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The QR Algorithm

and other methods to compute the eigenvalues of complex matrices

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The QR Algorithm

> ”[The QR algorithm is] one of the most remarkable algorithms in numerical mathematics”
> (Strang)
>
> ”Indeed it is quite remarkable that an algorithm, wich is both effective and easy to describe, has resisted, and stoutly continues to resist, a full mathematical analysis, to such an extent that no proof of convergence in the most general case (the matrix not Hermitian; the QR algorithm with shifts) exists at the present, at the same time that no counter-example to convergence exists”
> (Phillippe G. Ciarlet)

Abstract

This work deals with variants of the power and QR method to determine the eigenvalues of complex matrices. First, definitions and properties about matrices, the eigenvalues problem and matrix decompositions are presented. Then the methods are thoroughly discussed. All presented algorithms were implemented and tested in Java.

Introduction

At first the eigenvalue problem seems quite clear. The eigenvalues of a matrix A are exactly the roots of its characteristic polynomial p_A and in $\mathbb{C}$ one can find all the roots of p_A. So why all the excitement?

The reason is the numeric instability of the determinant function. In fact one rather tries to find the zeroes of a polynomial by applying the QR algorithm to its companion matrix (which has exactly the zeroes of the polynomial as eigenvalues) than to form the characteristic polynomial of a matrix and find its zeroes.

The correspondence between (arbitrary) polynomials and the eigenvalue problem shows also that one cannot find explicit solutions for the eigenvalues of a matrix with more than 4x4 entries. Hence, one has to use iterative solutions. The QR method is a simple algorithm that does that. It can be improved to make it efficient. Anyway it has some disadvantages: It has problems with multiple eigenvalues and eigenvalues of equal modulus. Although one can try to work around theses problems there is no all-embracing algorithm to solve the eigenvalue problem.

Remarks

The reader needs basic knowledge in linear algebra and analysis (as gained in the first or second year of studying mathematics).

A ”$\bullet$” indicates a definition, a ”$\diamond$” indicates a proposition or theorem. In the whole paper $\mathbb{K}$ can be considered as $\mathbb{R}$ or $\mathbb{C}$.

The notation $\begin{pmatrix} \bullet & \bullet \\ \cdot & \bullet \end{pmatrix}$ stands for a 2x2 matrix A with arbitrary entries A_{11}, A_{12}, A_{22} and zero entry A_{21}.

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1 Matrices

1.1 Basic Definitions

Let denote:
- $M_{nl}(\mathbb{K})$ the set of all n-l matrices over $\mathbb{K}$
- $M_n(\mathbb{K})$ the set of all n-n matrices over $\mathbb{K}$ (i.e. $M_n(\mathbb{K}) := M_{nn}(\mathbb{K})$)
- I_n the n-n identity matrix
- 0_{nl} the n-l zero matrix.

For abbreviation let M_n denote $M_n(\mathbb{C})$.

For a matrix $A=(A_{ij}) \in M_{nl}(\mathbb{K})$ one defines:
- the **transposed matrix** $A^T \in M_{nl}(\mathbb{K})$ as $A^T=(B_{ij})$ with $B_{ij} := A_{ji}$
- the **conjugate-transposed matrix** $A^H \in M_{nl}(\mathbb{K})$ as $A^H=(B_{ij})$ with $B_{ij} := \overline{A_{ji}}$

◇ For real matrices: $A^H = A^T$

A matrix $A \in M_n(\mathbb{K})$ is called:
- **symmetric** $:\Leftrightarrow A^T = A$
- **skew-symmetric** $:\Leftrightarrow A^T = -A$
- **Hermitian** $:\Leftrightarrow A^H = A$
- **skew-Hermitian** $:\Leftrightarrow A^H = -A$
- **regular** $:\Leftrightarrow$ A is invertible
- **unitary** $:\Leftrightarrow A^H A = E$
- **orthogonal** $:\Leftrightarrow A^T A = E$
- **normal** $:\Leftrightarrow AA^H = A^H A$

◇ If $A \in M_n(\mathbb{R})$ then: A is (skew-)symmetric $\Leftrightarrow$ A is (skew-)Hermitian
A is orthogonal $\Leftrightarrow$ A is unitary
◇ If A is Hermitian, skew-Hermitian or unitary then A is normal.
◇ If A is Hermitian then $x^H Ax$ is real for $x \in \mathbb{C}^n$ and A is called
- positive (semi)definit (write: $A > 0, A \geq 0$) $:\Leftrightarrow \forall x \neq 0 : x^H Ax > 0$ (≥ 0)
- negative (semi)definit (write: $A < 0, A \leq 0$) $:\Leftrightarrow \forall x \neq 0 : x^H Ax < 0$ (≤ 0)
  A positive (negative) semi-definit matrix A is also called positive (negative).
  A positive (negative) definit matrix A is also called strictly positive (negative).

One defines:
- $GL_n(\mathbb{K}) := \{A \in M_n(\mathbb{K}) : A \text{ regular } \}$ = general linear group
- $SL_n(\mathbb{K}) := \{A \in M_n(\mathbb{K}) : \det A = 1\}$ = special linear group
- $O_n(\mathbb{K}) := \{A \in M_n(\mathbb{K}) : A \text{ orthogonal } \}$ = orthogonal group
- $SO_n(\mathbb{K}) := \{A \in M_n(\mathbb{K}) : A \text{ orthogonal, } \det A = 1\}$ = special orthogonal group
- $Sym(\mathbb{K}) := \{A \in M_n(\mathbb{K}) : A \text{ symmetric } \}$
- $H_n := \{A \in M_n(\mathbb{C}) : A \text{ Hermetian } \}$
- $U_n := \{A \in M_n(\mathbb{C}) : A \text{ unitary } \}$
- $US_n := \{A \in M_n(\mathbb{C}) : A \text{ unitary, } \det A = 1\}$
- $HPD_n := \{A \in M_n(\mathbb{C}) : A \text{ Hermitian, positive definit } \}$
- $SPD_n := \{A \in M_n(\mathbb{R}) : A \text{ symmetric, positive definit } \}$

Two matrices $A, B \in M_{nl}(\mathbb{K})$ are called:
- **equivalent** $:\Leftrightarrow \exists P_1 \in Gl_n(\mathbb{K}), P_2 \in Gl_l(\mathbb{K})$ s.t. $A = P_1 B P_2$

Two matrices $A, B \in M_n(\mathbb{K})$ are called:
- **similar** $:\Leftrightarrow \exists P \in Gl_n(\mathbb{K})$ s.t. $A = P^{-1}BP$
- **unitarily similar** $:\Leftrightarrow \exists P \in U_n(\mathbb{K})$ s.t. $A = P^{-1}BP$

A matrix $A \in M_n(\mathbb{K})$ is called:
- **lower triangular** $:\Leftrightarrow A_{ij} = 0$ whenever $i < j$
- **upper triangular** $:\Leftrightarrow A_{ij} = 0$ whenever $i > j$
- **diagonal** $:\Leftrightarrow A_{ij} = 0$ whenever $i \neq j$
- **reducible** $:\Leftrightarrow$ a nontrivial partition $\{1, ..., n\} = I \cup J$ exists s.t.
  (i) $A_{ij} = 0$ whenever $(i, j) \in I \times J$
- **irreducible** $:\Leftrightarrow A$ is not reducible
- **projection** $:\Leftrightarrow A$ is idempotent $(A^2 = A)$
- **permutation matrix** $:\Leftrightarrow A_{ij} = \delta_{i,s(j)}$ for some permutation $s \in S_n$

Let denote:
- diag $(d_1, ..., d_n)$ the diagonal n-n-matrix D s.t. $D_{ii} = d_i$
- P_s the permutation matrix related to the permutation $s \in S_n$

◇ Permutation matrices are real, orthogonal and have in every row and column exactly one nonzero entry. Further: $P_s^{-1} = P_{s^{-1}} = P_s^T$

◇ $A \in M_n$ is reducible iff a permutation matrix P exists s.t. $P^{-1}AP = \begin{pmatrix} B & C \\ 0_{p,n-p} & D \end{pmatrix}$.

◇ Every Projection P can be characterized by its image $M := \Im P$ and kernel $W :=$ Ker P. We say that P projects on M along W. It holds $\mathbb{C}^n = M \oplus W$. On the other side: If $\mathbb{C}^n = M \oplus W$ then there is an unique projection on M along W.

Every matrix $A \in M_{nl}(\mathbb{K})$ can be considered as linear map from $\mathbb{K}^l$ to $\mathbb{K}^n$ (and vice versa) via $x \mapsto Ax$. One defines:
- **null space (kernel)** Ker $A := \{x \in \mathbb{C}^n : Ax = 0\}$
- **range space** $\Im A := A\mathbb{C}^n = \{Ax : x \in \mathbb{C}^n\}$
- **trace** tr $A := A_{11} + ... + A_{nn}$

1.2 Matrix Norms

Since $M_{nl}(\mathbb{K})$ is a $\mathbb{K}$-vector space, the definition of a matrix norm is very natural:
- **matrix norm** = function $\|.\| : M_{nl}(\mathbb{K}) \to \mathbb{R}^+$ s.t. $\forall A, B \in M_{nl}(\mathbb{K}), \alpha \in \mathbb{K}$:
  (i) $\|A + B\| \leq \|A\| + \|B\|$ (triangular inequality)
  (ii) $\|\alpha A\| = |\alpha| \cdot \|A\|$ (homogeneity)
  (iii) $\|A\| = 0 \Leftrightarrow A = 0$

One calls a matrix norm $\|\cdot\|$ on $M_n(\mathbb{K})$ submultiplicative if $\forall A, B \in M_n(\mathbb{K})$:
  (iv) $\|AB\| \leq \|A\| \cdot \|B\|$

- A matrix norm $\|\cdot\|$ is said to consistent with a vector norm $\|\cdot\|$ if
  (i) $\|AX\| \leq \|A\|\|x\|, \quad \forall A \in M_n(\mathbb{K}), x \in \mathbb{K}^n$

Some important norms on $M_n(\mathbb{K})$ are:
- the **operator norm** regarding a norm $\|.\|$ on $\mathbb{K}^n$: $\|A\| := \max_{0 \neq x \in \mathbb{K}^n} \frac{\|Ax\|}{\|x\|} = \max_{\|x\|=1} \|Ax\|$
- the **p-norms** are special operator norms: $\|A\|_p = \max_{0 \neq x \in \mathbb{K}^n} \frac{\|Ax\|_p}{\|x\|_p}$, $p = 1, 2, \ldots, \infty$
- the **Schatten p-norms**: $\|A\|_{<p>} = \left(\sum_{j=1}^n \sigma_j(A)^p\right)^{1/p}$
- the Schatten 2-norm is also called **Frobenius norm** and denoted by $\|A\|_F$
- the **Ky Fan k-norms**: $\|A\|_{(k)} := \sum_{j=1}^k \sigma_j(A)$
  ($\sigma_i(A)$ are the singular values of A, see also section 3)

◇ One has the following characterization of the various norms:

(1) $\|A\|_1 = \max_j \sum_i |a_{ij}|$
(2) $\|A\|_\infty = \max_i \sum_j |a_{ij}| = \|A^H\|_1$
(3) $\|A\|_{<2>} = \|A\|_F = (\text{tr } A^H A)^{1/2} = \left(\sum_{i,j} |A_{ij}|^2\right)^{1/2}$

◇ All norms on $M_n(\mathbb{K})$ are equivalent.
◇ $\|A\|_2$ and $\|A\|_F$ are invariant w.r.t. unitary transformations
(i.e. $\|QAR\|_2 = \|A\|_2$, $\|QAR\|_F = \|A\|_F$ for appropriate unitary matrices Q, R)
One usually denotes by $|||\cdot|||$ a unitarily invariant norm.

• One defines for $A \in GL_n(\mathbb{K})$ the **condition number** relative to inversion as $\kappa_p(A) := \|A\|_p \|A^{-1}\|_p$.

2 The Eigenvalue Problem

For $\lambda \in \mathbb{K}$ one considers $E_A^\lambda := \text{Ker } (A - \lambda I_n) = \{x \in \mathbb{K}^n : Ax = \lambda x\}$.
◇ For all λ: $E_A^\lambda \subseteq_{sub} X$
One is interested in $\lambda' s$ where $\dim E_A^\lambda > 0$, i.e. where E_A^λ does not only contain 0.

The **eigenvalue problem** for $A \in M_n(\mathbb{K})$ is to find $0 \neq x \in \mathbb{K}^n$ and $\lambda \in \mathbb{K}$ s.t. $Ax = \lambda x$. In other words: find $\lambda \in \mathbb{K}$ s.t. $\dim E_A^\lambda > 0$.
One then calls:
• λ an **eigenvalue** of A
• x an **eigenvector** of A (associated with λ)
• E_A^λ the **eigenspace** of A associated with λ
◇ For every eigenvalue λ exists a **left eigenvector** $\psi \neq 0 : \psi^H A = \lambda \psi^H \quad (\Leftrightarrow A^H \psi = \overline{\lambda} \psi)$
◇ The eigenspaces of distinct eigenvalues $\lambda_1, ...\lambda_r$ are in direct sum.
(i.e. if $x_1 \in E^{\lambda_1}, ..., x_r \in E^{\lambda_r}, x_1 + ... + x_r = 0$ then $x_1 = ... = x_r = 0$)

The **characteristic polynomial** of $A \in M_n$ is $p_A(z) := \det(A - zI_n), z \in \mathbb{C}$.
◇ λ is eigenvalue of A iff it is a root of $p_A(z)$.
◇ Therefore A has exactly n (maybe repeated) eigenvalues in $\mathbb{C}$.
Let $\lambda_1(A), ..., \lambda_n(A)$ denote these eigenvalues s.t. equal values stay together and $|\lambda_1(A)| \geq ... \geq |\lambda_n(A)|$ (if possible I will just write $\lambda_1, ..., \lambda_n$)
Let $\mu_1(A), ..., \mu_K(A)$ denote the different eigenvalues of A

One further defines for A:
• the **spectrum** $\sigma(A) := \{\lambda \in \mathbb{C} : \lambda \text{ eigenvalue of } A\} = \{\lambda_1(A), ..., \lambda_n(A)\}$
• the **spectral radius** $r_\sigma(A) := \max_{\lambda \in \sigma(A)} |\lambda|$

◇ $p_A(z) = c_n z^n + c_{n-1} z^{n-1} + ... + c_0$ with $c_n = (-1)^n, c_{n-1} = (-1)^{n-1} \text{tr } A, c_0 = \det(A)$
◇ If A is similar to B then $p_A(z) = p_B(z)$, then $\sigma(A) = \sigma(B)$, tr A = tr B, $\det A = \det B$.
◇ For $A \in M_n$: $\sigma(A) = \sigma(A^T)$ and $\lambda \in \sigma(A) \Leftrightarrow \overline{\lambda} \in \sigma(A^H)$, hence $r_\sigma(A) = r_\sigma(A^H)$.

For an eigenvalue λ of A one defines:
• the **algebraic multiplicity** $m_A^\lambda :=$ multiplicity of the root λ of p_A
• the **geometric multiplicity** $g_A^\lambda := \dim E_A^\lambda$
◇ For all $\lambda \in \sigma(A)$: $1 \leq g_A^\lambda \leq m_A^\lambda \leq n$

An eigenvalue λ is called:
- **defective** $:\Leftrightarrow g_A^\lambda < m_A^\lambda$
- **nondefective** $:\Leftrightarrow g_A^\lambda = m_A^\lambda$
- **simple** $:\Leftrightarrow m_A^\lambda = 1$
- **geometrically simple** $:\Leftrightarrow g_A^\lambda = 1$

- A matrix is called **nondefective** if all its eigenvalues are nondefective.

◇ $A \in M_n$ is nondefective
$\Leftrightarrow \bigoplus_{\lambda \in \sigma(A)} E_A^\lambda = E_A^{\mu_1} \oplus ... \oplus E_A^{\mu_K} = \mathbb{K}^n$
$\Leftrightarrow$ there is an eigenbasis of $\mathbb{K}^n$ (a basis consisting of eigenvectors of A)
$\Leftrightarrow$ A admits an eigen decomposition (see section ...)
$\Leftrightarrow$ A is diagonalizable (i.e. A is similar to a diagonal matrix)

- A subset $S \subset \mathbb{C}^n$ is called **invariant** w.r.t. $A \in M_n :\Leftrightarrow AS \subseteq S$

There are various propositions concerning eigenvalues:

◇ If A is Hermitian (or real and symmetric) then all eigenvalues of A are real. ($\sigma(A) \subset \mathbb{R}$)
One can then order the eigenvalues. Let $\lambda_1^\downarrow(A) \geq ... \geq \lambda_n^\downarrow(A)$ and $\lambda_1^\uparrow(A) \leq ... \leq \lambda_n^\uparrow(A)$ denote the
eigenvalues of A in descending and increasing order, respectively.

◇ If A is skew-Hermitian then all eigenvalues of A are pure complex. ($\sigma(A) \subset i\mathbb{R}$)

◇ If A is unitary (or real and orthogonal) then all eigenvalues of A are of modulus 1.
($\sigma(A) \subset \mathbb{T} = \{z \in \mathbb{C} : |c| = 1\}$)

◇ **Schur Decomposition**: Every matrix $A \in M_n$ is unitarily similar to an upper triangular matrix
(see also section 3.9)

◇ Normal matrices are unitarily diagonalizable: (and only normal matrices are)
$A \in M_n(\mathbb{K})$ normal $\Leftrightarrow \exists U \in U_n : UAU^H = \text{diag}\ (\lambda_1, ..., \lambda_n)$

◇ Real normal matrices are orthogonally block-diagonalizable with blocks of size 1x1 and 2x2:
$A \in M_n(\mathbb{R})$ normal $\Rightarrow \exists O \in O_n(\mathbb{R}) : OAO^T = \text{diag}\ (\lambda_1, ..., \lambda_r, M_{r+1}, ..., M_n)$
where λ_k are the real eigenvalues of A and every M_k has the form $M_k = \begin{pmatrix} a_k & b_k \\ -b_k & a_k \end{pmatrix}, b_k \neq 0$ for
the conjugate complex eigenvalues $a_k \pm b_k i$ of A.

◇ Real symmetric matrices are orthogonally diagonalizable.

◇ **Break Down**: If $A \in M_n$ can be decomposed as $A = \begin{pmatrix} M_{11} & M_{12} \\ 0_{pp} & M_{22} \end{pmatrix}$ then $\sigma(A) = \sigma(M_{11}) \cup \sigma(M_{22})$.

3 Matrix Decompositions and Factorizations

This section presents the most important matrix decompositions.

3.1 LU Decomposition

- A LU decomposition of $A \in M_n(\mathbb{K})$ is a pair (L, U) of matrices $L, U \in M_n(\mathbb{K})$ s.t.
  (i) L is unit lower triangular (i.e. $L_{ii} = 1$)
  (ii) U is upper triangular
  (iii) $A = LU$

⋄ $A \in GL_n(\mathbb{K})$ admits a (unique) LU decomposition iff its leading principal minors are nonzero. (i.e. iff $\det A[1:p][1:p] \neq 0 \quad (p = 1:n)$)

3.2 LDM$^{\mathrm{T}}$ and LDL$^{\mathrm{T}}$ Decomposition

- A LDM$^{\mathrm{T}}$ decomposition of $A \in M_n(\mathbb{K})$ is a triple (L, D, M) of matrices $L, D, M \in M_n(\mathbb{K})$ s.t.
  (i) L is unit lower triangular (i.e. $L_{ii} = 1$)
  (ii) D is diagonal
  (ii) M is unit lower triangular
  (iv) $A = LDM^T$

⋄ $A \in GL_n(\mathbb{K})$ admits a (unique) LDM$^{\mathrm{T}}$ decomposition iff its leading principal minors are nonzero.

- If (L, D, M) is a LDM$^{\mathrm{T}}$ decomposition of a symmetric $A \in M_n(\mathbb{K})$ then $L = M$ and one calls this the LDL$^{\mathrm{T}}$ decomposition of A.

3.3 QR Decomposition

- A QR decomposition of $A \in M_n(\mathbb{K})$ is a pair (Q, R) of matrices $Q, R \in M_n(\mathbb{K})$ s.t.
  (i) Q is unitary
  (ii) R is upper triangular with positive diagonal entries ($R_{ii} > 0$)
  (iii) $A = QR$

⋄ Every $A \in GL_n(\mathbb{K})$ admits a (unique) QR decomposition.

- A generalized QR decomposition of $A \in M_{nl}(\mathbb{K})$ is a pair (Q, R) of matrices $Q \in M_n(\mathbb{K}), R \in M_{nl}(\mathbb{K})$ s.t.
  (i) Q is unitary
  (ii) R is pseudo upper triangular ($R_{ij} = 0$ whenever $i > j$)
  (iii) $A = QR$

⋄ Every $A \in M_{nl}(\mathbb{K})$ admits a (nonunique) generalized QR decomposition.

3.4 Cholesky Decomposition

- A Cholesky decomposition of $A \in M_n(\mathbb{K})$ is a matrix $L \in M_n(\mathbb{K})$, s.t.
  (i) L is lower triangular with positive diagonal entries ($L_{ii} > 0$)
  (ii) $A = LL^H$

⋄ $A \in HPD_n$ admits a (unique) Cholesky decomposition. If $A \in SPD_n$ then $L \in M_n(\mathbb{R})$.

3.5 SVD - Singular Value Decomposition

• A SV decomposition of $A \in M_{nl}(\mathbb{K})$ is a triple (U, D, V) of matrices $U \in M_n(\mathbb{K}), D \in M_{nl}(\mathbb{K})$, $V \in M_l(\mathbb{K})$ s.t.

(i) U, V are unitary
(ii) $D = \text{diag } (\sigma_1, \dots, \sigma_p)$ with $\sigma_1 \geq ... \geq \sigma_p \geq 0$ and $p = \min(n, l)$
(iii) $A = UDV^H$

◇ Every $A \in M_{nl}(\mathbb{K})$ admits a (nonunique) SV decomposition. The $\sigma_1, \dots, \sigma_p$ are uniquely determined by A (and thus equal in all SVD's). In fact $\sigma_i^2(A) = \sigma_i^2(A^H) = \lambda_i(AA^H) = \lambda_i(A^H A)$ for $i = 1, \dots, p$.

• If $D = \text{diag } (\sigma_1, \dots, \sigma_n), U = [u_1, \dots, u_n], V = [v_1, \dots, v_n]$ then the σ_i are called **singular values** of A, the u_i, v_i are called left- and right **singular vectors**, respectively.

• One denotes by $|A|$ the unique positive square root of $A^H A$.

3.6 Polar Decomposition

• A **polar decomposition** of $A \in M_{nl}(\mathbb{K})$ is a pair (U, P) of matrices $U \in M_n(\mathbb{K}), P \in M_{nl}(\mathbb{K})$ s.t.

(i) U is unitary
(ii) P is positive

◇ Every $A \in M_{nl}(\mathbb{K})$ admits a (nonunique) polar decomposition. The matrix P is uniquely determined by A. In fact $P = |A|$. The matrix U is unique iff A is regular.

3.7 Block Diagonal Decomposition

• A **block diagonal decomposition** of $A \in M_n(\mathbb{K})$ is a pair (P, B) of matrices $P, B \in M_n$ s.t.

(i) P is regular
(ii) $B = \text{diag } (\lambda_1 I_{n_1} + N_1, ..., \lambda_K I_{n_K} + n_K)$ is block diagonal where the λ_1 are the distinct eigenvalues of A, $N_i \in M_{n_i}$ are strictly upper triangular
(ii) $A = PBP^{-1}$

◇ Every $A \in M_n(\mathbb{C})$ admits a (nonunique) block diagonal decomposition.

3.8 Jordan Decomposition

• A **Jordan box** is a matrix $J_m(\lambda) \in M_n(\mathbb{K})$ of the form:

$$J_m(\lambda) = \begin{pmatrix} \lambda & 1 & & & \bigcirc \\ & \lambda & \ddots & & \\ & & \ddots & 1 & \\ & & & \lambda & 1 \\ \bigcirc & & & & \lambda \end{pmatrix}$$

• A Jordan decomposition of $A \in M_n(\mathbb{K})$ is a pair (P, J) of matrices $P, J \in M_n(\mathbb{K})$ s.t.

(i) P is regular
(ii) J is block diagonal $J = \text{diag } (J_1, \dots, J_K)$ with J_i being Jordan boxes
(ii) $P^{-1}AP = J$

◇ Every $A \in M_n(\mathbb{C})$ admits a (nonunique) Jordan decomposition. The basic numbers of the

Jordan blocks are eigenvalues of A. The number and dimensions of Jordan blocks corresponding to an eigenvalue are unique, although P can be chosen s.t. they appear in any order.

3.9 Schur Decomposition

- A Schur decomposition of $A \in M_n(\mathbb{K})$ is a pair (U, T) of matrices $U, T \in M_n(\mathbb{K})$ s.t.
  - (i) U is unitary
  - (ii) T is upper triangular with the eigenvalues of A as diagonal entries
  - (ii) $A = UTU^H$

This means $T = D + N$ with $D = \text{diag}\,(\lambda_{s(1)}, \ldots, \lambda_{s(n)})$ for some permutation $s \in S_n$ and N strictly upper triangular.

◇ Every $A \in M_n(\mathbb{C})$ admits a (nonunique) Schur decomposition. U can be chosen so that λ_i appear in any order in the diagonal of D.

- The column vectors in U are called **Schur vectors**.

◇ Let (U, T) be a Schur decomposition of $A \in M_n$ and $U = \begin{pmatrix} u_1 & \ldots & u_n \end{pmatrix}$ a partitioning of U in its Schur vectors, $D = \text{diag}\,(\lambda_1, ..., \lambda_n)$. Then the subspaces $S_k = \text{span}\,\{u_1, ..., u_k\}$ are invariant under A. Further, if $U_k = \begin{pmatrix} u_1 & \ldots & u_k \end{pmatrix}$ then $\sigma(U_k^H A U_k) = \{\lambda_1, ..., \lambda_k\}$. Since the eigenvalues of A can be arranged in any order in the diagonal of the Schur decomposition it follows that for every k-dimensional subset S of eigenvalues there exists a k-dimensional invariant subspace associated with the eigenvalues in S.

- $\|N\|_F$ is independent of the choice of U and called **A's departure from normality**

3.10 Eigen Decomposition

- An eigen decomposition of $A \in M_n(\mathbb{K})$ is a pair (P, D) of matrices $P, D \in M_n(\mathbb{K})$ s.t.
  - (i) P is regular
  - (ii) D is diagonal
  - (iii) $A = PDP^{-1}$

◇ $A \in M_n(\mathbb{K})$ admits an (nonunique) eigen decomposition iff it is nondefective.

◇ If $A \in M_n(\mathbb{K})$ is nondefective with eigenvalues $\lambda_1, ..., \lambda_n \in \mathbb{K}$ and corresponding (distinct) eigenvectors $x_1, ..., x_n$ then for every permutation $s \in S_n$:

If one sets $D = \text{diag}\,(\lambda_{s(1)}, ..., \lambda_{s(n)})$ and $P = [x_{s(1)}, \ldots, x_{s(n)}]$ then $A = PDP^{-1}$.

4 Sensitivity of the Eigenvalue Problem, Perturbation Theory

The family of all eigenvalues of an $A \in M_n$ can be regarded as unordered n-tuple of complex numbers. All these tuples form the space $\mathbb{C}^n_{sym} = \mathbb{C}^n_{/\sim}$ with $(a_1, ..., a_n) \sim (b_1, ..., b_n) \Leftrightarrow \exists s \in S_n : b_i = a_{s(i)}, i = 1, ..., n$. It is a quotient space of $\mathbb{C}^n$ and has therefore an induced metric:

(1) $d(M_1, M_2) := \min_{a \in M_1, b \in M_2} \|a - b\|_\infty$ where $M_1 = [(a_1, ..., a_n)]_{/\sim}, M_2 = [(b_1, ..., b_n)]_{/\sim}$

One can easily verify that this is equal to the now defined

- **spectral variation** (=optimal matching distance) of $A, B \in M_n$:

(2) $d(\sigma(A), \sigma(B)) := \inf_{s \in S_n} \max_j |\lambda_j(A) - \lambda_{s(j)}(B)|$ (S_n is the group of permutations on $\{1, ..., n\}$)

Another distance function for the spectra of two matrices is now introduced:

- For closed subsets $A, B \subset \mathbb{C}$ one defines $s(A, B) = \sup_{a \in A} \text{dist } (a, B) = \sup_{a \in A} \inf_{b \in B} |a - b|$. Then one defines the **Hausdorff distance** of A and B as $h(A, B) := \max(s(A, B), s(B, A))$. One can think of the spectrum of a matrix as a subset of $\mathbb{C}$. This defines the Hausdorff distance of the spectra of two matrices.

◇ For arbitrary $A, B \in M_n$:

(3) $h(\sigma(A), \sigma(B)) \leq d(\sigma(A), \sigma(B))$

Only for $n = 2$ are the two distances equal.

4.1 Continuity of the Eigenvalue Problem

The next theorem states that the eigenvalues of a matrix are continuous functions of its entries:
◇ For $A \in M_n, \lambda \in \sigma(A)$ let $d := \text{dist } (\lambda, \sigma(A) \setminus \{\lambda\})$ be the distance of λ to the other eigenvalues. Then for every $0 < \rho < d$ there exists $\epsilon > 0$ s.t.

(4) $\|E\| < \epsilon \Rightarrow \sum_{\mu \in \sigma(A+E) \cap D} m_\mu(A + E) = m_\lambda(A)$

where $D = B(\lambda, \rho) = \{z \in \mathbb{C}^n : |z - \lambda| < \rho\}, E \in M_n$.

With the notation of spectral variation this can be formulated more elegantly:
◇ Let $A, B \in M_n$ then $\forall \alpha > 0 \ \exists \epsilon > 0$ s.t.

(5) $\|A - B\| < \epsilon \Rightarrow d(\sigma(A), \sigma(B)) < \alpha$

4.2 Spectral Variation of Nonnormal Matrices

In this section some important results for nonnormal matrices are presented. These results can be greatly improved when one works with normal or Hermitian matrices.

The following theorem answers the question how good the diagonal entries of a matrix approximate its eigenvalues:
◇ **Gershgorin Theorems**:
1. If $A \in M_n$ then $\sigma(A) \subseteq \mathcal{S}_\mathcal{R} \cap \mathcal{S}_\mathcal{C}$ where

(6) $\mathcal{S}_\mathcal{R} = \bigcup_{i=1}^n \mathcal{R}_i, \quad \mathcal{R}_i = \{z \in \mathbb{C} : |z - A_{ii}| \leq \sum_{j=1, j \neq i}^n |a_{ij}|\}$
(7) $\mathcal{S}_\mathcal{C} = \bigcup_{j=1}^n \mathcal{C}_j, \quad \mathcal{C}_j = \{z \in \mathbb{C} : |z - A_{jj}| \leq \sum_{i=1, i \neq j}^n |a_{ij}|\}$

The $\mathcal{R}_i$ are called row Gershgorin circles, the $\mathcal{C}_i$ column Gershgorin circles.
2. If $\mathcal{S}_1 = \bigcup_{i=1}^m \mathcal{R}_i, \mathcal{S}_2 = \bigcup_{i=m+1}^n \mathcal{R}_i$ and $\mathcal{S}_1 \cap \mathcal{S}_2 = \emptyset$ then $\mathcal{S}_1$ contains exactly m eigenvalues of A

(counted with algebraic multiplicity).

The next theorems establish bounds for the variation of the spectra of two matrices:
◇ If $A, B \in M_n$ then:

(8) $h(\sigma(A), \sigma(B)) \leq (\|A\|_2 + \|B\|_2)^{1-1/n} \|A - B\|_2^{1/n}$

(9) $d(\sigma(A), \sigma(B)) \leq 4(\|A\|_2 + \|B\|_2)^{1-1/n} \|A - B\|_2^{1/n}$

◇ **Bauer-Fike Theorem**: Assume $A \in M_n$ is diagonalizable with $X^{-1}AX = \text{diag}\ (\lambda_1, ..., \lambda_n)$. Then for any $B \in M_n$:

(10) $s(\sigma(B), \sigma(A)) \leq \kappa_p(X) \|A - B\|_p$ for any p-norm $\| \cdot \|_p$

◇ Let $U^H AU = T = D + N$ a Schur decomposition of $A \in M_n$ with D diagonal and N strictly upper triangular. If p is the smallest positive integer s.t. $|N|^p = 0$ the for any $B \in M_n$:

(11) $s(\sigma(B), \sigma(A)) \leq \max(\theta, \theta^{1/p})$ where $\theta = \|A - B\|_2 \sum_{k=0}^{p-1} \|N\|_2^k$

4.2.1 Eigenvalue Sensitivity

- If λ is a simple eigenvalue of $A \in M_n$ then on defines the **condition number** of λ as:

(12) $\kappa(\lambda) := \frac{1}{|y^H x|}$

The following proposition shows why this is justified:
◇ Assume $A \in M_n$ is diagonalizable and has a simple eigenvalue λ with associated normalized right and left eigenvectors x, y (i.e. $Ax = \lambda x, y^H A = \lambda y^H, \|x\|_2 = \|y\|_2 = 1$). Further, let $A(\epsilon) = A + \epsilon E$ be a perturbation of A with $\|E\|_2 = 1$. Then exist in a neighborhood of zero two differentiable functions $x(\epsilon)$ and $\lambda(\epsilon)$ with:

(13) $A(\epsilon)x(\epsilon) = \lambda(\epsilon)x(\epsilon)$

(14) $\|x(\epsilon)\|_2 = 1, \lambda(0) = \lambda, x(0) = x$

(15) $\left|\frac{\partial \lambda}{\partial \epsilon}(0)\right| = \left|\frac{y^H Ex}{y^H x}\right| \leq \frac{1}{|y^H x|} = \kappa(\lambda)$

This means roughly that order ϵ perturbations of A lead to $\epsilon\kappa(\lambda)$ perturbations of λ. Thus, if $\kappa(\lambda)$ is small then λ is regarded as well-conditioned.

The condition of an eigenvalue is not affected by unitary similarity transformations:
◇ Let λ be an simple eigenvalue of $A \in M_n$ with left- and right eigenvector x, y. For $U \in U_n$ let $\tilde{A}$ denote $U^H AU$. Then $\tilde{x} = U^H x$ and $\tilde{y} = U^H y$ are the right- and left eigenvectors of $\tilde{A}$ corresponding to λ. If $\kappa(\lambda)$ and $\tilde{\kappa}(\lambda)$ denote the condition of λ in A and $\tilde{A}$, respectively, then:

(16) $\kappa(\lambda) = \frac{1}{|y^H x|} = \frac{1}{|y^H UU^H x|} = \tilde{\kappa}(\lambda)$

4.2.2 Eigenvector Sensitivity

- If $A \in M_n$ has n distinct eigenvalues and x is the normalized eigenvector associated with $\lambda \in \sigma(A)$ then on defines the **condition number** of x as:

(17) $\kappa(x) := \frac{1}{\text{dist}\ (\lambda, \sigma(A) \setminus \{\lambda\})} = 1/(\min_{\mu \in \sigma(A), \mu \neq \lambda} |\mu - \lambda|)$

The following proposition shows why this is justified:
◇ Assume $A \in M_n$ has n distinct eigenvalues λ_i with associated normalized right and left

eigenvectors x_i, y_i (i.e. $Ax_i = \lambda_i x_i, y_i^H A = \lambda_i y_i^H, \|x_i\|_2 = \|y_i\|_2 = 1, i = 1, ..., n$). Further, let $A(\epsilon) = A + \epsilon E$ be a perturbation of A with $\|E\|_2 = 1$. Then exist in a neighborhood of zero differentiable functions $x_i(\epsilon), y_i(\epsilon)$ and $\lambda_i(\epsilon)$ with:

(18) $A(\epsilon)x_i(\epsilon) = \lambda_i(\epsilon)x_i(\epsilon)$
(19) $y_i(\epsilon)^H A(\epsilon) = \lambda_i(\epsilon)y_i(\epsilon)^H$
(20) $\|x_i(\epsilon)\|_2 = \|y_i(\epsilon)\|_2 = 1$, $\lambda_i(0) = \lambda_i, x_i(0) = x_i, y_i(0) = y_i$
(21) $\|x_k(\epsilon) - x_k\|_2 \leq \epsilon/(\min_{j\neq k} |\lambda_k - \lambda_j|)\|E\|_2 + \mathcal{O}(\epsilon^2) = \kappa(x_k)\|E\|_2\epsilon + \mathcal{O}(\epsilon^2)$

This means that the sensitivity of x_k depends upon the separation of λ_k from the other eigenvalues.

4.2.3 Invariant Subspace Sensitivity

Suppose

(22) $U^H AU = \begin{pmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{pmatrix}$ $, T_{11} \in M_p, T_{22} \in M_{n-p}$

is a Schur decomposition of $A \in M_n$ and $U = (U_1 U_2)$ with $U_1 \in M_{n,p}, U_2 \in M_{n,n-p}$.
It is known that span (U_1) is an invariant subspace of A. Its sensitivity should depend upon the separation of $\sigma(T_{11})$ and $\sigma(T_{22})$. The appropriate measure is defined now:

- Under the assumptions above one defines the separation of T_{11} and T_{22} as:
  (23) sep $(T_{11}, T_{22}) = \min_{x\neq 0} \frac{\|T_{11}X - XT_{22}\|_F}{\|X\|_F}$

◇ From [1]: Suppose that (22) holds and that for any matrix $E \in M_n$ we partition $U^H EU$ as follows:

(24) $U^H EU = \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix}$ $, E_{11} \in M_p, E_{22} \in M_{n-p}$

If $\delta =$ sep $(T_{11}, T_{22}) - \|E_{11}\|_2 - \|E_22\|_2 > 0$ and

(25) $\|E_{21}\|_2(\|T_{12}\|_2 + \|E_{21}\|_2) \leq \delta^2/4$

then there exists a $P \in M_{n-p,p}$ s.t.

(26) $\|P\|_2 \leq 2\|E_{21}\|_2/\delta$

and the columns of $\hat{U} = (U_1 + U_2 P)(I_p + P^H P)^{-1/2}$ form an orthonormal basis for a subspace that is invariant for $A + E$.

4.3 Normal Matrices

◇ Let $A \in M_n$ be normal and $B \in M_n$ arbitrary. Then:

(27) $s(\sigma(A), \sigma(B)) \leq \|A - B\|_2$

Thus, if A and B are normal then:

(28) $h(\sigma(A), \sigma(B)) \leq \|A - B\|_2$

If $n = 2$ then:

(29) $d(\sigma(A), \sigma(B)) \leq \|A - B\|_2$

◇ **Hoffman-Wielandt Theorem**: Let $A, B \in M_n$ be normal. Then:

(30) $\min_{s\in S_n} \left(\sum_{i=1}^n |\lambda_i(A) - \lambda_{s(i)}(B)|\right)^{1/2} \leq \|A - B\|_F \leq \max_{s\in S_n} \left(\sum_{i=1}^n |\lambda_i(A) - \lambda_{s(i)}(B)|\right)^{1/2}$

$\diamond$ Let $A \in M_n$ be normal and $B \in M_n$. If $\|A - B\|_2 \leq \frac{1}{2} \min_{\lambda,\mu\in\sigma(A),\lambda\neq\mu} |\lambda - \mu|$, Then:

(31) $d(\sigma(A), \sigma(B)) \leq \|A - B\|_2$

4.4 Hermitian and Skew-Hermitian Matrices

Let recall and invite some notations: A Hermitian matrix $A \in M_n$ has real eigenvalues that can be ordered as $\lambda_1^{\downarrow}(A) \geq \ldots \geq \lambda_n^{\downarrow}(A)$ and $\lambda_1^{\uparrow}(A) \leq \ldots \leq \lambda_n^{\uparrow}(A)$. One uses the denotation $\text{Eig}^{\downarrow}(A) = \text{diag}\,(\lambda_1^{\downarrow}(A), \ldots, \lambda_n^{\downarrow}(A))$ and $\text{Eig}^{\uparrow}(A) = \text{diag}\,(\lambda_1^{\uparrow}(A), \ldots, \lambda_n^{\uparrow}(A))$. Since the eigenvalues of skew - Hermitian matrices cannot be ordered (in a natural way) one introduces the denotation $\text{Eig}^{|\downarrow|}(A)$ and $\text{Eig}^{|\uparrow|}(A)$ for any diagonal matrix of the eigenvalues of A that are ordered with decreasing (increasing) modulus. I.e. $\text{Eig}^{|\downarrow|}(A) = \text{diag}\,(\mu_1, \ldots, \mu_n)$ with $|\mu_1| \geq \ldots \geq |\mu_n|$ and $\text{Eig}^{|\uparrow|}(A) = \text{diag}\,(\eta_1, \ldots, \eta_n)$ with $|\eta_1| \leq \ldots \leq |\eta_n|$ and the μ_i and η_i are the eigenvalues of A.

For Hermitian matrices one can formulate some strong perturbation theorems. But let us first consider a characterization of the eigenvalues of a Hermitian matrix. One therefore introduces Rayleigh quotients: • For $A \in M_n$ one defines the **Rayleigh quotient** (function) as $R_A : \mathbb{C}^n \setminus \{0\} \to \mathbb{C}$ s.t. $v \mapsto R_A(v) = \frac{v^H A v}{v^H v}$.
$\diamond$ If $A \in M_n$ is Hermitian then $R_A(v)$ is real and $R_A(\alpha v) = R_A(v)$ for $\alpha \in \mathbb{C} \setminus \{0\}$.

Now one can give the characterizations of the eigenvalues of a Hermitian matrix:
$\diamond$ Let $A \in M_n$ be Hermitian with eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$ and associated eigenvectors x_i that form an orthonormal basis of $\mathbb{C}^n$. With the notation $V_k := \text{span}\,\{x_1, \ldots, x_k\}$, $V_0 = \{0\}$ and
$\mathfrak{V}_k := \{V \subset_{sub} \mathbb{C}^n |\, \dim V = k\}$, $\mathfrak{V}_0 = \{V_0\}$ one has:

(32) $\lambda_k = R_A(x_k)$
(33) $\lambda_k = \min_{v\in V_k, v\neq 0} R_A(v) \quad = \min_{v\in V_k, \|v\|_2=1} v^H A v$
(34) $\lambda_k = \max_{v\perp V_{k-1}, v\neq 0} R_A(v)$
(35) $\lambda_k = \max_{W\in\mathfrak{V}_k} \max_{v\in W, v\neq 0} R_A(v) \quad = \max_{W\in\mathfrak{V}_k} \max_{v\in w, \|v\|_2=1} v^H A v$
(36) $\lambda_k = \min_{W\in\mathfrak{V}_{k-1}} \max_{v\perp W, v\neq 0} R_A(v) \quad = \min_{W\in\mathfrak{V}_{n-k+1}} \max_{v\in W, \|v\|_2=1} v^H A v$

Equation (35) and (36) are also called the **Minimax Principal**. Furthermore:

(37) $R_A(\mathbb{C}^n \setminus \{0\}) = \{R_A(v) | v \in \mathbb{C}^n, v \neq 0\} = [\lambda_1, \lambda_n] \subset \mathbb{R}$

$\diamond$ Let $A, B \in M_n$ be Hermitian. Then:

(38) $\lambda_j^{\downarrow}(A + B) \leq \lambda_i^{\downarrow}(A) + \lambda_{j-i+1}^{\downarrow}(B) \quad$ for $i \leq j$
(39) $\lambda_j^{\downarrow}(A + B) \geq \lambda_i^{\downarrow}(A) + \lambda_{j-i+n}^{\downarrow}(B) \quad$ for $i \geq j$
(40) $\lambda_j^{\downarrow}(A) + \lambda_n^{\downarrow}(B) \leq \lambda_j^{\downarrow}(A + B) \leq \lambda_j^{\downarrow}(A) + \lambda_1^{\downarrow}(B) \quad$ for $j = 1, \ldots, n$

$\diamond$ **Weyl's Monotonicity Theorem**: Let $A \in M_n$ be Hermitian and $H \in M_n$ be positive. Then:

(41) $\lambda_j^{\downarrow}(A + H) \geq \lambda_j^{\downarrow}(A) \quad$ for $j = 1, \ldots, n$

$\diamond$ **Weyl's Perturbation Theorem**: Let $A, B \in M_n$ be Hermitian. Then:

(42) $d(\sigma(A), \sigma(B)) = \max_j |\lambda_j^{\downarrow}(A) - \lambda_j^{\downarrow}(B)| \leq \|A - B\|_2 \leq \max_j |\lambda_j^{\downarrow}(A) - \lambda_j^{\uparrow}(B)|$

This can be generalized: For Hermitian $A, B \in M_n$ and any unitarily invariant norm $|||\cdot|||$:

(43) $|||\text{Eig}^{\downarrow}(A) - \text{Eig}^{\downarrow}(B)||| \leq \|A - B\|_2$

◇ **Lidskii's Theorem** Let $A, B \in M_n$ be Hermitian. Then:

(44) $\sum_{j=1}^{k} \lambda_{i_j}^{\downarrow}(A+B) \leq \sum_{j=1}^{k} \lambda_{i_j}^{\downarrow}(A) + \sum_{j=1}^{k} \lambda_{i_j}^{\downarrow}(B)$ for $1 \leq i_1 < \ldots < i_k \leq n$

◇ Let $A \in M_n$ be Hermitian and $B \in M_n$ skew-Hermitian. Let their eigenvalues $\lambda_i(A)$ and $\lambda_i(B)$ be arranged as $|\lambda_i(A)| \geq \ldots \geq |\lambda_n(A)|$ and $|\lambda_i(B)| \geq \ldots \geq |\lambda_i(B)|$. Then:

(45) $d(\sigma(A), \sigma(B)) \leq \max_j |\lambda_j(A) - \lambda_{n-j+1}(B)| \leq \|A - B\|_2$

◇ Let $A \in M_n$ be Hermitian and $B \in M_n$ skew-Hermitian.

Then for $2 \leq p \leq \infty$ inequality (46) and (47) hold while for $1 \leq p \leq 2$ inequality (48) and (49) hold:

(46) $\|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\uparrow|}(B)\|_{<p>} \leq \|A - B\|_{<p>} \leq 2^{\frac{1}{2}-\frac{1}{p}}\|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)\|_{<p>}$

(47) $\|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\uparrow|}(B)\|_{<p>} \leq \|\mathrm{Eig}(A) - \mathrm{Eig}_s(B)\|_{<p>} \leq \|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)\|_{<p>} \quad s \in S_n$

(48) $2^{\frac{1}{2}-\frac{1}{p}}\|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)\|_{<p>} \leq \|A - B\|_{<p>} \leq \|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\uparrow|}(B)\|_{<p>}$

(49) $\|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)\|_{<p>} \leq \|\mathrm{Eig}(A) - \mathrm{Eig}_s(B)\|_{<p>} \leq \|\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\uparrow|}(B)\|_{<p>} \quad s \in S_n$

Further:

(50) $\frac{1}{2}|||\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)||| \leq |||A - B||| \leq \sqrt{2}|||\mathrm{Eig}^{|\downarrow|}(A) - \mathrm{Eig}^{|\downarrow|}(B)|||$

◇ To sum up: If $A, B \in M_n$ and one one the following holds:

(i) A, B Hermitian
(ii) A Hermitian, B skew-Hermitian
(iii) A, B scalar multiples of unitary matrices
(iv) A, B normal and $n = 2$

then:

(51) $h(\sigma(A), \sigma(B)) \leq d(\sigma(A), \sigma(B)) \leq \|A - B\|_2$

4.5 Residuals

• Let $(\hat{\lambda}, \hat{x})$ be the estimation for an eigenvalue/eigenvector pair of $A \in M_n$. Then one defines its residual as:

(52) $\hat{r} = A\hat{x} - \hat{\lambda}\hat{x}$

The next two propositions give a posteriori estimates for eigenvalues and eigenvectors of a Hermitian matrix:

◇ Let $A \in M_n$ be Hermitian and let $\hat{r}$ be the residual of the estimated eigenvector/eigenvalue pair $(\hat{\lambda}, \hat{x})$. Then:

(53) $\min_{\mu \in \sigma(A)} |\hat{\lambda} - \mu| \leq \frac{\|\hat{r}\|_2}{\|\hat{x}\|_2}$

◇ Let $A \in M_n$ be Hermitian and let $\hat{r}$ be the residual of the estimated eigenvector/eigenvalue pair $(\hat{\lambda}, \hat{x})$. Suppose that $|\lambda_i(A) - \hat{\lambda}| \leq \|\hat{r}\|_2$ for $i = 1, \ldots, m$ and $|\lambda_i(A) - \hat{\lambda}| \geq \delta > 0$ for $i = m + 1, \ldots, n$. Then:

(54) $\mathrm{dist}_2(\hat{x}, U_m) = \inf_{u \in U_m} \|\hat{x} - u\|_2 \leq \frac{\|\hat{r}\|_2}{\delta}$

where $U_m = \mathrm{span}\ \{x_1, \ldots, x_m\}$ and x_i are the eigenvectors of A associated with $\lambda_i(A)$.

For Nonhermitian matrices one has:

◇ Let $A \in M_n$ be diagonalizable with $X^{-1}AX = \mathrm{diag}\ (\lambda_1, \ldots, \lambda_n)$. If $\|\hat{r}\|_2 \leq \epsilon\|\hat{x}\|_2$ for some $\epsilon > 0$ then:

(55) $\min_{\lambda \in \sigma(A)} |\hat{\lambda} - \lambda| \leq \epsilon\kappa_2(X) = \epsilon\|X\|_2\|X^{-1}\|_2$

5 Algorithms

Algorithms are presented in a pseudo java code. The assignment of objects (like vectors) should not be understand as the assignment of references. The following example makes that clear:

```
Vector $x = (0,2,3)^T$   // $x = (0,2,3)^T$
Vector $y = x$           // $y = (0,2,3)^T$
$y$ += $(1,1,1)^T$       // $y = (1,3,4)^T, x = (0,2,3)^T$
```

Complexity of algorithms is noted as "complexity $\leq [\ a\ ;\ b\ ;\ c\ ;\ d\ ]_{\mathbb{R}}$" which means that the computation needs less than or equal to a additions, b multiplications, c divisions and d roots (of real numbers).

5.1 Householder Transformations

- Define $H_n : \mathbb{C}^n \to M_n(\mathbb{C})$ as:

$$(1) \quad H_n(v) := \begin{cases} I_n - \frac{2}{v^H v} v v^H & \text{if } v \neq 0 \\ I_n & \text{if } v = 0 \end{cases}$$

and let $House_n = \Im H_n = H_n(\mathbb{C}^n)$ be the set of matrices that one then calls **Householder matrices** (also Householder reflection or transformation).

◇ Householder matrices are unitary and Hermitian.
◇ $H_n(v)$ describes for $v \neq 0$ a reflection in the hyperplane $\{v\}^{\perp}$.

The Householder Transformation can be used to zero all but one entries of a vector:
◇ Assume $x = (x_1, ..., x_n)^T \in \mathbb{C}^n$ and $1 \leq i \leq n$ are fixed. Set:

$$(2) \quad v = (x_1, ..., x_{i-1}, (1 \pm \tfrac{\|x\|_2}{|x_i|})x_i, x_{i+1}, ..., x_n)^T = x \pm \|x\|_2 \tfrac{x_i}{|x_i|} e_i \qquad \text{if } x_i \neq 0$$

$$(3) \quad v = (x_1, ..., x_{i-1}, \pm\|x\|_2 c, x_{i+1}, ..., x_n)^T = x + \|x\|_2 c e_i \text{ for some } c \in \mathbb{T} \qquad \text{if } x_i = 0$$

Then $H_n(v)x = \mp\|x\|_2 \frac{x_i}{|x_i|} e_i$ and $H_n(v)x = -\|x\|_2 c e_i$, respectively.
Proof: see appendix

- Define $h : \mathbb{C}^n \to \mathbb{C}^n$ as:

$$(4) \quad h(x) := \begin{cases} 0 & \text{if } x_2 = ... = x_n = 0 \\ x + \|x\|_2 e_1 & \text{if } x_1 = 0, x_2 \cdot \ldots \cdot x_n \neq 0 \\ x + \|x\|_2 \frac{x_1}{|x_1|} e_1 & \text{if } x_1 \neq 0, x_2 \cdot \ldots \cdot x_n \neq 0 \end{cases}$$

The Vector $h(x)$ will be called **Householder vector** for x. Then:

$$(5) \quad H_n(h(x))x := \begin{cases} x & \text{if } x_2 = ... = x_n = 0 \\ -\|x\|_2 e_1 & \text{if } x_1 = 0, x_2 \cdot \ldots \cdot x_n \neq 0 \\ -\|x\|_2 \frac{x_1}{|x_1|} e_1 & \text{if } x_1 \neq 0, x_2 \cdot \ldots \cdot x_n \neq 0 \end{cases}$$

If x is the $i - th$ column vector of X then $B = H_n(h(x))X$ will have zero entries $B_{i,2} = ... = B_{i,n} = 0$. One uses this to zero some entries of a matrix. First some important algorithms are presented.

One uses the special structure of $H_n(v)$ to compute the Householder pre- and post-multiplication $H_n(v)A$ and $AH_n(v)$ ($A \in M_{nl}, A \in M_{ln}$ respectively). The complexity is then $\leq [\ 8nl + 2n\ ;\ 8nl{+}2n{+}2l\ ;\ 1\ ]_{\mathbb{R}}$. An ordinary matrix multiplication would have complexity $[\ 4n^2l\ ;\ 4n^2l\ ]_{\mathbb{R}}$.

Listing 1: Householder Vector

```
requires: $x \in \mathbb{C}^n$
returns:  $h(x)$
complexity  $\leq [\, 2n+1\ ;\ 2n+4\ ;\ 1\ ;\ 1\,]_{\mathbb{R}}$

Vector getHouseVec(Vector $x$) {
    Vector $h = x$;
    if {$x[2:n]$ == 0) // If $x_2 = ... = x_n = 0$ then return zero vector
        return 0;
    if ($x_1 \neq 0$) {
        $h_1$ *= $(1 + \|x\|_2/|x_1|)$;
        return $h$;
    }
    $h_1$ += $\|x\|_2$;
    return $h$;
}
```

Listing 2: Householder Pre-Multiplication

```
requires: $A \in M_{nl}, v \in \mathbb{C}^n$
returns:  $H_n(v)^H A$   $(= H_n(v)A)$
complexity  $\leq [\, 8nl + 2n\ ;\ 8nl + 2n + 2l\ ;\ 1\,]_{\mathbb{R}}$

Matrix getTimesHouseMatPre(Matrix $A$, Vector $v$) {
    double norm2Sq = $\|v\|_2^2$; // compute $v_1^2 + ... + v_n^2$
    if (norm2Sq == 0) // if $v = 0$ then $H_n(v)A = I_nA = A$
        return $A$;
    double $b = -2./\mathrm{norm2Sq}$;
    Vector $w = bA^Hv$;
    return $A + vw^H$;
}
```

Listing 3: Householder Post-Multiplication

```
requires: $A \in M_{ln}, v \in \mathbb{C}^n$
returns:  $AH_n(v)$
complexity  $\leq [\, 8nl + 2n\ ;\ 8nl + 2n + 2l\ ;\ 1\,]_{\mathbb{R}}$

Matrix getTimesHouseMatPost(Matrix $A$, Vector $v$) {
    double norm2Sq = $\|v\|_2^2$; // compute $v_1^2 + ... + v_n^2$
    if (norm2Sq == 0) // if $v = 0$ then $AH_n(v) = AI_n = A$
        return $A$;
    double $b = -2./\mathrm{norm2Sq}$;
    Vector $w = bAv$;
    return $A + wv^H$;
}
```

Consider a matrix $A \in M_{nl}(\mathbb{C})$. One can zero the elements $A_{i_1,j}, ..., A_{i_2,j}$ for $1 < i_1 \leq i_2 \leq n$. To do so, compute the Householder vector v for $A[i_1 : i_2][j]$. Complete this vector with zero's to obtain a fitting vector h of length n: $h = (\underbrace{0 \, ... \, 0}_{i_1-1} v^T \underbrace{0 \, ... \, 0}_{n-i_2})^T$. One can easily verify that:

$$(6) \quad H_n(h) = \begin{pmatrix} I_{i_1-1} & & \bigcirc \\ & H_{i_2-i_1+1}(v) & \\ \bigcirc & & I_{n-i_2} \end{pmatrix}$$

Therefore the matrix $B = H_n(h)A$ has zero entries $B_{i_1+1,j} = ... = B_{i_2,j} = 0$.

Due to roundoff errors, it could happen that the $B_{i_1+1,j} ... B_{i_2,j}$ are only very small. The next algorithm zeros the entries $(i_1+1, j)...(i_2, j)$ of a given matrix by pre-multiplying it with the Householder matrix. The entries are explicitly zeroed. Vector h returns the Householder vector of the performed transformation for later usage.

Listing 4: Matrix Entry Zeroing

```
requires: $A \in M_{nl}, 1 \leq j \leq l, 1 \leq i_1 < i_2 \leq n$
returns:  $[H_n(h)A, h]$ where $h$ is chosen s.t. $(H_n(h)A)[i_1+1 : i_2][j] = 0$
complexity $\leq [\, 8st + 4s + 1 \,;\, 8st + 4s + 2t + 4 \,;\, 1 \,;\, 1 \,]_{\mathbb{R}}$ where $s = i_2 - i_1 + 1, t = n - j + 1$

[Matrix, Vector] applyHouse(Matrix $A$, int $j$, int $i_1$, int $i_2$) {
    Vector $v$ =getHouse($A[i_1 : i_2][j]$);
    Matrix $Sub = A[i_1 : i_2][j : n]$;
    $Sub$ =getTimesHouseMatPre($Sub$, $v$);
    $A[i_1 : i_2][j] = Sub$;
    $A[i_1+1 : i_2][j] = 0$; // set these entries to zero
    $h = (\overbrace{0 \, ... \, 0}^{i_1-1} v^T \underbrace{0 \, ... \, 0}_{n-i_2})^T$
    return $[A; h]$;
}
```

5.2 Givens Transformations

- For $c, s \in \mathbb{C}$ with $|c|^2 + |s|^2 = 1$ the n-n matrix $G_n(p,q,c,s)$ is called **Givens Matrix**:

$$(7) \quad G_n(p,q,c,s) = \begin{array}{cc} \left(\begin{array}{ccccc} I_{q-1} & & & & \bigcirc \\ & \text{c} & & \overline{s} & \\ & & I_{p-q-1} & & \\ & \text{-s} & & \overline{c} & \\ \bigcirc & & & & I_{n-p} \end{array}\right) & \begin{array}{l} \\ \leftarrow q \\ \\ \leftarrow p \\ \\ \end{array} \\ \begin{array}{ccccc} & \uparrow & & \uparrow & \\ & q & & p & \end{array} & \end{array} \quad (1 \leq q < p \leq n)$$

◇ Givens matrices are unitary.

The Givens Transformation can be used to zero one specific entry of a vector:

◇ Assume $\begin{pmatrix} a \\ b \end{pmatrix} \in \mathbb{C}^2$ and set $c = \frac{a}{\sqrt{|a|^2+|b|^2}}$, $s = \frac{-b}{\sqrt{|a|^2+|b|^2}}$. Then:

$$(8) \quad \begin{pmatrix} c & \overline{s} \\ -s & \overline{c} \end{pmatrix}^H \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \bullet \\ \cdot \end{pmatrix}$$

The following algorithm computes the Givens numbers:

Listing 5: Givens Numbers

```
requires: $a, b \in \mathbb{C}$
returns: $[c, s]$ s.t. $\begin{pmatrix} c & \overline{s} \\ -s & \overline{c} \end{pmatrix}^H \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \bullet \\ \cdot \end{pmatrix}$
complexity $\leq [\,3\,;\,8\,;\,1\,;\,1\,]_{\mathbb{R}}$

[C,C] getGivensNumbers(C $a$, C $b$) {
    if ($b$ == 0)
        return $[1;0]$;
    double $f = 1./\sqrt{|a|^2 + |b|^2}$;
    return $[fa; -fb]$;
}
```

Consider the product $B = G_n(p,q,c,s)^H A$ where $A \in M_{nl}$. Then only the $p-th$ and $q-th$ row of A changes, i.e.

$$(9) \quad B_{ij} = \begin{cases} sA_{qj} + cA_{pj} & \text{if } i = p \\ \overline{c}A_{qj} - \overline{s}A_{pj} & \text{if } i = q \\ A_{ij} & \text{else} \end{cases}$$

Similar, in the product $AG_n(p,q,c,s)$ only the $p-th$ and $q-th$ column changes. One uses this to compute the Givens pre- and post-multiplication:

Listing 6: Givens Pre-Multiplication

```
requires: $A \in M_{nl}; c, s \in \mathbb{C}; 1 \leq q < p \leq n$
returns:  $G_n(p, q, c, s)^H A$
complexity $\leq [\, 12l \,;\, 16l \,]_{\mathbb{R}}$

Matrix getTimesGivensMatPre(Matrix $A$, int $p$, int $q$, C $c$, C $s$) {
    Matrix $A^{(p)} = A[p][]$; // Row p of A
    Matrix $A^{(q)} = A[q][]$; // Row q of A
    Matrix $B = \overline{s}A^{(q)}$;
    $A^{(q)} = \overline{c}A^{(q)} - \overline{s}A^{(p)}$;
    $A^{(p)} = \overline{c}A^{(p)} + B$;
    Matrix $R = A$;
    $R[p][] = A^{(p)}$;
    $R[q][] = A^{(q)}$;
    return $R$;
}
```

Listing 7: Givens Post-Multiplication

```
requires: $A \in M_{nl}; c, s \in \mathbb{C}; 1 \leq q < p \leq n$
returns:  $AG_n(p, q, c, s)$
complexity $\leq [\, 12l \,;\, 16l \,]_{\mathbb{R}}$

Matrix getTimesGivensMatPost(Matrix $A$, int $p$, int $q$, C $c$, C $s$) {
    Matrix $A^{(p)} = A[][p]$; // Column p of A
    Matrix $A^{(q)} = A[][q]$; // Column q of A
    Matrix $B = sA^{(p)}$;
    $A^{(p)} = cA^{(p)} - sA^{(q)}$;
    $A^{(q)} = cA^{(q)} + B$;
    Matrix $R = A$;
    $R[][p] = A^{(p)}$;
    $R[][q] = A^{(q)}$;
    return $R$;
}
```

Because of roundoff errors we need another method to zero a specific entry of a matrix:

Listing 8: Matrix Entry Zeroing

```
requires: $A \in M_{nl}; 1 \leq q < p \leq n$
returns:  $[G_n(p, q, c, s)^H A, c, s]$ where $[c, s]$ =getGivensNumbers($A_{qq}, A_{pq}$)
complexity $\leq [\, 12l + 3 \,;\, 16l + 8 \,;\, 1 \,;\, 1 \,]_{\mathbb{R}}$

[Matrix, C, C] applyGivens(Matrix $A$, int $p$, int $q$) {
    C $c = 0$;
    C $s = 0$;
    [c, s] = getGivensNumbers($A_{qq}, A_{pq}$);
    Matrix $R$ = getTimesGivensMatPre($A, p, q, c, s$);
    $R_{pq} = 0$;
    return $[R, c, s]$;
}
```

5.3 QR Decomposition

One uses the Householder transformation to compute the (generalized) QR decomposition of a matrix:

Listing 9: QR Decomposition

```
requires: $A \in M_{nl}$
returns: $[U,R]$ s.t. $(U,R)$ is the (generalized) QR decomposition of $A$
complexity $\leq [\, 11n^3 + 3n \,;\, 11n^3 + 3n^2 + 5n \,;\, 2n-2 \,;\, n-1 \,]_{\mathbb{R}}$ for $n = l$

[Matrix, Matrix] getQR(Matrix $A$) {
    Matrix $R = A$;
    Matrix $U = I_n$;
    Vector $h = 0$;
    int $nStep = \min(n-1, l)$;
    for (int $k = 1; k \leq nStep; k{+}{+}$) {
        $[R,h]$ = applyHouse(R, k, k, n - 1);
        $U$ = getTimesHouseMatPost($U, h$);
    }
    return $[U,R]$;
}
```

5.4 Hessenberg Matrices

5.4.1 Definition and Properties

- A matrix $A \in M_n$ is called Hessenberg, if $A_{ij} = 0$ whenever $i \geq j+2$.

  It has the form: $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \cdot & \bullet & \bullet & \bullet & \bullet \\ \cdot & \cdot & \bullet & \bullet & \bullet \\ \cdot & \cdot & \cdot & \bullet & \bullet \end{pmatrix}$

◇ Every upper triangular matrix is Hessenberg.

5.4.2 Hessenberg Reduction

Every matrix is unitarily similar to a Hessenberg matrix:

◇ **Hessenberg Reduction**: For every $A \in M_n$ there exists a unitary U s.t. $U^H A U$ is Hessenberg. If $A \in M_n(\mathbb{R})$ one may take U real, orthogonal.

Listing 10: Hessenberg Reduction

```
Requires: $A \in M_{nl}$
Returns: $[U,H]$ s.t. $U$ is unitary, $H$ is a Hessenberg matrix and $H = U^H A U$
complexity $\leq [\, 19n^3 - 25n^2 \,;\, 19n^3 - 25n^2 \,;\, 3n-6 \,;\, n-2 \,]_{\mathbb{R}}$

[Matrix, Matrix] getHessenberg(Matrix $A$) {
    Matrix $H = A$;
    Matrix $U = I_n$;
    Vector $h = 0$;
    for (int $j = 1; j \leq n-2; j{+}{+}$) {
        $[H,h]$ = applyHouse($H, j, j+1, n-1$);
```

```
        H = getTimesHouseMatPost($H, h$);
        U = getTimesHouseMatPost($U, h$);
    }
    return [$H, U$];
}
```

5.4.3 QR Decomposition of Hessenberg Mastrices

The importance of Hessenberg matrices is due to the fast computability of their QR decomposition. Instead of complexity $[\ 19n^3\ ;\ 19n^3\ ;\ 3n\ ;\ n\ ]_{\mathbb{R}}$ it needs only $[\ 24n^2\ ;\ 32n^2\ ;\ n\ ;\ n\ ]_{\mathbb{R}}$:

Listing 11: QR Decomposition of Hessenberg Matrices

```
Requires: $H \in M_{nl}$ in Hessenberg form
Returns:  $[U, R]$ s.t. $(U, R)$ is the (generalized) QR decomposition of $H$
complexity $\leq [\ 24n^2 - 21n\ ;\ 32n^2 - 24n\ ;\ n-1\ ;\ n-1\ ]_{\mathbb{R}}$ for $n = l$

[Matrix, Matrix] getQR_Hess(Matrix $H$) {
    Matrix $R = H$;
    Matrix $U = I_n$;
    C $c, s = 0$;
    int $nStep = \min(n-1, l)$;
    for (int $k = 1; k \leq nStep; k{+}{+}$) {
        [$R, c, s$] = applyGivens($R, k+1, k$);
        getTimesGivensMatPost($U, k+1, k, c, s$);
    }
    return [$U, R$];
}
```

5.5 The Power Methods

5.5.1 The Simple Power Method

The simple power Method constructs for $A \in M_n(\mathbb{C}), q^{(0)} \in \mathbb{C}^n$ the sequence $q^{(k)} = \frac{A^k q^{(0)}}{\|A^k q^{(0)}\|_2}$. This can be used to compute the dominant eigenvalue of a matrix: Suppose $A \in M_n(\mathbb{C})$ is diagonalizable with $X^{-1}AX = \text{diag}\,(\lambda_1, \ldots, \lambda_n), X = [x_1, \ldots, x_n]$ and that A has a dominant eigenvalue, i.e. $|\lambda_1| > |\lambda_2| \geq \ldots \geq |\lambda_n|$. The x_i span $\mathbb{C}^n$ and so one can write every $q^{(0)} \in \mathbb{C}^n$ as $q^{(0)} = a_1 x_1 + \ldots + a_n x_n$. If $a_1 \neq 0$ then:

$$(10)\quad A^k q = a_1 \lambda_1^k \left(x_1 + \sum_{j=2}^{n} \frac{a_j}{a_1} \left(\frac{\lambda_j}{\lambda_1} \right)^k x_j \right) = a_1 \lambda_1^k (x_1 + s^{(k)})$$

$$(11)\quad q^{(k)} = \frac{A^k q^{(0)}}{\|A^k q^{(0)}\|_2} = \frac{a_1 \lambda_1^k (x_1 + s^{(k)})}{\|a_1 \lambda_1^k (x_1 + s^{(k)})\|_2} = \frac{a_1}{|a_1|} \left(\frac{\lambda_1}{|\lambda_1|} \right)^k \frac{x_1 + s^{(k)}}{\|x_1 + s^{(k)}\|_2}$$

with $s^{(k)} \to 0$ for $k \to \infty$. This means that $q^{(k)}$ tends to lie in span $\{x_1\}$. Further:

$$(12)\quad \|Ax^{(k)}\|_2 \quad \to r_\sigma(A) \quad (k \to \infty)$$

$$(13)\quad q(k)^H A q^{(k)} \to \lambda_1 \qquad (k \to \infty)$$

The results above are summarized in the following theorem:

◇ Suppose $A \in M_n(\mathbb{C})$ is diagonalizable with $X^{-1}AX = \text{diag}\,(\lambda_1, \ldots, \lambda_n), X = [x_1, \ldots, x_n]$ and that A has a dominant eigenvalue, i.e. $|\lambda_1| > |\lambda_2| \geq \ldots \geq |\lambda_n|$. Let further $q^{(0)} \in \mathbb{C}^n$ be an arbitrary vector. $q^{(0)}$ can be represented as $q^{(0)} = a + b$ with $a \in$ span $\{x_1\}$ and $b \in$ span $\{x_2, \ldots, x_n\}$. If $a \neq 0$ then construct the sequences:

$$(14) \quad q^{(k)} = \frac{Aq^{(k-1)}}{\|Aq^{(k-1)}\|_2}$$

$$(15) \quad \lambda^{(k)} = (q^{(k)})^H A q^{(k)}$$

Then:

$$(16) \quad \text{dist (span } \{q^{(k)}\}, \text{span } \{x_1\}) = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

$$(17) \quad |\lambda_1 - \lambda^{(k)}| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

Thus $\lambda^{(k)} \to \lambda_1$ $(k \to \infty)$.

It follows, that this method is well suited when $|\lambda_2|/|\lambda_1|$ is small. A possible stopping criterium is to monitor the differences between $\lambda^{(k)}$ and $\lambda^{(k-1)}$ and to stop when $|\lambda^{(k)} - \lambda^{(k-1)}|$ is small. Another stopping criterium uses the residual $r^{(k)} = Aq^{(k)} - \lambda^{(k)} q^{(k)}$:

$$(18) \quad |\lambda_1 - \lambda^{(k)}| \approx \frac{\|r^{(k)}\|_2}{|{w^{(k)}}^H q^{(k)}|}$$

where $w^{(k)}$ are approximate left eigenvectors $w^{(k)} = \frac{(A^H)^k w^{(0)}}{\|(A^H)^k w^{(0)}\|_2}$. The necessity to compute $w^{(k)}$ nearly doubles the costs for the power method.

An algorithm that uses the first stopping criterium is given in the following listing:

Listing 12: Power Method

```
Requires: $A \in M_{nl}(\mathbb{C}), q^{(0)} \in \mathbb{C}^n$
Returns:  $[\lambda^{(k)}, q^{(k)}]$ that were constructed as indicated above
complexity $\leq [\, 4n^2 + 4n \,;\, 4n^2 + 6n \,;\, 2n \,;\, 1 \,]_{\mathbb{R}}$ per iteration

[C, Vector] powerMethod(Matrix $A$, Vector $q^{(0)}$, double $acc$) {
    Vector $q_1 = q^{(0)}$;
    Vector $q_2 = 0$;
    C $\lambda_1 = 0$;
    C $\lambda_2 = 0$;
    for (int $k = 0; k < 1000; k{+}{+}$) {
        $q_2 = Aq_1$
        $\lambda_2 = q_1^H q_2$;
        $q_1 = q_2 / \|q_2\|_2$;
        if ($|\lambda_1 - \lambda_2| < acc$)
            break;
        $\lambda_1 = \lambda_2$;
    }
    return $[\lambda_2, q_2]$;
}
```

5.5.2 The Inverse Power Method

The inverse power method is a modification of the simple power method that finds the eigenvalue nearest to a given value. If λ_i are the eigenvalues of $A \in M_n$ then $\lambda_i - \mu$ are the eigenvalues of $A - \mu I_n$ and $\frac{1}{\lambda_i - \mu}$ are the eigenvalues of $(A - \mu I_n)^{-1}$. Thus, the closer μ is to one λ_i, the more dominant is the largest eigenvalue of $(A - \mu I_n)^{-1}$. The inverse power method uses that and applies the standard power method to $(A - \mu I_n)^{-1}$.

If the simple power method returns the approximate eigenvalue/eigenvector pair (λ, q) for $(A - \mu I_n)^{-1}$ then $(\frac{1}{\lambda} + \mu, q)$ is an approximate eigenvalue/eigenvector pair for A.

Listing 13: Inverse Power Method

```
Requires: $A \in M_{nl}(\mathbb{C}), q^{(0)} \in \mathbb{C}^n$
Returns:  $[\frac{1}{\lambda}, q]$ that were constructed as indicated above
complexity $\leq [\, 4n^2+4n\ ;\ 4n^2+6n\ ;\ 2n\ ;\ 1\,]_{\mathbb{R}}$ per iteration
    (+ complexity of one matrix inversion)

[C, Vector] powerMethod_Inv(Matrix $A$, Vector $q^{(0)}$, C $\mu$, double $acc$) {
    Matrix $B$ = $(A - \mu I_n)^{-1}$
    C $\lambda = 0$;
    Vector $q = 0$;
    $[\lambda, q]$ = powerMethod($B, q^{(0)}, acc$);
    return $[\frac{1}{\lambda} + \mu; q]$;
}
```

5.6 The QR Method

5.6.1 Definition and Properties

The simple QR method constructs for $A^{(0)} \in M_n(\mathbb{C})$ a sequence of unitarily similar matrices via successive QR decompositions. The following proposition shows how this can be used to compute all eigenvalues:

◇ Suppose $A \in M_n(\mathbb{C})$ is diagonalizable with $P^{-1}AP = \text{diag}\,(\lambda_1, \ldots, \lambda_n)$ and that all eigenvalues have distinct moduli, i.e. $|\lambda_1| > \ldots > |\lambda_n|$. Let further A admit an LU decomposition. Construct the sequence

$A^{(k)} = R^{(k-1)}Q^{(k-1)}$ where $A^{(k-1)} = Q^{(k-1)}R^{(k-1)}$ is the QR decomposition of $A^{(k-1)}$

Then:

$A^{(k)}_{ii} \to \lambda_i$

$A^{(k)}_{ij} \to 0 \quad \text{if } i > j$

That means the lower part of $A^{(k)}$ converges to diag $(\lambda_1, \ldots, \lambda_n)$. The convergence rate is:

$$|A^{(k)}_{i,i-1}| = \mathcal{O}\left(\left|\frac{\lambda_i}{\lambda_{i-1}}\right|^k\right)$$

An algorithm is given in the following listing:

Listing 14: Simple QR Method

```
Requires: $A \in M_n$
Returns:  $A^{(k)}$ that was constructed as indicated above
complexity $\leq [\, 15n^3+3n\ ;\ 15n^3+3n^2+5n\ ;\ 2n-2\ ;\ n-1\,]_{\mathbb{R}}$ per iteration

Matrix qr(Matrix $A$) {
    Matrix $B = A$;
    Matrix $U, R = 0$;
    for (int $k = 0; k < 1000; k{+}{+}$) {
        $[U, R]$ =getQR($B$);
        $B = RU$;
    }
    return $B$;
}
```

5.6.2 QR Method with Hessenberg Reduction

The QR method can be improved when one first reduces A to Hessenberg form. Then one can compute the QR decomposition much faster. An algorithm is given in the following listing:

Listing 15: Simple QR Method with Hessenberg Reduction

```
Requires: $A \in M_n$
Returns:  $A^{(k)}$ that was constructed as indicated above
complexity $\leq [\,24n^2\,;\,32n^2\,;\,n-1\,;\,n-1\,]_{\mathbb{R}}$ per iteration

Matrix qr_Hess(Matrix $A$) {
    Matrix $U_0, U, R, H = 0$;
    $[H, U_0]$ = getHessenberg($A$);
    for (int $k = 0; k < 100; k{+}{+}$) {
        // fast QR step:
        for (int $j = 1; j < n; j{+}{+}$) {
            applyGivens($H, j+1, j, c, s$);
            timesGivensMatPost($H, j+1, j, c, s$);
        }
    }
    return $H$;
}
```

5.6.3 QR Method with Shifts and Decoupling

A QR step with shift $\rho \in \mathbb{C}$ has the form: (H in Hessenberg form)

```
$H^{(k)} - \rho I = UR$ // QR factorization
$H^{(k+1)} = RU + \rho I$
```

Then $H^{(k+1)}$ is still orthogonally similar to $H^{(k)}$ since $H^{(k+1)} = RU + \rho I = U^H(UR + \rho I)U = U^H H^{(k)} U$. The shifted QR steps fasten the algorithm when ρ is near to an eigenvalue of H. If one orders the eigenvalues of H in such a way that $|\lambda'_1 - \rho| \geq \ldots \geq |\lambda'_h - \rho|$ then one sees that $|H^{(k)}_{i,i-1}| = \mathcal{O}\left(\left|\frac{\lambda'_i - \rho}{\lambda'_{i-1} - \rho}\right|^k\right)$. Thus, if $\rho \simeq \lambda'_i$ then $H^{(k)}_{i,i-1}$ tends to zero very fast.

It is useful to monitor the entries $A^{(k)}_{i,i+1}$. If $|A^{(k)}_{i+1,i}| \leq \epsilon(|A^{(k)}_{i,i}| + |A^{(k)}_{i+1,i+1}|)$ for some small ϵ than $A^{(k)}_{i,i+1}$ is set to zero. Then one decouples the matrix $A^{(k)}$ into two submatrices that are considered independently. The spectrum of the original matrix is the union of the spectra of the decoupled submatrices.

There are several strategies how to choose the shift. One can use always the entry $A^{(k)}_{nn}$ as shift. This is called the single shift strategy. One hopes that $A^{(k)}_{n,n-1}$ tends to zero. Then one would decouple $A^{(k)}$ into the matrices $A^{(k)}[1:n-1][1:n-1]$ and $A^{(k)}[n:n][n:n] = A^{(k)}_{nn}$. This is called deflating. The value $A^{(k)}_{nn}$ would be an approximate eigenvalue of A. This method works only as long as there is only one eigenvalue of minimal modulus.

Another method uses the smallest subdiagonal entry to find a shift. If $A^{(k)}_{p+1,p}$ is the smallest subdiagonal entry then one uses the shift $A^{(k)}_{p+1,p+1}$. The reason is that if $A_{p+1,p}$ is small then $A^{(k)}$ almost decouples at position p and one wants to fasten the convergence of $A^{(k)}_{p+1,p}$ to zero.

A Proofs

Proof: of Theorem 3 in Section 5.1 (for convenience: $\|.\| = \|.\|_2$)

$$\begin{aligned}
x_i \neq 0\text{: }\; v^H v &= \|v\|^2 = |x_1|^2 + ...|(1 \pm \tfrac{\|x\|_2}{|x_i|})x_i|^2 ... + |x_n|^2 \\
&= |x_1|^2 + ...(|x_i| \pm \|x\|)^2 ... + |x_n|^2 \\
&= |x_1|^2 + ... + |x_n|^2 \pm 2\|x\||x_i| + \|x\|^2 = 2(\|x\|^2 \pm |x_i|) \\
P(v)x &= x - \tfrac{1}{\|x\|^2 + |x_i|}(x \pm \|x\| \tfrac{x_i}{|x_i|} e_i)(x^H \pm \|x\| \tfrac{\overline{x_i}}{|x_i|} e_i^T)x \\
&= x - \tfrac{1}{\|x\|^2 + |x_i|}(x \pm \|x\| \tfrac{x_i}{|x_i|} e_i)(\|x\|^2 \pm \|x\| \tfrac{\overline{x_i}}{|x_i|} x_i) \\
&= x - \tfrac{\|x\|^2 + |x_i|}{\|x\|^2 + |x_i|}(x \pm \|x\| \tfrac{x_i}{|x_i|} e_i) \\
&= \mp \|x\| \tfrac{x_i}{|x_i|} e_i \\
x_i = 0\text{: }\; v^H v &= |x_1|^2 + ...| \pm \|x\| c|^2 ... + |x_n|^2 = 2\|x\|^2 \\
P(v)x &= x - \tfrac{1}{\|x\|^2}(x + \|x\| c e_i)(x^H + \|x\| \overline{c} e_i^T)x \\
&= x - \tfrac{1}{\|x\|^2}(x + \|x\| c e_i)(\|x\|^2 + \|x\| \overline{c} x_i) \\
&= x - \tfrac{\|x\|^2}{\|x\|^2}(x + \|x\| c e_i) = -\|x\|_2 c e_i
\end{aligned}$$

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