Computational Methods

Exam - 2020

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Rules of the game

Choose one of the four exercises and write a report of maximum 7 pages (including figures with captions) and send it in *.pdf format together with the Python codes used to generate the plots in a zipped directory.
The deadline for submitting the report is the 15th of January 2021.
The report must include a brief description of the physical or mathematical problem, followed by the answers to the points in the exercises. When necessary describe the method (or formula) used to find the solutions.
You can/must use the Python codes written during the course!

1. Driven-damped harmonic oscillator

Let us consider the equation of motion of an oscillator under the influence of a friction and also in the presence of a periodic external force

$$\ddot{x}(t) = -\omega^2 x(t) - \gamma \dot{x}(t) + f_0 \cos(\omega_0 t)$$

Write a brief introduction to the problem reporting the analytical solutions (do not demonstrate anything). Answer to the following questions:

1. At first set the external force to zero $f_0 = 0$. Use for example $\omega = 9$ and the initial conditions $x_0 = 1$ and $v_0 = 1$. Evolve the system using one of the following algorithms: Velocity-Verlet, second order Runge-Kutta second or fourth order Runge-Kutta. Compare the evolutions for different values of the friction parameter $\gamma = [0.0, 1.0, 2.0, 3.0, \ldots]$ and compute the period of the first oscillation $T(\gamma)$ as a function of the friction parameter γ. There exists a critical value of $\gamma = \gamma_c$ for which the spring is not able to complete its first oscillation. Determine this value numerically.

   Plot the evolution of the system for some values of γ around the critical value. Plot the values of the period $T(\gamma)$ as a function of γ. Discuss the results.

2. For $\gamma = \gamma_c$ and for $\gamma < \gamma_c$ (choose a value) how does the energy decrease with time? Given its numerical values, plot the evolution of the energy function in time, and make an hypothesis of the functional rule governing the decay of $E(t)$. Discuss the results.

3. Switch on the driving force $f_0 \neq 0$ and set $\gamma = 1$. Study the evolution of this system for $f_0 = 1.0, 1.5, 2.0$ and plot it for a finite time t. Discuss the results.

2. Quantum Monte Carlo for an infinite potential well

Consider the time-independent Schrödinger equation for an infinite potential well

$$\hat{H}\Psi(x) = E\Psi(x)$$

with the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

with

$$V(x) = \begin{cases} +\infty & x \leq -L \\ V_0 & -L < x < L \\ +\infty & x \geq L \end{cases}$$

For simplicity let us fix $\hbar = m = 1$. Consider the approximate trial solution of the type

$$\Psi_T(x) = A\cos(kx) + (1 - A)\sin(kx),$$

where A and k are variational parameters.
Write a brief introduction to the problem reporting the analytical solutions (do not demonstrate anything).
Answer to the following questions:

1. Write a Monte Carlo algorithm to compute the energy functional $E[\Psi_T]$ by defining the local energy and the probability density associated to the square modulus of the trial wave function $|\Psi_T|^2$.

2. Setting $A = 1$ our trial wave function approximates only the even solutions of the equation. Since the analytical expressions and thus the value of $k_0 = \frac{\pi}{2L}$ corresponding to the 'even' ground state's wave function are known, plot the energy with the associated statistical error for different values of k around the exact value $k = k_0$ by adding a shift Δk.

3. The error computed from consecutive values of the local energy is correlated. Study the auto-correlation function of the local energy and estimate the correlation time. Plot the values of the energy obtained for the previous values of k this time with the uncorrelated error. Discuss the results and about the auto-correlation time.

4. By fixing the value of k to k_0 change the parameter of A in the interval $[0, 1]$ and plot the energy and the corresponding uncorrelated statistical error. Show also how the variance of the local energy behaves as a function of A. Describe the behaviour of the Energy and of the Variance. Does the latter go to zero, why?

3. Shooting method for the quantum harmonic oscillator

Consider the time-independent Schrödinger equation of the one dimensional harmonic oscillator

$$\hat{H}\Psi(x) = E\Psi(x)$$

with the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

with

$$V(x) = \frac{1}{2}m\omega^2$$

For simplicity let us fix $\hbar = m = \omega = 1$.
Write a brief introduction to the problem reporting the analytical solutions (do not demonstrate anything).
Answer to the following questions:

1. Set the initial conditions $\Psi(0) = 1$ and $\frac{d\Psi(x)}{dx}\Big|_{x=0} = 0$ (even solutions) and use the Shooting method to evolve the solution until $\Psi(x) \approx 0$ for $x > 0$ (Initially use a small but positive value of E, for example $E = 0.1$). The boundary condition in this case will be $\Psi(x \to \infty) = 0$. Yet, one should observe that there is a region of the space x in which the solution rapidly decays to zero. The numerical solution will go to zero and then diverge to positive or negative values (thus changing sign), in between you have the correct eigenfunction. Do a plot with different shootings increasing E and discuss the results.

2. Write a function that changes the values of E and evolves the solution until $\Psi(x)$ becomes 'small enough' for a value of $x > 0$ and that computes the first eigenvalue with a precision of $\epsilon_{cut} = 10^{-5}$.

3. Write a function that progresses from the first eigenvalue and computes the second and third. Write a table that compares the exact eigenvalues with those obtained numerically, for the first three states. Plot the best numerical estimation of the first three eigenfunctions. Briefly comment on the results.

4. Kernel Ridge Regression (KRR)

Write a brief introduction on Kernel Ridge Regression (KRR) and describe the data contained in the attached files (First plot the data). The files "DATA_.dat" contain two columns of numbers. The first one (X) contains the features and the second (Y) contains the targets. In total there are 1000, 800, 500, and 200 observations. Using the data within these files, do the following:

1. Using only the file "DATA_1000.dat", do GridSearchCV with Scikit-learn to train KRR models for the gaussian (rbf), laplacian and polynomial kernels. Consider only 4 different values for each hyperparameter (for instance, for the case of the polynomial kernel you must consider 4 values of lambda [alpha in Scikit-learn], 4 values of degree, 4 values of gamma, and 4 values of coef0). You need to do K-fold cross validation with K = 5. Take the best models for each kernel and plot them together with the original data. Discuss the findings and the quality of the result obtained with the kernels.

2. Choose the best performing kernel function from task 1, and do GridSearchCV to train KRR models using each "DATA_.dat" file separately. You need again to do K-fold cross validation with K = 5. Compute the Mean Absolute Error (MAE) of all cross-validation tasks, and for each of the "DATA_.dat" files keep the lowest MAE value. Plot the MAE as a function of the size of the training set. Comment on the results.