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— Computational Quantum Physics —

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Sommersemester

Exercise 1

Task 1: Power method (4 points)

The *power method*[1] can be used to calculate the largest (in absolute value) eigenvalue of a (diagonalizable) matrix M. Given an initial vector v_0 and the recurrence relation $v_{n+1} = M v_n$, the series (v_n) converges to an eigenvector for the dominant eigenvalue.
Implement the power method and compare the results of your implementation to the value obtained with the `eigvals` function. For this, use random, real $N \times N$ matrices.

Task 2: Numerical integration (3 points)

Calculate the integral

$$\int_0^1 \mathrm{e}^x \, \mathrm{d}x$$

using (a) the midpoint rule and (b) Simpson's rule. Compare the results for different interval lengths to the exact value.

Task 3: Monte-Carlo π (3 points)

Create N pairs $r_i = (x_i, y_i)$ of random numbers that are uniformly distributed on the unit square $[0,1)^2$ (i.e., x_i and y_i are each uniformly distributed on $[0,1)$), and count how many pairs N_{inside} are inside the unit circle $x_i^2 + y_i^2 \leq 1$. Since

$$\frac{N_{\text{inside}}}{N} \xrightarrow{N \to \infty} \frac{A_{\text{unit circle}}/4}{A_{\text{unit square}}} = \frac{\pi}{4} \,,$$

this method can be used to calculate an approximate value of π.
Implement the method described above and check the accuracy of the calculated value for π for different N.

[1] cf. `https://en.wikipedia.org/wiki/Power_iteration`