16/20

Homework 1

Deadline: Monday 24 March 2024 (by 19h00)

Credits: 20 points

Instructions:

- When you finish, please submit a single **.ipynb** file via email to wbanda@yachaytech.edu.ec (mailto:wbanda@yachaytech.edu.ec)
- The homework is **individual**. Please include your name in the notebook.
- Within a **single python notebook**, solve the following problems.

Name:

In [1]:

✓

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.optimize import fsolve
import sympy as sp
from scipy.integrate import solve_ivp
from scipy.optimize import brentq
```

1. Population dynamics (8 points)

The system of ordinary differential equations (ODEs) describing the population dynamics of two prey species (x and y) and one predator species (z) is given by:

$$\frac{dx}{dt} = g_1\, x \left(1 - \frac{x}{c_1}\right) - p_1\, x\, z,$$
$$\frac{dy}{dt} = g_2\, y \left(1 - \frac{y}{c_2}\right) - p_2\, y\, z,$$
$$\frac{dz}{dt} = e_1\, p_1\, x\, z + e_2\, p_2\, y\, z - d\, z.$$

where:

- g_1, g_2 are the intrinsic growth rates (e.g. birth rates) of the prey populations,
- c_1, c_2 are the carrying capacities of the prey populations (the carrying capacity of an environment is the maximum population size of a biological species that can be sustained by that specific environment),
- p_1, p_2 are the predation rates of the predator on each prey (e.g. how successful a hunt is),
- e_1, e_2 are the conversion efficiencies of consumed prey into predator biomass (the conversion efficiency tells us how efficiently a predator can use the energy from its prey to reproduce),

- d is the natural death rate of the predator. Note that the death rates of the two prey species are intrinsically given by their individual carrying capacities.

This system models the interactions where both prey species grow logistically but are

State vector and slope:

(a) Write down this system of ODEs in terms of the system state vector $S(t)$, i.e. $\frac{dS}{dt} = F(S)$. Identify the slope function $F(S)$ and indicate whether or not it can be explicitly written as a function of S. Create a python function for the slope $F(S)$.

The same notation should be used as in the instructions.

$$\frac{d\mathbf{x}}{dt} = \begin{bmatrix} g_1 x\left(1 - \frac{x}{c_1}\right) - p_1 x z \\ g_2 y\left(1 - \frac{y}{c_2}\right) - p_2 y z \\ e_1 p_1 x z + e_2 p_2 y z - d z \end{bmatrix}$$

-0.25 It is not indicated if the function can be explicitly solved.

ODE integration methods:

(b) Create a python function that implements a trapezoidal Euler method for ODE integration.

(c) Design your own third-order RK method (RK3), and create a python function for this integrator.

(d) Write a python function for the **Butcher's Runge-Kutta method**, which is a popular method for integrating ODEs with a high order of accuracy. It is obtained by following a similar approach to the one we discussed in class. This method uses six points k_1, k_2, k_3, k_4, k_5, and k_6. A weighted average of these points is used to produce the approximation of the solution. The algorithm relies on computing the following slopes:

$$\begin{aligned}
k_1 &= F(t_j, S(t_j)) \\
k_2 &= F\left(t_j + \frac{h}{4}, S(t_j) + \frac{1}{4}k_1 h\right) \\
k_3 &= F\left(t_j + \frac{h}{4}, S(t_j) + \frac{1}{8}k_1 h + \frac{1}{8}k_2 h\right) \\
k_4 &= F\left(t_j + \frac{h}{2}, S(t_j) - \frac{1}{2}k_2 h + k_3 h\right) \\
k_5 &= F\left(t_j + \frac{3h}{4}, S(t_j) + \frac{3}{16}k_1 h + \frac{9}{16}k_4 h\right) \\
k_6 &= F\left(t_j + h, S(t_j) - \frac{3}{7}k_1 h + \frac{2}{7}k_2 h + \frac{12}{7}k_3 h - \frac{12}{7}k_4 h + \frac{8}{7}k_5 h\right)
\end{aligned}$$

The solution is then constructed with the step size (h, same as `dt`)as follows:

$$S(t_{j+1}) = S(t_j) + \frac{h}{90}(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6)\,.$$

In [ ]:

```python
import numpy as np
from scipy.optimize import fsolve
import matplotlib.pyplot as plt

def system(t, state, params):
    """
    Defines the system of ODEs for the predator-prey model.

    Parameters:
    t (float): Time variable.
    state (list): List containing the current state [x, y, z].
    params (dict): Dictionary containing model parameters.

    Returns:
    list: Derivatives [dx/dt, dy/dt, dz/dt].
    """
    x, y, z = state
    g1 = params['g1']
    c1 = params['c1']
    p1 = params['p1']
    g2 = params['g2']
    c2 = params['c2']
    p2 = params['p2']
    e1 = params['e1']
    e2 = params['e2']
    d = params['d']

    dxdt = g1 * x * (1 - x / c1) - p1 * x * z
    dydt = g2 * y * (1 - y / c2) - p2 * y * z
    dzdt = e1 * p1 * x * z + e2 * p2 * y * z - d * z
    return np.array([dxdt, dydt, dzdt])

def trapezoid(f, t0, t_end, x0, h, params):
    """
    Implements the trapezoidal Euler method for ODE integration.

    Parameters:
    f (function): Function defining the system of ODEs.
    t0 (float): Initial time.
    t_end (float): End time.
    x0 (list): Initial state.
    h (float): Time step size.
    params (dict): Parameters for the system of ODEs.

    Returns:
    tuple: Arrays of time values and state values.
    """
    t_values = np.arange(t0, t_end + h, h)
    x_values = np.zeros((len(t_values), len(x0)))
    x_values[0] = x0

    for i in range(1, len(t_values)):
        t_n = t_values[i-1]
        t_np1 = t_values[i]

        # Predictor step (Forward Euler for initial guess)
        x_guess = x_values[i-1] + h * f(t_n, x_values[i-1], params)

        # Implicit correction using fsolve
        def implicit_eq(x_next):
            return x_next - x_values[i-1] - 0.5 * h * (
                f(t_n, x_values[i-1], params) + f(t_np1, x_next, param
            )

        x_values[i] = fsolve(implicit_eq, x_guess)

    return t_values, x_values

def RK3(f, t0, t_end, x0, h, params):
    """
    Implements the third-order Runge-Kutta (RK3) method for ODE integ

    Parameters:
    f (function): Function defining the system of ODEs.
    t0 (float): Initial time.
    t_end (float): End time.
    x0 (list): Initial state.
    h (float): Time step size.
    params (dict): Parameters for the system of ODEs.

    Returns:
    tuple: Arrays of time values and state values.
    """
    t_values = np.arange(t0, t_end + h, h)
    x_values = np.zeros((len(t_values), len(x0)))
    x_values[0] = x0

    for i in range(1, len(t_values)):
        t_n = t_values[i-1]

        k1 = f(t_n, x_values[i-1], params)
        k2 = f(t_n + h/2, x_values[i-1] + h/2 * k1, params)
        k3 = f(t_n + h, x_values[i-1] - h * k1 + 2 * h * k2, params)

        x_values[i] = x_values[i-1] + (h / 6) * (k1 + 4 * k2 + k3)

    return t_values, x_values

def butcher(f, t0, t_end, x0, h, params):
    """
    Implements Butcher's Runge-Kutta method for ODE integration.

    Parameters:
    f (function): Function defining the system of ODEs.
    t0 (float): Initial time.
    t_end (float): End time.
    x0 (list): Initial state.
    h (float): Time step size.
    params (dict): Parameters for the system of ODEs.

    Returns:
    tuple: Arrays of time values and state values.
    """
    t_values = np.arange(t0, t_end + h, h)
    x_values = np.zeros((len(t_values), len(x0)))
    x_values[0] = x0

    for i in range(1, len(t_values)):
        t_n = t_values[i-1]

        k1 = f(t_n, x_values[i-1], params)
        k2 = f(t_n + h/4, x_values[i-1] + h/4 * k1, params)
```

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```
        k3 = f(t_n + h/4, x_values[i-1] + h/8 * k1 + h/8 * k2, params
        k4 = f(t_n + h/2, x_values[i-1] - h/2 * k2 + h * k3, params)
        k5 = f(t_n + 3/4 * h, x_values[i-1] + 3/16 * h * k1 + 9/16 *
        k6 = f(t_n + h, x_values[i-1] - 3/7 * h * k1 + 2/7 * h * k2 +

        x_values[i] = x_values[i-1] + h/90 * (7 * k1 + 32 * k3 + 12 *

    return t_values, x_values
```

Settings and initial conditions:

(e) Create a dictionary that allocates all the user-defined initial conditions needed for integration, including an option for the user to select the integration method. The default parameters in the dictionary should be:

Parameter	Value	Description
g1	1.0	Growth rate of prey 1
c1	200.0	Carrying capacity of prey 1
p1	0.01	Predation rate of predator on prey 1
g2	1.2	Growth rate of prey 2
c2	150.0	Carrying capacity of prey 2
p2	0.008	Predation rate of predator on prey 2
e1	0.08	Conversion efficiency of prey 1 to predator
e2	0.07	Conversion efficiency of prey 2 to predator
d	0.15	Death rate of predator
x0	100.0	Initial population of prey 1
y0	80.0	Initial population of prey 2
z0	20.0	Initial population of predator
t_span	(0, 200)	Time span for simulation
dt	0.01	Time step size ($= h$)
method	RK3	Integration method

In [ ]:
```python
def create_default_parameters():
    """
    Creates a dictionary with default parameters for the predator-prey

    Returns:
    dict: Dictionary containing default parameters.
    """
    params = {
        # Growth parameters
        'g1': 1.0,           # Growth rate of prey 1
        'c1': 200.0,         # Carrying capacity of prey 1
        'p1': 0.01,          # Predation rate of predator on prey 1
        'g2': 1.2,           # Growth rate of prey 2
        'c2': 150.0,         # Carrying capacity of prey 2
        'p2': 0.008,         # Predation rate of predator on prey 2
        'e1': 0.08,          # Conversion efficiency of prey 1 to pred
        'e2': 0.07,          # Conversion efficiency of prey 2 to pred
        'd': 0.15,           # Death rate of predator

        # Initial conditions
        'x0': 100.0,         # Initial population of prey 1
        'y0': 80.0,          # Initial population of prey 2
        'z0': 20.0,          # Initial population of predator

        # Simulation parameters
        't_span': (0, 200),  # Time span for simulation
        'dt': 0.01,          # Time step size
        'method': 'RK3'      # Integration method
    }

    return params

def get_user_parameters(default_params=None):
    """
    Allow users to modify the default parameters.

    Parameters:
    default_params (dict, optional): Dictionary containing default pa

    Returns:
    dict: Dictionary containing user-defined or default parameters.
    """
    if default_params is None:
        default_params = create_default_parameters()


    params = default_params.copy()

    print("Enter new parameter values (press Enter to keep default):")
    for key, value in params.items():
        user_input = input(f"{key} [{value}]: ")
        if user_input:
            if isinstance(value, int):
                params[key] = int(user_input)
            elif isinstance(value, float):
                params[key] = float(user_input)
            elif isinstance(value, tuple) and key == 't_span':
                # Special handling for t_span tuple
                t_values = user_input.strip('()').split(',')
                params[key] = (float(t_values[0]), float(t_values[1]))
            else:
                params[key] = user_input

    print(params)
    return params
```

Time stepping:

(f) Create a python function that integrates the system of ODEs using the settings and initial conditions as arguments. The function should perform integration for all three methods (according to the option `method`) and return the resulting times (t) and system states $S(t)$ as arrays.

In [ ]:
```python
def integrator(f, params):
    """
    Integrates a system of ODEs using the specified method.

    Parameters:
    f (function): Function defining the system of ODEs.
    params (dict): Dictionary containing parameters for the system of

    Returns:
    tuple: Arrays of time values and state values.
    """
    params_f = {key: params[key] for key in params if key not in ['x0

    # Initial conditions
    x0 = [params['x0'], params['y0'], params['z0']]

    method = params['method']

    t0, t_end = params['t_span']
    dt = params['dt']

    # Call the integrator function
    if method == 'trapezoid':
        t_values, x_values = trapezoid(f, t0, t_end, x0, dt, params_f
        method = 'Trapezoidal Euler'
    elif method == 'RK3':
        t_values, x_values = RK3(f, t0, t_end, x0, dt, params_f)
    elif method == 'butcher':
        t_values, x_values = butcher(f, t0, t_end, x0, dt, params_f)
        method = 'Butcher RK'
    else:
        raise ValueError(f"Invalid method: {method}")

    return t_values, x_values, method
```

Plotting function:

(g) Create a python function that takes the times (t) and system states $S(t)$ as arguments and returns a 3-panel figure showing the evolution of each species (x, y, and z) in the system as a function of time, t.

In [5]:

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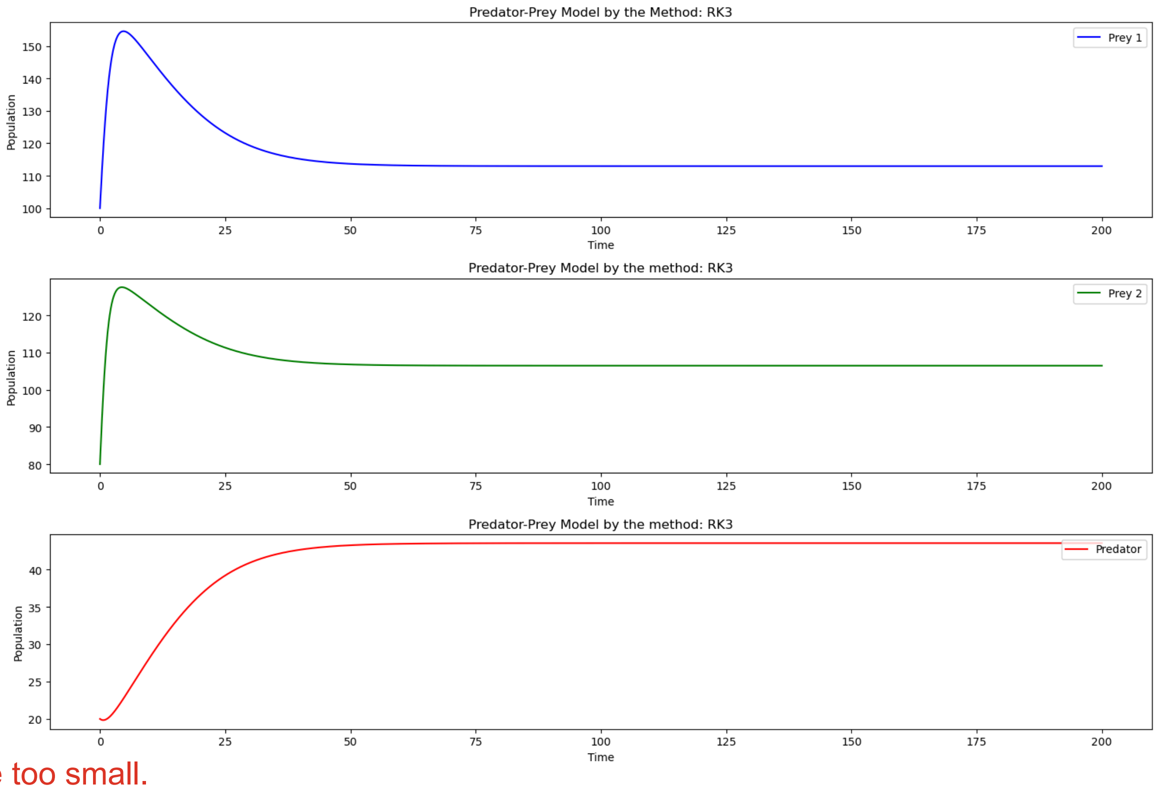
```
def plotter(t_values, x_values, method):
    """
    Plots the state variables as a function of time.

    Parameters:
    t_values (array): Array of time values.
    x_values (array): Array of state values.
    """
    fig, ax = plt.subplots(3, 1, figsize=(15, 10))
    ax[0].plot(t_values, x_values[:, 0], label='Prey 1', color='blue')
    ax[1].plot(t_values, x_values[:, 1], label='Prey 2', color='green
    ax[2].plot(t_values, x_values[:, 2], label='Predator', color='red
    ax[0].set_xlabel('Time')
    ax[1].set_xlabel('Time')
    ax[2].set_xlabel('Time')
    ax[0].set_ylabel('Population')
    ax[1].set_ylabel('Population')
    ax[2].set_ylabel('Population')
    ax[0].set_title(f'Predator-Prey Model by the Method: {method}')
    ax[1].set_title(f'Predator-Prey Model by the method: {method}')
    ax[2].set_title(f'Predator-Prey Model by the method: {method}')
    ax[0].legend(loc = 1)
    ax[1].legend(loc = 1)
    ax[2].legend(loc = 1)
    plt.tight_layout()
    plt.show()
```

Simulation:

(h) Call your time-stepping and plotting functions to run and display the results of three simulations (one per integration method), using the default settings and initial conditions from the table in (e). Based on your simulations, does the system reach equilibrium?

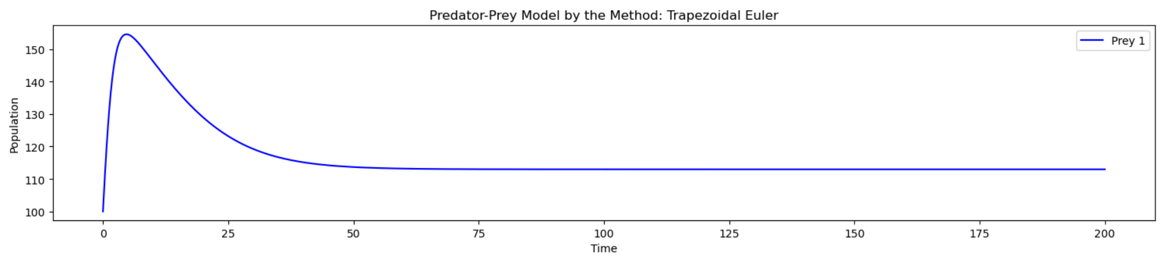
```
In [6]: params = get_user_parameters(create_default_parameters())
        t_values, x_values, method = integrator(system, params)
        plotter(t_values, x_values, method)

        params_2 = get_user_parameters()
        t_values_2, x_values_2, method_2 = integrator(system, params_2)
        plotter(t_values_2, x_values_2, method_2)

        params_3 = get_user_parameters()
        t_values_3, x_values_3, method_3 = integrator(system, params_3)
        plotter(t_values_3, x_values_3, method_3)
```

```
Enter new parameter values (press Enter to keep default):
{'g1': 1.0, 'c1': 200.0, 'p1': 0.01, 'g2': 1.2, 'c2': 150.0, 'p2':
0.008, 'e1': 0.08, 'e2': 0.07, 'd': 0.15, 'x0': 100.0, 'y0': 80.0,
'z0': 20.0, 't_span': (0, 200), 'dt': 0.01, 'method': 'RK3'}
```



The labels are too small.

```
Enter new parameter values (press Enter to keep default):
{'g1': 1.0, 'c1': 200.0, 'p1': 0.01, 'g2': 1.2, 'c2': 150.0, 'p2':
0.008, 'e1': 0.08, 'e2': 0.07, 'd': 0.15, 'x0': 100.0, 'y0': 80.0,
'z0': 20.0, 't_span': (0, 200), 'dt': 0.01, 'method': 'trapezoid'}
```



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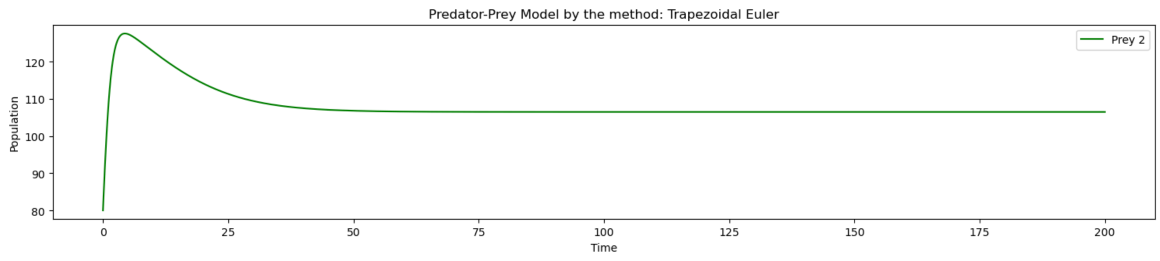
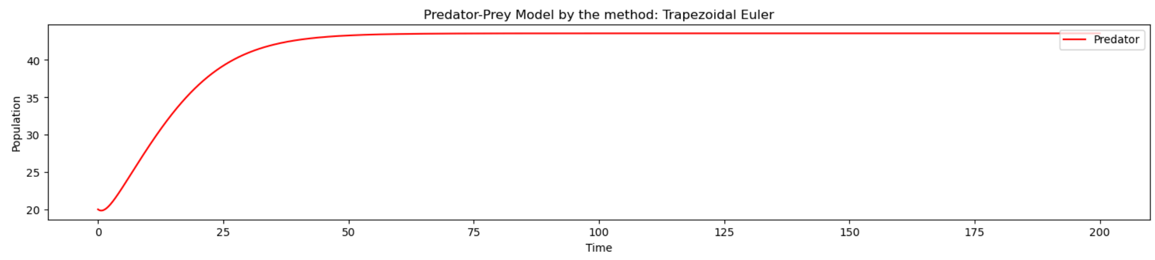
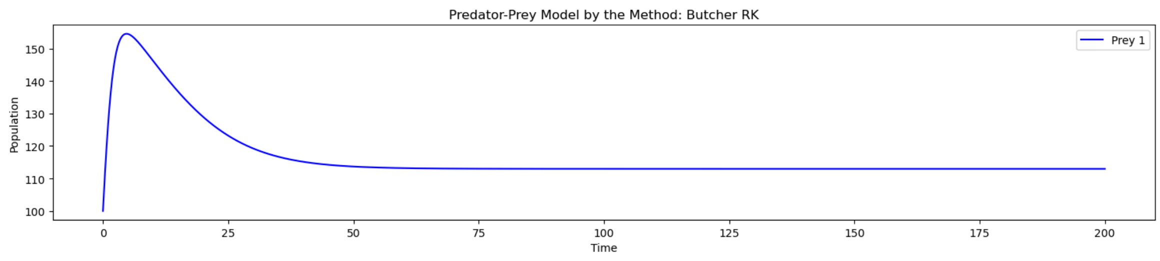




```
Enter new parameter values (press Enter to keep default):
{'g1': 1.0, 'c1': 200.0, 'p1': 0.01, 'g2': 1.2, 'c2': 150.0, 'p2':
0.008, 'e1': 0.08, 'e2': 0.07, 'd': 0.15, 'x0': 100.0, 'y0': 80.0,
'z0': 20.0, 't_span': (0, 200), 'dt': 0.01, 'method': 'butcher'}
```



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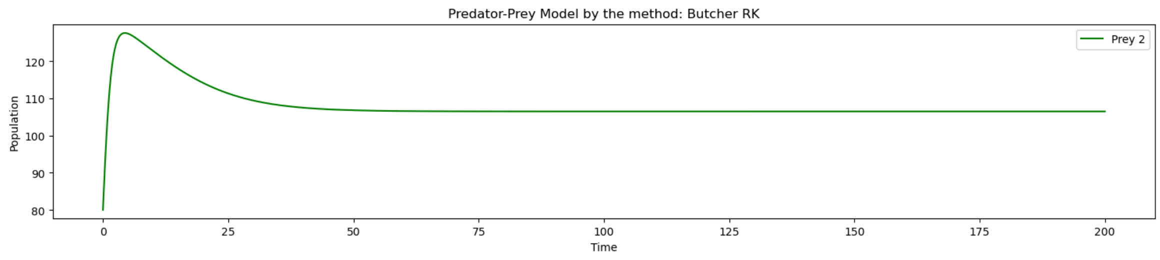
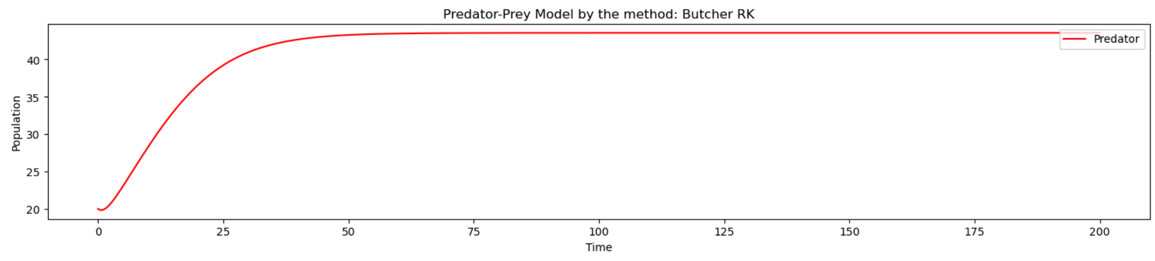




-0.25 There is no answer to the question provided.

2. Dynamical systems and equilibrium (5 points)

Python class:

(a) Reorganise all your code from problem 1 into a single python class that contains attributes and methods. The settings and initial conditions should be attributes and all the

[illegible]

In [ ]:
```python
import numpy as np
from scipy.optimize import fsolve
import matplotlib.pyplot as plt

class PredatorPreyModel:
    def __init__(self, params):
        """
        Initializes the PredatorPreyModel with the given parameters.

        Parameters:
        params (dict): Dictionary containing model parameters.
        """
        self.params = params
        self.x0 = np.array([params['x0'], params['y0'], params['z0']])
        self.t0, self.t_end = params['t_span']
        self.dt = params['dt']
        self.method = params['method']

    def system(self, t, state):
        """
        Defines the system of ODEs for the predator-prey model.

        Parameters:
        t (float): Time variable.
        state (list): List containing the current state [x, y, z].

        Returns:
        list: Derivatives [dx/dt, dy/dt, dz/dt].
        """
        x, y, z = state
        g1 = self.params['g1']
        c1 = self.params['c1']
        p1 = self.params['p1']
        g2 = self.params['g2']
        c2 = self.params['c2']
        p2 = self.params['p2']
        e1 = self.params['e1']
        e2 = self.params['e2']
        d = self.params['d']

        dxdt = g1 * x * (1 - x / c1) - p1 * x * z
        dydt = g2 * y * (1 - y / c2) - p2 * y * z
        dzdt = e1 * p1 * x * z + e2 * p2 * y * z - d * z
        return np.array([dxdt, dydt, dzdt])

    def trapezoid(self):
        """
        Implements the trapezoidal Euler method for ODE integration.

        Returns:
        tuple: Arrays of time values and state values.
        """
        t_values = np.arange(self.t0, self.t_end + self.dt, self.dt)
        x_values = np.zeros((len(t_values), len(self.x0)))
        x_values[0] = self.x0

        for i in range(1, len(t_values)):
            t_n = t_values[i-1]
            t_np1 = t_values[i]

            # Predictor step (Forward Euler for initial guess)
            x_guess = x_values[i-1] + self.dt * self.system(t_n, x_va

            # Implicit correction using fsolve
            def implicit_eq(x_next):
                return x_next - x_values[i-1] - 0.5 * self.dt * (
                    self.system(t_n, x_values[i-1]) + self.system(t_n
                )

            x_values[i] = fsolve(implicit_eq, x_guess)
        return t_values, x_values

    def RK3(self):
        """
        Implements the third-order Runge-Kutta (RK3) method for ODE i

        Returns:
        tuple: Arrays of time values and state values.
        """
        t_values = np.arange(self.t0, self.t_end + self.dt, self.dt)
        x_values = np.zeros((len(t_values), len(self.x0)))
        x_values[0] = self.x0

        for i in range(1, len(t_values)):
            t_n = t_values[i-1]

            k1 = self.system(t_n, x_values[i-1])
            k2 = self.system(t_n + self.dt/2, x_values[i-1] + self.dt
            k3 = self.system(t_n + self.dt, x_values[i-1] - self.dt *

            x_values[i] = x_values[i-1] + (self.dt / 6) * (k1 + 4 * k

        return t_values, x_values

    def butcher(self):
        """
        Implements Butcher's Runge-Kutta method for ODE integration.

        Returns:
        tuple: Arrays of time values and state values.
        """
        t_values = np.arange(self.t0, self.t_end + self.dt, self.dt)
        x_values = np.zeros((len(t_values), len(self.x0)))
        x_values[0] = self.x0

        for i in range(1, len(t_values)):
            t_n = t_values[i-1]

            k1 = self.system(t_n, x_values[i-1])
            k2 = self.system(t_n + self.dt/4, x_values[i-1] + self.dt
            k3 = self.system(t_n + self.dt/4, x_values[i-1] + self.dt
            k4 = self.system(t_n + self.dt/2, x_values[i-1] - self.dt
            k5 = self.system(t_n + 3/4 * self.dt, x_values[i-1] + 3/1
            k6 = self.system(t_n + self.dt, x_values[i-1] - 3/7 * sel

            x_values[i] = x_values[i-1] + self.dt/90 * (7 * k1 + 32 *

        return t_values, x_values

    def integrate(self):
        """
        Integrates the system of ODEs using the specified method.
        Returns:
        tuple: Arrays of time values and state values.
        """
        if self.method == 'trapezoid':
            return self.trapezoid()
        elif self.method == 'RK3':
            return self.RK3()
        elif self.method == 'butcher':
            return self.butcher()
        else:
            raise ValueError(f"Invalid method: {self.method}")

    def plot(self, t_values, x_values):
        """
        Plots the results of the integration.

        Parameters:
        t_values (array): Array of time values.
        x_values (array): Array of state values.
        """
        plt.figure(figsize=(10, 6))
        plt.plot(t_values, x_values[:, 0], label='x (prey)')
        plt.plot(t_values, x_values[:, 1], label='y (predator)')
        plt.plot(t_values, x_values[:, 2], label='z (super-predator)'
        plt.xlabel('Time')
        plt.ylabel('Population')
        plt.legend()
        plt.title('Predator-Prey Model')
        plt.show()

    def calculate_l2_norm(self, numerical_solution, reference_solutio
        """
        Calculates the L2-norm error between the numerical solution a

        Parameters:
        numerical_solution (array): Array of numerical solution value
        reference_solution (array): Array of reference solution value

        Returns:
        float: L2-norm error.
        """
        error = numerical_solution - reference_solution
        l2_norm = np.sqrt(np.sum(error**2))
        return l2_norm

    @staticmethod
    def get_user_parameters():
        """
        Prompts the user to input parameters for the model.

        Returns:
        dict: Dictionary containing user-defined parameters.
        """
        params = {}
        params['x0'] = float(input("Enter initial population of prey (
        params['y0'] = float(input("Enter initial population of predat
        params['z0'] = float(input("Enter initial population of super-
        params['g1'] = float(input("Enter growth rate of prey (g1): ")
        params['c1'] = float(input("Enter carrying capacity of prey (
        params['p1'] = float(input("Enter predation rate of prey by su
```

✓

```
        params['g2'] = float(input("Enter growth rate of predator (g2
        params['c2'] = float(input("Enter carrying capacity of predat
        params['p2'] = float(input("Enter predation rate of predator 
        params['e1'] = float(input("Enter efficiency of prey to super-
        params['e2'] = float(input("Enter efficiency of predator to su
        params['d'] = float(input("Enter death rate of super-predator 
        t_start = float(input("Enter start time (t0): "))
        t_end = float(input("Enter end time (t_end): "))
        params['t_span'] = (t_start, t_end)
        params['dt'] = float(input("Enter time step size (dt): "))
        params['method'] = input("Enter integration method (trapezoid,
        return params
```

Error analysis:

(b) Call the methods from your python class above to run 15 simulations (5 simulations per integration method) for 5 decreasing values of the time step size, `dt` (i.e. h). Then, compute the L_2-norm errors for all these 15 runs and report the results in a single figure with the L_2-norm errors in the Y axis and h in the X axis. Which method produces the most accurate results?

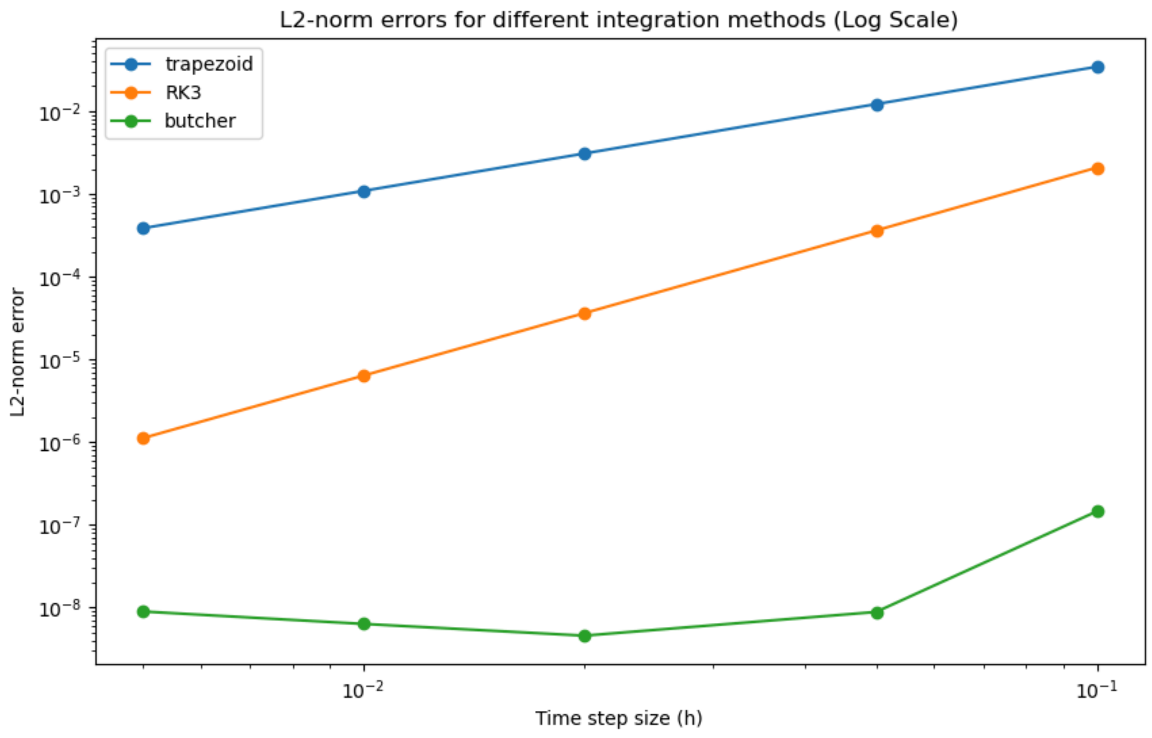
```
In [ ]: # Define the reference solution
        params = create_default_parameters()
        params['dt'] = 0.001
        params['method'] = 'RK3'
        model = PredatorPreyModel(params)
        t_ref, x_ref = model.integrate()

        # Define the time step sizes to test
        time_steps = [0.1, 0.05, 0.02, 0.01, 0.005]

        methods = ['trapezoid', 'RK3', 'butcher']
        l2_errors = {method: [] for method in methods}

        # Run the simulations and compute the L2-norm errors
        for method in methods:
            for dt in time_steps:
                params['dt'] = dt
                params['method'] = method
                model = PredatorPreyModel(params)
                t_values, x_values = model.integrate()

                x_ref_interp = np.interp(t_values, t_ref, x_ref[:, 0]), np.int
                x_ref_interp = np.vstack(x_ref_interp).T

                l2_error = model.calculate_l2_norm(x_values, x_ref_interp)
                l2_errors[method].append(l2_error)


        plt.figure(figsize=(10, 6))
        for method in methods:
            plt.plot(time_steps, l2_errors[method], label=method, marker='o')
        plt.xlabel('Time step size (h)')
        plt.ylabel('L2-norm error')
        plt.xscale('log')
        plt.yscale('log')
        plt.legend()
        plt.title('L2-norm errors for different integration methods (Log Scale
        plt.show()
```

✓

✓

There is an issue somewhere in the error calculation.

✓



-0.25

The errors in the butcher method should follow a similar slope as the other two methods.

Equilibrium conditions:

(c) Write down the equilibrium condition for the system, $S(t)$. Then, create a python function that uses sympy to study the equilibrium populations of x, y, and z for a range of values of the natural death rate of the predator, d. The function should accept a range of d values and return the equilibrium populations for all the d values in the range. Ensure that the solutions are filtered to exclude extinction cases.

(d) After computing equilibrium solutions for multiple values of the predator mortality d, you should create a high-quality figure of the equilibrium populations of x, y, and z (on the Y axis) versus d (on the x-axis), and label what happens in the parameter regions outside of equilibrium conditions.

(e) Based on your analysis, for what range of d values the system reaches equilibrium? What happens outside of that range? Call your class again to run and compare equilibrium versus extinction scenarios using 3 different values of d.

The equilibrium conditions for the system occur when the derivatives of the state variables are zero. For the predator-prey model, this means:

$$\frac{dx}{dt} = 0$$
$$\frac{dy}{dt} = 0$$
$$\frac{dz}{dt} = 0$$

✓

Given the system of ODEs:

$$\frac{dx}{dt} = g1 \cdot x \cdot \left(1 - \frac{x}{c1}\right) - p1 \cdot x \cdot z$$
$$\frac{dy}{dt} = g2 \cdot y \cdot \left(1 - \frac{y}{c2}\right) - p2 \cdot y \cdot z$$
$$\frac{dz}{dt} = e1 \cdot p1 \cdot x \cdot z + e2 \cdot p2 \cdot y \cdot z - d \cdot z$$

✓

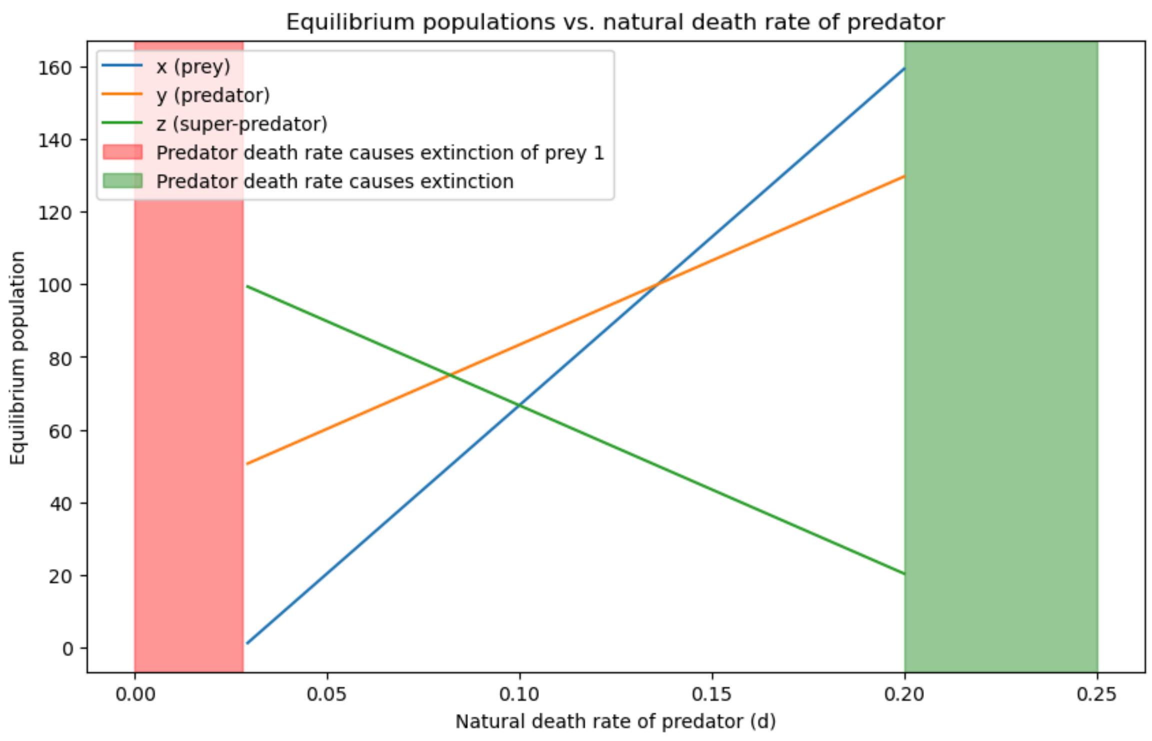
At equilibrium, these equations become: $$ 0 = g1 \cdot x \cdot \left(1 - \frac{x}{c1}\right) - p1 \cdot x \cdot z \\\ 0 = g2 \cdot y \cdot \left(1 - \frac{y}{c2}\right) - p2 \cdot y \cdot z \\\

0 = e1 \cdot p1 \cdot x \cdot z + e2 \cdot p2 \cdot y \cdot z - d \cdot z $$

The equations should be properly displayed.

```
In [ ]: def find_equilibrium_populations(params, d_values):
            """
            Finds the equilibrium populations of x, y, and z for a range of va

            Parameters:
  ✓         params (dict): Dictionary containing model parameters.
            d_values (array): Array of d values to test.

            Returns:
            list: List of equilibrium populations [x_eq, y_eq, z_eq] for each
            """
            # Define symbols
            x, y, z, d = sp.symbols('x y z d')

            # Define parameters
            g1 = params['g1']
            c1 = params['c1']
            p1 = params['p1']
  ✓         g2 = params['g2']
            c2 = params['c2']
            p2 = params['p2']
            e1 = params['e1']
            e2 = params['e2']

            # Define the system of equations
  ✓         eq1 = sp.Eq(g1 * x * (1 - x / c1) - p1 * x * z, 0)
            eq2 = sp.Eq(g2 * y * (1 - y / c2) - p2 * y * z, 0)
            eq3 = sp.Eq(e1 * p1 * x * z + e2 * p2 * y * z - d * z, 0)

            # Solve the system of equations for each value of d
            equilibrium_pops = []
            for d_val in d_values:
                solutions = sp.solve([eq1, eq2, eq3.subs(d, d_val)], (x, y, z)
                for sol in solutions:
  ✓                 x_eq, y_eq, z_eq = sol[x], sol[y], sol[z]
                    # Filter out extinction cases
                    if x_eq > 0 and y_eq > 0 and z_eq > 0:
                        equilibrium_pops.append((d_val, float(x_eq), float(y_e

            return equilibrium_pops

        params = create_default_parameters()
  ✓     d_values = np.linspace(0.01, 0.2, 50)
        equilibrium_pops = find_equilibrium_populations(params, d_values)

  ✓     # Extract equilibrium populations for plotting
        d_vals, x_eq_vals, y_eq_vals, z_eq_vals = zip(*equilibrium_pops)

        plt.figure(figsize=(10, 6))
        plt.plot(d_vals, x_eq_vals, label='x (prey)')
        plt.plot(d_vals, y_eq_vals, label='y (predator)')  Prey 2
        plt.plot(d_vals, z_eq_vals, label='z (super-predator)')  Predator
        plt.axvspan(0, 0.028, color='red', alpha=0.4, label='Predator death ra
        plt.axvspan(0.20, 0.25, color='green', alpha=0.4, label='Predator deat
        plt.xlabel('Natural death rate of predator (d)')
        plt.ylabel('Equilibrium population')
        plt.legend()
  ✓     plt.title('Equilibrium populations vs. natural death rate of predator
        plt.show()
```

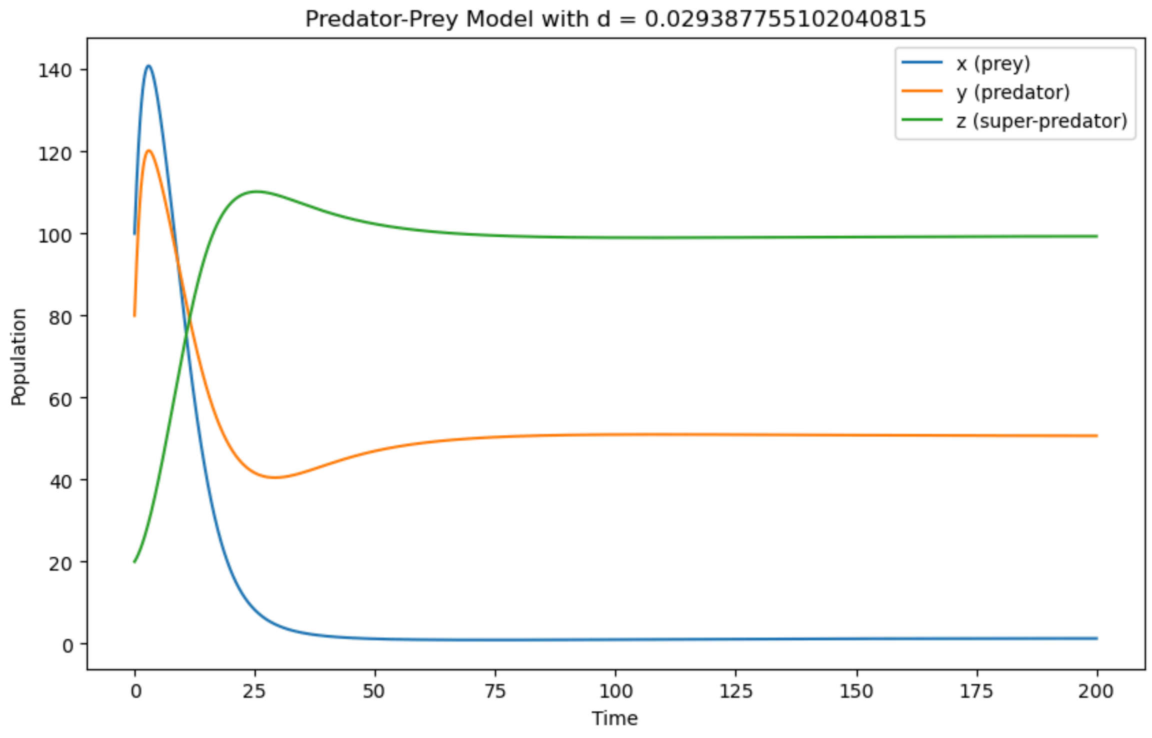
✓


Equilibrium populations vs. natural death rate of predator
x (prey)
y (predator)
z (super-predator)
Predator death rate causes extinction of prey 1
Predator death rate causes extinction
Equilibrium population
Natural death rate of predator (d)
0
20
40
60
80
100
120
140
160
0.00
0.05
0.10
0.15
0.20
0.25

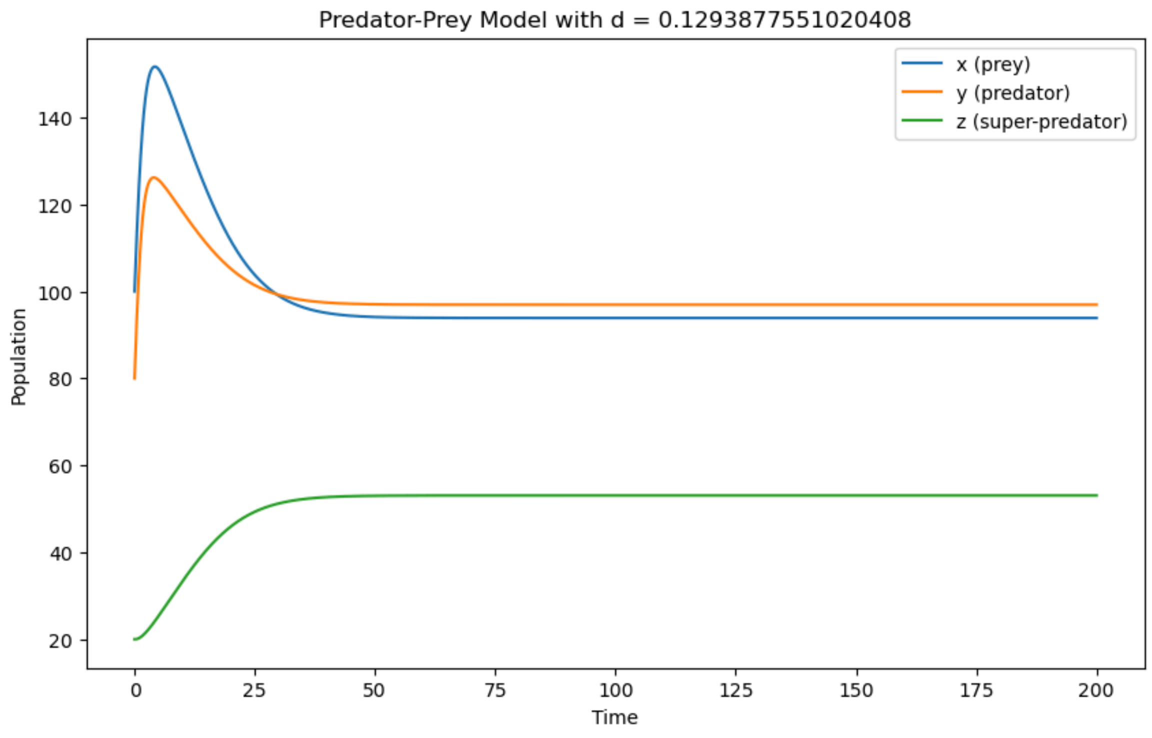
In [35]:
```
  # Extract the range of d values where the system reaches equilibrium
  eq_range = [d for d, x, y, z in equilibrium_pops if x > 0 and y > 0 ar
✓ print(f'The system reaches equilibrium for d values in the range: {mir

  # Define test values for d, including the minimum, midpoint, maximum,
✓ d_test = [min(eq_range), min(eq_range) + max(eq_range) / 2, max(eq_rar

  # Loop through the test values of d
  for d in d_test:
      # Update the parameter dictionary with the current value of d
      params['d'] = d
✓     # Initialize the PredatorPreyModel with the updated parameters
      model = PredatorPreyModel(params)
      # Integrate the system of ODEs
      t_values, x_values = model.integrate()

      # Plot the results
      plt.figure(figsize=(10, 6))
      plt.plot(t_values, x_values[:, 0], label='x (prey)')
      plt.plot(t_values, x_values[:, 1], label='y (predator)') prey 2
✓     plt.plot(t_values, x_values[:, 2], label='z (super-predator)')
      plt.xlabel('Time')                                          predator
      plt.ylabel('Population')
      plt.legend()
      plt.title(f'Predator-Prey Model with d = {d}')
      plt.show()
```

✓
```
The system reaches equilibrium for d values in the range: 0.02938775
5102040815 to 0.2
```

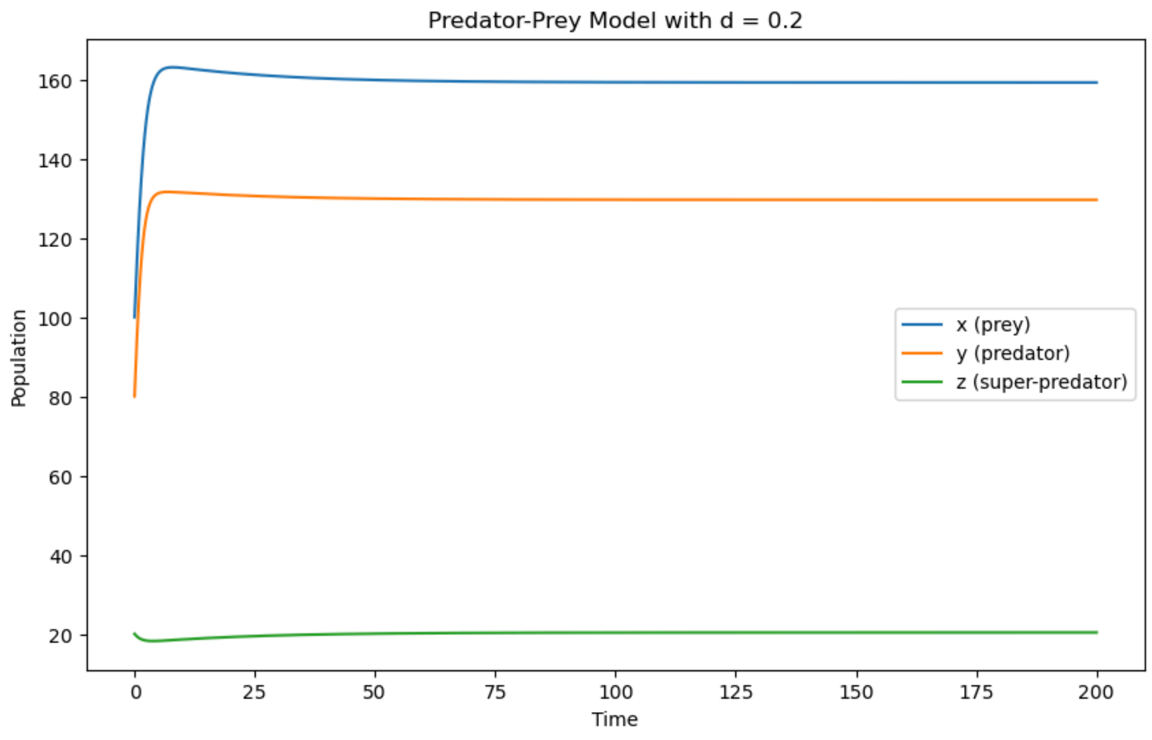
✓

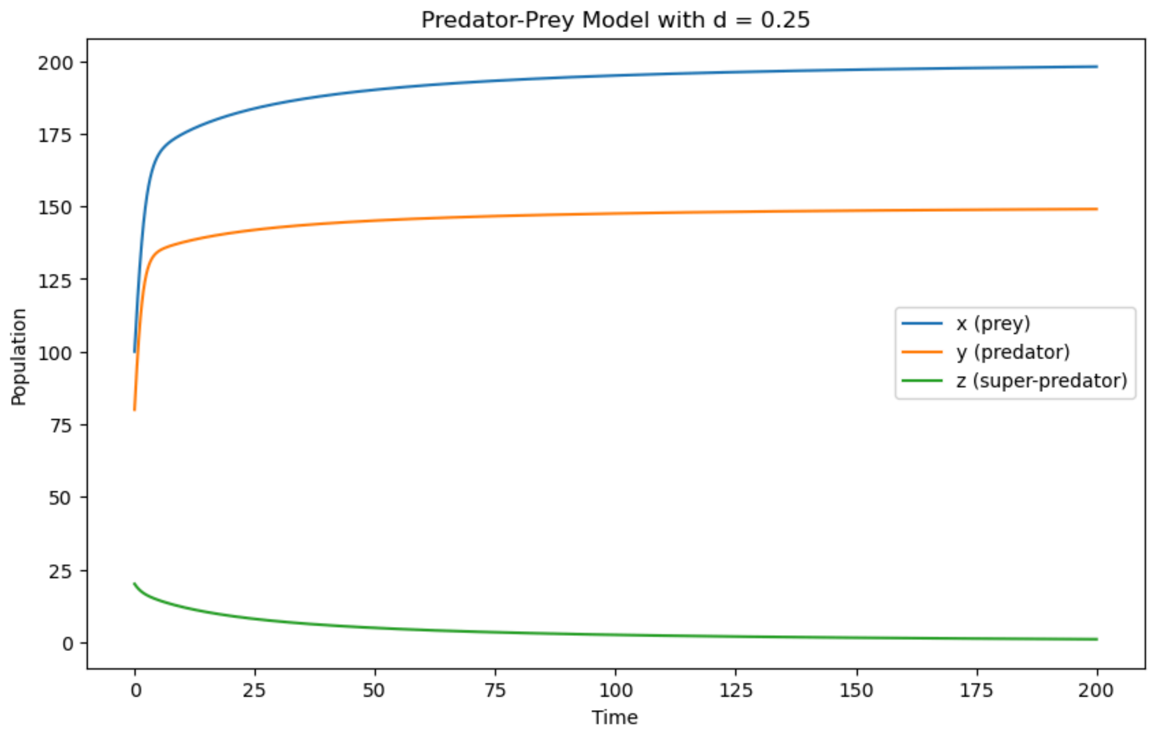


✓


Predator-Prey Model with d = 0.1293877551020408
x (prey)
y (predator)
z (super-predator)
Population
Time
0
25
50
75
100
125
150
175
200
20
40
60
80
100
120
140

✓


Predator-Prey Model with d = 0.2
x (prey)
y (predator)
z (super-predator)
Population
Time
0
25
50
75
100
125
150
175
200
20
40
60
80
100
120
140
160



✓

3. Quantum Harmonic Oscillator (7 points)

The Schrödinger equation for the quantum harmonic oscillator is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

It can be rewritten, in terms of a new variable, $\xi \equiv \sqrt{\frac{m\,\omega}{\hbar}}x$, as follows:

$$\frac{d^2\psi}{d\xi^2}=\left(\xi^2-K\right)\psi$$

where $K \equiv \frac{2E}{\hbar\omega}$ is the energy in units of $\frac{1}{2}\hbar\omega$.

Order reduction and slope function:

(a) Reduce the above ODE to first order. Write down the resulting slope function.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

With new variable $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$, the equation becomes:

$$\frac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi$$

Where $K \equiv \frac{2E}{\hbar\omega}$ is the energy in units of $\frac{1}{2}\hbar\omega$.

Order Reduction

✓ Let $\psi(\xi)=u(\xi)$, and define $y_1=u$, $y_2=\frac{du}{d\xi}$

Then the first-order system is:

✓

1. $\frac{dy_1}{d\xi} = y_2$
2. $\frac{dy_2}{d\xi} = (\xi^2 - K)y_1$

The slope function would be:

✓

$$f_1(y_1, y_2, \xi) = y_2$$
$$f_2(y_1, y_2, \xi) = (\xi^2 - K)y_1$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

=

✓

$$\begin{bmatrix} 0 & 1 \\ \xi^2 - K & 0 \end{bmatrix}$$
$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

Shooting method class:

(b) Carefully read the tasks (c-g) below and design a suitable python class with attributes and methods that solves the above ODE using **the shooting method** with the slope computed in (a). You may use scipy integrators; there is no need to design your own integrators in this problem.

Tasks to be performed by your python class:

(c) Find the **ground state energy** of the harmonic oscillator, to six significant digits, by using **the shooting method.** That is, solve the above equation numerically, varying K until you get a wave function that goes to zero at large ξ. The appropriate boundary conditions for the ground state (and any even state) are $\psi(0) = 1$, $\psi'(0) = 0$.

(d) Make a few illustrative panels showing plots of the wave function for different values of K as it converges to the solution. What does the tail of the wave function does when the values are slightly above or below the correct solution?

(e) Find the **first four excited state energies** (to six significant digits) for the harmonic oscillator, using **the shooting method.** For the first (and third) excited state you will need to set $\psi(0) = 0$, $\psi'(0) = 1$).

(f) Make a few illustrative panels showing plots of the wave functions for different values of K as they converge to their respective solutions.

(g) Make a single plot showing the **harmonic potential** joinly with the **energy ladder** of the quantum harmonic oscillator (include the ground state plus the first four excited states that you calculated above, each with their **respective wave functions**). Consider the particle to be an electron and choose appropriate units for any physical parameters you may need.

Setting xi max to 3 or 4 makes the shape of the wave function visible.

-0.25

```
In [ ]: class QuantumHarmonicOscillatorSolver:
            def __init__(self, xi_max=10, num_points=1000):
                """
                Initializes the solver with the given maximum xi value and nur

                Parameters:
                xi_max (float): Maximum value of xi.
                num_points (int): Number of points in the xi range.
                """
✓               self.xi_max = xi_max
                self.num_points = num_points
                self.xi_range = np.linspace(0, xi_max, num_points)

✓           def slope_function(self, xi, y, K):
                """
                Defines the slope function for the ODE system.

                Parameters:
✓               xi (float): Independent variable.
                y (list): List containing the current state [psi, psi'].
                K (float): Energy parameter.

                Returns:
                list: Derivatives [dpsi/dxi, d^2psi/dxi^2].
                """
✓               return [y[1], (xi**2 - K) * y[0]]

            def shoot(self, K, initial_conditions, target_value=0):
                """
                Implements the shooting method to find the wave function value

                Parameters:
                K (float): Energy parameter.
✓               initial_conditions (list): Initial conditions [psi(0), psi'(0)
                target_value (float): Target value for the wave function at x

                Returns:
                float: Difference between the computed wave function value at
                """
                sol = solve_ivp(self.slope_function, [0, self.xi_max], initia
                    args=(K,),
                    max_step=self.xi_max/self.num_points
                )
                return sol.y[0, -1] - target_value

            def find_energy(self, initial_conditions, guess_range=(0, 10)):
                """
                Finds the energy parameter K that results in the wave function

✓               Parameters:
                initial_conditions (list): Initial conditions [psi(0), psi'(0)
                guess_range (tuple): Range of K values to search for the root.

                Returns:
                float: Energy parameter K that satisfies the boundary conditio
                """
                a, b = guess_range
                fa = self.shoot(a, initial_conditions)
✓               fb = self.shoot(b, initial_conditions)
                if fa * fb > 0:
                    raise ValueError("The shoot function has the same sign at
                                    "Adjust the guess_range to bracket a root.
                K_solution = brentq(self.shoot, a, b, args=(initial_conditions
                return K_solution

            def solve_wave_function(self, K, initial_conditions):
                """
                Solves the wave function for a given energy parameter K.

                Parameters:
                K (float): Energy parameter.
                initial_conditions (list): Initial conditions [psi(0), psi'(0)

                Returns:
                tuple: Arrays of wave function values and xi values.
                """
                sol = solve_ivp(self.slope_function, [0, self.xi_max], initia
                    args=(K,),
                    max_step=self.xi_max/self.num_points
                )
                return sol.y, sol.t

            def plot_wave_function_convergence(self, K_values, initial_condit
                """
                Plots the convergence of the wave function for different K va

                Parameters:
                K_values (list): List of K values to plot.
                initial_conditions (list): Initial conditions [psi(0), psi'(0)
                title (str, optional): Title of the plot.
                """
                plt.figure(figsize=(10, 6))
                for K in K_values:
                    psi, xi = self.solve_wave_function(K, initial_conditions)
                    plt.plot(xi, psi[0], label=f'K = {K:.4f}')
                plt.title(title or 'Wave Function Convergence')
                plt.xlabel(r'$\xi$')
                plt.ylabel(r'$\psi(\xi)$')
                plt.xlim(9.4, 10)
                plt.legend()
                plt.grid(True)
                plt.show()

            def plot_energy_ladder(self, energies, wave_functions):
                """
                Plots the energy ladder of the quantum harmonic oscillator.

                Parameters:
                energies (list): List of energy values.
                wave_functions (list): List of wave function arrays.
                """
                plt.figure(figsize=(12, 8))
                xi = np.linspace(0, 5, 200)
                potential = 0.5 * xi**2
                plt.plot(xi, potential, 'k--', label='Harmonic Potential')
                colors = ['r', 'g', 'b', 'purple', 'orange']
                for i, (E, (psi, xi_vals)) in enumerate(zip(energies, wave_fun
                    if psi is None:
                        continue
                    scaled_psi = 0.5 * psi[0] / np.max(np.abs(psi[0]))
                    plt.plot(xi_vals, scaled_psi + E, color=colors[i % len(co
                             label=f'E{i} = {E:.4f}')
                    plt.axhline(y=E, color=colors[i % len(colors)], linestyle=
                plt.title('Quantum Harmonic Oscillator Energy Ladder')
                plt.xlabel(r'$\xi$')
                plt.ylabel('Energy')
                plt.legend()
                plt.grid(True)
                plt.show()
```

In [ ]:
```
solver = QuantumHarmonicOscillatorSolver()

# Ground state energy
ground_energy = solver.find_energy([1, 0], (0, 2))
print(f"Ground state energy: {ground_energy:.6f}")
```

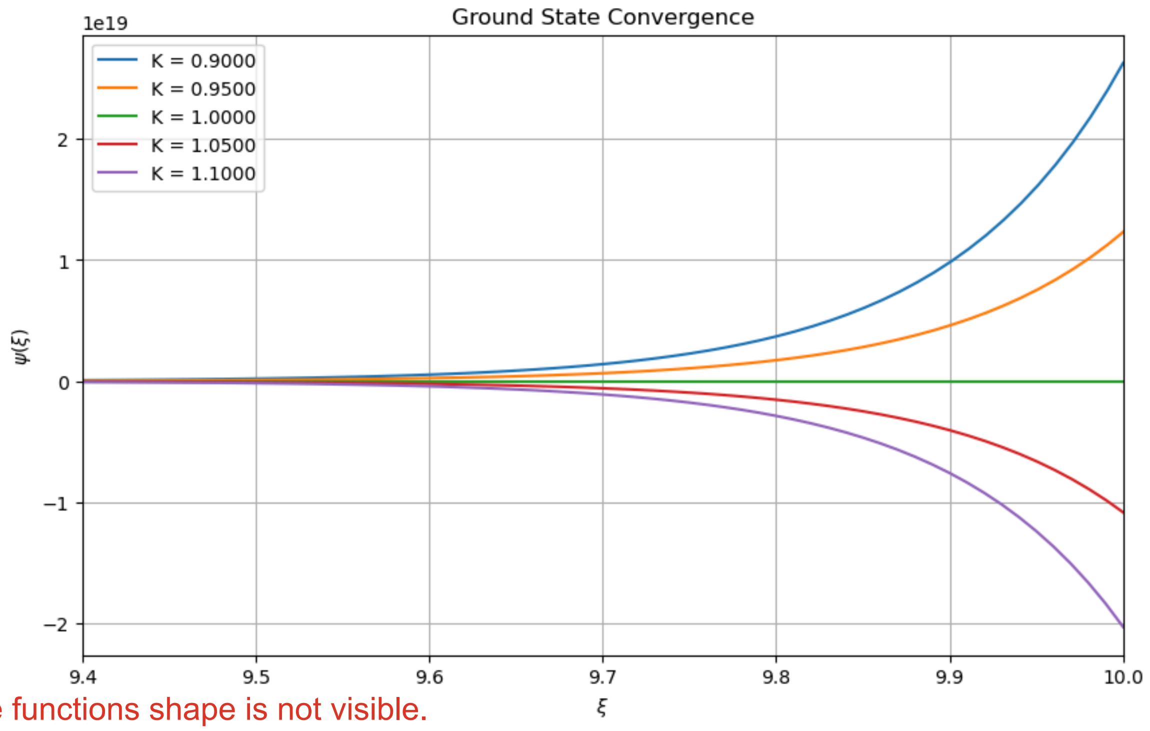
✓

```
Ground state energy: 1.000000
```

✓

In [23]:
```
# Ground state convergence plot
solver.plot_wave_function_convergence(np.linspace(ground_energy - 0.1,
                                       title='Ground State Convergence'
```

✓



The wave functions shape is not visible.

In [ ]:
```
# First four excited states
excited_energies = []
conditions = [[0, 1], [1, 0], [0, 1], [1, 0]]
for cond in conditions:
    energy = solver.find_energy(cond, (0, 20))
    excited_energies.append(energy)
    print(f"Excited state energy: {energy:.6f}")
```

-1

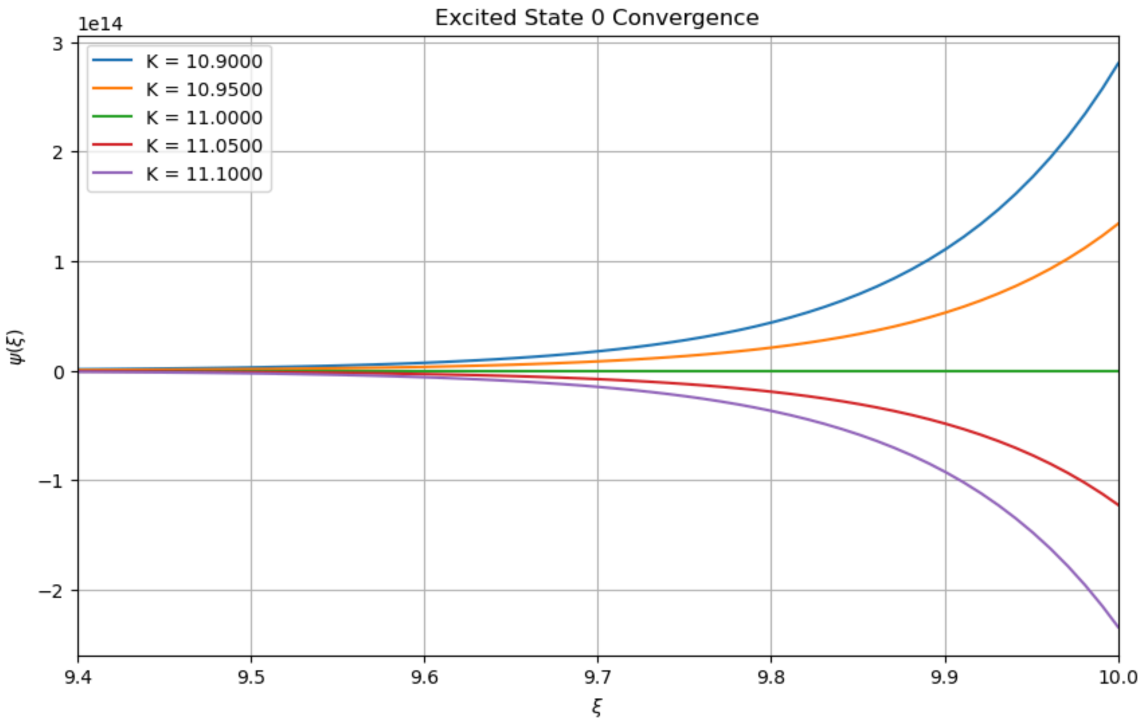
✗

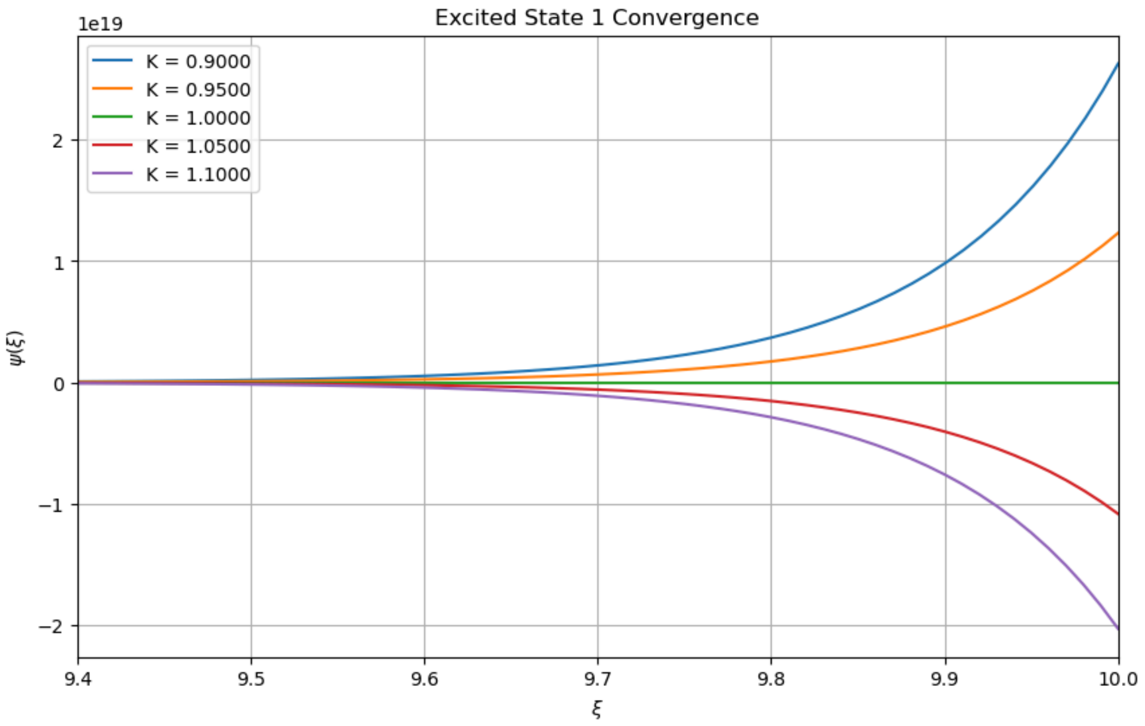
```
Excited state energy: 11.000000
Excited state energy: 1.000000
Excited state energy: 11.000000
Excited state energy: 1.000000
```

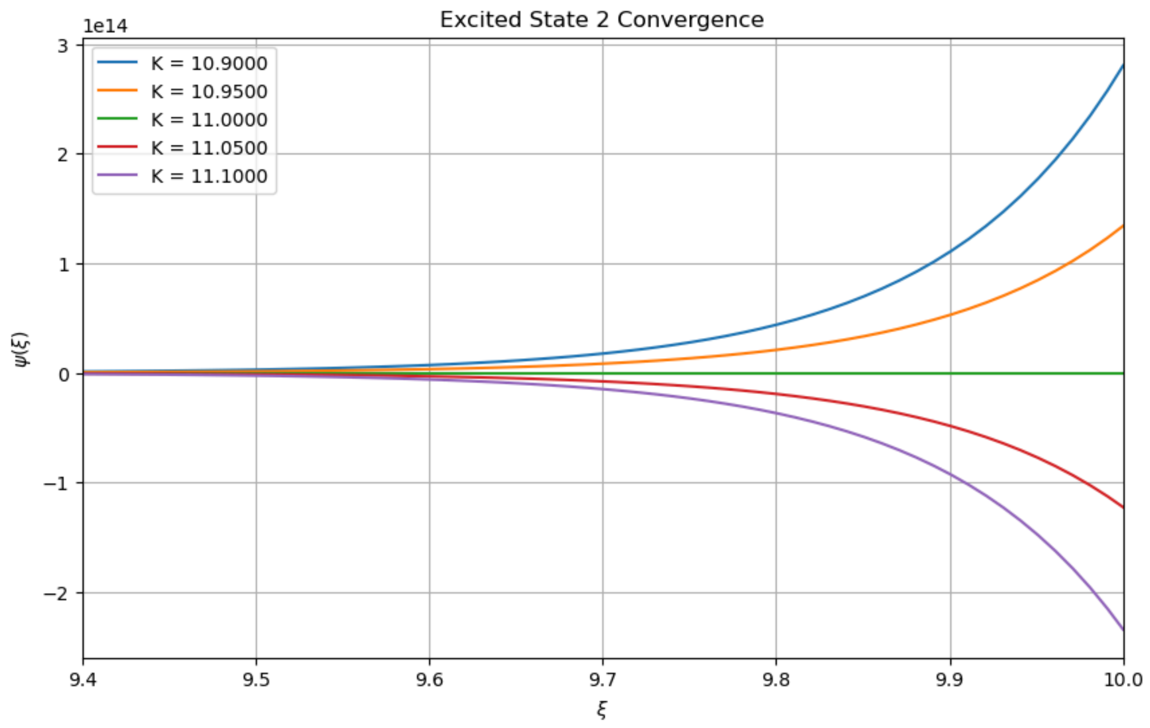
This are not physical results, because of the uneven space between solutions, but I couldnt get to know where the error was :c

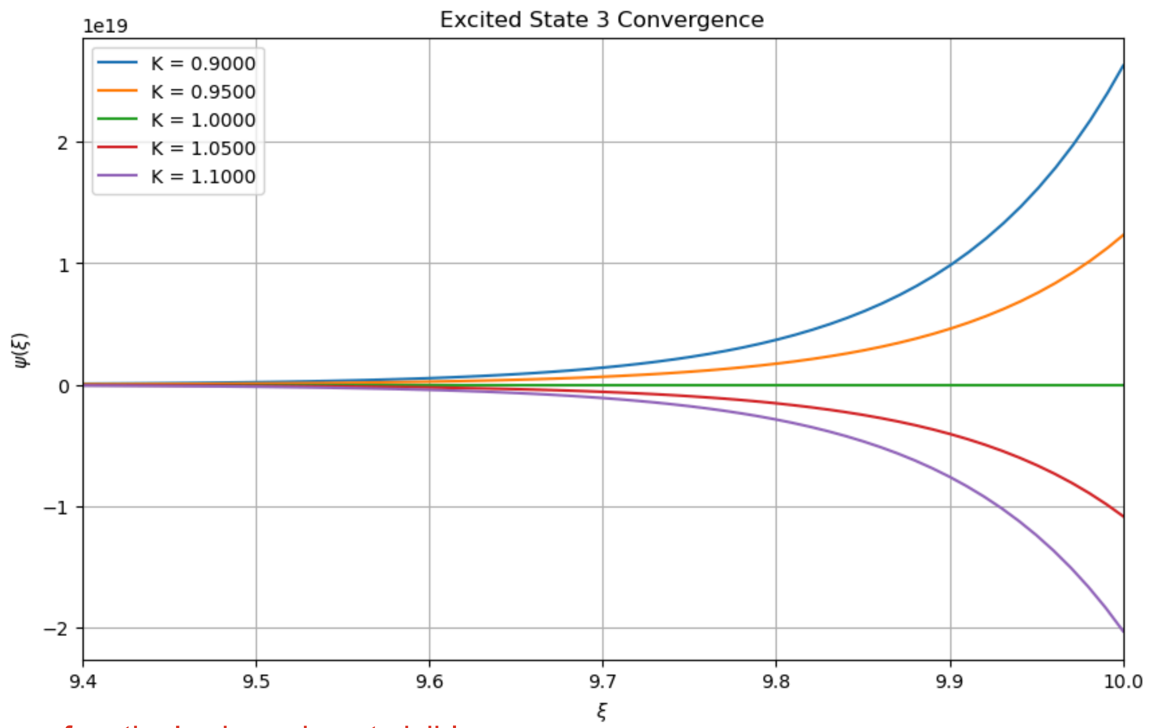
The problem is likely at the setting of the initial conditions.

```
In [29]: # Excited state convergence plots
         for i, cond in enumerate(conditions):
             solver.plot_wave_function_convergence(np.linspace(excited_energies
                                                   cond, title=f'Excited State 
```







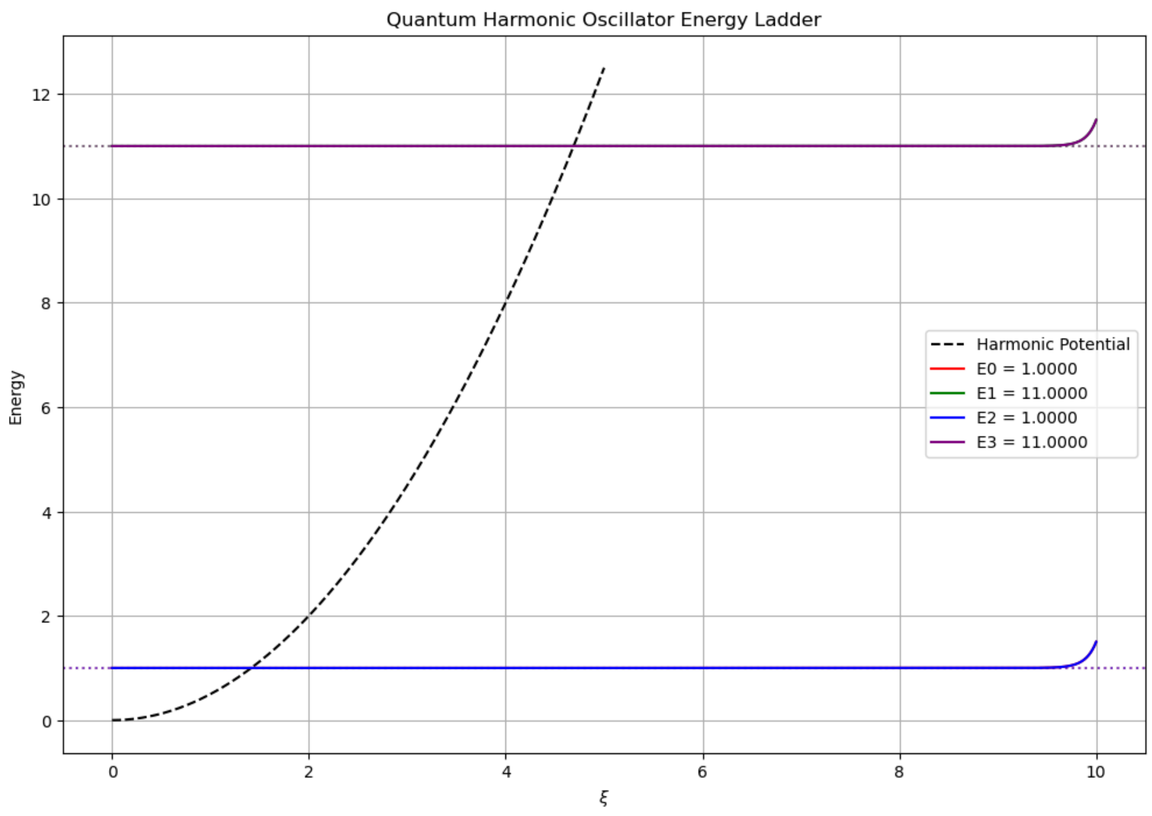


-1

The wave function's shape is not visible.

In [30]:
```
# Energy ladder plot
wave_functions = [solver.solve_wave_function(energy, conditions[i]) fo
solver.plot_energy_ladder([ground_energy] + excited_energies, wave_fu
```

×



×

-1

The discrepancies suggest numerical errors in the computational approach, possibly due to:

- Insufficient numerical precision
- Inappropriate boundary conditions
- Improper step size or integration method
- Convergence issues in the shooting method algorithm

To obtain physically meaningful results, lookinf forward, I should:

- Proper implementation of boundary conditions
- Appropriate numerical integration techniques
- Careful handling of the differential equation's singularities
- Verification against known analytical solutions