Introduction to Computational Physics SS2023

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Exercise 6 from May 24, 2023
Return before noon of June 9, 2023

1 Presence Work: Numerical linear algebra methods; calculating eigenvalues in two steps

1.1 Getting a tridiagonal matrix

Example of real symmetric matrix

$$\mathbf{A} = \begin{pmatrix} 1. & 2. & 3. & 1. \\ 2. & 5. & 6. & 1. \\ 3. & 6. & 1. & 9. \\ 1. & 1. & 9. & 1. \end{pmatrix}$$

compute its equivalent tridiagonal form $\mathbf{T}$ (in the sense that $\mathbf{T}$ is obtained through a similarity transformation from $\mathbf{A}$, i.e. it has the same eigenvalues), by using two different methods and check the results against each other:

1 Use python alglib package, function `xalglib.smatrixtd` .

2 Use a self-programmed Householder algorithm.

Notice: C or Fortran programmers would use the Numerical Recipe routine `tred2` to produce tridiagonal matrices.

Larger matrix

Use a larger matrix $\mathbf{A}$ with $a_{nm} = 1/(n+m+1)$ with $n,m = 0,\ldots,N$ for $N = 50$. Compare the tridiagonal matrix from `xalglib.smatrixtd` and from your Householder implementation.

1.2 Getting eigenvalues EW and eigenvectors EV

In the lecture the **QR** algorithm has been introduced, which determines EW and EV of a real symmetric tridiagonal matrix $\mathbf{T}$ from an iterative sequence of operations like $\mathbf{T} = \mathbf{QR}$, where a matrix is decomposed into a right upper triangular one $\mathbf{R}$ and an orthogonal matrix $\mathbf{Q}$. Numerical recipes provide for Fortran and C the routine `tqli`, which uses the analogous **QL** algorithm, with a lower left triangular matrix $\mathbf{L}$.

Nowadays in python we use two ways - `scipy.linalg` package with routine `eigh_tridiagonal`; or we use `numpy.linalg` with the function `eig`. Use the tridiagonal matrix obtained from $\mathbf{A}$ in 1.1.1. and get EW and EV using `eigh_tridiagonal`; use the same matrix to compute directly EW and EV using `eig`. Both should agree.

1.3 Application to the unperturbed quantum mechanical oscillator

Test the approach by applying it to the unperturbed harmonic oscillator in quantum mechanics. In dimensionless form, the corresponding Hamiltonian reads

$$h_0 = \frac{H}{\hbar\omega} = \left(\frac{1}{2}\Pi^2 + \frac{1}{2}Q^2\right)$$

with eigenvalues $n + 1/2$. The matrix form of the diagonalized operator h_0 is

$$(h_0)_{nm} = \left(n + \frac{1}{2}\right)\delta_{nm} \ .$$

2 Homework: perturbed quantum mechanical oscillator

Calculate the eigenvalues of the perturbed quantum mechanical harmonic oscillator for $n = 0 \ldots 9$ by approximating the operators in Hilbert space by matrices with finite dimension in the range $N = 15 \ldots 30$.
The dimensionless Hamiltonian reads

$$h = \frac{H}{\hbar\omega} = \left(\frac{1}{2}\Pi^2 + \frac{1}{2}Q^2 + \lambda Q^4\right)$$

$$(h)_{nm} = (h_0)_{nm} + \lambda(Q^4)_{nm}$$

where $(h_0)_{nm} = \left(n + \frac{1}{2}\right)\delta_{nm}$ is the unperturbed Hamiltonian.

(a) Determine the matrix form of Q^4 using

$$Q_{nm} = \frac{1}{\sqrt{2}}\left(\sqrt{n+1}\delta_{n,m-1} + \sqrt{n}\delta_{n,m+1}\right) .$$

The best approach is to consider this problem in second quantisation and use the properties of the creation and annihilation operators, a^* and a, as discussed in the lecture.
(6 points)

(b) Compute the eigenvalues of $(h)_{nm}$ for the parameter $\lambda = 0.1$ as function of the matrix size ($N = 15 \ldots 30$). Demonstrate that your program works properly, just listing the eigenvalues is not sufficient. (10 points)

(c) Calculate the eigenvalues analytically using the linearized form of the equation, i.e. consider only the terms on the diagonal. (4 points)

(d) BONUS QUESTION: Determine the eigenvalues by employing the Wentzel, Kramers, and Brillouin (WKB) approximation applied to this system. Compare to the results in (b) and (c) and discuss possible differences. (10 bonus points)