Numerical Methods in Scientific Computing, spring 2023

Problem sheet 11: differential equations

Return code and solutions by **Monday 17.4.2023** 23:59 to Moodle.

Note: the analytical energy was wrong in problem 3.

1. (computer, 6 points) Write a function `runge_kutta_solver(a,b,N,y0,yp0)` which solves the equation $y''(x) + y(x) = 0$ with the fourth-order Runge–Kutta method (RK4) from the lecture notes, where `N` is the number of grid points in the range $x \in (a, b)$ and `y0` and `yp0` are the initial values $y(a)$ and $y'(a)$, . (You have to write the solvers yourself.)

   Find the numerical solution in $x \in [0, 10]$ with the initial values $y(0) = 1$, $y'(0) = 0$ with

   (a) $N = 30$

   (b) $N = 100$

   (c) $N = 300$

   The analytical solution is $y(x) = \cos x$.

2. (computer, 6 points) Write a function `shooting_solver(a,b,N,y0,y1)` which solves the equation $y''(x) + y(x) = 0$ with the shooting method, where `N` is the number of grid points in the range $x \in (a, b)$ and `y0` and `y1` are the boundary values $y(a)$ and $y(b)$. (You have to write the solvers yourself.)

   Using the boundary conditions $y(0) = 1$, $y(1) = 1$, what is the solution you find with

   (a) $N = 10$

   (b) $N = 30$

   (c) $N = 100$

   The analytical solution is $y(x) = \cos x + c \sin x$ with $c = \frac{1-\cos 1}{\sin 1} \approx 0.5460$.

   Hint: convert the boundary value problem $y(a) = \alpha$, $y(b) = \beta$ to an initial value problem $y(a) = \alpha$, $y'(a) = k$ with k being a shooting angle; this problem can now be solved with the routine of problem 1 in the interval $x \in [0, 1]$. What you get out from this solution is a curve that depends on the used value for k, $y = y(x; k)$. Next, you just have to find a value for k that yields the other boundary condition $y(1) = 1$ by solving for the root of $g(k) := y(1; k) - 1$ i.e. for $g(k^*) = 0$.

3. (computer, 6 points) Solve the particle-in-a-box problem using a three-point finite difference stencil. The dimensionless Schrödinger equation is $\psi''(x) + 2E\psi(x) = 0$, with the boundary conditions $\psi(-1) = 0$ and $\psi(1) = 0$. Use the three-point stencil given in the lecture notes.

   There are several values of E which satisfy the differential equation and the boundary conditions; an analytical solution to the problem yields the spectrum $E_n = n^2\pi^2/8$.

   Find the first 5 eigenstates, and plot the wave functions. Remember to check that you are using a sufficient number of points in the solution by doubling the number of points until the wanted eigenvalues E have converged.

   Hint: write the equation as an eigenproblem $\boldsymbol{D}\boldsymbol{\psi} = \boldsymbol{E}\boldsymbol{\psi}$, from which you can get the energies $\boldsymbol{E}_i$ and the corresponding wave functions $\boldsymbol{\psi}_i$ with a call to the eig() function in Octave/Matlab or linalg.eig() in NumPy. (You are allowed to use library routines for the diagonalization.)

4. (computer, 6 points) Similar to problem 3, only now there is a potential in the box given by

$$V(x) = V_0\left(1 - x^2\right),$$

where V_0 controls the strength of the potential. The differential equation to solve is now $\psi''(x)+2[E-V(x)]\psi(x) = 0$, with the same boundary conditions $\psi(-1) = 0 = \psi(1)$. Again, there is an infinite number of allowed solutions with increasing values for E.

Calculate the lowest value of E for the following strengths of the parabolic potential

(a) $V_0 = 1$

(b) $V_0 = 10$

(c) $V_0 = 30$

In each case, how much does the lowest value of E differ from the estimate given by perturbation theory

$$E = E_0 + \frac{\int_{-1}^{1} |\psi_0(x)|^2 \, V(x)\mathrm{d}x}{\int_{-1}^{1} |\psi_0(x)|^2 \, \mathrm{d}x}$$

where $\psi_0(x)$ is the solution with $V_0 = 0$?