November 28, 2022

Recommended reading:

- Lectures 24, 25, 27 in [4]
- Sections I.6 in [3]
- Sections 6.1, 6.2, 6.4 in [2]
- Kapitel 7 in [1]

Literature:


[1] R. Rannacher.
*Numerik 0 - Einführung in die Numerische Mathematik.*
Heidelberg University Publishing, 2017.

[2] G. Strang.
*Introduction to Linear Algebra.*
Wellesley-Cambridge Press, 2003.

[3] G. Strang.
*Linear Algebra and Learning from Data.*
Wellesley-Cambridge Press, 2019.

[4] L.N. Trefethen and D. Bau.
*Numerical linear algebra.*
SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

# 3 Eigenvalues: Theory and Algorithms

## 3.1 Introduction

## 3.2 Eigenvalues and Eigendecompositon

**Definition 3.2 (*Eigenvalues and -vectors*)** *Let $A \in \mathbb{F}^{n \times n}$ be a matrix. A number $\lambda \in \mathbb{C}$ is called an* ***eigenvalue*** *of $A$, if*

$$\exists v \in \mathbb{F}^n, v \neq 0: \; Av = \lambda v.$$

*In that case, $v$ is called an* ***eigenvector*** *and $(\lambda, v)$ an* ***eigenpair***. *The set of all eigenvalues is denoted by*

$$\sigma(A) := \{\lambda \in \mathbb{C} : \lambda \text{ is eigenvalue of } A\}$$

*and called the* ***spectrum of*** *$A$.*

1) Assume we knew an eigenvalue $\lambda$:

2) Assume we had an eigenvector $v$:

## The determinant and eigenvalues

Let $A \in \mathbb{F}^{n \times n}$. Then:

**Lemma 3.4 (*Matrix and Eigenvalue Properties*)**

i) *Power of a matrix:* $A \in \mathbb{F}^{n\times n},\ \lambda \in \sigma(A) \quad \Rightarrow \quad \lambda^k \in \sigma(A^k)$ *for any* $k \in \mathbb{N}$

ii) *Inverse matrix:* $A \in GL_n(\mathbb{F}),\ \lambda \in \sigma(A) \quad \Rightarrow \quad \lambda \neq 0,\ \frac{1}{\lambda} \in \sigma(A^{-1})$

iii) *Scaling:* $A \in \mathbb{F}^{n\times n},\ \lambda \in \sigma(A) \quad \Rightarrow \quad \alpha\lambda \in \sigma(\alpha A)$ *for any* $\alpha \in \mathbb{F}$

iv) $A \in \mathbb{F}^{n\times n}$ *hermitian* $(A = A^H) \quad \Rightarrow \quad \sigma(A) \subset \mathbb{R}$.

v) $Q \in \mathbb{F}^{n\times n}$ *unitary* $(Q^H Q = I)$, $\lambda \in \sigma(Q) \quad \Rightarrow \quad |\lambda| = 1$

vi) $A \in \mathbb{F}^{n\times n}$ *positive definite (semi-definite)* $(x^H A x > 0\ (\geq 0)) \quad \Leftrightarrow \quad \forall \lambda \in \sigma(A):\ \lambda > 0\ (\lambda \geq 0)$

vii) *The eigenvalues of an upper (lower) triangular matrix are sitting on the diagonal.*

viii) *Similarity transformation:* $A \in \mathbb{F}^{n\times n},\ T \in GL_n(\mathbb{F}) \quad \Rightarrow \quad \sigma(A) = \sigma(T^{-1}AT)$

ix) *Shifts:* $A \in \mathbb{F}^{n\times n},\ (\lambda, v)$ *eigenpair of* $A \quad \Rightarrow \quad \forall s \in \mathbb{F}:\ (\lambda + s, v)$ *eigenpair of* $A + sI$

**Attention:** The following rules do not hold in general:

- $\lambda \in \sigma(A), \mu \in \sigma(B) \quad \not\Rightarrow \quad (\lambda + \mu) \in \sigma(A + B)$
- $\lambda \in \sigma(A), \mu \in \sigma(B) \quad \not\Rightarrow \quad (\lambda \cdot \mu) \in \sigma(A \cdot B)$

*Proof.* Exercise.

# Diagonalizing a matrix

Let us first revisit the example from above (see Examples ?? and ??)

In the previous Example **??** the matrix $V$ of eigenvectors turned out to be orthogonal. The next theorem states, that this is true for any real symmetric matrix.

**Theorem 3.6 (*Eigendecomposition of real symmetric matrices*)** *For any symmetric matrix $A \in \mathbb{R}^{n \times n}$, there is an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ (i.e., $Q^\top Q = I$) such that*

$$Q^\top A Q = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix} =: \mathit{diag}(\lambda_1, \ldots, \lambda_n) \quad (= \textit{diagonal matrix})$$

*and $\lambda_i \in \mathbb{R}, i \in \{1, \ldots, n\}$, are the eigenvalues of $A$. The columns of $Q$ are the normalized eigenvectors.*

*Proof.* In the exercises we will prove this statement for the special case that the matrix has $n$ distinct eigenvalues. The general proof is rather technical and can be found in any standard textbook.

$\rightarrow$ **Thus:** "knowing the eigenpairs = knowing the matrix"

An immediate consequence of Theorem 3.6 is this:
**Corollary 3.7** *A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is invertible, if and only if all its eigenvalues are nonzero.*

Geometry of the eigendecomposition:

## 3.3 Eigenvalue Algorithms: Solving the eigenvalue problem

**Aim:** Solving the ***eigenvalue problem*** defined by

$$\textit{Given } A \in \mathbb{F}^{n\times n}, \textit{ find eigenpairs } (\lambda_i, v_i) \textit{ so that, for all } i = 1, \ldots, n,$$

$$v_i \neq 0 \;\; \textit{and} \;\; Av_i = \lambda_i v_i.$$

Sometimes we are only interested in a few eigenpairs $(\lambda_i, v_i)$ (for example the one with largest eigenvalue in magnitude). In this case we call it a *partial* eigenvalue problem.

### Overview

1. **A first naive approach: Direct method**
   $\rightarrow$ only feasible for very small matrices: $n \in \{2, 3, 4\}$

2. **Partial eigenvalue problem: Simple iterative methods** (here: The Power Method)
   $\rightarrow$ determine a *single* eigenpair

3. **A second advanced approach: General iterative method** (here: The $QR$ algorithm)
   $\rightarrow$ determine *all* eigenpairs

## 3.3.1 A first naive approach: Direct method

**Recipe:**

a) Eigenvalues:
Solving **root finding problem** for the characteristic polynomial

$$\chi_A(\lambda) := \det(A - \lambda I) = 0$$

yields the eigenvalues $\lambda_i$.

b) Eigenvectors:
Solving the homogeneous **linear system**

$$(A - \lambda_i I)v_i = 0$$

for each distinct $\lambda_i$, gives the corresponding eigenvectors $v_i$ (or more precisely, eigenspaces).

**Example:** $n = 2$

Consider a general $(2 \times 2)$-matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$.

a) Root finding problem:
Above, we have derived a closed formula for the determinant of a $(2 \times 2)$-matrix, which applied to $A - \lambda I$ gives

$$0 = \chi_A(\lambda) = \det(A - \lambda I) = \det\left(\begin{pmatrix} a-\lambda & b \\ c & d-\lambda \end{pmatrix}\right) = (a-\lambda)(d-\lambda) - cb = \lambda^2 - (a+d)\lambda + (ad - cb)$$

$$\to \lambda_{1/2} = \frac{a+d}{2} \pm \sqrt{\left(\frac{a+d}{2}\right)^2 - (ad - cb)}.$$

b) Linear system:
We then have to solve

$$\begin{pmatrix} a-\lambda_i & b \\ c & d-\lambda_i \end{pmatrix} \begin{pmatrix} v_1^i \\ v_2^i \end{pmatrix} \quad \text{for} \quad i = 1, 2.$$

$$\to v^1, v^2$$

Note: For $n = 3$ we can proceed similarly by applying the rule of Sarrus in step a).

**Problem:**

In practice, for general, potentially very large, matrices the root finding problem is infeasible, because:

$$A \text{ with large dimension } n \quad \Rightarrow \quad \chi_A \text{ high polynomial degree} \quad \Rightarrow \quad \text{high risk of rounding errors}$$

See for example:
https://en.wikipedia.org/wiki/Root-finding_algorithms#Roots_of_polynomials

**Abel–Ruffini theorem** (see related discussion in [4, Theorem 25.1]):
*There are no "closed formulas" for the roots of general polynomials with degree higher than* $4$*.*

**As a consequence**:

We cannot solve the eigenvalue problem in finitely many steps.
Instead, any eigenvalue algorithm has to be iterative!

### 3.3.2 Simple Iterative Method: The Power Iteration

$\rightarrow$ basis for PageRank algorithm from Google and the WTF algorithm from Twitter

**Theorem 3.10 (*Convergence of power iteration*)** *Let $A \in \mathbb{R}^{n\times n}$ be a matrix with eigenvalues $\lambda_i$ for $i \in \{1,\dots,n\}$ which satisfy $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ and whose eigenvectors form a basis of $\mathbb{R}^n$. Also, let the sequence of vectors $\{w^k\}_{k=0}^{\infty}$ be defined by the so-called* ***power iteration***

$$w^{k+1} := \frac{Aw^k}{\|Aw^k\|_p},\ k \geq 0, p \geq 1, \quad \text{with} \quad w^0 \text{ such that } (v^1, w^0)_2 \neq 0,$$

*where $v^1$ is the normalized (i.e., $\|v^1\|_p = 1$) eigenvector corresponding to $\lambda_1$. Then, for $k \to \infty$, we find $w^k \longrightarrow \pm v^1$ and also the so-called Rayleigh quotients*

$$\mu_k := \frac{(w^k, Aw^k)_2}{(w^k, w^k)_2} \longrightarrow \lambda_1.$$

*Proof.* See, e.g., [1, Satz 7.3] or [4, Theorem 27.1 ].

*Remark:*

- A variant of this approach is given by the so-called **inverse power method**, which can estimate any eigenpair, assumed a good initial guess for the eigenvalue is available.
- The assumption on the eigenvectors is satisfied, e.g., for real symmetric matrices (see Theorem 3.6)
- From the proof idea one finds that the convergence speed is determined by the fraction $\left(\frac{\lambda_2}{\lambda_1}\right)^k$ (potentially very slow)

### 3.3.3 A second advanced approach: General iterative method

**Recall:** (Lemma 3.4)

a) Similar matrices have the same eigenvalues:

$$\sigma(A) = \sigma(T^{-1}AT) \quad \text{for} \quad T \in GL_n(\mathbb{F}).$$

b) Simple matrices: Eigenvalues of an upper triangular matrix $U$ (e.g., a diagonal matrix) are found on its diagonal, i.e.,

$$\sigma(U) = \{u_{11}, \ldots, u_{nn}\}.$$

**Recipe:**

a) Iteratively applying similarity transformations $T_k \in GL_n(\mathbb{F})$ to $A =: A_0$ thereby producing a sequence

$$A_k = T_k^{-1} A_{k-1} T_k.$$

b) Choose $T_k$ so that this sequence converges to a simple matrix (triangular or even diagonal)

$$A_\infty := \lim_{k \to \infty} A_k.$$

$\rightarrow$ **Question:** Choice of the $T_k$'s?

**Requirements** on the transformations $T_k$:

1. easily constructed from $A_{k-1}$
2. easy to invert (e.g., orthogonal matrix)
3. $(A_k)_k$ converges to something simple

**One Implementation:**

a) The $QR$-**Algorithmn** defines such transformations $T_k$ through

$$
\begin{aligned}
&A_0 = A \\
&\textbf{for } k = 1, \dots, \infty : \\
&\qquad Q_k R_k := A_{k-1} \\
&\qquad A_k := R_k Q_k
\end{aligned}
$$

b) We find: $A_k = \overline{Q}_k^T A \overline{Q}_k \xrightarrow[k\to\infty]{} U$, where $U$ is (quasi) upper triangular; given as follows:

**Theorem 3.11 ($QR$ *Algorithm*)** *Consider a matrix $A \in \mathbb{R}^{n\times n}$ with distinct eigenvalues $\lambda_i$ for $i = 1, \ldots, n$, i.e., $|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n|$. Then the iterates $A_k \in \mathbb{R}^{n\times n}$ produced by the $QR$ algorithm converge to the diagonal matrix $\Lambda := diag(\lambda_1, \ldots, \lambda_n)$ which consists of the eigenvalues of $A$, i.e.,*

$$\lim_{k\to\infty} A_k = \Lambda.$$

*Proof.* See, e.g., [1, Satz 7.8].

Finally: **What about the eigenvectors?**

One can further show that similar to the power iteration, we find that the columns of

$$\overline{Q}_\infty := \lim_{k\to\infty} \overline{Q}_k$$

are normalized eigenvectors of $A$.

### 3.3.4 In Practice: Combined Iterative Methods

**Problems:**

- $QR$ decomposition for general and very large matrices too expensive
- Exact Schur complement is not reached in finitely many steps ( $=$ many $QR$ decompositions needed)

**However:**

- Any matrix can be reduced to a Hessenberg matrix ($=$ simple matrix) in *finitely many* steps
- $QR$ decomposition for this type of matrix is cheap

This leads to:

**(3) A third state-of-the-art approach: Combined iterative methods**

a) **Similarity transformation via reduction** (e.g., Householder, Wilkinson, Givens) to something simple such as Hessenberg or even tridiagonal
*($\rightarrow$ finite steps)*

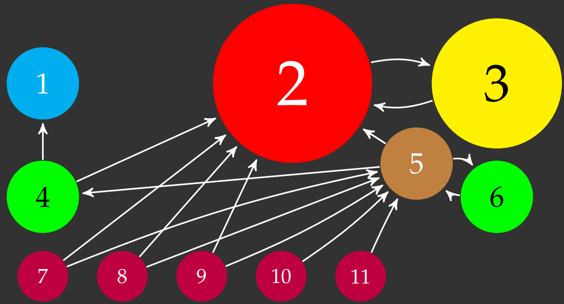
b) **Similarity transformation via iterative method** (e.g., $QR$ or $LR$ algorithm)
*($\rightarrow$ potentially infinitely many steps)*

Standard: $QR$ Algorithm (with performance optimized modifications (shifts etc...))

c) Determine eigenvalues from the limiting simple matrix (and eigenvectors from the similarity transformations).

Common combination in practice: (a) Householder reflection + (b) $QR$ algorithm
$\rightarrow$ Works pretty well for matrices up to 1 mio. columns $n \approx 10^6$
$\rightarrow$ for larger matrices one needs to develop problem-tailored structure exploiting methods

## 3.4 Example: The PageRank Algorithm from Google




**Aim:** Rank search enginge results according to the *"importance"* of the web pages.

**1998:** For this purpose, Larry Page and Sergei Brin develop the PageRank algorithm as the basis of the Google empire.

**Assumption:** *"important"* means more links from other (important) web pages.

→ More details on the sheet and in the video.