- **3** Eigenvalues: Theory and Algorithms
 - Introduction
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 - Eigenvalue Algorithms: Solving the eigenvalue problem
 - Example: The PageRank Algorithm from Google

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.

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

[3] G. Strang.

Linear Algebra and Learning from Data.

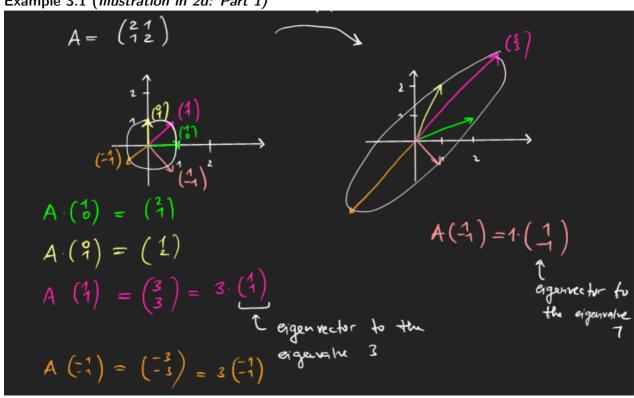
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3 Eigenvalues: Theory and Algorithms

3.1 Introduction

Example 3.1 (Illustration in 2d: Part 1)



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

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

In that case, v is called an **eigenvector** and (λ, 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 λ : Then we find a corresponding eigenvector by solving the linear equation

$$(A - \lambda I_n)v = 0$$

Observation:

v eigenvector $\Rightarrow \alpha v$ eigenvector $\forall \alpha \in \mathbb{F}$

We often normalize the eigenvector by $\frac{v}{\|v\|_2}$.

2) Assume we had an eigenvector v: Then the corresponding eigenvalue is uniquely determined by the so-called *Rayleigh-Quotient*

$$\lambda = \frac{v^T A v}{v^T v}$$

The determinant and eigenvalues

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

1) Relation between the determinant and eigenvalues:

$$\lambda \in \mathbb{C}$$
 eigenvalue of $A \Leftrightarrow \exists v \neq 0 \colon Av = \lambda v \Leftrightarrow \exists v \neq 0 \colon (A - \lambda I_n)v = 0$ $\Leftrightarrow \exists v \neq 0 \colon v \in \ker(A - \lambda I_n) \Leftrightarrow (A - \lambda I_n) \text{ not injective}$ $\Leftrightarrow (A - \lambda I_n) \notin \operatorname{GL}(n, \mathbb{F}) \Leftrightarrow \det(A - \lambda I_n) = 0$

2) Implication:

By invoking the Laplace formula (see Def.??) for the determinant we can show that the function

$$\lambda \mapsto \chi_A(\lambda) := \det(A - \lambda I_n)$$

is a **polynomial of degree** $\leq n$. Thus, we can state:

The eigenvalues of A are the roots of the polynomial $\chi_A(\lambda)$.

The fundamental theorem of algebra then assures the existence of eigenvalues (at most n distinct ones).

Definition: The polynomial $\chi_A(\lambda)$ is called characteristic polynomial of A.

Example 3.3 (Illustration in 2d: Part 2)

Let us consider the (2×2) matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

from Example 3.1 above.

• We compute its eigenvalues by solving the following root finding problem:

$$0 = \chi_A(\lambda) = \det(A - \lambda I) = \det\left(\begin{pmatrix} 2 - \lambda & 1\\ 1 & 2 - \lambda \end{pmatrix}\right) = (2 - \lambda)^2 - 1$$

$$\Leftrightarrow \lambda \in \{3, 1\} =: \{\lambda_1, \lambda_2\} = \sigma(A)$$

- Now that we have the eigenvalues we can find corresponding eigenvectors by solving the following homogeneous linear systems:
 - For $\lambda_1 = 3$:

$$(A - \lambda_1 I)v^1 = 0 \Leftrightarrow \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}v^1 = 0 \Rightarrow v_1^1 - v_2^1 = 0$$

Thus, the set of all eigenvectors corresponding to the eigenvalue λ_1 is given by

$$E(\lambda_1):=\{v\in\mathbb{R}^2:\ Av=\lambda_1v\}\quad =\quad \{v\in\mathbb{R}^2:\ v_1^1=v_2^1\}=\quad \{\binom{\alpha}{\alpha}\in\mathbb{R}^2:\ \alpha\in\mathbb{R}\}=\quad \operatorname{span}\left(\binom{1}{1}\right)$$

Sometimes it is reasonable to choose eigenvectors of length 1, so that we normalize: $v^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

- For $\lambda_2 = 1$:

$$(A - \lambda_2 I)v^2 = 0 \iff \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} v^2 = 0 \iff v_1^2 + v_2^2 = 0$$

Thus, the set of all eigenvectors corresponding to the eigenvalue λ_2 is given by

$$E(\lambda_2):=\{v\in\mathbb{R}^2:\ Av=\lambda_2v\}=\{v\in\mathbb{R}^2:\ v_1^2=-v_2^2\}=\{\begin{pmatrix}\alpha\\-\alpha\end{pmatrix}\in\mathbb{R}^2:\ \alpha\in\mathbb{R}\}=\operatorname{span}\left(\begin{pmatrix}1\\-1\end{pmatrix}\right)$$

Normalization: Choose $v^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Remark:

The set of all eigenvectors corresponding to the eigenvalue $\lambda \in \sigma(A)$, i.e.,

$$E(\lambda) = \ker(A - \lambda I) \subset \mathbb{F}^n$$

is called eigenspace to the eigenvalue λ of A.

Lemma 3.4 (Matrix and Eigenvalue Properties)

- i) Power of a matrix: $A \in \mathbb{F}^{n \times n}$, $\lambda \in \sigma(A) \Rightarrow \lambda^k \in \sigma(A^k)$ for any $k \in \mathbb{N}$
- ii) Inverse matrix: $A \in GL_n(\mathbb{F})$, $\lambda \in \sigma(A) \Rightarrow \lambda \neq 0$, $\frac{1}{\lambda} \in \sigma(A^{-1})$
- iii) Scaling: $A \in \mathbb{F}^{n \times n}$, $\lambda \in \sigma(A) \Rightarrow \alpha \lambda \in \sigma(\alpha A)$ for any $\alpha \in \mathbb{F}$
- iv) $A \in \mathbb{F}^{n \times n}$ hermitian $(A = A^H) \Rightarrow \sigma(A) \subset \mathbb{R}$.
- v) $Q \in \mathbb{F}^{n \times n}$ unitary $(Q^H Q = I)$, $\lambda \in \sigma(Q) \Rightarrow |\lambda| = 1$
- vi) $A \in \mathbb{F}^{n \times n}$ positive definite (semi-definite) $(x^H Ax > 0 \ (\geq 0)) \Leftrightarrow \forall \lambda \in \sigma(A) : \lambda > 0 \ (\lambda \geq 0)$
- vii) The eigenvalues of an upper (lower) triangular matrix are sitting on the diagonal.
- viii) Similarity transformation: $A \in \mathbb{F}^{n \times n}$, $T \in GL_n(\mathbb{F}) \Rightarrow \sigma(A) = \sigma(T^{-1}AT)$
 - ix) Shifts: $A \in \mathbb{F}^{n \times n}$, (λ, v) eigenpair of $A \Rightarrow \forall s \in \mathbb{F}$: $(\lambda + s, v)$ eigenpair of A + sI

Attention: The following rules do not hold in general:

- $\lambda \in \sigma(A)$, $\mu \in \sigma(B)$ \Rightarrow $(\lambda + \mu) \in \sigma(A + B)$
- $\lambda \in \sigma(A), \mu \in \sigma(B) \implies (\lambda \cdot \mu) \in \sigma(A \cdot B)$

Proof. Exercise. Here, we exemplary prove viii):

Diagonalizing a matrix

Let us consider a matrix $A \in \mathbb{F}^{n \times n}$ with eigenpairs $(\lambda_i, v_i) \in \mathbb{F} \times \mathbb{F}^n$, so that

$$Av_i = \lambda_i v_i$$
, for $1 \le i \le n$.

Using matrix notation this can be written as

$$A \cdot \underbrace{\begin{pmatrix} \mid & \mid & & \mid \\ v_1 & v_2 & \cdots & v_n \\ \mid & \mid & & \mid \end{pmatrix}}_{=:V \in \mathbb{F}^{n \times n}} = \begin{pmatrix} \mid & \mid & & \mid \\ \lambda_1 v_1 & \lambda_2 v_2 & \cdots & \lambda_n v_n \\ \mid & \mid & & \mid \end{pmatrix} = \begin{pmatrix} \mid & & \mid \\ v_1 & \cdots & v_n \\ \mid & & \mid \end{pmatrix} \underbrace{\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}}_{=:\Lambda \in \mathbb{F}^{n \times n}}$$

which is equivalent to

$$AV = V\Lambda$$
.

If V is invertible (note that this is not necessarily the case!), then we can rearrange this into the following decomposition

$$V^{-1}AV = \Lambda \Leftrightarrow A = V\Lambda V^{-1}.$$

One central question arises: When is V invertible?

Let us first revisit the example from above (see Examples 3.1 and 3.3)

Example 3.5 (Illustration in 2d: Part 3)

Let us again consider the real symmetric matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

with eigenpairs

$$\lambda_1 = 3, \ v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \lambda_2 = 1, \ v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Assembling the normalized eigenvectors into the matrix V yields

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Since for the columns we have

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 1 - 1 = 0$$

and by construction

$$\|v_1\|_2 = \frac{1}{\sqrt{2}} \underbrace{\| \begin{pmatrix} 1 \\ 1 \end{pmatrix} \|}_{\sqrt{2}} = 1$$
, and similarly $\|v_2\|_2 = 1$,

we find that V is orthogonal and thus in particular invertible.

In the previous Example 3.5 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

$$Q^{ op}AQ = egin{pmatrix} \lambda_1 & & & & & \\ & \lambda_2 & & & & \\ & & \ddots & & & \\ & & & \lambda_n \end{pmatrix} =: \textit{diag}(\lambda_1,\ldots,\lambda_n) \ \ \textit{(= diagonal matrix)}$$

and $\lambda_i \in \mathbb{R}, i \in \{1, ..., n\}$, 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.

Let us again continue our example:

Example 3.8 (Illustration in 2d: Part 4)

For the symmetric matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

with eigenpairs

$$\lambda_1 = 3, \ v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \lambda_2 = 1, \ v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

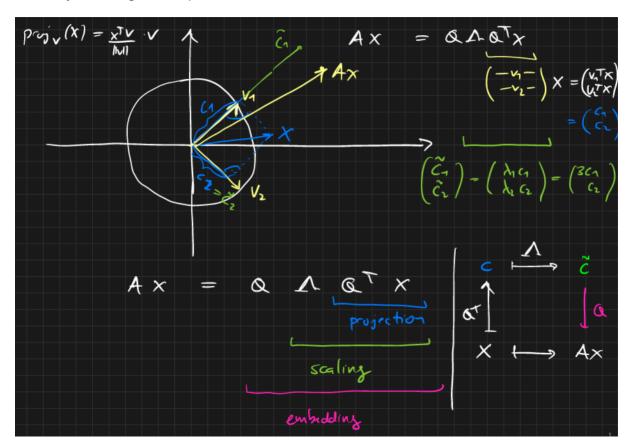
let us set

$$Q:=V=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}\quad\text{and}\quad \Lambda:=\begin{pmatrix}3&0\\0&1\end{pmatrix}.$$

Indeed, we can verify

$$A = Q\Lambda Q^{T} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \underbrace{\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{=\begin{pmatrix} 3 & 3 \\ 1 & -1 \end{pmatrix}}$$
$$= \begin{pmatrix} 4 & 2 \\ 2 & 4 \end{pmatrix}$$
$$= \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Geometry of the eigendecomposition:



3.3 Eigenvalue Algorithms: Solving the eigenvalue problem

Aim: Solving the eigenvalue problem defined by

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

$$v_i \neq 0$$
 and $Av_i = \lambda_i v_i$.

Sometimes we are only interested in a few eigenpairs (λ_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
 - ightarrow 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 λ_i .

b) Eigenvectors:
Solving the homogeneous linear system

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

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

Example: n=2

Consider a general (2×2) -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 (2×2) -matrix, which applied to $A - \lambda I$ gives

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

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

b) Linear system:

We then have to solve

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

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 with large dimension $n \Rightarrow \chi_A$ high polynomial degree \Rightarrow 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!

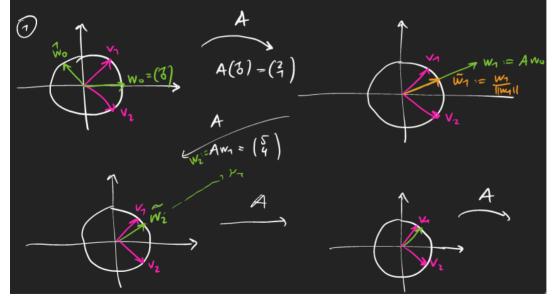
3.3.2 Simple Iterative Method: The Power Iteration

ightarrow basis for PageRank algorithm from Google and the WTF algorithm from Twitter

Example 3.9 (Illustration in 2d: Part 5)

Again, let us consider
$$A=\begin{pmatrix}2&1\\1&2\end{pmatrix}$$
, $\lambda_1=3$, $v_1=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$, $\lambda_2=1$, $v_2=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$.

Let us successively apply the matrix A to an initial guess $w^0 \in \mathbb{R}^n$:



Note: The normalization step can be performed with respect to any norm.

Theorem 3.10 (Convergence of power iteration) Let $A \in \mathbb{R}^{n \times n}$ be a matrix with eigenvalues λ_i for $i \in \{1, \ldots, n\}$ which satisfy $|\lambda_1| > |\lambda_2| \geq \ldots \geq |\lambda_n|$ 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**

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

where v^1 is the normalized (i.e., $||v^1||_p = 1$) eigenvector corresponding to λ_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]. The idea: Let $v^i \in \mathbb{R}^n$ be the corresponding eigenvectors. Then we can write the initial guess as linear combination $w^0 = \sum_{j=1}^n \mu_j v^j (\mu_1 \neq 0)$, so that with $c_k := \frac{1}{\|Aw^k\|_n}$ we find

$$w^{k} = c_{k}A^{k}w^{0} = c_{k}\sum_{j=1}^{n}\mu_{j}A^{k}v^{j} = c_{k}\sum_{j=1}^{n}\mu_{j}\lambda_{j}^{k}v^{j} = c_{k}\lambda_{1}^{k}\left(\mu_{1}v^{1} + \sum_{j=2}^{n}\mu_{j}\left(\frac{\lambda_{j}}{\lambda_{1}}\right)^{k}v^{j}\right).$$

The fractions $\left(\frac{\lambda_j}{\lambda_1}\right)^k$ vanish as $k \to \infty$ and the limit vector is in $\mathrm{span}(v^1)$. Since $\|w^k\|_p = \|v^1\|_p = 1$ the result follows.

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:

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

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

$$A_0 = A$$

for $k = 1, ..., \infty$:
 $Q_k R_k := A_{k-1}$
 $A_k := R_k Q_k$

Thus, inserting the first equation $R_k = Q_k^T A_{k-1}$ into the second gives

$$A_k = R_k Q_k = Q_k^T A_{k-1} Q_k = Q_k^T Q_{k-1}^T A_{k-2} Q_{k-1} Q_k = \dots = \overline{Q}_k^T A \overline{Q}_k$$

where

$$\overline{Q}_k := Q_1 \cdot Q_2 \cdots Q_{k-1} \cdot Q_k$$

Here: $T_k = Q_{k-1}$, where Q_{k-1} is derived from the QR decomposition of A_{k-1} .

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 λ_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 $\Lambda:=\operatorname{diag}(\lambda_1,\ldots,\lambda_n)$ 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

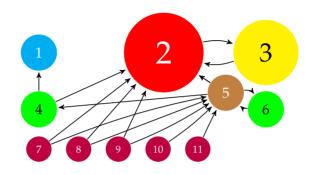
This leads to:

- (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
 (→ finite steps)
 - b) Similarity transformation via iterative method (e.g., QR or LR algorithm)
 (→ 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 $n \approx 10^6$
- ightarrow 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.

 \rightarrow More details on the sheet and in the video.