Lab 6: Advanced Plotting and SciPy

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Exercise 1: Wave Function for a 2D Infinite Square Well

AIM:

The normalized wave functions for a particle in a 2D infinite square well located in the region $0 \le x \le L$, $0 \le y \le L$ are

$$\psi_{m,n}(x, y) = \frac{2}{L}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{L}\right)$$

where (x, y) is the position of the particle, $m = 1, 2, 3, \ldots$ and $n = 1, 2, 3, \ldots$ are the quantum numbers of the state. Write a Python program that uses the `matplotlib` module to make the 3D surface plot and the 3D wireframe plot of the wave function $\psi_{4,3}(x, y)$ over the region $0 \le x \le L$, $0 \le y \le L$ side-by-side inside the same figure.

ALGORITHM:

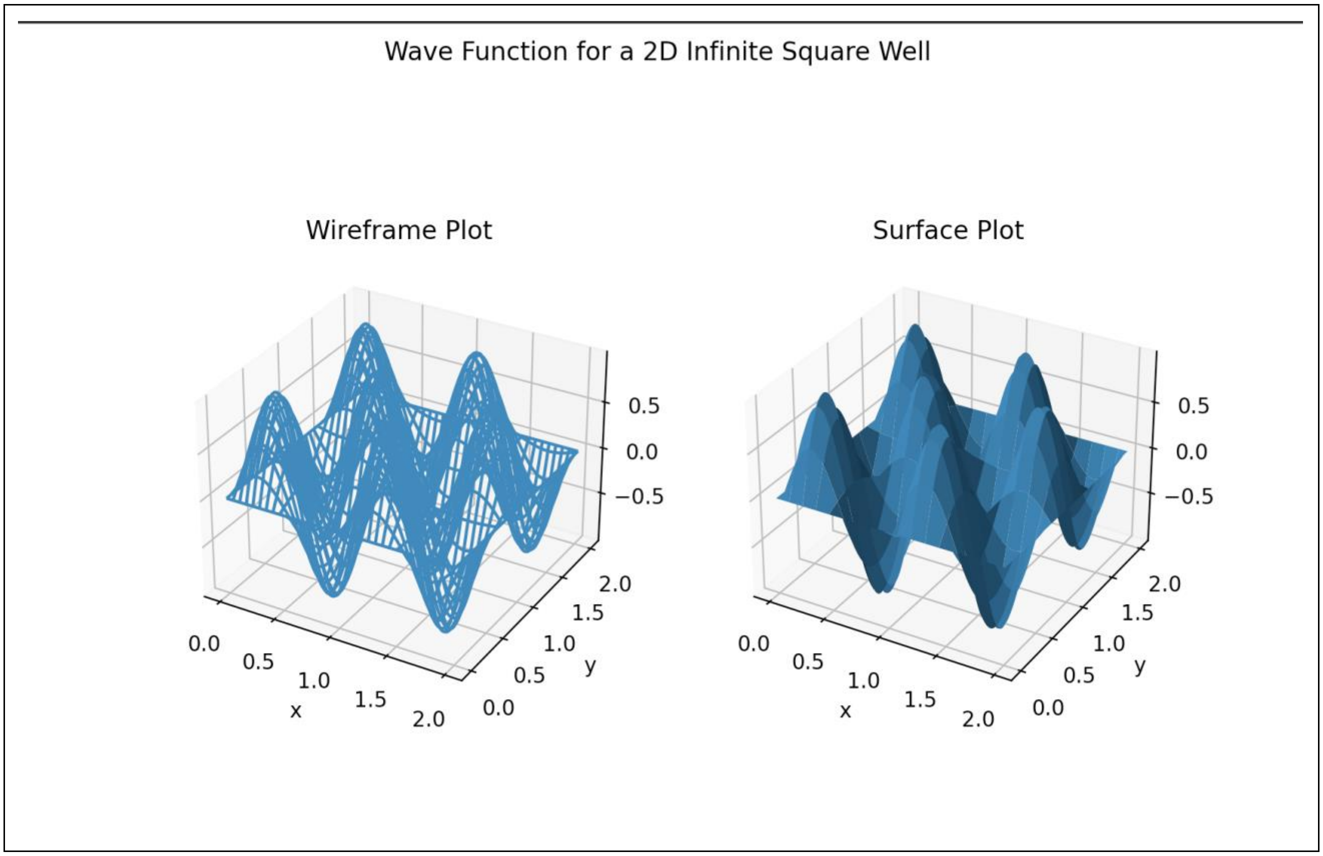
- Prepare the values for x & y using numpy's linspace and meshgrid functions
- The range for both is $0 \le x \le L$, where L is set to 2 in this program.
- Obtain the Z values for the wave function setting m, n = 4, 3.
- Plot the wireframe and surface plot using the data obtained.
- Label axes and figures.

PROGRAM:

```
# 3D Surface & Wirefram Plots
# Created by Shaheer Ziya

import matplotlib.pyplot as plt
import matplotlib.cm as cm
import numpy as np

# Constant
L, steps = 2, 500
# Parameters for Wave Fucntion
m, n = 4, 3

```

```
def psi(x, y):
    return (2/L) * np.sin(m * np.pi * (x/L)) * np.sin(n * np.pi * (y/L))


def main():
    x = np.linspace(0, L, steps)
    y = x.copy()

    X, Y = np.meshgrid(x, y)
    Z = psi(X, Y)

    fig, axs = plt.subplots(1, 2, subplot_kw={"projection": "3d"})

    axs[0].plot_wireframe(X, Y, Z, rstride=15, cstride=15)
    axs[0].set_title("Wireframe Plot")
    axs[0].set_xlabel("x")
    axs[0].set_ylabel("y")

    axs[1].plot_surface(X, Y, Z, rstride=30, cstride=30)
    axs[1].set_title("Surface Plot")
    axs[1].set_xlabel("x")
    axs[1].set_ylabel("y")

    fig.suptitle("Wave Function for a 2D Infinite Square Well")

    plt.show()


main()
```

OUTPUT:


Wave Function for a 2D Infinite Square Well
Wireframe Plot
Surface Plot
0.5
0.0
−0.5
0.0
0.5
1.0
1.5
2.0
x
y

Exercise 2: Mass, Center of Mass, and Moment of Inertia of a Laminar

AIM:

For a lamina occupying a region D in the x-y plane with mass density $\sigma(x, y)$, the mass M, the center of mass (x_{cm}, y_{cm}), as well as the moment of inertia about the x-axis I_x and about the y-axis I_y are given by the double integrals

$$M = \iint_D \sigma(x, y)\, dA,$$

$$x_{\text{cm}} = \frac{1}{M}\iint_D x\,\sigma(x, y)\, dA, \qquad y_{\text{cm}} = \frac{1}{M}\iint_D y\,\sigma(x, y)\, dA,$$

$$I_x = \iint_D y^2\,\sigma(x, y)\, dA, \qquad I_y = \iint_D x^2\,\sigma(x, y)\, dA.$$

Write a Python program that uses the `scipy.integrate` function `dblquad` to compute M, x_{cm}, y_{cm}, I_x, and I_y for a lamina occupying the region $0 \le x \le 2$, $0 \le y \le xe^{-x}$ with mass density $\sigma(x, y) = x^2y^2$ and then outputs the results. Assume all the quantities are expressed in SI units.

ALGORITHM:

- Set up the limits of integration for the lamina along with the required density functions for integration.
- Calculate all the required properties by calling dblquad from scipy.integrate
- Print these results to the screen

PROGRAM:

```
# Mass, Center of Mass, and Moment of Inertia of a Laminar
# Created by Shaheer Ziya


import matplotlib.pyplot as plt
import scipy.integrate as intgr
import numpy as np


# Bounds for the lamina
x = 2
y = x * np.exp(-x)


# The density function for the lamina
```

```python
def sigma(x, y):
  return (x * y) ** 2

# Functions for Centre of Mass
def xsigma(x, y):
  return x * sigma(x, y)
def ysigma(x, y):
  return y * sigma(x, y)
# Functions for Moments of Inertia
def x2sigma(x, y):
  return (x ** 2) * sigma(x, y)
def y2sigma(x, y):
  return (y ** 2) * sigma(x, y)

def main():

  M = intgr.dblquad(sigma, 0, x, 0, y)[0]
  xm = (1/M) * intgr.dblquad(xsigma, 0, x, 0, y)[0]
  ym = (1/M) * intgr.dblquad(ysigma, 0, x, 0, y)[0]
  Ix = intgr.dblquad(y2sigma, 0, x, 0, y)[0]
  Iy = intgr.dblquad(x2sigma, 0, x, 0, y)[0]

  print(f"The mass of the lamina is ~{M:.3f} kg")
  print(f"The centre of mass of the lamina is ({xm:.2f}, {ym:.2f}) (upto 2 d.p. in metres)")
  print(f"The moments of inertia of the lamina are {Ix:.5f} kgm^2 and {Iy:.5f} kgm^2")


main()
```

OUTPUT:

```
y"
The mass of the lamina is ~0.018 kg
The centre of mass of the lamina is (0.20, 1.50) (upto 2 d.p. in metres)
The moments of inertia of the lamina are ~0.04230 kgm^2 and` 0.00077 kgm^2
```

Exercise 3: Series *LRC* Circuit

AIM:

A series *LRC* circuit is composed of an inductor of inductance L, a resistor of resistance R, and a capacitor of capacitance C connected in series with an alternating emf $\xi(t)$. It can be shown that the charge q on the capacitor obeys the differential equation:

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{q}{C} = \xi(t)$$

where the current in the circuit $I(t) = q'(t)$. Write a Python program to solve this equation subject to the initial conditions $q(0) = 0$ C, $I(0) = 6$ A from time $t = 0$ to 5s for the case $L = 0.5$ H, $R = 20\ \Omega$, $C = 0.001$ F, and $\xi(t) = 100 \sin 60t$ V by using the `scipy.integrate.odeint` method. Your program should also use the `matplotlib` module to plot the numerical solutions of $q(t)$ and $I(t)$ versus t as separate plots sharing the same horizontal axis.

ALGORITHM:

- Define the constants in the function
- Define the necessary relevant functions like the one to define the alternating emf
- Define the original ODE as a set simultaneous of ODEs dependent on t. (q, I)
- Initialize the initial conditions for q(0) and I(0).

$$\frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \left[I(t), \frac{1}{L}\left(\xi(t) - Rt - \frac{q}{C}\right)\right]^T$$

- Solve the ODEs using scipy.odeint
- Plot the resultant solution functions with the same horizontal axis on the interval they were solved on.

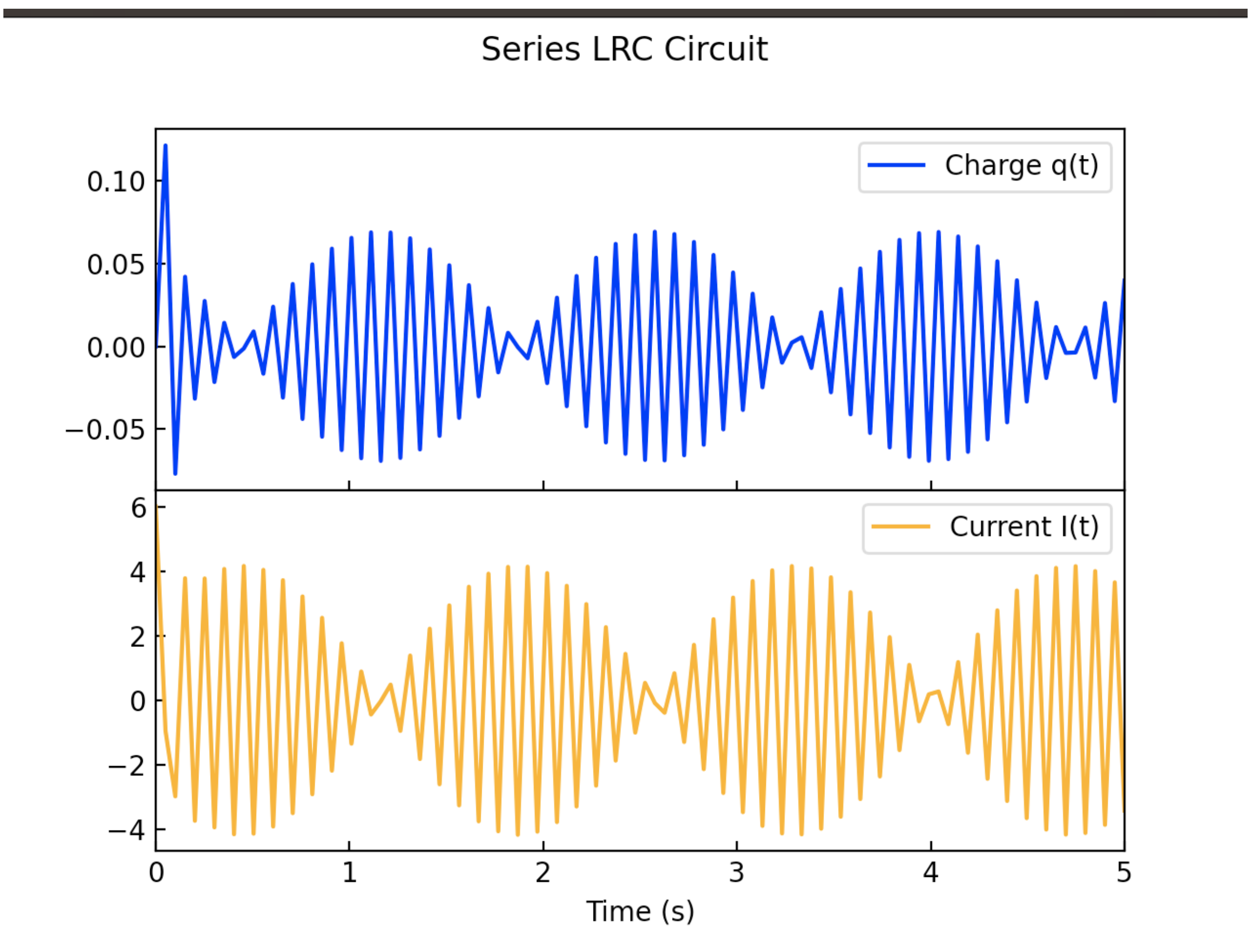
PROGRAM:

```python
# Series LRC Circuit
# Created by Shaheer Ziya


import matplotlib.pyplot as plt
from scipy.integrate import odeint
import numpy as np
```

```
# L = 0.5 H, R = 20 ohms,C = 0.001 F
L, R, C = 0.5, 20, 0.001

def emf(t):
 return 100 * np.sin(60 * t)

def dr_dt(r, t: float) -> float:
 q, I = r
 dq_dt = I
 dI_dt = 1/L * (emf(t) - (R * I) - (q/C))
 return np.array([dq_dt, dI_dt])


def main():
 # r = q, I
 # Interval to solve for and plot in
 start, end = 0, 5
 # Number of partitions of the interval
 STEPS = 100
 # The array holding the partitions
 t = np.linspace(start, end, STEPS)

 # Initial conditions
 r0 = 0, 6

 # Solve the differential equation
 sol = odeint(dr_dt, r0, t)

 ### Plotting th Solution ###
 fig, axs = plt.subplots(2)
 fig.suptitle('Series LRC Circuit')
 fig.subplots_adjust(hspace=0)
 axs[0].plot(t, sol[:,0], color='blue', label='Charge q(t)')
 axs[1].plot(t, sol[:, 1], color='orange', label='Current I(t)')

 # Visual Aspects
 for i in (0,1):
```

```
        if i == 0:
            axs[i].set_xticklabels("")
        axs[i].set_xlim(start, end)
        axs[i].set_xlabel('Time (s)')
        axs[i].tick_params(direction="in")
        axs[i].legend()

    plt.show()

main()
```

OUTPUT:



Exercise 4: Legendre Polynomial

AIM:

Below is a table listing the data set drawn from the Legendre polynomial of degree 4, $P_4(x)$, with some noise added.

x	−1.0	−0.8	−0.6	−0.4	−0.2	0
y	0.91695	−0.19706	−0.29293	−0.04645	0.24494	0.44410
x	0.2	0.4	0.6	0.8	1.0	
y	0.31141	-0.04369	−0.42651	−0.39541	1.14994	

Write a Python program that uses the `scipy.optimize` function `curve_fit` to fit the data set to a degree-4 polynomial of x with the initial guesses of all fitting parameters set to 1, prints out the fitting parameters, as well as plots the data set, fitting result, and the polynomial $P_4(x)$ on the same graph using the `matplotlib` module and the `scipy.special` function `eval_legendre`.

ALGORITHM:

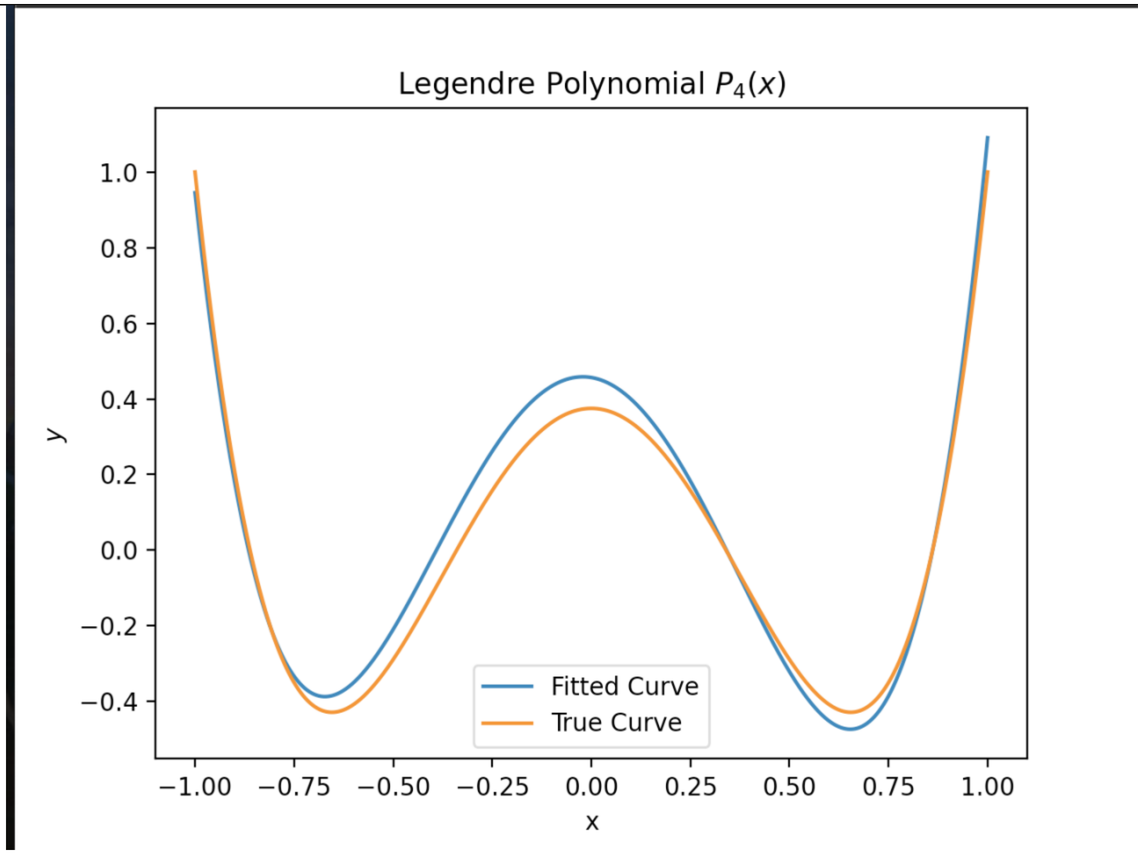
- Init the data
- Fit the data to a degree 4 polynomial using a user-defined function representing a degree 4 polynomial
- Create the data set for the fitted polynomial and the true legendre polynomial
- Plot the two on the same plot
- The initial fitting parameters are set to 1 by default

PROGRAM:

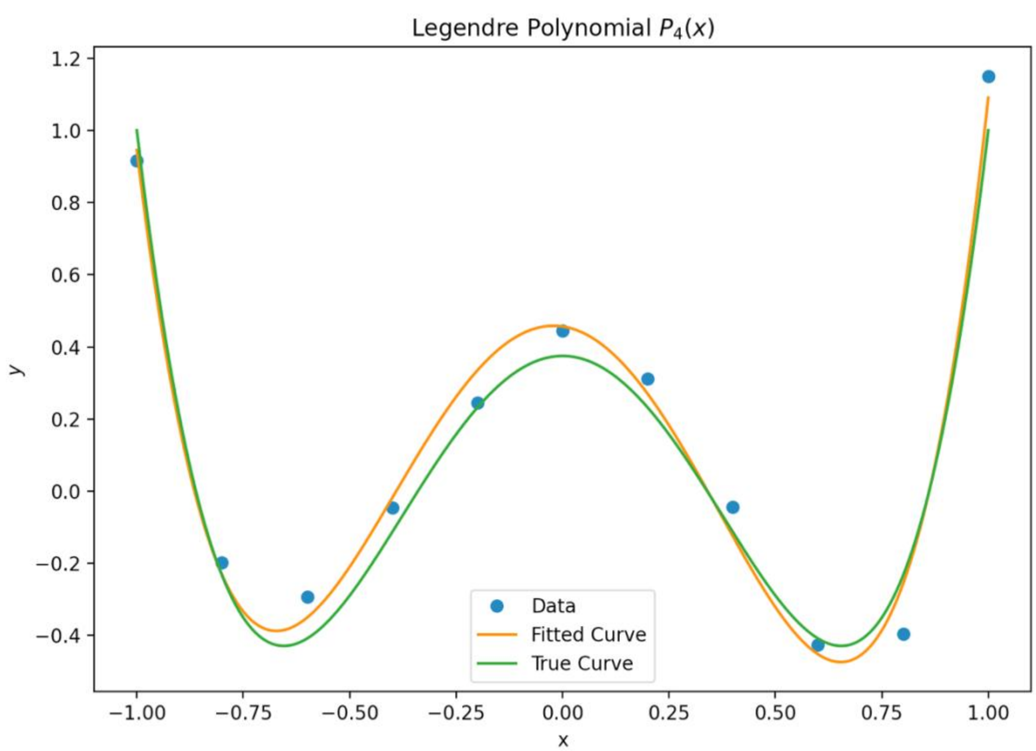
```
# Legendre Polynomial
# Created by Shaheer Ziya


import matplotlib.pyplot as plt
import numpy as np
from scipy.optimize import curve_fit
from scipy.special import eval_legendre


x_data = np.linspace(-1, 1, 11)
y_data = np.array([0.91695, -0.19706, -0.29293, -0.04645,
          0.24494, 0.44410, 0.31141, -0.04369, -0.42651, -0.39541, 1.14994])


def try_fit(x, a, b, c, d, e):
```

```
    '''Degree 4 polynomial'''
    return a * (x ** 4) + b * (x ** 3) + c * (x ** 2) + d * x + e

def main():
    fitted_paramters = curve_fit(try_fit, x_data, y_data)[0]
    print(fitted_paramters)

    fig, axs = plt.subplots()



    X = np.linspace(-1, 1, 1000)

    fitted_curve = try_fit(X, *fitted_paramters)
    # axs.plot(x_data, y_data, 'o', label='Data')
    axs.plot(X, fitted_curve, '-', label='Fitted Curve')

    true_curve = eval_legendre(4, X)
    axs.plot(X, true_curve, '-', label='True Curve')

    plt.title("Legendre Polynomial $P_4(x)$")
    plt.xlabel("x")
    plt.ylabel("$y$")

    plt.legend()
    plt.show()



main()
```

OUTPUT:



Legendre Polynomial $P_4(x)$
y
x
Fitted Curve
True Curve



Legendre Polynomial $P_4(x)$
y
x
Data
Fitted Curve
True Curve