Metodes Numerics II. Curs 2023-24. Semestre de tardor.
Pràctica 1

Mathematical/Physical background.

In Quantum Mechanics, Heisenberg's uncertainty principle implies that on the quantum level, the position, $\vec{r}$, and momentum, p, of a particle cannot be determined. Therefore, the quantum state of particle is described by the wave function $\Psi(\vec{r}, t)$ which depends on the spacial coordinates $\vec{r}$ and time t and whose interpretation is the probability amplitude. In particular, $|\Psi(\vec{r}, t)|^2$ is interpreted as the probability density of a particle to be at a given position at a given time.

The time-dependent Schrödinger equation determines that the wave function $\Psi(\vec{r}, t)$ evolves over time as follows

$$i\hbar\frac{\partial\Psi}{\partial t}(\vec{r}, t) = \hat{H}\Psi(\vec{r}, t), \quad \vec{r} \in \mathbb{R}^n, t \in \mathbb{R},$$

where $\hbar$ is the reduced Planck's constant and $\bar{H}$ is the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}, t)$$

with mass of the particle m, potencial function V, and ∇^2 being the Laplacian operator.

If $V(\vec{r}, t) = V(\vec{r})$ is time-independent, we can find the solution by separation of variables $\Psi(\vec{r}, t) = \psi(\vec{r}) \cdot f(t)$. We obtain 2 equations

$$\begin{aligned} i\hbar\frac{df(t)}{dt} &= Ef(t) \\ \left[-\frac{\hbar}{2m}\nabla^2 + V(\vec{r}, t)\right]\psi(\vec{r}) &= E\psi(\vec{r}). \end{aligned}$$

The first equation can be solved as $f(t) = \exp(-iEt/\hbar)$. The second equation is the time-independent Schrödinger equation at which we can look as equation of eigenvalues E_n and eigenfunctions $\psi_n(\vec{r})$ of $\hat{H}$:

$$\hat{H}\psi_n = E_n\psi_n, \quad n \in \mathbb{Z}$$

which actually gives the energy quantization.

Then the general solution is

$$\Psi(\vec{r}, t) = \sum c_n\psi_n(\vec{r})\exp(-iE_nt/\hbar).$$

One of the most famous examples in mathematics and physics is the harmonic oscillator when

$$V(\vec{r}) = \frac{1}{2}m\omega^2|\vec{r}|^2,$$

where ω is the oscillation frequency.

Problem: 1D shifted harmonic oscillator

Let us consider the one-dimensional shifted harmonic oscillator $V(x) = \frac{1}{2}m\omega^2 x^2 + V_0$ for $x \in [-L, L]$ and look for the eigenvalues and eigenfunctions of $\hat{H}$:

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + (\frac{1}{2}m\omega^2 x^2 + V_0)\psi_n(x) = E_n\psi_n(x).$$

We can make the equation dimensionless after a change of variable and reparametrization as follows

$$-\frac{1}{2}\frac{d^2\psi_n(x)}{dx^2} + (\frac{1}{2}x^2 + V_0)\psi_n(x) = E_n\psi_n(x), \tag{1}$$

with new potential function $\tilde{V}(x) = \dfrac{1}{2}x^2 + V_0$.

We assume zero boundary conditions $x(-L) = x(L) = 0$, where L is a given longitude for the interval of x.

We solve this problem numerically using a finite difference method. We discretizate the interval $[-L, L]$ in $N + 1$ points x_i with the constant step $\Delta x = 2L/N$, $x_i = -L + \Delta x$. Suppose that $\psi_n(x_i) = f_i$ (unknown) and $V_i = \tilde{V}(x_i) = \frac{1}{2}x_i^2 + V_0$. We also approximate the second derivatives as

$$\frac{d^2\psi(x_i)}{dx^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

Therefore, equation (1) becomes the following three-diagonal linear system

$$Af = E_n f,$$

on

$$A = \begin{pmatrix} \frac{1}{\Delta x^2} + V_1 & -\frac{1}{2\Delta x^2} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + V_2 & -\frac{1}{2\Delta x^2} & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & \\ \vdots & & & & & \\ \vdots & & \ddots & & \ddots & \ddots \\ & & & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + V_{N-1} & -\frac{1}{2\Delta x^2} \\ 0 & & & 0 & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + V_N \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} \tag{2}$$

The task is to find the eigenvalues E_n. It is known that the eigenvalues of A should be close to the values $n + \frac{1}{2} + V_0$, $n = 0, 1, 2, \ldots$.

Enunciat

La pràctica consteix en trobar el valor propi mínim E_0 i el valor propi màxim E_N de la matriu tridiagonal A definida a (2). Per això,

1. Fixeu els valors N, L, V_0 prou grans (per exemple, $N = 50$, $L = 5$, $V_0 = 5$) i *tol* prou petit.

2. Programeu una funció que faci el producte de la matriu tridiagonal per un vector

$$\begin{pmatrix} a_1 & b & 0 & \dots & \dots & 0 \\ b & a_2 & b & \dots & \dots & 0 \\ 0 & b & a & b & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \\ & & & b & a_{n-1} & b \\ 0 & & & 0 & b & a_n \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} v'_1 \\ v'_2 \\ \vdots \\ v'_N \end{pmatrix}$$

sense assignar memòria per a la matriu.

3. Programeu **el mètode de Gauss-Seidel** per resoldre el sistema

$$\begin{pmatrix} a_1 & b & 0 & \dots & \dots & 0 \\ b & a_2 & b & \dots & \dots & 0 \\ 0 & b & a_3 & b & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \\ & & & b & a_{n-1} & b \\ 0 & & & 0 & b & a_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

sense assignar memòria per a matrius.

4. Programeu **el mètode de la potència** per trobar el valor propi més gran de la matriu tridiagonal donada a (2).

5. Programeu **el mètode de la potència inversa** per trobar el valor propi més petit fent servir el mètode de Gauss-Seidel per resoldre $Ay^{(k)} = z^{(k-1)}$.

Heu de penjar els fitxers .c a les tasques preparades al CV, abans de les 23:59h del 6 de novembre de 2023.