i) = \sum_{i=1}^k \mu_A(\lambda_i) = n$ lin.indep. eigenvectors $x_1, \ldots, x_n \in \mathbb{C}^n\backslash\{0\}$ for A. Then, $X := (x_1|\ldots|x_n)$ is invertible and, setting $D := \mathrm{diag}_{n\times n}(d_1, \ldots, d_n)$ with $d_1, \ldots, d_n \in \mathbb{C}$ satisfying $Ax_i = d_i x_i$, there holds $AX = XD$ and hence $A = XDX^{-1}$. $\square$

Theorem (Characterization of unitary diagonalizable matrices)

A matrix $A \in \mathbb{C}^{n\times n}$ is unitary diagonalizable iff it is normal. In particular, every hermitian matrix is unitary diagonalizable.

Remark: If $A \in \mathbb{R}^{n\times n}$ is symmetric, then $\exists$ a real eigenvalue decomposition $A = XDX^{-1} = XDX^{\mathrm{T}}$ with $X \in \mathbb{R}^{n\times n}$ orthogonal and $D \in \mathbb{R}^{n\times n}$ diagonal. We call real symmetric matrices orthogonally diagonalizable.

Any symmetric matrix is orthogonally equivalent to a diagonal matrix.

Definition (Orthogonally equivalent matrices)

Two matrices $A, B \in \mathbb{R}^{n\times n}$ are called **orthogonally equivalent** iff there exists an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ such that $A = QBQ^{\mathrm{T}}$.

Eigenvalue-revealing factn 2: Schur factorization

Drawback of eigenvalue decompn: it only exists for non-defective matrices.

Definition (Schur factorization)

Let $A \in \mathbb{C}^{n\times n}$. If there exists a unitary matrix $Q \in \mathbb{C}^{n\times n}$ and an upper-triangular matrix $T \in \mathbb{C}^{n\times n}$ such that

$$A = QTQ^*,$$

then we call this factorization a **Schur factorization** of A.

Theorem (Existence of Schur factorization)

Every matrix $A \in \mathbb{C}^{n\times n}$ has a Schur factorization.

Remark 1: If $A = QTQ^*$ is a Schur factn, then $\Lambda(A) = \Lambda(T)$.
$\Longrightarrow$ we can read off the eigenvalues of A from the diagonal of T.
Remark 2: If $A \in \mathbb{C}^{n\times n}$ is normal and $A = QTQ^*$ is a Schur factn of A, then T must be diagonal. (exercise)

Claim: Every matrix $A \in \mathbb{C}^{n\times n}$ has a Schur factorization $A = QTQ^*$.

Proof: (induction on $n \in \mathbb{N}$). For the case $n = 1$, i.e., $A = (a) \in \mathbb{C}^{1\times 1}$, we have that $A = (a) = (1)(a)(1) = I_1 A I_1^*$ is a Schur factorization of A. As induction hypothesis suppose the claim is true for some $n \in \mathbb{N}$.

Let $A \in \mathbb{C}^{(n+1)\times(n+1)}$. Our goal is to construct a Schur factorization of A. Let $\lambda \in \Lambda(A)$ and $x \in \mathbb{C}^{n+1}\backslash\{0\}$ with $x^*x = 1$ and $Ax = \lambda x$. We can find $U = (u_1|\dots|u_n|u_{n+1}) \in \mathbb{C}^{(n+1)\times(n+1)}$ unitary with $u_1 = x$. Then,

$$U^*AU = \left(\begin{array}{c|c} \lambda & w^* \\ \hline 0_{n\times 1} & B \end{array}\right) \in \mathbb{C}^{(n+1)\times(n+1)}$$

for some $w \in \mathbb{C}^n$ and $B \in \mathbb{C}^{n\times n}$. By hypothesis, $\exists$ Schur factn $B = VRV^*$ ($V \in \mathbb{C}^{n\times n}$ unitary, $R \in \mathbb{C}^{n\times n}$ upper-triangular). Then,

$$\left[U \left(\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & V \end{array}\right)\right]^* A \left[U \left(\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & V \end{array}\right)\right] = \left(\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & V^* \end{array}\right)\left(\begin{array}{c|c} \lambda & w^* \\ \hline 0_{n\times 1} & B \end{array}\right)\left(\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & V \end{array}\right)$$
$$= \left(\begin{array}{c|c} \lambda & w^*V \\ \hline 0_{n\times 1} & R \end{array}\right) =: T \in \mathbb{C}^{(n+1)\times(n+1)}.$$

$\Longrightarrow A = QTQ^*$ with $Q := U \left(\begin{array}{c|c} 1 & 0_{1\times n} \\ \hline 0_{n\times 1} & V \end{array}\right)$ is a Schur factn of A. $\square$

6.3 Transformation into upper-Hessenberg form

Eigenvalue solvers must be iterative

"Bad news": there is no algorithm which can compute the eigenvalues of an arbitrary matrix in a finite number of steps.
$\Longrightarrow$ Any eigenvalue solver must be iterative.

Let $a := (a_0, \ldots, a_{n-1})^{\mathrm{T}} \in \mathbb{C}^n$. Observe that the problem of finding the roots of the monic polynomial $p : \mathbb{C} \to \mathbb{C}$, $p(z) = z^n + \sum_{i=0}^{n-1} a_i z^i$ is equivalent to finding the eigenvalues of the matrix

$$A := \big(e_2 | e_3 | \cdots | e_n | -a\big) \in \mathbb{C}^{n \times n}.$$

(Pf: Denoting the roots of p by $z_1, \ldots, z_n \in \mathbb{C}$, $(1, z_i, z_i^2, \ldots, z_i^{n-1})^{\mathrm{T}} \in \mathbb{C}^n$ is an eigenvector of A^{T} with eigenvalue z_i for $i \in \{1, \ldots, n\}$. Hence, since $\Lambda(A) = \Lambda(A^{\mathrm{T}})$, we find that $\Lambda(A) = \{z_1, \ldots, z_n\}$.)

$\Longrightarrow$ If there were an algorithm which can compute the exact eigenvalues of an arbitrary matrix in finite steps, we would have a formula for computing the roots of any arbitrary polynomial. However, this is impossible since it is known that no such formula exists for polynomials of degree greater than or equal to 5.

We cannot find a Schur factn in finite time, but ...

We can transform a given matrix into an "almost" triangular matrix via unitary similarity transformations in a finite number of steps:

$$A = \begin{pmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \end{pmatrix} \quad \Longrightarrow \quad H = Q^*AQ = \begin{pmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & 0 & * & * \end{pmatrix}.$$

Definition (upper-Hessenberg matrix)

A square matrix $A = (a_{ij}) \in \mathbb{C}^{n\times n}$ is called an **upper-Hessenberg matrix** iff $a_{ij} = 0$ whenever $i > j + 1$.

Definition (Hessenberg decomposition)

Let $A \in \mathbb{C}^{n\times n}$. If there exist a unitary matrix $Q \in \mathbb{C}^{n\times n}$ and an upper-Hessenberg matrix $H \in \mathbb{C}^{n\times n}$ such that $A = QHQ^*$, then we call this a **Hessenberg decomposition** of A.

Hessenberg decomposition

Definition (Hessenberg decomposition)

Let $A \in \mathbb{C}^{n \times n}$. If there exist a unitary matrix $Q \in \mathbb{C}^{n \times n}$ and an upper-Hessenberg matrix $H \in \mathbb{C}^{n \times n}$ such that $A = QHQ^*$, then we call this a **Hessenberg decomposition** of A.

Theorem (Existence of Hessenberg decomposition)

Any square matrix $A \in \mathbb{C}^{n \times n}$ has a Hessenberg decomposition. Moreover, if $A \in \mathbb{R}^{n \times n}$ is real, then there exists a Hessenberg decomposition $A = QHQ^{\mathrm{T}}$ with $Q \in \mathbb{R}^{n \times n}$ orthogonal and $H \in \mathbb{R}^{n \times n}$ upper-Hessenberg.

Transformation into upper-Hessenberg form via unitary similarity transformations is typically the first phase of any eigenvalue algorithm.

Example: Transformation into upper-Hessenberg form

Consider $A := \begin{pmatrix} 1 & 1 & 0 & -1 & 0 \\ -2 & -1 & 1 & 1 & 0 \\ 1 & 1 & -1 & 1 & 0 \\ 2 & 1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{pmatrix}$.

Step 1: Find $Q_1 \in \mathbb{R}^{5\times 5}$ orthogonal s.t. $A_1 := Q_1^{\mathrm{T}} A Q_1 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \end{pmatrix}$.

We take $Q_1^{\mathrm{T}} = Q_1$ to be a Householder reflector that leaves the first row unchanged and introduces the desired zeros. Set $x_1 := (-2, 1, 2, 0)^{\mathrm{T}}$ and $v_1 := \mathrm{sign}(\langle x_1, e_1\rangle)\|x_1\|_2 e_1 + x_1 = (-5, 1, 2, 0)^{\mathrm{T}}$, and take

$$Q_1 := \left(\begin{array}{c|c} 1 & 0_{1\times 4} \\ \hline 0_{4\times 1} & I_4 - 2\frac{v_1 v_1^{\mathrm{T}}}{\|v_1\|_2^2} \end{array}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -\frac{2}{3} & \frac{1}{3} & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & \frac{14}{15} & -\frac{2}{15} & 0 \\ 0 & \frac{2}{3} & -\frac{2}{15} & \frac{11}{15} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then, $Q_1 A = Q_1^{\mathrm{T}} A$ has the desired zero-entries in first column, and so does $Q_1^{\mathrm{T}} A Q_1$ (right-multpcn by Q_1 leaves first column unchanged).

We have $A_1 := Q_1^{\mathrm{T}} A Q_1 = \begin{pmatrix} 1 & -\frac{4}{3} & * & * & * \\ 3 & -\frac{17}{9} & * & * & * \\ 0 & \frac{17}{45} & * & * & * \\ 0 & \frac{19}{45} & * & * & * \\ 0 & \frac{1}{3} & * & * & * \end{pmatrix}$.

Step 2: Find $Q_2 \in \mathbb{R}^{5\times 5}$ orthogonal s.t. $A_2 := Q_2^{\mathrm{T}} A_1 Q_2 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \end{pmatrix}$.

We take $Q_2^{\mathrm{T}} = Q_2$ to be a Householder reflector that leaves the first two rows unchanged and introduces the desired zeros. Set $x_2 := (\frac{17}{45}, \frac{19}{45}, \frac{1}{3})^{\mathrm{T}}$ and $v_2 := \mathrm{sign}(\langle x_2, e_1\rangle)\|x_2\|_2 e_1 + x_2 = \frac{1}{45}(17 + 5\sqrt{35}, 19, 15)^{\mathrm{T}}$, and take

$$Q_2 := \left(\begin{array}{c|c} I_2 & 0_{2\times 3} \\ \hline 0_{3\times 2} & I_3 - 2\frac{v_2 v_2^{\mathrm{T}}}{\|v_2\|_2^2} \end{array}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -\frac{17}{5\sqrt{35}} & -\frac{19}{5\sqrt{35}} & -\frac{3}{\sqrt{35}} \\ 0 & 0 & -\frac{19}{5\sqrt{35}} & \frac{39375+6137\sqrt{35}}{102550} & -\frac{9975-969\sqrt{35}}{20510} \\ 0 & 0 & -\frac{3}{\sqrt{35}} & -\frac{9975-969\sqrt{35}}{20510} & \frac{2527+153\sqrt{35}}{4102} \end{pmatrix}.$$

Then, $Q_2 A_1 = Q_2^{\mathrm{T}} A_1$ has the desired zero-entries in its second column, and so does $A_2 := Q_2^{\mathrm{T}} A_1 Q_2$.

We have $A_2 := Q_2^{\mathrm{T}} A_1 Q_2 = \begin{pmatrix} 1 & -\frac{4}{3} & -\frac{4}{3\sqrt{35}} & * & * \\ 3 & -\frac{17}{9} & -\frac{26}{9\sqrt{35}} & * & * \\ 0 & -\frac{\sqrt{35}}{9} & \frac{523}{315} & * & * \\ 0 & 0 & \frac{2565\sqrt{35}-8721}{20510} & * & * \\ 0 & 0 & -\frac{6885+3249\sqrt{35}}{20510} & * & * \end{pmatrix}.$

Step 3: Find $Q_3 \in \mathbb{R}^{5\times 5}$ orthogonal s.t. $A_3 := Q_3^{\mathrm{T}} A_2 Q_3 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{pmatrix}.$

We take $Q_3^{\mathrm{T}} = Q_3$ Householder reflector that leaves first 3 rows unchanged and introduces the desired zeros. Set $x_3 := (\frac{2565\sqrt{35}-8721}{20510}, -\frac{6885+3249\sqrt{35}}{20510})^{\mathrm{T}}$ and $v_3 := \operatorname{sign}(\langle x_3, e_1\rangle)\|x_3\|_2 e_1 + x_3$, and take

$$Q_3 := \left(\begin{array}{c|c} I_3 & 0_{3\times 2} \\ \hline 0_{2\times 3} & I_2 - 2\frac{v_3 v_3^{\mathrm{T}}}{\|v_3\|_2^2} \end{array}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\frac{285\sqrt{910}-969\sqrt{26}}{15236} & \frac{765\sqrt{26}+361\sqrt{910}}{15236} \\ 0 & 0 & 0 & \frac{765\sqrt{26}+361\sqrt{910}}{15236} & \frac{285\sqrt{910}-969\sqrt{26}}{15236} \end{pmatrix}.$$

Then, $Q_3 A_2 = Q_3^{\mathrm{T}} A_2$ has the desired zero-entry in its third column, and so does $Q_3^{\mathrm{T}} A_2 Q_3$.

We have

$$A_3 = Q_3^{\mathrm{T}} Q_2^{\mathrm{T}} Q_1^{\mathrm{T}} A Q_1 Q_2 Q_3 = \begin{pmatrix} 1 & -\frac{4}{3} & -\frac{4}{3\sqrt{35}} & -\frac{4}{\sqrt{910}} & -\frac{2}{\sqrt{26}} \\ 3 & -\frac{17}{9} & -\frac{26}{9\sqrt{35}} & -\frac{\sqrt{910}}{105} & 0 \\ 0 & -\frac{\sqrt{35}}{9} & \frac{523}{315} & \frac{8\sqrt{26}}{105} & 0 \\ 0 & 0 & -\frac{9\sqrt{26}}{35} & \frac{8}{35} & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix} =: H.$$

This is in upper-Hessenberg form. We find that $A = QHQ^{\mathrm{T}}$ with H as above and

$$Q := Q_1 Q_2 Q_3 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -\frac{2}{3} & -\frac{11}{3\sqrt{35}} & -\frac{11}{\sqrt{910}} & \frac{1}{\sqrt{26}} \\ 0 & \frac{1}{3} & -\frac{8}{3\sqrt{35}} & -\frac{8}{\sqrt{910}} & -\frac{4}{\sqrt{26}} \\ 0 & \frac{2}{3} & -\frac{7}{3\sqrt{35}} & -\frac{7}{\sqrt{910}} & \frac{3}{\sqrt{26}} \\ 0 & 0 & -\frac{3}{\sqrt{35}} & \frac{26}{\sqrt{910}} & 0 \end{pmatrix}$$

is a Hessenberg decomposition of A (note Q is orthogonal as a product of orthogonal matrices).

Existence and (non-)uniqueness of Hessenberg decompn

Using this methodology, any arbitrary square matrix $A \in \mathbb{C}^{n\times n}$ can be transformed into upper-Hessenberg form via unitary similarity transformations in (at most) $n-2$ steps. We are now able to find a Hessenberg decomposition to any given square matrix.

The Hessenberg decomposition is **not unique**. Consider, e.g., a 2×2 matrix $A \in \mathbb{C}^{2\times 2}$. Then, for any unitary $Q \in \mathbb{C}^{2\times 2}$, we have that $A = Q(Q^*AQ)Q^*$ is a Hessenberg decomposition of A (note any 2×2 matrix is upper-Hessenberg).

Let $A \in \mathbb{C}^{n\times n}$ be hermitian, and let $A = QHQ^*$ be a Hessenberg decomposition of A. Then, $H^* = (Q^*AQ)^* = Q^*A^*Q = Q^*AQ = H$, i.e., H is hermitian upper-Hessenberg and thus, H must be tridiagonal.

$\Longrightarrow$ *we can transform any hermitian matrix via unitary similarity transformations into a hermitian tridiagonal matrix.*

$\Longrightarrow$ *we can transform any real symmetric matrix via orthogonal similarity transformations into a symmetric tridiagonal matrix.*

Algorithm: Transformation into upper-Hessenberg form

Let $A \in \mathbb{R}^{n\times n}$. To obtain the factor H of a Hessenberg decomposition $A = QHQ^{\mathrm{T}}$, do as follows:

for $i = 1, \ldots, n-2$ **do**

$x = A_{i+1:n,i}$

$v_i = \mathrm{sign}(\langle x, e_1\rangle)\|x\|_2 e_1 + x$

$v_i = \frac{v_i}{\|v_i\|_2}$

$A_{i+1:n,i:n} = A_{i+1:n,i:n} - 2v_i\left(v_i^{\mathrm{T}} A_{i+1:n,i:n}\right)$

$A_{1:n,i+1:n} = A_{1:n,i+1:n} - 2\left(A_{1:n,i+1:n} v_i\right) v_i^{\mathrm{T}}$

end for.

The algorithm stores the result H in place of A. Note that Q is not explicitly formed, but can be obtained from the vectors $v_1, \ldots, v_{n-2}$.

Theorem

The above algorithm requires $\sim \frac{10}{3}n^3$ *flops.*

If $A \in \mathbb{R}^{n\times n}$ is symmetric, clever modifications are used in practice to transform into tridiagonal form using only $\sim \frac{4}{3}n^3$ flops.

Backward stability of Hessenberg via Householder

Theorem

Suppose we apply the above algorithm to a matrix $A \in \mathbb{R}^{n\times n}$, leading to outputs $\tilde{H} \in \mathbb{R}^{n\times n}$ and $\tilde{v}_1, \dots, \tilde{v}_n \in \mathbb{R}^n$ (the computed factor H and reflection vectors v_i in floating point computation). Writing $\tilde{Q} := \tilde{Q}_1 \tilde{Q}_2 \dots \tilde{Q}_{n-2}$ with $\tilde{Q}_i$ denoting the orthogonal matrix corresponding to the reflection vector $\tilde{v}_i$, there holds

$$\tilde{Q}\tilde{H}\tilde{Q}^{\mathrm{T}} = A + \Delta A \quad \text{for some } \Delta A \in \mathbb{R}^{n\times n} \text{ with } \frac{\|\Delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{\mathrm{machine}})$$

for all matrix norms $\|\cdot\|$ on $\mathbb{R}^{n\times n}$.

6.4 Some classical algorithms

For simplicity, ...

Restriction: Assume from now on that $A = A^{\mathrm{T}} \in \mathbb{R}^{n \times n}$, i.e., A is a real symmetric matrix.

$\Longrightarrow \exists\ Q \in \mathbb{R}^{n \times n}$ orthogonal and $D = \mathrm{diag}_{n \times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A) \subseteq \mathbb{R}$ s.t. $A = QDQ^{\mathrm{T}}$.
(The i-th column of Q is an eigenvec to the eigenval λ_i.)

Rayleigh quotient: connection between eigvecs and eigvals

Definition (Rayleigh quotient)

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix. We define the map

$$R_A : \mathbb{R}^n \backslash \{0\} \to \mathbb{R}, \qquad x \mapsto \frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} = \frac{\langle Ax, x\rangle}{\|x\|_2^2} = \left\langle A\frac{x}{\|x\|_2}, \frac{x}{\|x\|_2}\right\rangle.$$

For $x \in \mathbb{R}^n\backslash\{0\}$, call $R_A(x)$ **Rayleigh quotient** of x (corresponding to A).

Theorem (Properties of the Rayleigh quotient)

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix.

(i) *If $x \in \mathbb{R}^n\backslash\{0\}$ is eigvec of A, then $R_A(x)$ is its corresponding eigval.*

(ii) *R_A is differentiable on $\mathbb{R}^n\backslash\{0\}$ with gradient $\nabla R_A : \mathbb{R}^n\backslash\{0\} \to \mathbb{R}^n$ given by $\nabla R_A(x) = 2\,\frac{Ax-(R_A(x))x}{\|x\|_2^2}$.*
For $x \in \mathbb{R}^n\backslash\{0\}$, have $\nabla R_A(x) = 0$ iff x is eigvec of A.

(iii) *If $q \in \mathbb{R}^n\backslash\{0\}$ eigvec of A: $|R_A(x) - R_A(q)| = \mathcal{O}(\|x-q\|_2^2)$ as $x \to q$.*

$A = A^{\mathrm{T}} \in \mathbb{R}^{n\times n}$. (i) If $x \in \mathbb{R}^n \backslash \{0\}$ eigvec of A, then $R_A(x)$ is corresponding eigval.
(ii) $\nabla R_A(x) = 2\,\frac{Ax-(R_A(x))x}{\|x\|_2^2}$, stationary pts of R_A are the eigvecs of A.
(iii) If $q \in \mathbb{R}^n \backslash \{0\}$ eigvec of A: $|R_A(x) - R_A(q)| = \mathcal{O}(\|x-q\|_2^2)$ as $x \to q$.

Proof: (i) Let $x \in \mathbb{R}^n \backslash \{0\}$ eigvec of A and let $\lambda \in \mathbb{R}$ be its corresponding eigval, i.e., $Ax = \lambda x$. Then,

$$R_A(x) = \frac{\langle Ax, x\rangle}{\|x\|_2^2} = \frac{\langle \lambda x, x\rangle}{\|x\|_2^2} = \lambda \frac{\langle x, x\rangle}{\|x\|_2^2} = \lambda.$$

(ii) Define $f, g : \mathbb{R}^n \to \mathbb{R}$, $f(x) := x^{\mathrm{T}} A x = \sum_{i,j=1}^n a_{ij} x_i x_j$, $g(x) := x^{\mathrm{T}} x = \sum_{i=1}^n x_i^2$. Note $R_A(x) = \frac{f(x)}{g(x)}$ $\forall x \in \mathbb{R}^n \backslash \{0\}$. Compute

$$\nabla f(x) = \sum_{i,j=1}^n a_{ij}\,(x_j e_i + x_i e_j) = 2\sum_{i,j=1}^n a_{ij} x_j e_i = 2\sum_{i=1}^n (Ax)_i e_i = 2Ax$$

and $\nabla g(x) = 2x$. Therefore, for any $x \in \mathbb{R}^n \backslash \{0\}$, we have

$$\nabla R_A(x) = \left(\frac{g\,\nabla f - f\,\nabla g}{g^2}\right)(x) = \frac{2\|x\|_2^2 Ax - 2(x^{\mathrm{T}}Ax)x}{\|x\|_2^4} = 2\,\frac{Ax - (R_A(x))x}{\|x\|_2^2}.$$

For $x \in \mathbb{R}^n \backslash \{0\}$: $\nabla R_A(x) = 0 \Leftrightarrow Ax = (R_A(x))x \Leftrightarrow x$ is eigvec of A.

(iii) Taylor: $R_A(x) = R_A(q) + \underbrace{(\nabla R_A(q))^{\mathrm{T}}}_{=0} x + \mathcal{O}(\|x-q\|_2^2)$ as $x \to q$. $\square$

Power iteration (Von Mises iteration)

$\Longrightarrow$ Algorithm for computing largest (in absolute value) eigval and a corresponding eigenvec (under suitable assumptions)

Given $A \in \mathbb{R}^{n\times n}$ symmetric.

Choose $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\|_2 = 1$, and do the following:

for $k = 1, 2, 3, \ldots$ **do**

$w = Av^{(k-1)}$

$v^{(k)} = \frac{w}{\|w\|_2}$

$\lambda^{(k)} = \langle Av^{(k)}, v^{(k)} \rangle$

end for

Observations:

- $\forall k \in \mathbb{N}$: $v^{(k)} = \frac{Av^{(k-1)}}{\|Av^{(k-1)}\|_2}$, and therefore,

$$v^{(k)} = \frac{A^k v^{(0)}}{\|A^k v^{(0)}\|_2}.$$

- $\forall k \in \mathbb{N}$: $\lambda^{(k)} = R_A(v^{(k)})$.

(Note: In practice, a suitable stopping criterion is necessary.)

Theorem (Convergence of power iteration)

Let $A \in \mathbb{R}^{n\times n}$ *symmetric with eigval decomposition* $A = QDQ^{\mathrm{T}}$, *where* $Q = (q_1|\cdots|q_n) \in \mathbb{R}^{n\times n}$ *orthogonal,* $D = \mathrm{diag}_{n\times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n\times n}$ *with* $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$ *and* $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$.

Let $v^{(0)} \in \mathbb{R}^n$ *with* $\|v^{(0)}\|_2 = 1$, *and let* $(v^{(k)}) \subseteq \mathbb{R}^n$ *and* $(\lambda^{(k)})_{k\in\mathbb{N}}$ *be the sequences produced by power iteration. If*

$$|\lambda_1| > |\lambda_2|, \qquad \langle v^{(0)}, q_1\rangle \neq 0,$$

then there holds

$$\lambda^{(k)} \to \lambda_1 \quad \textit{with} \quad |\lambda^{(k)} - \lambda_1| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right) \quad \textit{as} \quad k \to \infty,$$

$$\|v^{(k)} - s_k q_1\|_2 = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{k}\right) \quad \textit{as} \quad k \to \infty,$$

for some $(s_k)_{k\in\mathbb{N}} \subseteq \{-1, 1\}$. *("*$\mathrm{span}(v^{(k)})$ *converges to* $\mathrm{span}(q_1)$*")*

Proof: Suppose $|\lambda_1| > |\lambda_2|$ and $\langle v^{(0)}, q_1 \rangle \neq 0$. Write

$$v^{(0)} = \sum_{i=1}^{n} c_i q_i$$

with $c_1, \dots, c_n \in \mathbb{R}$. Note that $c_i = \langle v^{(0)}, q_i \rangle \ \forall \ i \in \{1, \dots, n\}$ and in particular, $c_1 \neq 0$. Then,

$$v^{(k)} = \frac{A^k v^{(0)}}{\|A^k v^{(0)}\|_2} = \frac{Q D^k Q^{\mathrm{T}} v^{(0)}}{\|Q D^k Q^{\mathrm{T}} v^{(0)}\|_2} = \frac{\sum_{i=1}^n c_i \lambda_i^k q_i}{\left\|\sum_{i=1}^n c_i \lambda_i^k q_i\right\|_2}$$

$$= \frac{c_1 \lambda_1^k}{|c_1 \lambda_1^k|} \frac{q_1 + \sum_{i=2}^n \frac{c_i}{c_1} \left(\frac{\lambda_i}{\lambda_1}\right)^k q_i}{\left\|q_1 + \sum_{i=2}^n \frac{c_i}{c_1} \left(\frac{\lambda_i}{\lambda_1}\right)^k q_i\right\|_2}.$$

If $\lambda_1 > 0$: $v^{(k)} \to \mathrm{sign}(c_1) q_1, \quad \|v^{(k)} - \mathrm{sign}(c_1) q_1\|_2 = \mathcal{O}(\left|\frac{\lambda_2}{\lambda_1}\right|^k)$.

If $\lambda_1 < 0$: $\|v^{(k)} - (-1)^k \mathrm{sign}(c_1) q_1\|_2 = \mathcal{O}(\left|\frac{\lambda_2}{\lambda_1}\right|^k)$.

$\Longrightarrow$

$|\lambda^{(k)} - \lambda_1| = |R_A(v^{(k)}) - R_A(s_k q_1)| = \mathcal{O}(\|v^{(k)} - s_k q_1\|_2^2) = \mathcal{O}(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k})$. $\square$

Drawbacks of power iteration

- It only computes the normalized eigenvector for the largest eigenvalue (and it computes only this largest eigenvalue).
- The rate of convergence for $\mathrm{span}(v^{(k)})$ to $\mathrm{span}(q_1)$ is only linear, i.e., the error in each step is reduced by a constant factor ($\approx |\frac{\lambda_1}{\lambda_2}|$).
- If $|\lambda_1| > |\lambda_2|$, but $|\lambda_1|$ is close to $|\lambda_2|$, then convergence is very slow (as $|\frac{\lambda_2}{\lambda_1}|$ is only slightly below 1).

Can we only compute "largest" eigval? An observation:

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix with an eigenvalue decomposition $A = QDQ^{\mathrm{T}}$ with $Q = (q_1|\cdots|q_n) \in \mathbb{R}^{n\times n}$ orthogonal and $D = \operatorname{diag}_{n\times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n\times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$.

Observation: For $\mu \in \mathbb{R}\backslash\Lambda(A)$, $A - \mu I_n \in \mathbb{R}^{n\times n}$ is invertible and

$$\Lambda\left((A-\mu I_n)^{-1}\right) = \left\{(\lambda_1-\mu)^{-1}, \ldots, (\lambda_n-\mu)^{-1}\right\}.$$

Indeed, for $i \in \{1, \ldots, n\}$, we have $(A-\mu I_n)^{-1} q_i = (\lambda_i - \mu)^{-1} q_i$ since

$$(A-\mu I_n)\left((\lambda_i-\mu)^{-1}q_i\right) = (\lambda_i-\mu)^{-1}\left(Aq_i - \mu q_i\right) = (\lambda_i-\mu)^{-1}(\lambda_i-\mu)q_i = q_i,$$

i.e., q_i is an eigenvec to $(A-\mu I_n)^{-1}$ with eigval $(\lambda_i-\mu)^{-1}$.

We observe that the eigenvalue of $(A-\mu I_n)^{-1}$ with the largest absolute value is $(\lambda_j-\mu)^{-1}$, where λ_j is the eigenvalue of A closest to μ.

$\Longrightarrow$ Apply power iteration to $(A-\mu I_n)^{-1}$ to find eigval of A closest to μ.

Inverse iteration: Power iteration for $(A - \mu I_n)^{-1}$

Let $A \in \mathbb{R}^{n \times n}$ symmetric and $\mu \in \mathbb{R} \backslash \Lambda(A)$.

Choose $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\|_2 = 1$, and do the following:

for $k = 1, 2, 3, \ldots$ **do**

  Solve $(A - \mu I_n) w = v^{(k-1)}$ for w $\quad (\Longleftrightarrow w = (A - \mu I_n)^{-1} v^{(k-1)})$

  $v^{(k)} = \frac{w}{\|w\|_2}$

  $\lambda^{(k)} = \langle A v^{(k)}, v^{(k)} \rangle$

end for

Theorem (Convergence of inverse iteration)

Let $A \in \mathbb{R}^{n \times n}$ *symmetric,* $A = QDQ^{\mathrm{T}}$ *with* $Q = (q_1 | \cdots | q_n) \in \mathbb{R}^{n \times n}$ *orthogonal and* $D = \mathrm{diag}_{n \times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n}$ *with* $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$. *Let* $\mu \in \mathbb{R} \backslash \Lambda(A)$, *let* $v^{(0)} \in \mathbb{R}^n$ *with* $\|v^{(0)}\|_2 = 1$. *Suppose* $\lambda_j, \lambda_k \in \Lambda(A)$ *are s.t.* $|\mu - \lambda_j| < |\mu - \lambda_k| \le |\mu - \lambda_i| \ \forall i \in \{1, \ldots, n\} \backslash \{j\}$ *and* $\langle v^{(0)}, q_j \rangle \neq 0$. *Then,*

$$|\lambda^{(k)} - \lambda_j| = \mathcal{O}\left(\left| \frac{\lambda_j - \mu}{\lambda_k - \mu} \right|^{2k} \right), \quad \|v^{(k)} - s_k q_j\|_2 = \mathcal{O}\left(\left| \frac{\lambda_j - \mu}{\lambda_k - \mu} \right|^{k} \right) \quad \textit{as} \quad k \to \infty$$

for some $(s_k)_{k \in \mathbb{N}} \subseteq \{-1, 1\}$.

Theorem (Convergence of inverse iteration)

Let $A \in \mathbb{R}^{n\times n}$ *symmetric,* $A = QDQ^{\mathrm{T}}$ *with* $Q = (q_1|\cdots|q_n) \in \mathbb{R}^{n\times n}$ *orthogonal and* $D = \operatorname{diag}_{n\times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n\times n}$ *with* $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$. *Let* $\mu \in \mathbb{R}\backslash\Lambda(A)$, *let* $v^{(0)} \in \mathbb{R}^n$ *with* $\|v^{(0)}\|_2 = 1$. *Suppose* $\lambda_j, \lambda_k \in \Lambda(A)$ *are s.t.* $|\mu - \lambda_j| < |\mu - \lambda_k| \leq |\mu - \lambda_i|\ \forall i \in \{1, \ldots, n\}\backslash\{j\}$ *and* $\langle v^{(0)}, q_j\rangle \neq 0$. *Then,*

$$|\lambda^{(k)} - \lambda_j| = \mathcal{O}\left(\left|\frac{\lambda_j - \mu}{\lambda_k - \mu}\right|^{2k}\right), \quad \|v^{(k)} - s_k q_j\|_2 = \mathcal{O}\left(\left|\frac{\lambda_j - \mu}{\lambda_k - \mu}\right|^{k}\right) \quad \text{as} \quad k \to \infty$$

for some $(s_k)_{k\in\mathbb{N}} \subseteq \{-1, 1\}$.

$\Longrightarrow$ If we have a good estimate for a certain eigval of A, can apply inverse iteration to produce this eigval and a corresponding eigvec.

$\Longrightarrow$ In particular, inverse iteration is the go-to method if one wants to find eigvecs to eigvals which are already known.

Drawback of inverse iteration: slow speed of convergence.

Rayleigh quotient iteration

Idea: Combine Rayleigh quotient (a way to find an eigval from an eigvec) and inverse iteration (a way to find an eigenvec from an eigenval).

Let $A \in \mathbb{R}^{n \times n}$ symmetric.

Choose $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\|_2 = 1$, set $\lambda^{(0)} := \langle Av^{(0)}, v^{(0)} \rangle$ and do:

for $k = 1, 2, 3, \dots$ **do**

  Solve the linear system $(A - \lambda^{(k-1)} I_n)w = v^{(k-1)}$

  $v^{(k)} = \frac{w}{\|w\|_2}$

  $\lambda^{(k)} = \langle Av^{(k)}, v^{(k)} \rangle$

end for

Choose $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\|_2 = 1$, set $\lambda^{(0)} := \langle Av^{(0)}, v^{(0)} \rangle$ and do:

for $k = 1, 2, 3, \ldots$ **do**

Solve the linear system $(A - \lambda^{(k-1)} I_n) w = v^{(k-1)}$

$v^{(k)} = \frac{w}{\|w\|_2}$

$\lambda^{(k)} = \langle Av^{(k)}, v^{(k)} \rangle$

end for

Theorem (Convergence of Rayleigh quotient iteration)

Let $A \in \mathbb{R}^{n \times n}$ symmetric, $A = QDQ^{\mathrm{T}}$ with $Q = (q_1 | \cdots | q_n) \in \mathbb{R}^{n \times n}$ orthogonal and $D = \operatorname{diag}_{n \times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$. Then, for almost all $v^{(0)} \in \mathbb{R}^n$ with $\|v^{(0)}\|_2 = 1$, the sequences $(v^{(k)}) \subseteq \mathbb{R}^n$ and $(\lambda^{(k)}) \subseteq \mathbb{R}$ converge to an eigvec and eigval of A. Further, in this case and if $\lambda_j \in \Lambda(A)$ is such that $v^{(0)}$ is sufficiently close to q_j, then

$$|\lambda^{(k+1)} - \lambda_j| = \mathcal{O}\left(|\lambda^{(k)} - \lambda_j|^3\right), \quad \|v^{(k+1)} - s_{k+1} q_j\|_2 = \mathcal{O}\left(\|v^{(k)} - s_k q_j\|_2^3\right)$$

for some $(s_k)_{k \in \mathbb{N}} \subseteq \{-1, 1\}$.

$\Longrightarrow$ **Cubic order of convergence!** (extremely quick)

Example: Let $A := \begin{pmatrix} -1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$. Choose $v^{(0)} := \frac{1}{3}\begin{pmatrix} 1 \\ -2 \\ 2 \end{pmatrix}$.

Step 0: Compute

$$\lambda^{(0)} := \langle Av^{(0)}, v^{(0)} \rangle = -\tfrac{17}{9} = -1.8888\ldots$$

Step 1: Solve $(A - \lambda^{(0)} I_3)w^{(1)} = v^{(0)}$. Find $w^{(1)} = \frac{3}{70}(191, -265, 184)^{\mathrm{T}}$.

$$v^{(1)} := \frac{w^{(1)}}{\|w^{(1)}\|_2} = \begin{pmatrix} \frac{191}{3\sqrt{15618}} \\ \frac{-265}{3\sqrt{15618}} \\ \frac{184}{3\sqrt{15618}} \end{pmatrix} = \begin{pmatrix} 0.5094\ldots \\ -0.7068\ldots \\ 0.4907\ldots \end{pmatrix},$$

$$\lambda^{(1)} := \langle Av^{(1)}, v^{(1)} \rangle = -\frac{128518}{70281} = -1.8286\ldots$$

Step 2: Solve $(A - \lambda^{(1)} I_3)w^{(2)} = v^{(1)}$ and compute

$$v^{(2)} := \frac{w^{(2)}}{\|w^{(2)}\|_2} = \begin{pmatrix} 0.49999838\ldots \\ -0.70710677\ldots \\ 0.50000162\ldots \end{pmatrix}, \quad \lambda^{(2)} := \langle Av^{(2)}, v^{(2)} \rangle = -1.82842712475\ldots$$

Rk: $\lambda^{(k)} \to 1 - 2\sqrt{2}$ and $\mathrm{span}(v^{(k)})$ converges to $\mathrm{span}((\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2})^{\mathrm{T}})$.

6.5 The QR algorithm

Restriction: Assume from now on that $A = A^{\mathrm{T}} \in \mathbb{R}^{n \times n}$, i.e., A is a real symmetric matrix.

$\Longrightarrow$ there exist an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ and a diagonal matrix $D = \mathrm{diag}_{n \times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A) \subseteq \mathbb{R}$ s.t. $A = QDQ^{\mathrm{T}}$. (The i-th column of Q is an eigenvec to the eigenval λ_i.)

Recall: If $A \in \mathbb{R}^{n \times n}$ symmetric, we can find a Hessenberg decomposition

$$A = QHQ^{\mathrm{T}}$$

with $Q \in \mathbb{R}^{n \times n}$ orthogonal and $H \in \mathbb{R}^{n \times n}$ symmetric and tridiagonal.

$\Longrightarrow$ Work with H instead of A.

QR algorithm

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric tridiagonal matrix. Set $A^{(0)} := A$ and do:

for $k = 1, 2, 3, \ldots$ **do**

Compute a QR factorization $A^{(k-1)} = Q^{(k)} R^{(k)}$ of $A^{(k-1)}$

$A^{(k)} = R^{(k)} Q^{(k)}$

end for

Note that for any $k \in \mathbb{N}$ we have

$$A^{(k)} = (Q^{(k)})^{\mathrm{T}} A^{(k-1)} Q^{(k)},$$

i.e., the QR algorithm consists of orthogonal similarity transformations.

We are going to see that the sequence $(A^{(k)})_{k \in \mathbb{N}}$ converges under suitable assumptions to a Schur form of A (here, as A is symmetric, this means to a diagonal matrix containing the eigenvalues of A on the diagonal).

Simultaneous iteration

Suppose we are given a symmetric tridiagonal matrix $A \in \mathbb{R}^{n \times n}$ (i.e., Hessenberg reduction has already been performed).

Consider the following approach: Take linearly independent vectors $v_1^{(0)}, \ldots, v_n^{(0)} \in \mathbb{R}^n$ and apply power iteration to these vectors simultaneously in the following sense:

Setting $V^{(0)} := (v_1^{(0)} | \cdots | v_n^{(0)})$, compute $V^{(k)} := A^k V^{(0)}$ and write

$$(v_1^{(k)} | \cdots | v_n^{(k)}) = V^{(k)} = (A^k v_1^{(0)} | \cdots | A^k v_n^{(0)}),$$

and orthogonalize in the sense of computing a QR factn $V^{(k)} = Q^{(k)} R^{(k)}$.

Under suitable assumptions, the span of the first l columns of $Q^{(k)}$ will converge to the span of eigvecs $q_1, \ldots, q_l$ to the l largest (in $|\cdot|$) eigvals.

In practice, in view of numerical stability, the following normalized version of simultaneous iteration is used (orthonormalize at each step):

Simultaneous iteration

Let $A \in \mathbb{R}^{n\times n}$ symmetric, tridiagonal. Choose $Q^{(0)} \in \mathbb{R}^{n\times n}$ orthogonal.

for $k = 1, 2, 3, \ldots$ **do**

$Z = AQ^{(k-1)}$

Compute a QR factorization $Z = Q^{(k)}R^{(k)}$ of Z

$A^{(k)} = (Q^{(k)})^{\mathrm{T}} A Q^{(k)}$

end for

Theorem (Convergence of simultaneous iteration)

Let $A \in \mathbb{R}^{n\times n}$ symmetric, tridiagonal, with eigenvalue decompn $A = QDQ^{\mathrm{T}}$ with $Q = (q_1|\cdots|q_n) \in \mathbb{R}^{n\times n}$ orthogonal and $D = \mathrm{diag}_{n\times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n\times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$. Suppose $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$. Then, if

$$\det(M_{1:i,1:i}) \neq 0 \quad \forall i \in \{1, \ldots, n\}, \text{ where } \quad M := Q^{\mathrm{T}}Q^{(0)},$$

and writing $Q^{(k)} = (q_1^{(k)}|\ldots|q_n^{(k)})$, we have for any $j \in \{1, \ldots, n\}$ that for some $(s_k)_{k\in\mathbb{N}} \subseteq \{-1, 1\}$ there holds

$$\|q_j^{(k)} - s_k q_j\|_2 = \mathcal{O}\left(\left(\max_{i\in\{1,\ldots,n-1\}} \left|\frac{\lambda_{i+1}}{\lambda_i}\right|\right)^k\right).$$

QR algorithm $\Longleftrightarrow$ simultaneous iteration

Theorem (Equivalence of QR algorithm and simultaneous iteration)

The QR algorithm and simultaneous iteration with $Q^{(0)} := I_n$ produce the same sequences $(A^{(k)})_{k\in\mathbb{N}}$. Further, we have that

$$\begin{aligned} Q_{\mathrm{sIt}}^{(k)} &= Q_{\mathrm{QR}}^{(1)} Q_{\mathrm{QR}}^{(2)} \cdots Q_{\mathrm{QR}}^{(k)} =: \tilde{Q}_{\mathrm{QR}}^{(k)}, \\ \tilde{R}_{\mathrm{sIt}}^{(k)} := R_{\mathrm{sIt}}^{(k)} \cdots R_{\mathrm{sIt}}^{(2)} R_{\mathrm{sIt}}^{(1)} &= R_{\mathrm{QR}}^{(k)} \cdots R_{\mathrm{QR}}^{(2)} R_{\mathrm{QR}}^{(1)} =: \tilde{R}_{\mathrm{QR}}^{(k)} \end{aligned}$$

for any $k \in \mathbb{N}$, and there holds

$$\begin{aligned} A^{(k)} &= (\tilde{Q}_{\mathrm{QR}}^{(k)})^{\mathrm{T}} A \, \tilde{Q}_{\mathrm{QR}}^{(k)}, \\ A^k &= \tilde{Q}_{\mathrm{QR}}^{(k)} \tilde{R}_{\mathrm{QR}}^{(k)}. \end{aligned}$$

(Here, the subscript sIt refers to the iterates from simultaneous iteration and the subscript QR refers to the iterates from the QR algorithm.)

Convergence of QR algorithm

Theorem (Convergence of QR algorithm)

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric tridiagonal matrix with an eigenvalue decomposition $A = QDQ^{\mathrm{T}}$ with $Q = (q_1|\cdots|q_n) \in \mathbb{R}^{n\times n}$ orthogonal and $D = \mathrm{diag}_{n\times n}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n\times n}$ with $\{\lambda_1, \ldots, \lambda_n\} = \Lambda(A)$. Suppose

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$$

and that

$$\det(Q_{1:i,1:i}) \neq 0 \quad \forall i \in \{1, \ldots, n\}.$$

Let $(A^{(k)})_{k\in\mathbb{N}}$ and $(Q^{(k)})_{k\in\mathbb{N}}$ be the sequences produced by the QR algorithm, and let $\tilde{Q}^{(k)} := (\tilde{q}_1^{(k)}|\cdots|\tilde{q}_n^{(k)}) := Q^{(1)}Q^{(2)}\cdots Q^{(k)}$ for $k \in \mathbb{N}$. Then, as $k \to \infty$, $A^{(k)} \to D$, and for any $j \in \{1, \ldots, n\}$ we have for some $(s_k)_{k\in\mathbb{N}} \subseteq \{-1, 1\}$ that $\tilde{q}_j^{(k)} - s_k q_j \to 0$. The speed of convergence is linear with constant $\max_{i\in\{1,\ldots,n-1\}} \left|\frac{\lambda_{i+1}}{\lambda_i}\right|$.

Observation: the iterates $A^{(k)}$ are Rayleigh quotients:

$$a_{ii}^{(k)} = \langle e_i, A^{(k)} e_i\rangle = \langle e_i, (\tilde{Q}^{(k)})^{\mathrm{T}} A \tilde{Q}^{(k)} e_i\rangle = \langle \tilde{Q}^{(k)} e_i, A\tilde{Q}^{(k)} e_i\rangle = \langle \tilde{q}_i^{(k)}, A\tilde{q}_i^{(k)}\rangle = R_A(\tilde{q}_i^{(k)})$$

for any $i \in \{1, \ldots, n\}$.

Example: QR algorithm

Consider $A := \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$. The matrix A has the eigenvalue decomposition $A = QDQ^{\mathrm{T}}$ with

$$D := \mathrm{diag}_{3\times 3}(\lambda_1, \lambda_2, \lambda_3) := \begin{pmatrix} 1+\sqrt{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1-\sqrt{2} \end{pmatrix} = \begin{pmatrix} 2.414\ldots & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -0.414\ldots \end{pmatrix}$$

$$Q := (q_1|q_2|q_3) := \begin{pmatrix} -\frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -0.5 & 0.707\ldots & -0.5 \\ 0.707\ldots & 0 & -0.707\ldots \\ 0.5 & 0.707\ldots & 0.5 \end{pmatrix}.$$

Let us perform the QR algorithm:

Step $k = 1$

We need to compute a QR factorization of $A^{(0)} := A$. Take the QR factorization $A^{(0)} = Q^{(1)}R^{(1)}$ with

$$Q^{(1)} := \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}, \qquad R^{(1)} := \begin{pmatrix} \sqrt{2} & -\sqrt{2} & -\frac{1}{\sqrt{2}} \\ 0 & 1 & 1 \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

We compute

$$A^{(1)} := R^{(1)}Q^{(1)} = \begin{pmatrix} 2 & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} = \begin{pmatrix} 2 & -0.707\ldots & 0 \\ -0.707\ldots & 1 & 0.707\ldots \\ 0 & 0.707\ldots & 0 \end{pmatrix}$$

$$\tilde{Q}^{(1)} := Q^{(1)} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0.707\ldots & 0 & 0.707\ldots \\ -0.707\ldots & 0 & 0.707\ldots \\ 0 & 1 & 0 \end{pmatrix}.$$

Step $k = 2$

We need to compute a QR factorization of $A^{(1)}$. We omit the details and take the QR factorization $A^{(1)} = Q^{(2)}R^{(2)}$ with

$$Q^{(2)} := \begin{pmatrix} \frac{2\sqrt{2}}{3} & \frac{1}{3\sqrt{2}} & \frac{1}{3\sqrt{2}} \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}, \qquad R^{(2)} := \begin{pmatrix} \frac{3}{\sqrt{2}} & -1 & -\frac{1}{3\sqrt{2}} \\ 0 & 1 & \frac{\sqrt{2}}{3} \\ 0 & 0 & \frac{\sqrt{2}}{3} \end{pmatrix}.$$

We compute

$$A^{(2)} := R^{(2)}Q^{(2)} = \begin{pmatrix} \frac{7}{3} & -\frac{1}{3} & 0 \\ -\frac{1}{3} & 1 & \frac{1}{3} \\ 0 & \frac{1}{3} & -\frac{1}{3} \end{pmatrix} = \begin{pmatrix} 2.333\ldots & -0.333\ldots & 0 \\ -0.333\ldots & 1 & 0.333\ldots \\ 0 & 0.333\ldots & -0.333\ldots \end{pmatrix},$$

$$\tilde{Q}^{(2)} := \tilde{Q}^{(1)}Q^{(2)} = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} \end{pmatrix} = \begin{pmatrix} 0.666\ldots & 0.666\ldots & -0.333\ldots \\ -0.666\ldots & 0.333\ldots & -0.666\ldots \\ -0.333\ldots & 0.666\ldots & 0.666\ldots \end{pmatrix}.$$

Step $k = 3$

We need to compute a QR factorization of $A^{(2)}$. We omit the details and take the QR factorization $A^{(2)} = Q^{(3)} R^{(3)}$ with

$$Q^{(3)} := \begin{pmatrix} \frac{7}{5\sqrt{2}} & \frac{2}{15} & \frac{1}{15\sqrt{2}} \\ -\frac{1}{5\sqrt{2}} & \frac{14}{15} & \frac{7}{15\sqrt{2}} \\ 0 & \frac{1}{3} & -\frac{2\sqrt{2}}{3} \end{pmatrix}, \qquad R^{(3)} := \begin{pmatrix} \frac{5\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & -\frac{1}{15\sqrt{2}} \\ 0 & 1 & \frac{1}{5} \\ 0 & 0 & \frac{3}{5\sqrt{2}} \end{pmatrix}.$$

We compute

$$A^{(3)} := R^{(3)} Q^{(3)} = \begin{pmatrix} \frac{12}{5} & -\frac{1}{5\sqrt{2}} & 0 \\ -\frac{1}{5\sqrt{2}} & 1 & \frac{1}{5\sqrt{2}} \\ 0 & \frac{1}{5\sqrt{2}} & -\frac{2}{5} \end{pmatrix} = \begin{pmatrix} 2.4 & -0.141\ldots & 0 \\ -0.141\ldots & 1 & 0.141\ldots \\ 0 & 0.141\ldots & -0.4 \end{pmatrix},$$

$$\tilde{Q}^{(3)} := \tilde{Q}^{(2)} Q^{(3)} = \begin{pmatrix} \frac{4}{5\sqrt{2}} & \frac{3}{5} & \frac{4}{5\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{3}{5\sqrt{2}} & \frac{4}{5} & -\frac{3}{5\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0.565\ldots & 0.6 & 0.565\ldots \\ -0.707\ldots & 0 & 0.707\ldots \\ -0.424\ldots & 0.8 & -0.424\ldots \end{pmatrix}.$$

Step $k = 4$

We need to compute a QR factorization of $A^{(3)}$. We omit the details and take the QR factorization $A^{(3)} = Q^{(4)}R^{(4)}$ with

$$Q^{(4)} := \begin{pmatrix} \frac{12\sqrt{2}}{17} & \frac{7}{85\sqrt{2}} & \frac{1}{85\sqrt{2}} \\ -\frac{1}{17} & \frac{84}{85} & \frac{12}{85} \\ 0 & \frac{1}{5\sqrt{2}} & -\frac{7}{5\sqrt{2}} \end{pmatrix}, \qquad R^{(4)} := \begin{pmatrix} \frac{17}{5\sqrt{2}} & -\frac{1}{5} & -\frac{1}{85\sqrt{2}} \\ 0 & 1 & \frac{\sqrt{2}}{17} \\ 0 & 0 & \frac{5\sqrt{2}}{17} \end{pmatrix}.$$

We compute

$$A^{(4)} := R^{(4)}Q^{(4)} = \begin{pmatrix} \frac{41}{17} & -\frac{1}{17} & 0 \\ -\frac{1}{17} & 1 & \frac{1}{17} \\ 0 & \frac{1}{17} & -\frac{7}{17} \end{pmatrix} = \begin{pmatrix} 2.411\ldots & -0.058\ldots & 0 \\ -0.058\ldots & 1 & 0.058\ldots \\ 0 & 0.058\ldots & -0.411\ldots \end{pmatrix},$$

$$\tilde{Q}^{(4)} := \tilde{Q}^{(3)}Q^{(4)} = \begin{pmatrix} \frac{9}{17} & \frac{12}{17} & -\frac{8}{17} \\ -\frac{12}{17} & \frac{1}{17} & -\frac{12}{17} \\ -\frac{8}{17} & \frac{12}{17} & \frac{9}{17} \end{pmatrix} = \begin{pmatrix} 0.529\ldots & 0.705\ldots & -0.470\ldots \\ -0.705\ldots & 0.058\ldots & -0.705\ldots \\ -0.470\ldots & 0.705\ldots & 0.529\ldots \end{pmatrix}.$$

We see that after 4 steps of the QR algorithm, we have obtained the following approximations to the eigenvalues:

$$\begin{aligned}
&\lambda_1 \approx \tfrac{41}{17} = 2.411\ldots, && (\text{recall } \lambda_1 = 1+\sqrt{2} = 2.414\ldots)\\
&\lambda_2 \approx 1, && (\text{recall } \lambda_2 = 1)\\
&\lambda_3 \approx -\tfrac{7}{17} = -0.411\ldots, && (\text{recall } \lambda_3 = 1-\sqrt{2} = -0.414\ldots)
\end{aligned}$$

and the following approximations to the (subspaces spanned by the) eigenvectors:

$$\mathrm{span}(q_1) \approx \mathrm{span}(\begin{pmatrix} \frac{9}{17} \\ -\frac{12}{17} \\ -\frac{8}{17} \end{pmatrix}) = \mathrm{span}(\begin{pmatrix} 0.529\ldots \\ -0.705\ldots \\ -0.470\ldots \end{pmatrix}), \quad (\text{recall } q_1 = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix})$$

$$\mathrm{span}(q_2) \approx \mathrm{span}(\begin{pmatrix} \frac{12}{17} \\ \frac{1}{17} \\ \frac{12}{17} \end{pmatrix}) = \mathrm{span}(\begin{pmatrix} 0.705\ldots \\ 0.058\ldots \\ 0.705\ldots \end{pmatrix}), \quad (\text{recall } q_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix})$$

$$\mathrm{span}(q_3) \approx \mathrm{span}(\begin{pmatrix} -\frac{8}{17} \\ -\frac{12}{17} \\ \frac{9}{17} \end{pmatrix}) = \mathrm{span}(\begin{pmatrix} -0.470\ldots \\ -0.705\ldots \\ 0.529\ldots \end{pmatrix}) \quad (\text{recall } q_3 = \begin{pmatrix} -\frac{1}{2} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix})$$

QR algorithm with Rayleigh quotient shift

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric tridiagonal matrix. Set $A^{(0)} := A$ and do the following:

for $k = 1, 2, 3, \dots$ **do**

$\mu^{(k)} = A^{(k-1)}_{nn}$ [here, $A^{(k-1)}_{nn}$ is the (n,n)-entry of $A^{(k-1)}$]

Compute a QR factorization $A^{(k-1)} - \mu^{(k)} I_n = Q^{(k)} R^{(k)}$

$A^{(k)} = R^{(k)} Q^{(k)} + \mu^{(k)} I_n$

end for

Remarks:

(i) For $k \in \mathbb{N}$ define $\tilde{Q}^{(k)} := Q^{(1)} Q^{(2)} \cdots Q^{(k)}$ and $\tilde{R}^{(k)} := R^{(k)} \cdots R^{(1)}$. Then, for any $k \in \mathbb{N}$ we have

$$A^{(k)} = (\tilde{Q}^{(k)})^{\mathrm{T}} A \tilde{Q}^{(k)}, \quad (A - \mu^{(k)} I_n)(A - \mu^{(k-1)} I_n) \cdots (A - \mu^{(1)} I_n) = \tilde{Q}^{(k)} \tilde{R}^{(k)}.$$

The first result follows from the fact that

$$\begin{aligned} A^{(k)} &= (Q^{(k)})^{\mathrm{T}} Q^{(k)} (R^{(k)} Q^{(k)} + \mu^{(k)} I_n) = (Q^{(k)})^{\mathrm{T}} \left((Q^{(k)} R^{(k)}) Q^{(k)} + \mu^{(k)} Q^{(k)} \right) \\ &= (Q^{(k)})^{\mathrm{T}} \left((A^{(k-1)} - \mu^{(k)} I_n) Q^{(k)} + \mu^{(k)} Q^{(k)} \right) = (Q^{(k)})^{\mathrm{T}} A^{(k-1)} Q^{(k)} \end{aligned}$$

for any $k \in \mathbb{N}$. The proof of the second result is omitted.

(ii) The first column of $\tilde{Q}^{(k)}$ is the result of applying k steps of shifted power iteration to e_1 with shifts $\mu^{(1)}, \dots, \mu^{(k)}$, and the last column of $\tilde{Q}^{(k)}$ is the result of applying k steps of shifted inverse iteration to e_n with shifts $\mu^{(1)}, \dots, \mu^{(k)}$. To see the latter, define $P := (e_n| \cdots |e_2|e_1) \in \mathbb{R}^{n \times n}$ and note that

$$(A - \mu^{(k)} I_n)^{-1}(A - \mu^{(k-1)} I_n)^{-1} \cdots (A - \mu^{(1)} I_n)^{-1} P = ((\tilde{Q}^{(k)} \tilde{R}^{(k)})^{-1})^{\mathrm{T}} P$$
$$= \left((\tilde{R}^{(k)})^{-1}(\tilde{Q}^{(k)})^{\mathrm{T}}\right)^{\mathrm{T}} P = (\tilde{Q}^{(k)} P)(P((\tilde{R}^{(k)})^{-1})^{\mathrm{T}} P)$$

is a QR factorization of the left-hand side.

(iii) For any $k \in \mathbb{N}$, we have

$$A^{(k)}_{nn} = \langle e_n, A^{(k)} e_n \rangle = \langle e_n, (\tilde{Q}^{(k)})^{\mathrm{T}} A \tilde{Q}^{(k)} e_n \rangle = \langle \tilde{Q}^{(k)} e_n, A \tilde{Q}^{(k)} e_n \rangle$$
$$= \langle \tilde{q}^{(k)}_n, A \tilde{q}^{(k)}_n \rangle = R_A(\tilde{q}^{(k)}_n),$$

where $\tilde{q}^{(k)}_n := \tilde{Q}^{(k)} e_n$ denotes the last column of $\tilde{Q}^{(k)}$.

(iv) The approximation $\mu^{(k)}$ to the eigenvalue corresponding to the eigenvector approximated by $\tilde{q}^{(k)}_n$, and the approximated eigenvector $\tilde{q}^{(k)}_n$, are the result of Rayleigh quotient iteration applied to e_n. It follows that we have cubic convergence for the convergence of $\mathrm{span}(\tilde{q}^{(k)}_n)$ to the span of an eigenvector.

QR algorithm in practice: shift and deflation

Let A be a real symmetric tridiagonal square matrix. Set $A^{(0)} := A$ and do the following:

for $k = 1, 2, 3, \dots$ **do**

Choose a shift $\mu^{(k)}$, e.g., the final diagonal entry of $A^{(k-1)}$

Compute a QR factorization $A^{(k-1)} - \mu^{(k)} I_n = Q^{(k)} R^{(k)}$

$A^{(k)} = R^{(k)} Q^{(k)} + \mu^{(k)} I_n$

If an off-diagonal element $A^{(k)}_{i,i+1}$ *is sufficiently close to* 0*, set* $A^{(k)}_{i,i+1} := 0$*,* $A^{(k)}_{i+1,i} := 0$ *so that* $A^{(k)} = \left(\begin{array}{c|c} A_1 & 0 \\ \hline 0 & A_2 \end{array}\right)$ *is block-diagonal and apply the algorithm to* A_1 *and* A_2*.*

end for

End of “Chapter 6: Eigenvalue Problems”.