Assignment 8 - Finite Difference Method

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Theory

(a) Explain Finite Difference Method for solving Schrodinger wave Equation in 1-D.

Ans. The schrodinger wave equation of quantum mechanics in 1-D is:

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

~~Take~~ here

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

$$H\psi = E\psi$$

This is eigen value equation, where H is eigen vector and E represents eigen values

Taking Schrodinger Wave Equation,
We know there is no first derivative term in Schrodinger Wave Equation, so we'll use taylor expansion to approximate $\psi''(x)$ and ignore $\psi'(x)$

$$\psi(x+h) = \psi(x) + \frac{h\psi'(x)}{1!} + \frac{h^2\psi''(x)}{2!} + \frac{h^3\psi'''(x)}{3!} + \cdots$$

$$\psi(x-h) = \psi(x) - \frac{h\psi'(x)}{1!} + \frac{h^2\psi''(x)}{2!} - \frac{h^3\psi'''(x)}{3!} + \cdots$$

$$\psi(x+h) + \psi(x-h) = 2h\psi'(x) + \cancel{\frac{2h^3\psi'''(x)}{3!}} \quad \frac{2h^2\psi''(x)}{2!}$$

$$\psi'(x) = 0$$

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} = \psi''(x)$$

The dimensionless S.E is $-\frac{d^2\psi}{d\xi^2} + V(\xi)\psi = E\psi$

$$-\left(\frac{\psi(\xi_i+h) + \psi(\xi_i-h) - 2\psi(\xi_i)}{h^2}\right) + V\psi(\xi_i) = E\psi(\xi_i) \quad -(1)$$

Now, if we have multiple schrodinger wave equations to solve, then there will be multiple corresponding eigen values and eigen vectors, So writing S.E. in terms of indexes

Take $\psi(\xi+h) = \psi_{i+1}$ $\psi(\xi-h) = \psi_{i-1}$ $\psi(\xi) = \psi_i$

Equation (1) becomes

$$-\left(\frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{h^2}\right) + V\psi_i = \varepsilon\psi_i$$

Now let's take we want to solve for N eigen values with $(N=1)$ grid points

$i=1$

$$-\left(\frac{\psi_2 + \psi_0 - 2\psi_1}{h^2}\right) + V\psi_1 = \varepsilon\psi_1$$

$i=2$ $$-\left(\frac{\psi_3 + \psi_1 - 2\psi_2}{h^2}\right) + V\psi_2 = \varepsilon\psi_2$$

$i=N$ $$-\left(\frac{\psi_{N+1} + \psi_{N-1} - 2\psi_N}{h^2}\right) + V\psi_N = \varepsilon\psi_N$$

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$$-\frac{1}{h^2}\begin{bmatrix} -2\psi_1 & \psi_2 & & & \\ \psi_1 & -2\psi_2 & \psi_3 & & \\ & & \ddots & & \\ & & & -2\psi_{N-2} & \psi_{N-1} \end{bmatrix} + \begin{bmatrix} V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_{N-1} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

$$= \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_{N-1} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

$$= \underbrace{-\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & -2 & 1 \end{bmatrix}}_{KE}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix} + \underbrace{\begin{bmatrix} V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_{N-1} \end{bmatrix}}_{V}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

$$= \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_{N-1} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{bmatrix}$$

Here we will take $H = KE + V$

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(b) Electron confined in 1-D box from $x = -a/2$ to $a/2$. Show numerical steps for finding its first two energy eigen values and corresponding stationary state wave function using finite difference method with $N=3$. Perform calculation upto four significant digits & compare it with analytical ones.

Ans: $N = 3$ $\quad x_{min} = \frac{-a}{2}$ $\quad x_{max} = \frac{a}{2}$ $\quad$ Take $a = 1$

$$h = \frac{x_{max} - x_{min}}{N} = \frac{a}{3} = \frac{1}{N} = 0.33$$

$$-\frac{1}{h^2}\left[\psi_0 - 2\psi_1 + \psi_2\right] + V_1\psi_1 = E_1\psi_1$$

$$-\frac{1}{h^2}\left[\psi_1 - 2\psi_2 + \psi_3\right] + V_2\psi_2 = E_2\psi_2$$

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$$\frac{-1}{h^2}\begin{bmatrix} -2u_1 & u_2 \\ u_1 & -2u_2 \end{bmatrix} \Rightarrow \frac{-1}{h^2}\begin{bmatrix} -2 & 1 \\ 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$\Rightarrow \frac{-1}{(0.33)^2}\begin{bmatrix} -2 & 1 \\ 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} u \end{bmatrix}$$

$$\frac{-1}{h^2}\begin{bmatrix} -2 & 1 \\ 1 & -2 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 18.3654 & -9.1827 \\ -9.1827 & 18.3654 \end{bmatrix}}_{K}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}}_{V}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

To calculate Eigen values, take λ and put

$$|(K+V) - \lambda I| = 0$$

$$\begin{vmatrix} 18.3654-\lambda & -9.1827 \\ -9.1827 & 18.3654-\lambda \end{vmatrix} = 0$$

$$(18.365-\lambda)^2 - (9.1827)^2 = 0$$

$$(18.365-\lambda)^2 = (9.1827)^2$$

$18.365 - \lambda = 9.1827$ $\qquad\qquad$ $18.365 - \lambda = -9.1827$

$\lambda_1 = 9.1827$ $\qquad\qquad$ $\lambda_2 = 27.5481$

~~Analytical eigen value~~

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To find Eigen Vectors:
when $\lambda = 9.1827$

$$\begin{pmatrix} 9.1827 & -9.1827 \\ -9.1827 & 9.1827 \end{pmatrix}\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$x_1 = y_1$

$$X_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.7071 \\ 0.7071 \end{pmatrix}$$

Take $\lambda = 27.5481$ $\begin{pmatrix} -9.1827 & -9.1827 \\ -9.1827 & -9.1827 \end{pmatrix}\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

$$X_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -0.7071 \\ 0.7071 \end{pmatrix}$$

$-x_2 = +y_2$

Eigen Vectors: $\begin{bmatrix} 0.7071 & -0.7071 \\ 0.7071 & 0.7071 \end{bmatrix}$

Comparison with Analytical Values:

V	Theoretical	Analytical ($n^2\pi^2$)
1	9.1827	9.8596
2	27.5481	39.4384

Eigen vectors after normalisation

Theoretical

$$\begin{bmatrix} 0.7071 & -0.7071 \\ 0.7071 & 0.7071 \end{bmatrix}$$

Analytical

$$\begin{bmatrix} 0.7071 & -0.7071 \\ 0.7071 & 0.7071 \end{bmatrix}$$

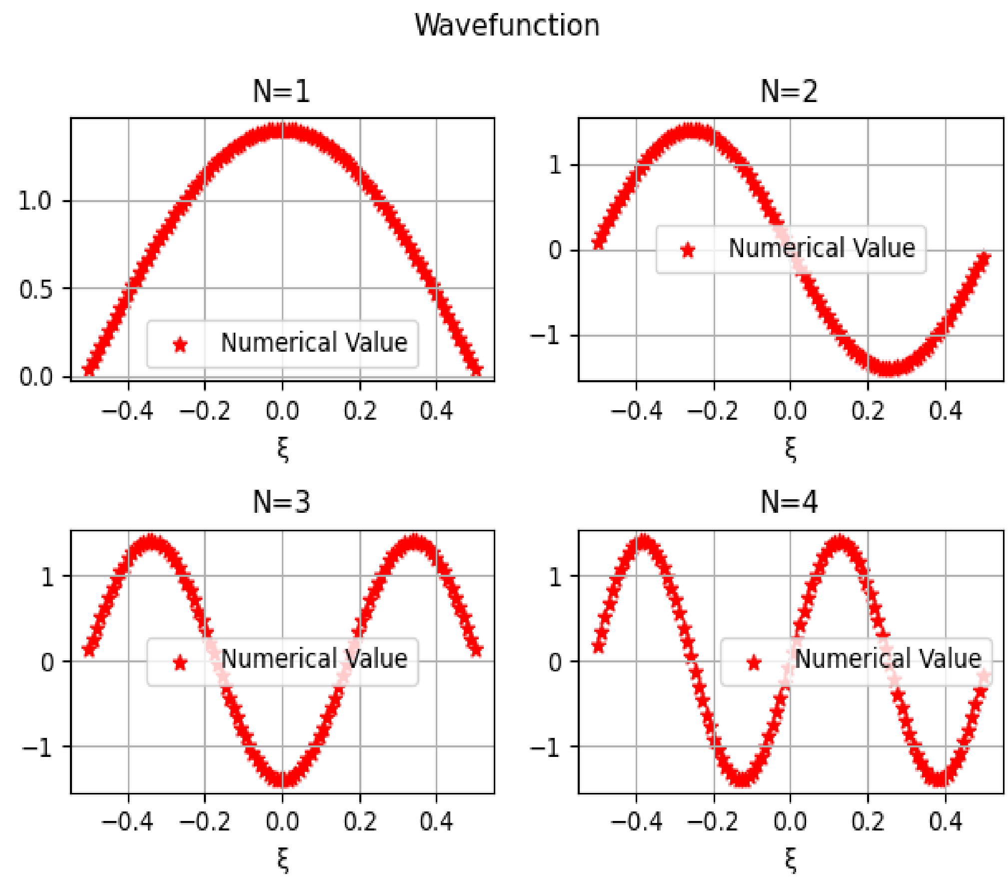
Programming

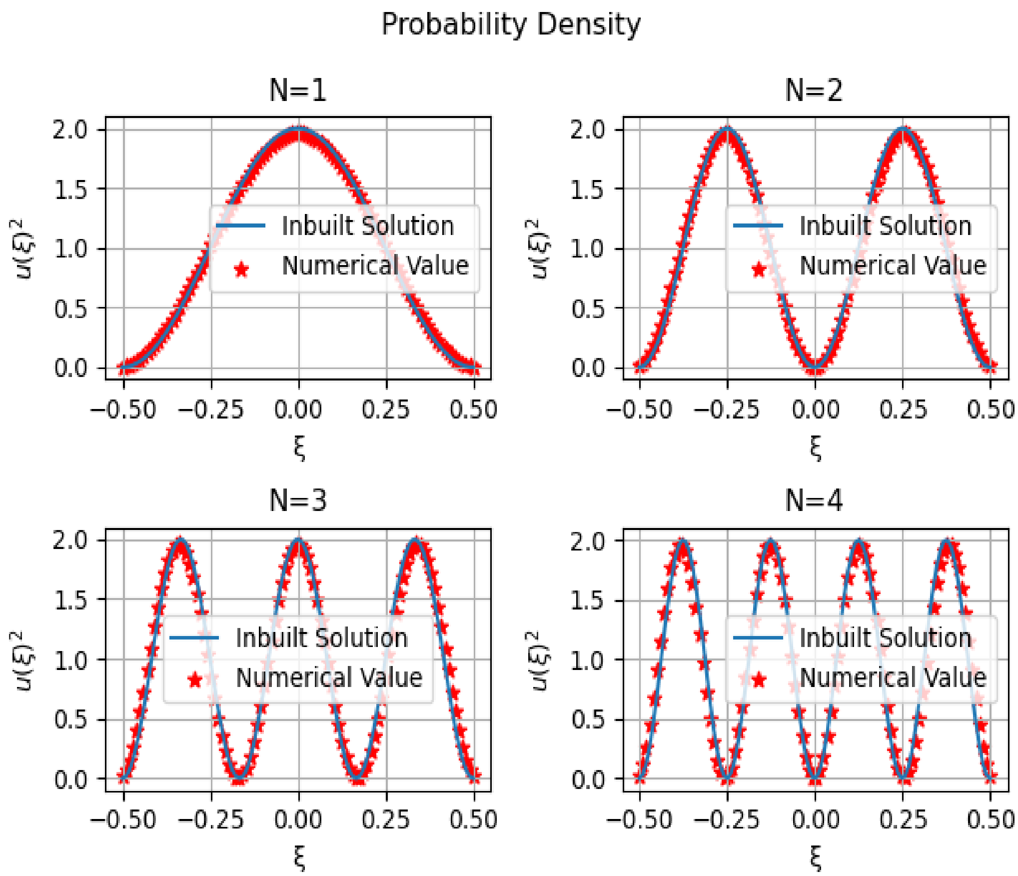
```
import numpy as np
from scipy.linalg import eigh
import matplotlib.pyplot as plt
import scipy.integrate as integrate
import pandas as pd
def V():
    return 0
def analytical(x,n):
        if (i%2)== 0:
            return 2*(np.cos(n*np.pi*x))**2
        else:
            return 2*(np.sin(n*np.pi*x))**2
def analytical_1(x,n):
        if (i%2)== 0:
            return np.sqrt(2)*(np.cos(n*np.pi*x))
        else:
            return np.sqrt(2)*(np.sin(n*np.pi*x))

def sub_plot(ax,a,b,d,title,x_label,y_label,key=1):
    ax.scatter(a,b,label="Numerical Value",marker="*",color="red")
    if key == 1:
        ax.plot(a,d,label="Inbuilt Solution")
        ax.set_ylabel(y_label)
    ax.set_title(title)
    ax.set_xlabel(x_label)
    ax.legend()
    ax.grid(True)

def diag_mat(n,xi,xf):
    h = (xf-xi)/(N+1)
    a,v,e=np.zeros((n,n)),np.zeros((n,n)),np.zeros((n,n))
    for i in range(n):
        for j in range(n):
            if i==j:
                a[i][i]=-2
                a[i][i-1]=1
                a[i-1][i]=1
                v[i][i]=V()
            else:
                a[i][j]=0
                v[i][j]=V()
                e[i][i]=1
    A=a*(-1/(h**2))+v
    eig = eigh(A)
    return eig

n=2;N=2
xi=-1/2;xf=1/2
x=np.linspace(xi,xf,N)
U=diag_mat(n,xi,xf)[0]
data={
    "Eigen Value": diag_mat(n,xi,xf)[0],
    "Eigen Vector 1":diag_mat(n,xi,xf)[1][0],
    "Eigen Vector 2":diag_mat(n,xi,xf)[1][1]
}
print(pd.DataFrame(data))


n=100;N=100
xi=-1/2;xf=1/2
x=np.linspace(xi,xf,N)
print("First 11 Eigen Values")
data={
    "Eigen Value": diag_mat(n,xi,xf)[0][:11],
}
```

```
print(pd.DataFrame(data))


fig2, ((axx1, axx2), (axx3, axx4)) = plt.subplots(2,2)
fig2.suptitle("Probability Density")
dict = {'0': axx1,'1': axx2,'2': axx3,'3': axx4}
for i in range(0,4,1):
    U=diag_mat(n,xi,xf)[1][:,i]
    u_norm=U/np.sqrt(integrate.simps(np.power(U,2),x))
    sub_plot(dict[str(int(i))],x,np.power(u_norm,2),analytical(x,i+1),f'N={i+1}',"\
    u03BE","$u(\u03BE)^2$")
plt.tight_layout()
plt.show()

fig2, ((axx1, axx2), (axx3, axx4)) = plt.subplots(2,2)
fig2.suptitle("Wavefunction")
dict = {'0': axx1,'1': axx2,'2': axx3,'3': axx4}
for i in range(0,4,1):
    U=diag_mat(n,xi,xf)[1][:,i]
    u_norm=U/np.sqrt(integrate.simps(np.power(U,2),x))
    sub_plot(dict[str(int(i))],x,np.power(u_norm,1),analytical_1(x,i+1),f'N={i+1}',
    "\u03BE","$u(\u03BE)^2$",key=0)
plt.tight_layout()
plt.show()
```

Result and Discussion

```
    Eigen Value  Eigen Vector 1  Eigen Vector 2
0           9.0       -0.707107       -0.707107
1          27.0       -0.707107        0.707107
First 11 Eigen Values
     Eigen Value
0       9.868809
1      39.465687
2      88.762003
3     157.710064
4     246.243168
5     354.275666
6     481.703042
7     628.402018
8     794.230674
9     979.028580
10   1182.616957
```




Probability Density
N=1
N=2
N=3
N=4
Inbuilt Solution
Numerical Value
$u(\xi)^2$
ξ
2.0
1.5
1.0
0.5
0.0
−0.50
−0.25
0.00
0.25
0.50