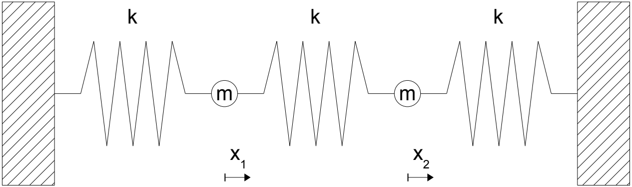
7. The Symmetric Eigenvalue Problem

A ‘must’ for engineering applications . . .

7.1. Motivation

7.1.1. An Example from Physics

Consider the following system, consisting of two bodies B_1, B_2 with mass m, connected by springs with spring constant k. Let $x_1(t), x_2(t)$ denote the displacement of the bodies B_1, B_2 at time t.



From Newton's law ($F = m\ddot{x}$) and Hooke's law ($F = mk$), we have the following **linear second-order differential equations with constant coefficients**:

$$\begin{aligned} m\ddot{x}_1 &= -kx_1 + k(x_2 - x_1) \\ m\ddot{x}_2 &= -k(x_2 - x_1) - kx_2 \end{aligned}$$

- From calculus, we know that we can use the following complex ansatz to find a (non-trivial) solution of this differential equation:

$$x_j(t) = c_j e^{i\omega t},$$

  $c_j, \omega \in \mathbb{R}$, $j = 1, 2$.

- Since $\ddot{x}_j(t) = -c_j \omega^2 e^{i\omega t}$, we have:

$$\begin{aligned} -mc_1\omega^2 &= -kc_1 + k(c_2 - c_1) = k(-2c_1 + c_2) \\ -mc_2\omega^2 &= -k(c_2 - c_1) - kc_2 = k(c_1 - 2c_2) \end{aligned}$$

- We substitute $\lambda := -m\omega^2/k$:

$$\begin{aligned} \lambda c_1 &= -2c_1 + c_2 \\ \lambda c_2 &= c_1 - 2c_2 \end{aligned}$$

  Or, with $c := (c_1, c_2)^T$,

$$\begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix} c = \lambda c$$

  We have an instance of the **symmetric eigenvalue problem**!

- For given **initial values**, the solution is unique.
- We can obtain similar instances of the symmetric eigenvalue problem for systems with a higher number of bodies.

7.1.2. Eigenvalues in Numerics

- A common problem in numerics is to solve systems of linear equations of the form $Ax = b$ with $A \in \mathbb{R}^{n \times n}$ symmetric, $b \in \mathbb{R}^n$.
- An important question is the **condition** of this problem, i.e. to which extent an error in b affects the value of the correct solution x^*.
- The maximum ratio of the relative error in the solution x^* to the relative error in b (measured using the Euclidean norm) is the **condition number** $\kappa(A)$ of solving $Ax = b$. It can be shown that, for symmetric A,

$$\kappa(A) = \left| \frac{\lambda_{max}(A)}{\lambda_{min}(A)} \right| .$$

  That means the condition depends directly on the eigenvalues of A!
- This number plays an important role in iterative solution of linear equation systems, for example:
  - Assume we have an approximate solution $\hat{x}$.
  - This means we have exactly solved the system $Ax = \hat{b}$ with $\hat{b} := A\hat{x}$.
  - However, if $\kappa(A)$ is large, this means that even if $\hat{b} - b$ is small, our solution may be far away from the solution of $Ax = b$!
- Finally, also the **convergence speed** of common iterative solvers is greatly affected by the eigenvalues of A.

7.2. Condition

- Before trying to develop numerical algorithms for the symmetric eigenvalue problem, we should have a look at its **condition**!
- Assume that instead of A we have a disturbed matrix $A + \varepsilon B$, where $||B||_2 = 1$. Since A is symmetric, we assume that B is also symmetric (usually only one half of A is stored in memory).
- Let λ be an eigenvalue of A and x an eigenvector to this eigenvalue, i.e. $Ax = \lambda x$. Let $x(\varepsilon)$ and $\lambda(\varepsilon)$ be the disturbed values of x and λ, implicitly given by the equality:

$$(A + \varepsilon B)x(\varepsilon) = \lambda(\varepsilon)x(\varepsilon)$$

$$\underset{\downarrow \atop (A+\varepsilon B)}{A}x = \lambda x$$

- Using Taylor series expansion around $\varepsilon_0 = 0$, we have:

$$\begin{aligned}(A + \varepsilon B)(x + x'(0)\varepsilon + \tfrac{1}{2}x''(0)\varepsilon^2 + \ldots) = \; & (\lambda + \lambda'(0)\varepsilon + \tfrac{1}{2}\lambda''(0)\varepsilon^2 + \ldots) \\ & (x + x'(0)\varepsilon + \tfrac{1}{2}x''(0)\varepsilon^2 + \ldots)\end{aligned}$$

- We are interested in the value of $\lambda'(0)$. Comparing coefficients of ε, we have:

$$\begin{aligned} Bx + Ax'(0) &= \lambda'(0)x + \lambda x'(0) \\ x^T Bx + x^T Ax'(0) &= \lambda'(0)x^T x + \lambda x^T x'(0) \\ x^T Bx + \lambda x^T x'(0) &= \lambda'(0)x^T x + \lambda x^T x'(0) \\ \frac{x^T Bx}{x^T x} &= \lambda'(0) \end{aligned}$$

- It follows that

$$\lambda(\varepsilon) - \lambda(0) = \frac{x^T B x}{x^T x}\varepsilon + O(\varepsilon^2).$$

- Since $\left|\frac{x^T B x}{x^T x}\right| \le \|B\|_2$, we get

$$|\lambda(\varepsilon) - \lambda(0)| \le |\varepsilon| \, \|B\|_2 + O(\varepsilon^2)$$

$A = PDP^{-1}$

$A = A^T \qquad A^T = (P^{-1})^T D^T P^T$

- Finally, with our assumption $\|B\|_2 \le 1$ for the perturbation matrix B, we have

$$|\lambda(\varepsilon) - \lambda(0)| = O(\varepsilon)$$

$\Rightarrow \boxed{D = D^T}$ ✓

$P = (P^{-1})^T$

$\boxed{P^T = P^{-1}}$

- Thus, the **symmetric** eigenvalue problem is a **well-conditioned** problem!

Remark: The **asymmetric** eigenvalue problem is **ill-conditioned**! Consider the asymmetric matrices

$$A = \begin{pmatrix} 1 & 1 \\ 0 & 1 + 10^{-10} \end{pmatrix}, \quad A + \varepsilon B = \begin{pmatrix} 1 - \lambda & 1 \\ \boxed{10^{-10}} & 1 + 10^{-10} - \lambda \end{pmatrix}.$$

A has eigenvalues $\lambda_1 = 1, \lambda_2 = 1 + 10^{-10}$ while $A + \varepsilon B$ has eigenvalues $\mu_{1/2} = 1 \pm 10^{-5}$. This means the error in the eigenvalues is about 10^5 times larger than the error in the matrix!

$(1-\lambda)(1+10^{-10}-\lambda) - 10^{-10} = 0$

$\Rightarrow (1-\lambda)(1+10^{-10}-\lambda) = 10^{-10}$

Naive Computation

- A naive method to compute eigenvalues could be to determine the characteristic polynomial $p(\lambda)$ of A, then using an iterative method for solving $p(\lambda) = 0$, e.g. Newton's iteration.
- However, this reduces the well-conditioned symmetric eigenvalue problem to the **ill-conditioned** problem of determining the roots of a polynomial!
- Example: Consider a 12×12 matrix with the eigenvalues $\lambda_i = i$. Its characteristic polynomial is

$$\boxed{p(\lambda)} = \prod_{i=1}^{12} (\lambda - i)$$

The coefficient of λ^7 is -6926634. Assume we have the polynomial $q(\lambda) = p(\lambda) - 0.001\lambda^7$, i.e. the relative error of the coefficient of λ^7 is $\varepsilon \approx 1.44 \cdot 10^{-10}$. However, the relative error of the eigenvalue λ_9 in this case is ≈ 0.02!

- $\Rightarrow$ We need better ideas ...

7.3. Vector Iteration

7.3.1. Power Iteration

Let $A \in \mathbb{R}^{n\times n}$ be symmetric. Then A has n eigenvectors $u_1, \dots, u_n$ that form a basis of $\mathbb{R}^n$, and we can write any vector $x \in \mathbb{R}^n$ as a linear combination of $u_1, \dots, u_n$:

$$x = c_1u_1 + c_2u_2 + \dots + c_nu_n \quad (c_1, \dots, c_n \in \mathbb{R})$$

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A corresponding to the eigenvectors $u_1, \dots, u_n$. Then

$$\begin{aligned} Ax &= \lambda_1c_1u_1 + \lambda_2c_2u_2 + \dots + \lambda_nc_nu_n \\ A^2x &= \lambda_1^2c_1u_1 + \lambda_2^2c_2u_2 + \dots + \lambda_n^2c_nu_n \\ &\vdots \\ A^kx &= \lambda_1^kc_1u_1 + \lambda_2^kc_2u_2 + \dots + \lambda_n^kc_nu_n \\ &= \lambda_1^k\left[c_1u_1 + \overset{<1}{\left(\frac{\lambda_2}{\lambda_1}\right)^k}c_2u_2 + \dots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_nu_n\right] c_1u_1 \end{aligned}$$

$\#\ \lambda_1 u_1 = A u_1$

$\#$ 当 $k \to \infty$

$$A^k x = \lambda_1^k c_1 u_1$$

$$\frac{A^k x}{\lambda_1^k}$$

Assume that λ_1 is **dominant** (i.e. $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$). $\Rightarrow \frac{\lambda_2}{\lambda_1} < 1 \quad \frac{\lambda_n}{\lambda_1} < 1$

Then for $k \to \infty$, we have $\left(\frac{\lambda_2}{\lambda_1}\right)^k, \dots, \left(\frac{\lambda_n}{\lambda_1}\right)^k \to 0$, and thus $\frac{1}{\lambda_1^k}A^kx \to c_1u_1$.

$$\begin{cases} x = c_1u_1 + c_2u_2 + c_3u_3 \\ A\ x = Ac_1u_1 + Ac_2Au_2 + Ac_3u_3 = \lambda_1c_1u_1 + \lambda_2c_2u_2 + \lambda_3c_3u_3 \\ A^3 = \lambda_1^3 c_1 u_1 + \dots \end{cases}$$

$\Rightarrow$ 可求 λ_1

- By choosing an appropriate start vector $x^{(0)} \in \mathbb{R}^n$ and performing the iteration

$$x^{(k+1)} = Ax^{(k)},$$

  we can calculate an approximation of an eigenvector of A belonging to the eigenvalue λ_1.

- "Appropriate" means that $u_1^T x^{(0)} \neq 0$. (Otherwise, $x^{(k)}$ will converge to the first eigenvector u_i where $u_i^T x^{(0)} \neq 0$.) If $x^{(0)}$ is chosen randomly with uniform probability, then the probability that $u_1^T x^{(0)} = 0$ is negligible (mathematically, it is zero).
- The values of the iteration vector get arbitrarily large (if $\lambda_1 > 1$) or small (if $\lambda_1 < 1$). To avoid numerical problems, we should therefore normalize the value of x_k after each iteration step.
- Calculating eigenvalues from eigenvectors: Let $\boxed{x}$ be an eigenvector of A belonging to the eigenvalue $\boxed{\lambda}$. Then

$$\begin{aligned} Ax &= \lambda x \\ \frac{x^T Ax}{x^T x} &= \lambda \end{aligned}$$

$$\frac{x^T Ax}{x^T x}$$

  If x is normalized, i.e. $\|x\| = 1$, then $\lambda = x^T Ax$.

- The term

$$\boxed{\frac{x^T Ax}{x^T x}}$$

  is also called **Rayleigh quotient**.

Power Iteration: Algorithm

- Choose a random $x^{(0)} \in \mathbb{R}^n$ such that $\left\|x^{(0)}\right\| = 1$
- for $k = 0, 1, 2, \cdots$:
  1. $w^{(k)} := Ax^{(k)}$
  2. $\lambda^{(k)} := (x^{(k)})^T w^{(k)}$
  3. $x^{(k+1)} := \frac{w^{(k)}}{\left\|w^{(k)}\right\|}$
  4. stop if approximation “sufficiently accurate”

Remarks:

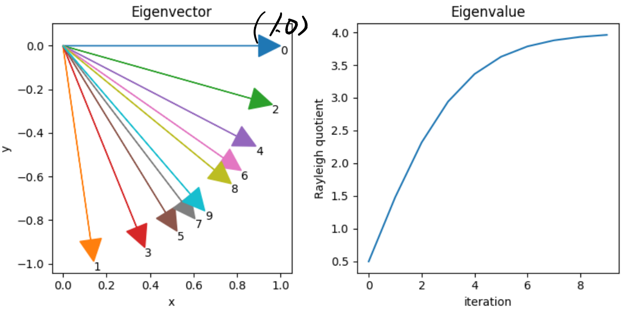
- We can consider our approximation $x^{(k)}$ “sufficiently accurate” if

$$\left\|w^{(k)} - \lambda^{(k)} x^{(k)}\right\| \leq \varepsilon \left\|w^{(k)}\right\|.$$

- The **cost** per iteration step is determined by the cost of computing the matrix-vector product $Ax^{(k)}$, which is at most $O(n^2)$.

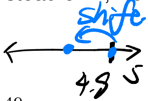
Example

- We consider the matrix $A = \begin{pmatrix} 0.5 & -3.5 \\ -3.5 & 0.5 \end{pmatrix}$.
- The matrix A has the eigenvalues $\lambda_{1,2} = -3, 4$ with corresponding eigenvectors $v_{1,2} = \begin{pmatrix} \sqrt{2}/2 \\ \sqrt{2}/2 \end{pmatrix}, \begin{pmatrix} \sqrt{2}/2 \\ -\sqrt{2}/2 \end{pmatrix}$
- We start a power iteration with the initial guess $\underline{x^{(0)} = \begin{pmatrix} 1 & 0 \end{pmatrix}^T}$.
- We see the convergence $x^{(i)} \to v_2, \lambda^{(i)} \to \lambda_2$:



Convergence

- The **convergence order** of the sequence $\{x^{(k)}\}$ is **linear** with convergence rate $q = \lambda_2/\lambda_1$.
- The convergence order of the sequence $\{\lambda^{(k)}\}$ is **quadratic** with convergence rate q.
- Thus, if λ_2 is only slightly smaller than λ_1, convergence will be very slow. We can address this problem by **shifting** the eigenvalues:
  - Assume we have guessed an approximation $\mu \approx \lambda_2$.
  - Consider the matrix $A - \mu I$. It is easy to see that this matrix has eigenvalues $\lambda_1 - \mu, \dots, \lambda_n - \mu$.
  - By performing the iteration with the matrix $A' = A - \mu I$ instead of A, we can greatly speed up convergence.
  - Example: $n = 2, \lambda_1 = 5, \lambda_2 = 4.9$.
    Using $\mu = 4.85$, we have convergence rate $\frac{\lambda_2-\mu}{\lambda_1-\mu} = \frac{1}{3}$.
    Compare this to the "original" convergence rate $\lambda_2/\lambda_1 = \frac{49}{50}$!



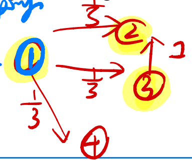
  - In general, we have a convergence rate $\frac{\lambda_j-\mu}{\lambda_i-\mu}$, where $\lambda_i - \mu$ is the largest and $\lambda_j - \mu$ the second largest shifted eigenvalue, regarding the modulus, i.e. $|\lambda_i - \mu| \geq |\lambda_j - \mu| \geq |\lambda_k - \mu| \;\; \forall\, k \in \{1, \dots, n\} \setminus \{i, j\}$.

Remarks

- The algorithm also works for a slightly weaker condition on the eigenvalues of A: If A has no dominant eigenvalue, but there exists an $r \in \{1, \dots, n\}$ such that $\lambda_1 = \dots = \lambda_r$ and $|\lambda_r| > |\lambda_i|$ for all $i \in \{r+1, \dots, n\}$, then the sequence $\{x^{(k)}\}$ converges to a linear combination of $u_1, \dots, u_r$.
- Power iteration can be used to successively compute several eigenvalues in descending order:
  - It is a standard result in linear algebra that, if v_1 is an eigenvector belonging to the eigenvalue λ_1, the matrix $A - \lambda_1 v_1 v_1^T$ has the same eigenvalues and eigenvectors as A, but λ_1 has been replaced by 0.
  - After eigenvalue λ_1 and a corresponding eigenvector v_1 have been computed with sufficient precision, we continue the iteration with the matrix $A - \lambda_1 v_1 v_1^T$ to find λ_2 and so on.
- Prominent areas of application of power iteration are found in statistics (Google's PageRank algorithm, Principal Component Analysis).

Page Ranking

Los! 1



$$\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{pmatrix} 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \boxed{\frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4} \quad \frac{1}{4}} \\ 0 & 1 & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix} = A$$

Summe : 1

random walk

Schritt 1: $(1\ 0\ 0\ 0)\,A = (0\ \ \frac{1}{3}\ \ \frac{1}{3}\ \ \frac{1}{3})$ $\Big\}\ (1,0,0,0)A^k$

② ② ④

Schritt 2: $(0\ \frac{1}{3}\ \frac{1}{3}\ \frac{1}{3})\,A = (\frac{1}{6}\ \ \frac{1}{2}\ \ \frac{1}{6}\ \ \frac{1}{6})$

7.3.2. Inverse Iteration

- We now look for a method to compute a **specific** eigenvalue λ^* of a symmetric matrix $A \in \mathbb{R}^{n\times n}$, given the approximation $\mu \approx \lambda^*$. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A.
- Remember that A^{-1} has eigenvalues $\lambda_1^{-1}, \ldots, \lambda_n^{-1}$, such that we could compute the **smallest** eigenvalue of A by perfoming power iteration with A^{-1}.
- We can combine this with the shifting technique we saw before: If μ is closer to λ^* than to any other eigenvalue, $\lambda^* - \mu$ is the smallest eigenvalue of $A - \mu I$.
- We can therefore perform power iteration with $(A - \mu I)^{-1}$ to calculate an approximation for $\lambda^* - \mu$!
- However, we do not have to calculate $(A - \mu I)^{-1}$ explicitly since the recurrence

  $$x^{(k+1)} = (A - \mu I)^{-1} x^{(k)}$$

  is equivalent to

  $$(A - \mu I) x^{(k+1)} = x^{(k)}.$$

  This means that we can calculate the value of $x^{(k+1)}$ by using a solver for linear systems of equations in each iteration step.

Inverse Iteration: Algorithm

- Choose a random $x^{(0)} \in \mathbb{R}^n$ such that $\left\|x^{(0)}\right\| = 1$
- for $k = 0, 1, 2, \cdots$:
  1. solve $(A - \mu I)w^{(k)} = x^{(k)}$
  2. $x^{(k+1)} := \frac{w^{(k)}}{\left\|w^{(k)}\right\|}$
  3. Stop if approximation “sufficiently accurate”

Remarks:

- The cost of each iteration step is dominated by the complexity of solving the linear system with coefficient matrix $A - \mu I$.
- Since this matrix does not change during iteration, we can compute its LU factorization in the beginning, thereby reducing the cost of each iteration step to $O(n^2)$ operations.
- As we are essentially performing power iteration, the same remarks about convergence apply.

7.3.3. Rayleigh Quotient Iteration

λ_1
λ_2
λ_3

- In our implementation of power iteration, we used the Rayleigh quotient to compute an approximation of λ_1 in each iteration step.
- We can make use of this value to refine our approximation μ in each step!
- This gives the following algorithm:
  - Choose a random $x^{(0)} \in \mathbb{R}^n$ such that $\|x^{(0)}\| = 1$
  - for $k = 0, 1, 2, \cdots$:
    1. $\mu^{(k)} := (x^{(k)})^T A x^{(k)}$
    2. solve $(A - \mu^{(k)} I) w^{(k)} = x^{(k)}$
    3. $x^{(k+1)} := \frac{w^{(k)}}{\|w^{(k)}\|}$
    4. Stop if approximation “sufficiently accurate”
- This algorithm is usually known as **Rayleigh quotient iteration**.

Remarks

- It can be shown that the convergence order of the sequence $\{\lambda^{(k)}\}$ is now **cubic**! Still, the sequence of the eigenvectors converges linearly.
- However, since we have to solve a different system of linear equations in each iteration step, the **cost** per step is usually significantly higher than for power iteration!
- Rayleigh quotient iteration is the method of choice if we have a good approximation of the eigenvalue we look for – then only a few iteration steps are needed due to the high convergence order.
- If we already have an eigenvalue and only want to compute a corresponding eigenvector, “standard” inverse iteration has an advantage over Rayleigh quotient iteration, since the sequence of eigenvectors converges linearly for both methods, but Rayleigh quotient iteration is more costly.

$$Av=\lambda v \rightarrow AV=V\Lambda$$

$$y=Ax \qquad V^TAV=\Lambda=\text{dig}$$

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

Nullstelle.

应用:

Quantenmechanik

PCA.

Graphen

Pagerank

7.4. QR Iteration

- **Factorization methods** such as the QR iteration [Francis 1961] compute **all** eigenvalues of a symmetric matrix $A \in \mathbb{R}^{n\times n}$ at once.
- The idea is to compute a sequence of matrices $\{A_k\}$ that are **similar** to A. This sequence should converge to a matrix in triangular form, such that the diagonal of A_k is an approximation for the eigenvalues of A.
- The QR iteration is based on the QR decomposition which factorizes a given matrix A such that $A = QR$, with Q an orthogonal and R an upper triangular matrix. Then the matrix

  $$RQ = \underline{Q^{-1}}AQ = \underline{Q^T}AQ$$

  is similar to A.
- It can be shown that the sequence $\{A^{(k)}\}$ defined by

  $$\begin{array}{rcl} A^{(0)} & = & A, \\ A^{(k+1)} & = & R^{(k)}Q^{(k)}, \\ & & Q^{(k)} \text{ orthogonal, } R^{(k)} \text{ upper triangular, } A^{(k)} = Q^{(k)}R^{(k)} \end{array}$$

  converges to a diagonal matrix.

QR Iteration: Algorithm

- Thus, we have the following algorithm:
  - $A^{(0)} := A$
  - for $k = 0, 1, 2, \dots$:
    1. Compute a factorization $A^{(k)} = QR$ using QR decomposition
    2. $A^{(k+1)} := RQ$
    3. if $a^{(k+1)}_{n,n-1}$ sufficiently small:
       output $\lambda_n \approx a^{(k+1)}_{n,n}$
       remove row and column n
- We consider the subdiagonal element $a^{(k+1)}_{n,n-1}$ "sufficiently small" if its absolute value is $\leq \varepsilon \cdot |a^{(k+1)}_{n,n}|$.
- We still need to know how to implement the QR decomposition!

7.4.1. QR Decomposition

- Remember: We want to decompose a matrix A into an orthogonal matrix Q and an upper triangular matrix R such that $A = QR$.
- This problem is equivalent to the following: Find an orthogonal matrix G such that $GA = R$, i.e. G “zeroes out” the subdiagonal part of A. Then $A = G^T R$.
- We first have a look at the two-dimensional case: Given a vector $x = (x_1, x_2)^T$, find an orthogonal matrix G such that $Gx = (r, 0)^T$ for some $r \in \mathbb{R}$.
- It is easy to see that

$$G = \frac{1}{\sqrt{x_1^2 + x_2^2}} \begin{pmatrix} x_1 & x_2 \\ -x_2 & x_1 \end{pmatrix}$$

  does the job.
- Geometrically, the matrix G describes a rotation by $\theta = \arctan(x_2/x_1)$ radians in the (x_1, x_2) plane.
- G is called a **Givens** rotation matrix [Givens 1958].

- Generalization to the n-dimensional case: When multiplied with A,

$$G_{ij} = \begin{pmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & \rho \cdot a_{jj} & \cdots & \rho \cdot a_{ij} & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & -\rho \cdot a_{ij} & \cdots & \rho \cdot a_{jj} & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{pmatrix}, \quad \rho = \frac{1}{\sqrt{a_{ij}^2 + a_{jj}^2}}$$

  affects rows i and j of A and eliminates entry a_{ij}. G_{ij} differs from the identity matrix in only four entries.

- To zero out the entire subdiagonal part, we use the product

$$G = G_{n,n-1} \cdot G_{n,n-2} \cdot G_{n-1,n-2} \cdot \cdots \cdot G_{n,2} \cdots G_{3,2} \cdot G_{n,1} \cdots G_{2,1},$$

  i.e. we eliminate the matrix entries column-wise from left to right, top to bottom, in order not to introduce additional non-zero entries!

- Since the product of two orthogonal matrices is orthogonal, G is orthogonal and GA is an upper triangular matrix for any matrix A.

QR Iteration: Implementation

- We now have a method to compute the QR decomposition of A: $R = GA$, $Q = G^T$.
- The naive computation of G via $n(n-1)/2$ matrix multiplications costs $O(n^5)$ operations!
- However, the **effect** of the multiplication with a Givens rotation matrix can be computed with $O(n)$ operations due to its special structure. This leads to a total of $O(n^3)$ operations for the QR decomposition.
- For QR iteration, we are not even interested in the value of G. We only need to compute the product $A^{(k+1)} = GA^{(k)}G^T$!
- Since matrix multiplication is associative and $(M_1M_2)^T = M_2^T M_1^T$, we can use the following scheme for computation of $A^{(k+1)}$:

$$A^{(k+1)} = \ldots G_{3,1} \left(G_{2,1}\, A^{(k)}\, G_{2,1}^T \right) G_{3,1}^T \ldots$$

Remarks

- QR iteration is the method of choice if **all** eigenvalues of a matrix are needed.
- The convergence order of the sequence $\{A^{(k)}\}$ is **linear**.
- As with power iteration, convergence is slow if any of the eigenvalues are close together. By using a shift operation, similar to the one in Rayleigh quotient iteration, we can achieve **quadratic** convergence order.
- Our algorithm does not calculate eigenvectors. Eigenvectors to specific eigenvalues can be retrieved using inverse iteration.
- QR decomposition can also be used as an **exact solver** for systems of linear equations: Let $A \in \mathbb{R}^{n\times n}, b \in \mathbb{R}^n$. Then

$$\begin{array}{rrcl} & Ax & = & b \\ \Longleftrightarrow & QRx & = & b \\ \Longleftrightarrow & Rx & = & Q^Tb \end{array}$$

  - Since R is upper triangular, the system $Rx = Q^Tb$ can be solved with $O(n^2)$ operations.
  - As the computation of the QR decomposition can take $O(n^3)$ operations, this method – as LU factorization – is especially useful when a set of systems with the same matrix A but many different vectors b_i has to be solved.

7.5. Reduction Algorithms

- The cost of all three algorithms presented so far depends largely on the number of non-zero entries in the matrix A:
  - Cost of an iteration step in power iteration is dominated by the complexity of the matrix-vector product Ax.
  - Cost of an iteration step in inverse iteration is dominated by the complexity of solving $Ax = b$.
  - Cost of an iteration step in QR iteration depends on the number of Givens rotations that we have to use to eliminate non-zero entries in the iteration matrix A_k.
- Therefore, for numerical computation of eigenvalues, we are interested in matrices that are **similar** to A but have a significantly lower number of non-zero entries.

- We try to develop an algorithm that transforms a symmetric matrix $A \in \mathbb{R}^{n\times n}$ into a similar **tridiagonal** symmetric matrix:

$$A \to \begin{pmatrix} * & * & 0 & 0 & \cdots & \cdots & 0 \\ * & * & * & 0 & 0 & \cdots & 0 \\ 0 & * & * & * & 0 & \cdots & 0 \\ & & & \vdots & & & \\ 0 & \cdots & 0 & * & * & * & 0 \\ 0 & \cdots & 0 & 0 & * & * & * \\ 0 & \cdots & \cdots & 0 & 0 & * & * \end{pmatrix}$$

- Observation: Matrix $A \in \mathbb{R}^{n\times n}$ is tridiagonal and symmetric if and only if it is of the form

$$\begin{pmatrix} \alpha & \rho & 0 & \cdots & 0 \\ \rho & & & & \\ 0 & & A' & & \\ \vdots & & & & \\ 0 & & & & \end{pmatrix}$$

with $A' \in \mathbb{R}^{(n-1)\times(n-1)}$ tridiagonal and symmetric.

- This leads to a “dynamic programming” approach: Use a similarity transformation to transform A to a matrix in the above form, then continue with A' recursively.

Transformation Algorithm

- If we had a matrix $H' \in \mathbb{R}^{(n-1)\times(n-1)}$ such that

$$H' \begin{pmatrix} a_{12} \\ a_{13} \\ \vdots \\ a_{1n} \end{pmatrix} = \begin{pmatrix} \rho \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

  for some $\rho \in \mathbb{R}$, then

$$HA := \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ 0 & & H' & \\ \vdots & & & \\ 0 & & & \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{12} & & & \\ a_{13} & & & \\ \vdots & & \ddots & \vdots \\ a_{1n} & & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \rho & & & \\ 0 & & B & \\ \vdots & & & \\ 0 & & & \end{pmatrix}$$

  ($B \in \mathbb{R}^{(n-1)\times(n-1)}$).

- We already know that such a H' exists – for example, it can be described as the product of $n-2$ Givens rotations.

- By transposing the result, we can use the effect of multiplication with H again:

$$H(HA)^T = H \begin{pmatrix} a_{11} & \rho & 0 & \cdots & 0 \\ a_{12} & & & & \\ a_{13} & & B^T & & \\ \vdots & & & & \\ a_{1n} & & & & \end{pmatrix} = \begin{pmatrix} a_{11} & \rho & 0 & \cdots & 0 \\ \rho & & & & \\ 0 & & A_2 & & \\ \vdots & & & & \\ 0 & & & & \end{pmatrix}$$

- Since $H(HA)^T = HA^TH^T = HAH^T$, this is a similarity transformation if and only if H is orthogonal.
- For that, it is important that the application of H does not destroy the first *row* of A. Therefore, we can only eliminate everything below the subdiagonal element of the first column, and produce a triadiagonal matrix only (instead of a diagonal one).
- With basic linear algebra, one can also show that A_2 is symmetric.
- Our task is now to find an appropriate matrix H'!

Householder Transformations

- A first idea could be to choose H' as a product of Givens rotations, as previously indicated.
- However, in practice **Householder transformations** [Householder 1958] are used more frequently.
- For any vector $x \in \mathbb{R}^n$, **Householder matrix** $H \in \mathbb{R}^{n \times n}$ is defined by

  $$H = I - 2vv^T,$$

  with $v := \frac{u}{\|u\|_2}$ and $u := x - \|x\|_2 \, e_1$, such that

  $$Hx = \begin{pmatrix} \rho \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

  for some $\rho \in \mathbb{R}$.
- Geometrically, H describes a **reflection** of x in the hyperplane defined by the vector v which is orthogonal to the hyperplane.

Remarks

- As with Givens rotation matrices, Householder matrices are usually not explicitly computed. When using an appropriate implementation, the effect of multiplication with a Householder matrix can be computed with $O(n^2)$ operations.
- In that case, the transformation algorithm described above takes $O(n^3)$ steps, rather than $O(n^4)$ steps for a naive implementation with $O(n)$ matrix multiplications.
- Householder transformations can also be used to compute the QR decomposition, since the product of $n-1$ Householder matrices transforms a matrix into upper triangular form.
- We could therefore also use them for QR iteration!
- However, it is more efficient to first reduce a matrix to tridiagonal form using Householder transformations (cost: $O(n^3)$), then perform QR iteration using Givens rotations on the reduced matrix.
- Then, in each iteration step, only $O(n)$ elements need to be zeroed using Givens rotations, which results in a cost of $O(n^2)$ per iteration step, vs. $O(n^3)$ when using Householder transformations.