Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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Exercise sheet 9

To be handed in on 13.12.2023 and discussed on 15.12.2023 and 18.12.2023.

Exercise 1 [*Volume of the unit sphere in d dimensions*] (6 pts.)

Using the Monte-Carlo integration method discussed in the lecture, compute the volume of a d dimensional unit sphere

$$V_d \equiv \int_{-1}^{+1} \mathrm{d}x_1 \int_{-1}^{+1} \mathrm{d}x_2 \cdots \int_{-1}^{+1} \mathrm{d}x_d \, \Theta(1 - x_1^2 - x_2^2 - \ldots - x_d^2) \quad ,$$

with $d \in \{2, 3, 10\}$. For each d, use $N_1 = 10^6$ and $N_2 = 10^8$ random points to evaluate the integral and estimate the statistical error of your result. Compare what you obtained with the expected analytical result and try to explain how and why the statistical error varies as function of N_i and of d.

Exercise 2 [*Eigenvalues of the Schroedinger equation*] (1+2+7+2+2 pts.)

Consider a 1-dimensional quantum mechanical system particle with mass m in the infinite potential well

$$V(x) \quad = \quad \begin{cases} 0 & \text{if } 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases} \quad .$$

(i) Write down the Schroedinger equation. Introduce dimensionless quantities $\hat{x}, \hat{E}$ to treat the equation numerically.

(ii) Discretize the interval $[0, L]$ using N lattice points and rewrite the Schroedinger equation as an eigenvalue equation

$$A\boldsymbol{\psi}_n = \hat{E}_n \boldsymbol{\psi}_n \tag{1}$$

where A is a symmetric and real matrix.
Hint: You can proceed in a very similar way as done, when discretizing the Poisson equation on exercise sheet 6 and in the lecture in section 7.7.2.

(iii) Implement the Jacobi algorithm to determine the eigenvalues and the eigenvectors of a real and symmetric matrix. To test your program properly, use the matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad A = \begin{pmatrix} -1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$

and compare numerical and analytical results.

(iv) Use your code from (iii) to solve Eq. (1). Plot the analytically known continuum $\hat{E}_n$ and your numerical results for $N = 20, 50, 100, 150, 200$ against $n \in [0, 40]$. Additionally, plot the relative error $\Delta\hat{E}_{n,\mathrm{rel}}$. Is it sufficient to use a small N if you are only interested in the low-lying eigenvalues? How would you choose N in order to obtain the first 10 eigenvalues with an error of $\Delta\hat{E}_{n,\mathrm{rel}} < 3\%$.

(v) Now plot and compare the wavefunctions $\psi_n(x)$ for $N = 50, 100, 150$ and $n = 1, 2, 5, 10, 30, 50$. Also include the analytical result in your plots and discuss the results. In particular, explain the reason, why higher energy eigenvalues have larger errors.