Problems for credits (Zápočtové úlohy) 2017

Problem 1: Particle in circular potential well

(integration of function, nonlinear equation solution)

Particle is moving inside infinitely deep two dimensional potential well of circular shape. Your task is to find energy of the first three bound states with zero angular momentum by solving the equation for boundary condition of radial part of wave function

$$\psi(a) = J_0(ka) = 0,$$

where $a = 1$ is radius of the potential well. Bessel function $J_0(kr)$ is radial part of solution of Schrödinger equation in 2D and it can be calculated from its integral representation

$$J_0(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos(z \cos x) \mathrm{d}x.$$

More detailed instructions:

- Calculate the integral in the definition of the Bessel function using the trapezoidal rule. Test the speed of convergence of the method and plot the dependence of the decadic logarithm of the estimated error on the number of integration points. Explain the results.
- Based on this analysis select suitable number of integration points and plot the Bessel function $J_0(z)$ for $z \in \langle 0, 15 \rangle$.
- Find the energies of the first three bound states (as roots of $J_0(z)$) as accurate as you can.

Output: you should present graph of convergence of the integral, graph of the Bessel function and the three energies including your estimate of their accuracy.

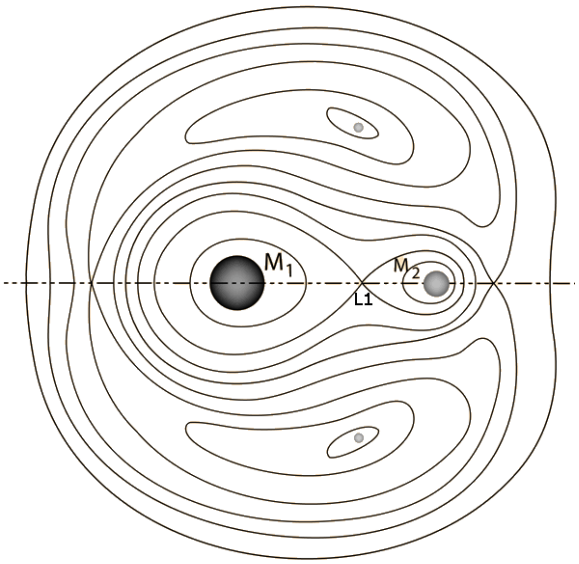
Problem 2: Length of equipotential line around Roche lobes

(nonlinear equation solution, extrapolation)

In binary star systems Roche lobe is defined as volume around star 1 that can be filled with gas, before it starts to flow to star 2. The border of this volume is given by equipotential surface in the coordinate system co-rotating with the two mutually orbiting stars where the potential energy is equal to potential in the Lagrange point L_1 (point on the line connecting the two stars, where the sum of gravitational forces and the centrifugal force is zero). In this problem we will restrict the motion of stars to the case of circular orbit and we will consider only the plane of the orbit. Your task is to find the curve in this plane that defines the border of the Roche lobe and to calculate its length. In the following we will consider the coordinate system with origin in star 1 and the x-axis pointing towards star 2. The lengths will be given in units of R, that is the distance of the two stars. More detailed instructions:

- Find the position of the point L1 (see the equation below) and the value of the potential V_L in this point.
- For the values $\theta = 2\pi n/N$, $n = 0, 1, ..., N$ find the points $x_n = r\cos\theta$, $y_n = r\sin\theta$ on the equipotential line in question. Using a numerical method of your choice for each fixed θ solve the equation $V(r) = V_L$. Try to find the points x, y with accuracy close to machine ϵ.
- Calculate length D_N of polygon (x_1, y_1), (x_2, y_2), ... (x_N, y_N). Investigate the speed of convergence in limit $N \to \infty$. Try to identify N where the equilibrium between truncation and round off errors is achieved.
- Try to improve precision of the result using (Richardson) extrapolation of truncation error.

You should produce figure showing polygon (x_1, y_1), (x_2, y_2), ... (x_N, y_N), and another figure documenting speed of convergence of D_N as an output of your work. Furthermore you should find the value $D = \lim_{N\to\infty} D_N$ and estimate size of the error of this value.



Equation for determination of coordinate x_L of the Lagrange point L_1, given by equilibrium of forces:

$$x_L - m_2 + \frac{m_2}{(1-x_L)^2} - \frac{m_1}{x_L^2} = 0,$$

where $m_1 = M_1/M$ and $m_2 = M_2/M$ are masses of the two stars in units of total mass $M = M_1 + M_2$ of the binary star. Gravitational potential (in units of $\kappa M/R$ in co-rotating system (including centrifugal force) is

$$V(x,y) = -\frac{m_1}{r} - \frac{m_2}{r_2} - \tfrac{1}{2}r_0^2,$$

where $r = \sqrt{x^2+y^2}$, $r_2 = \sqrt{r^2 - 2r\cos\theta + 1}$ and $r_0 = \sqrt{r^2 - 2m_2 r\cos\theta + m_2^2}$ are distances of point (x, y) from star 1, star 2 and from the center of mass (i.e. from rotation axis).

Problem 3: Model of chemical oscillator

(numerical solution of ordinary differential equations)

The following set of equations provides one of the possible models of coupled chemical reactions, that produce concentrations of products oscillating in time (you can search "chemical oscillator" or "Belousov–Zhabotinsky reaction" on youtube). In this model (Lotka-Voltera model) chemical substance A is gradually changing into product substance B and the intermediate products X and Y are also formed according to scheme

$$\begin{aligned} \mathrm{A} + \mathrm{X} &\rightarrow 2\mathrm{X} \\ \mathrm{X} + \mathrm{Y} &\rightarrow 2\mathrm{Y} \\ \mathrm{Y} &\rightarrow \mathrm{B} \end{aligned}$$

With k_1, k_2 and k_3 we denote rates of these reactions. Time dependences of concentrations A, X, Y and B satisfy

$$\begin{aligned} \tfrac{d}{dt}A &= -k_1AX, \\ \tfrac{d}{dt}X &= k_1AX - k_2XY, \\ \tfrac{d}{dt}Y &= k_2XY - k_3Y, \\ \tfrac{d}{dt}B &= k_3Y, \end{aligned} \qquad \begin{aligned} \tfrac{d}{d\tau}a &= -\kappa ax, \\ \tfrac{d}{d\tau}x &= \kappa ax - xy, \\ \tfrac{d}{d\tau}y &= xy - y, \\ \tfrac{d}{d\tau}b &= y. \end{aligned}$$

In the right column we wrote the same equations in terms of dimensionless quantities $\tau = tk_3$, $b = B/A_0$, $y = Y/A_0$, $x = k_2X/k_3$ and $\kappa = k_1/k_2$, with A_0 denoting the initial concentration of the reactant A.

Solve these equations numerically for $\kappa = 0.002$ and initial values $a = 498.4$, $x = 1.5$, $y = 0.1$, $b = 0$. *More detailed instructions:*

- Write procedure for integration of this system of differential equation with order of precision 4. Verify the speed of convergence with decreasing values of h for the concentrations at fixed time $t = 100$. Also verify the conservation of quantity $a + b + x + y$.
- Plot $a(t)$ and $b(t)$ in one graph and find the value of time t_0, when concentration of reactants and product is equal $a(t_0) = b(t_0)$. Estimate the precision of your value of t_0.
- Plot the concentration of intermediate products $x(t)$ a $y(t)$ and determine the period T of their oscillations. Estimate the precision of your value of T.

Note: the oscillations work as a "chemical pump". Part of the cycle with high x leads to high consumption of A and part of the cycle with high y leads to high production of B.

Output: You should produce three graphs (speed of convergence, time dependence of $a(t), b(t)$ and time dependence of intermediate products) and two numbers (times t_0 and T).

Problem 4: WKB approximation

(modification of Romberg integration)

In quantum mechanics, the condition for the energies of bound states in WKB approximation reads

$$\oint p(x)dx = 2\gamma \int_{x_1}^{x_2} \sqrt{E - V(x)} = 2\pi(n + \tfrac{1}{2}),$$

where E is the bound state energy, $V(x)$ the potential energy function and γ is constant. Integration limits x_1 a x_2 (turning points) are vales of x for which the integrand vanishes. Your first task is to find analytical formula for x_1 a x_2 for Morse potential $V(x) = e^{-2x} - 2e^{-x}$ and energies $E \in (-1, 0)$. Calculate integral

$$I(E) = \int_{x_1}^{x_2} \sqrt{E - V(x)}$$

using N-point trapezoid rule I_N and plot the dependence of error $|I_N - I_\infty|$ on N for $N = 2, 4, 8, ..., 1024$ in log/log scale. As an exact value (for plotting the graph) take $I_\infty = I_{1024}$. Compare this dependence with estimate N^{-2} from Euler-Maclaurin formula. Why is the dependence different? Try to find the correct behavior $N^{-\alpha}$ of the error. Improve the accuracy of the calculation using the method of Richardson extrapolation

$$I_{2N}^{(1)} = \frac{2^\alpha I_{2N} - I_N}{2^\alpha - 1}.$$

What is a new order α of the error of $I_{2N}^{(1)}$. Try to generalize method of Romberg integration for this case. Find the value of $I(E = -0.5)$ as precisely as possible.

Output: Plot demonstrating speed of convergence of trapezoidal rule for the integral of interest. Plot showing speed of convergence of $I_{2N}^{(1)}$. Your best approximation of I for $E = -0.5$.

Problem 5: WKB approximation once more

(Gauss-Chebyshev integration)

Calculate the integral from the Problem 4 using the Gauss-Chebyshev quadrature.

- First notice that the integrand in the turning points x_1, x_2 behaves as $\sqrt{x-x_1}$ and $\sqrt{x_2-x}$ i. e. it has singular first derivative. The singular behavior is corrected by multiplying with $\sqrt{(x-x_1)(x_2-x)}$. Fist find linear map $x \mapsto y$, transforming the integral to interval $\langle -1, 1\rangle$ and then calculate the integral using the Gauss-Chebyshev quadrature

$$\int_{-1}^{1} f(y)\frac{\mathrm{d}y}{\sqrt{1-y^2}} = \sum_{i}^{N} f(y_i)w_i.$$

- Study the speed of convergence of the integral $I(-0.5)$ for $N \to \infty$.
- Plot the graph of function $2\gamma I(E)$ for $E \in (-1, 0)$ and $\gamma = 16.65$ (approximately corresponds to vibrations of the molecule H_2). Estimate the value of the energy of the ground state (see the Problem 4 for the condition for bound states).

Output: graph of error of determination of I as it depends on N (use logscale if needed) and graph of function $2\gamma I(E)$ showing the approximate position of the ground state energy.
Optional extension: try to find this energy with precision close to machine epsilon.
Note: Values of weights for Gauss-Chebyshev quadrature are $w_i = \pi/N$ and the nodes are given by

$$y_i = \cos\frac{\pi(i-\frac{1}{2})}{N}.$$

Problem 6: Legendre polynomials

(QR-factorization, integration)

Write your own procedure for QR-factorization of rectangular matrix (modified Gram-Schmidt or Hausholder method) and verify by matrix multiplication, that the factorization is correct. Apply the procedure on the Vandermode matrix

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^N \\ 1 & x_1 & x_1^2 & \dots & x_1^N \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_M & x_M^2 & \dots & x_M^N \end{pmatrix},$$

which Gram-Schmidt orthogonalization yields approximation to Legendre polynomial (columns of matrix Q).

More detailed instructions:

- Chose nodes x_0, ... x_M with regular spacing on the interval $\langle -1, 1\rangle$ with step 0.02 (i. e. $M = 101$). Plot resulting polynomials $P_l(x)$ pro $l = 0, 1, ..., 5$, using the normalization condition $P_l(1) = 1$.
- Write independent function calculating the polynomial using Bonnet formula

  $$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$$

  and plot the result in the same graph.
- Discuss the differences of both methods. Try the same test for $M = 1001$. Discuss the difference of results for $M = 101$ and $M = 1001$ in terms of error estimate of the trapezoidal rule (Euler-Maclaurin formula). Modify the matrix in such a way, that the error of polynomials found from QR factorization is smaller.

Hint: Orthogonality of columns in matrix Q is not exactly identical to orthogonality of polynomials in L^2 space. Compare the orthogonality of columns of Q with L_2 orthogonality expressed using trapezoidal rule.

Problem 7: Chaotic dynamics

(integration of system of ordinary differential equations)

Solve the motion of particle with mass $m = 1$ in the potential field described by Hénon-Hailes potential

$$V(x, y) = \tfrac{1}{2}(x^2 + y^2) + x^2 y - \tfrac{1}{3}y^3.$$

Find the trajectory of the particle by solving Hamilton equations of motion

$$\begin{aligned} \dot{x} &= p_x, & \dot{p_x} &= -\tfrac{\partial}{\partial x}V(x, y), \\ \dot{y} &= p_y, & \dot{p_y} &= -\tfrac{\partial}{\partial y}V(x, y) \end{aligned}$$

for Hamiltonian

$$H(x, y, p_x, p_y) = \tfrac{1}{2}(p_x^2 + p_y^2) + V(x, y).$$

More detailed instructions:

- Choose convenient method of the order of precision 4 or higher for the solution of the equations of motion. Plot graph of convergence of the error of the solution at $t = 1$ for decreasing integration step $h \to 0$ in log/log scale. As an alternative to plotting error of solution you can plot convergence of the error in energy $H(x, y, p_x, p_y)$ which should be conserved but will contain discretization and round off error.

- Based on this analysis choose a suitable length of step h and try to draw Poincare map defined as follows. For given initial condition (you can choose $x = x_0 \in (0.3, 0.6)$, $y = 0$, $p_x = 0$, $p_y = 0.03$) integrate the trajectory $(x(t), y(t), p_x(t), p_y(t))$ in phase space. Find the coordinates (x, p_x, p_y) where the trajectory intersects the plane $y = 0$. Integrate the trajectory for sufficiently long time to produce enough intersection points (hundreds). Finally plot the two of the coordinates (for example x, p_x) of the intersection points in the planar graph. Observe the changes of this graph with changes of the initial coordinate x_0.

Output: Graph demonstrating that the local discretization error of your method is of at lest order of 4, selected set of graphs of Poincare maps showing the change of the character of the dynamics with the changes of value x_0.

Problem 8: Energies of the bound states using DVR method

(matrix diagonalization)

Your task is to find energies of bound states in one dimensional potential well from solution of Schrödinger equation, which (in dimensionless units) reads

$$-\frac{d^2}{dx^2}\psi(x) + \gamma^2[E - V(x)]\psi(x) = 0.$$

Consider Morse potential $V(x)$ and value γ from problems 4 and 5. Energies are found from diagonalization of the operator

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

using the following method. First we chose suitable interval $\langle a, b\rangle$ where we expect the bound states are localized (for example $a = -3$, $b = 5$) and we define the basis in the space of quadratically integrable functions in this interval

$$\phi_k(x) = \sqrt{\frac{2}{b-a}}\sin\frac{k\pi(x-a)}{b-a} \qquad k = 1, 2, ...$$

(k goes to infinity, but practically we have to introduce cut off value k_{max}). In this basis we express the matrix elements of hamiltonian $H_{kl} = \langle\phi_k|H|\phi_l\rangle$. Kinetic energy part can be calculated analytically

$$\int_a^b \phi_k(x)\left[-\gamma^{-2}\frac{d^2}{dx^2}\right]\phi_l(x)\mathrm{d}x = \gamma^{-2}\left[\frac{k\pi}{b-a}\right]^2\delta_{kl}.$$

You can calculate the matrix elements of the potential energy $V(x)$ using the trapezoidal quadrature rule. Next you should diagonalize matrix H_{kl} numerically. Find the three lowest eigenvalues (ground and first two excited states) using a suitable numerical method. What is your estimate of the accuracy of obtained values? Try to find this out by systematic variation of values of a, b, number of quadrature points in trapezoidal rule and the cut off value k_{max}, i. e. the size of the matrix representation of H.
Output: tree numbers (energies) and estimate of their error.

Note: For students interested in numerical quantum mechanics I suggest following modification. The above procedure is not DVR (discrete variable) method. In real DVR method the matrix elements of potential $V(x)$ are calculated differently. First we calculate matrix elements of the operator x analytically. For odd values of $k + l$ we get

$$X_{kl} = \int x\phi_k(x)\phi_l(x)\mathrm{d}x = -\frac{8kl(b-a)}{\pi^2(k+l)^2(k-l)^2}.$$

and zero otherwise. Matrix X is then diagonalized numerically $\lambda = Q^\dagger XQ$. In the diagonal reprezentation the potential matrix is also diagonal $V(\lambda)$ and we transform it back to original basis $V = QV(\lambda)Q^\dagger$. If you choose to implement this method of evaluation of the potential energy you do not have to integrate numerically and you get more precise energies of bound states. The presented method is called Fourier-DVR since we started with the Fourier basis on the interval $\langle a, b\rangle$. Similar method can be used for other basis, for example for eigenstates of the linear harmonic oscillator.

Problem 9: Statistics of errors of Gauss elimination

(solution of systems of linear equations, conditioning number of matrix)

As you know from the lecture, the solution of the system of linear equations

$$A\mathbf{x} = \mathbf{b},$$

where A is given matrix $N \times N$, $\mathbf{b}$ given vector and $\mathbf{x}$ the vector of solutions, is influenced by round off error. Its size depends on the method that we use and on the conditioning number of the matrix A.

- Write procedure for solution of the system of linear equations using the Gauss elimination without pivoting.
- Write the second procedure with row-pivoted Gauss elimination.
- For given N generate random matrix A with matrix elements $a_{ij} \in \langle -1, 1 \rangle$, random vector $\mathbf{x_0}$ and from them calculate the right hand side $\mathbf{b} = A\mathbf{x_0}$.
- Now solve the system $A\mathbf{x} = \mathbf{b}$ and calculate the error of the solution as $\epsilon = \|\mathbf{x} - \mathbf{x_0}\|$. Repeat this numerical experiment many (>100) times and plot the column diagram of number of occurrences of the error $e > 1$; $e \in \langle 10^k, 10^{k-1} \rangle$ for $k = 0, -1, -2, ..., -15$ and $e < 10^{-16}$

Output: Column diagrams for Gauss elimination with and without pivoting for $N = 10, 50, 100, 200$.

Problem 10: Singular values of random matrixes

(Matrix diagonalization, SVD, conditioning number of matrix)

- Write your own procedure for diagonalization of real symmetric matrix. Propose convenient method to test that the procedure works correctly.
- Use this procedure to find the singular values of real square matrix A from diagonalization of the auxiliary matrix

$$\left(\begin{array}{c|c} 0 & A \\ \hline A^\dagger & 0 \end{array}\right)$$

- Generate random matrix $N \times N$ with integer sized elements $a_{ij} \in \{-99, -98, -97, ..., 99\}$ and find its singular values σ_i.
- Repeat this numerical experiment many (>100) times and plot the column diagram of the distribution of the conditioning number of the random matrix, i. e. find how many times the given conditioning number occurs in the interval $\kappa(A) \in \langle 10^k, 10^{k+1} \rangle$ pro $k = 0, 1, ..., 18$.

Output: Column diagrams for conditioning number of the matrixes of the size $N = 10, 30, 100$.

Problem 11: Calculation of the Hilbert transform

(use of FFT for calculation of the convolution)

The Hilbert transform of the function $f(x)$ is defined as the principal value integral

$$g(y) = p.v. \int \frac{f(x)}{y-x} \mathrm{d}x.$$

Write program to calculate the Hilbert transform of the given function. Use the fact that the definition of the Hilbert transform is a convolution of the given function with the distribution $p.v.1/x$ for which we know the Fourier transform analytically by integration in the complex plane using the fact that

$$p.v.\frac{1}{x} = \mathrm{Re}\frac{1}{x+i\epsilon}.$$

First test the program for FFT by calculating the derivative a suitable function analytically and using forward and backward FFT. Finally calculate the Hilbert transform of the function $\theta(x)xe^{-x}$ ($\theta(x)$ is the Heavyside step function). Test the dependence of result on the sampling frequency and the length of the interval where you calculate the transform.