Numerical Programming 2 (CSE) 2015

Worksheet 10

Exercise 1 (Stationary Schrödinger) eq.

Let's consider the stationary Schrödinger equation

$$H\psi(x) = E\psi(x),\ x \in (-a, a) \qquad \psi(-a) = \psi(a) = 0$$

with $H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$. Let the potential $V(x)$ be the finite square well on $[-L, L]$:

$$\begin{cases} V(x) = 0 \ \text{ for } \ -L \leq x \leq L \\ V(x) = U > 0 \ \text{ otherwise} \end{cases}$$

By discretizing the space with a uniform grid define the finite dimensional matrix corresponding to H (use central finite difference to approximate the second derivative operator). Compute the eigenvectors and eigenvalues of H. The entries of each eigenvector v_i represent approximations of the exact solution at the grid points for each quantum state and the corresponding eigenvalues E_i are the energy levels of the quantum states.

The squares of the absolute values of the entries of the eigenvectors give information regarding the probability of finding the system at each grid point of the domain.

Compute and visualize this probability distribution for the ground state, i.e. the quantum state belonging to the lowest energy, for $a = 1$, $L = 0.1$ and varying potential barriers $U = 10^k$, $k = 1, 2, \ldots, 6$.

Is the probability equal to zero outside $[-L, L]$ as expected in a classical system?

Exercise 2 (Spectral method for Schrödinger eq.)

The behavior of diatomic molecules in which one atom is fixed at position x_m is essentially one-dimensional and well describe by the Morse potential

$$V(x) = U\left(e^{-2\alpha(x-x_m)} - 2e^{-\alpha(x-x_m)}\right).$$

The corresponding Hamiltonian can be decomposed into

$$H = -\frac{1}{2}\frac{\partial}{\partial x^2} + V(x) = \underbrace{-\frac{1}{2}\frac{\partial}{\partial x^2} + \frac{1}{2}x^2}_{:=D} + \underbrace{V(x) - \frac{1}{2}x^2}_{:=W}$$

Using the fact that the Hermite functions ϕ_k defined in the lecture fulfill $D\phi_k = (k + 1/2)\phi_k$, write a MATLAB function that discretizes the Hamilton operator

H using the spectral Hermite method. Use the first 40 Hermite functions and parameter values $\alpha = 0.8$, $x_m = -3$, $U = 10$.

MATLAB functions that compute the parameters of Gauss-Hermite quadrature and the values of the Hermite functions ϕ_k are available on the course website.

Exercise 3 (Chebyshev method)

The Clenshaw algorithm for computing the approximation

$$P_{m-1}(\tau A)v \approx e^{-i\tau A}v$$

of the exponential of a matrix A with eigenvalues in $[a, b]$ is given by

$$X = \frac{2}{b-a}\left(A - \frac{a+b}{2}I\right)$$

$$d_{m+1} = d_m = 0$$

$$d_k = c_k v + 2X d_{k+1} - d_{k+2} \text{ for } k = m-1, m-2, \ldots, 0$$

$$c_k = (-i)^k J_k(\tau(b-a)/2)$$

$$P_{m-1}(\tau A)v = d_0 - d_2.$$

The Bessel function J_k can be computed in MATLAB as $J_k(x) = \texttt{besselj}(k, x)$.

Consider again the diatomic molecule from Exercise 2. After the space discretization the Schrödinger equation with Gaussian initial condition

$$\begin{cases} i\dfrac{\partial}{\partial t}\psi(x,t) = \left(-\dfrac{1}{2}\dfrac{\partial}{\partial x^2} + V(x)\right)\psi(x,t) \\ \psi(x,0) = \dfrac{1}{\pi^{1/4}}e^{-(x-x_0)^2} \end{cases}$$

is reduced to the linear system $i\frac{d}{dt}y = Ay$ where A is the matrix computed in Exercise 2. The solution is given by the matrix exponential $y = e^{-itA}y(0)$ where $y(t)$ is the vector of coefficients in $\psi(x,t) \approx \sum_{j=0}^{K} y_k(t)\phi_k(x)$.

- Implement the Clenshaw algorithm.
- Use the Chebyshev method to approximate the value of the matrix exponential and compute the approximate solution of the above Schrödinger equation with time step $\tau = 0.02$. Visualize the evolution of the probability density $|\psi(\cdot, t)|^2$.

  Use $x_0 = -1$ for the initial condition. For the Chebyshev method use $m = 1000$ and determine the interval $[a, b]$ with MATLAB's `eig` function.