Computational Physics — SuSe 2023
7. Exercise Sheet

Handing out: 05.06.2023 — Prof. H. Jelger Risselada
Submission: 09.06.2023 8 pm

Exercise 0: Matrix diagonalization - Power method — 8 Points

Many physical systems can be described by matrices whose eigenvalues correspond to the eigenfrequencies of these systems. Therefore, matrix diagonalization is an important tool in physics, and the power method is a simple and significant technique.

Given the symmetric 4×4-matrix:

$$A = \begin{pmatrix} 1 & -2 & -3 & 4 \\ -2 & 2 & -1 & 7 \\ -3 & -1 & 3 & 6 \\ 4 & 7 & 6 & 4. \end{pmatrix} \tag{1}$$

a) Determine the eigenvalues of the matrix using numpy.linalg.eig or the C++ library Eigen (http://www.eigen.tuxfamily.org).

b) Determine the eigenvalues a second time by implementing the power method. Choose a suitable initial vector $\vec{v}_0$ and an appropriate number of iterations. Compare your results with the ones from the first part of the task.

Exercise 1: Householder with QR Iteration — 12 Points

In the following, you are asked to become familiar with the Householder algorithm and the QR iteration. Using this method, it is possible to efficiently diagonalize even large matrices.

Given the symmetric N × N matrix:

$$A_{k,l} = k + l + k\delta_{k,l} \quad 0 \leq k, l < N. \tag{2}$$

a) Use Householder transformations to transform matrix A into tridiagonal form.

b) Determine the eigenvalues of A using QR iteration.

c) Diagonalize matrix A also using the power method that you implemented in Task 1. Compare the results and runtimes.

Do this for $N = 10$, $N = 100$ and $N = 1000$.