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The time required to reach a particular conversion X in a reactor is given by this integral equation:

$$t = \int_0^X \frac{1}{kC_{A0}(1-X)^2} dX$$

 $t=\int_0^X \frac{1}{kC_{A0}(1-X)^2} dX$ In this problem, k=1e-3 L/mol/min, and $C_{A0}=1$ mol/L.

We aim to find the uncertainty in the amount of time required to reach a conversion of 0.9. The uncertainty is estimated by:

$$\sigma_t = \sqrt{\frac{\partial t}{\partial k}^2 \sigma_k^2 + \frac{\partial t}{\partial C_{A0}}^2 \sigma_{C_{A0}}^2}$$
with $\sigma_k = 1e - 4$ and $\sigma_{C_{A0}} = 0.01$.

To evaluate those derivatives, we need a differentiable integrator. You can use this implementation of the trapezoid rule for that. You cannot use the quad function.

```
import autograd.numpy as np
def trapz(y, x):
    d = np.diff(x)
    return np.sum((y[0:-1] + y[1:]) * d / 2)
```

First, use the equation above and the provided trapz function to find the time required to reach 90% conversion for this reactor.

Next, use the formula for σ_t to estimate the uncertainty in this time.

solution 1.1 solution

```
import autograd.numpy as np
1
2
    k = 1e-3
    sigma_k = 1e-4
    Ca0 = 1.0
6
    sigma_Ca0 = 0.01
    X = np.linspace(0.0, 0.9, 5000)
10
11
    def trapz(y, x):
        d = np.diff(x)
12
        return np.sum((y[0:-1] + y[1:]) * d / 2)
13
14
    def t(k, Ca0):
15
16
         integrand = 1./(k*Ca0)*(1./(1-X)**2)
17
         return trapz(integrand, X)
18
    print(t(k, Ca0))
```

9000.00539675

```
dtdk = grad(t, 0)
dtdC = grad(t, 1)
```

```
3
4 sigma_t = np.sqrt(dtdk(k, Ca0)**2 * sigma_k**2 + dtdC(k, Ca0)**2 * sigma_Ca0**2)
5 sigma_t
```

904.48881132260317

2 ASSIGNED exam3-2 eigenvalue LA:p2:3:mingjie

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We have mostly focused on numerical solutions to ODEs. Sometimes, it is possible to leverage Python to obtain analytical solutions though. This problem will focus on a way to do that. We will focus on these equations:

$$y_1'(t) = -0.02y_1 + 0.02y_2$$

$$y_2'(t) = 0.02y_1 - 0.02y_2$$

with the initial conditions that $y_1(0) = 0$ and $y_2(0) = 150$.

We can rewrite the equations in matrix form:

$$\mathbf{v}' = \mathbf{A}\mathbf{v}$$

Here we have
$$\mathbf{y}' = \begin{bmatrix} y_1'(t) \\ y_2'(t) \end{bmatrix}$$
 and $\mathbf{y} = \begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix}$. **A** is the array of coefficients.

This is a set of constant coefficient, coupled ODEs. We can try a solution of the form:

 $\mathbf{y} = \mathbf{x}e^{\lambda t}$, where we have an unknown vector \mathbf{x} and λ , and we seek to find values for these that solve the equations.

If you plug this in to the equations then we find:

$$\mathbf{v}' = \lambda \mathbf{x} e^{\lambda t} = \mathbf{A} \mathbf{x} e^{\lambda t}$$

Or, with some minor rearrangement:

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

This is an eigenvalue problem, and the solutions to it are the pairs of eigenvalues (λ) and corresponding eigenvectors (\mathbf{x}).

Find the eigenvalues and eigenvectors of this system of equations:

The solution to the system of ODEs is then a linear combination defined by:

$$\mathbf{y}(\mathbf{t}) = c_1 \mathbf{x_1} e^{\lambda_1 t} + c_2 \mathbf{x_2} e^{\lambda_2 t}$$

where c_i are arbitrary constants, and $\mathbf{x_i}$ is the ith eigenvector that corresponds to the ith eigenvalue λ_i . To find the values of c_i we must use the initial conditions. At t = 0 we can express this in the form:

$$\begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} \mathbf{x_1} & \mathbf{x_2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$
 (1)

where $[\begin{array}{ccc} \mathbf{x_1} & \mathbf{x_2} \end{array}]$ is an array with $\mathbf{x_i}$ in the ith column, in other words it is an array of the eigenvectors in column form.

Solve this linear equation for the unknown coefficients c.

Finally, combine all of this information to get the complete solution

 $\mathbf{y}(\mathbf{t}) = c_1 \mathbf{x_1} e^{\lambda_1 t} + c_2 \mathbf{x_2} e^{\lambda_2 t}$. There is not a simple matrix algebra way to do this, so I suggest you do it as:

```
y1(t) = c_1 \mathbf{x_1}[0] e^{\lambda_1 t} + c_2 \mathbf{x_2}[0] e^{\lambda_2 t}
and
y2(t) = c_1 \mathbf{x_1}[1] e^{\lambda_1 t} + c_2 \mathbf{x_2}[1] e^{\lambda_2 t}
and plot the solution for y_1(t) and y_2(t) from t=0 to t=100.
```

2.1 solution solution

[0. -0.04] [0.70710678 -0.70710678] [0.70710678 0.70710678]

```
c = np.linalg.solve(evecs, [0, 150])
c
```

array([106.06601718, 106.06601718])

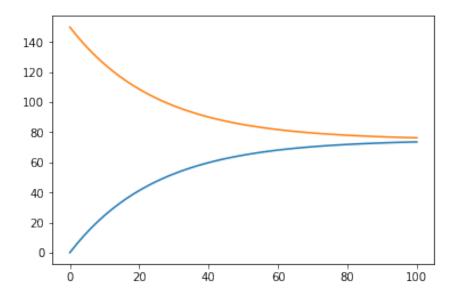
```
t = np.linspace(0, 100)

x1 = evecs[:, 0]
x2 = evecs[:, 1]

y1 = c[0] * x1[0] * np.exp(evals[0] * t) + c[1] * x2[0] * np.exp(evals[1] * t)
y2 = c[1] * x1[1] * np.exp(evals[0] * t) + c[1] * x2[1] * np.exp(evals[1] * t)

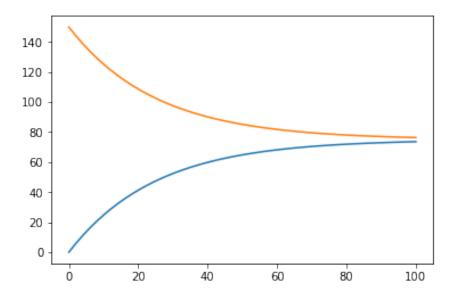
plt.plot(t, y1, t, y2)
```

[<matplotlib.lines.Line2D at 0x1193c9d68>, <matplotlib.lines.Line2D at 0x118c65668>]



Here is the numpy way of writing this solution. It is more advanced syntax than we have used in class and involves combinations of matrix algebra, elementwise operations and broadcasting.

[<matplotlib.lines.Line2D at 0x11a168d30>, <matplotlib.lines.Line2D at 0x11a168f28>]



ASSIGNED exam3-3 nla - continuation 3 autograd:ode:p3:3:john

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A common problem in solving nonlinear problems is how to make the initial quess?

Let's consider finding the solution to the following nonlinear equations:

$$2 + x + y - x^{2} + 8xy + y^{3} = 0$$
$$1 + 2x - 3y + x^{2} + xy - ye^{x} = 0$$

$$1 + 2x - 3y + x^2 + xy - ye^x = 0$$

The strategy we work on here is to reformulate these equations with a new variable λ

$$2 + x + y + \lambda(-x^2 + 8xy + y^3) = 0$$

$$1 + 2x - 3y + \lambda(x^2 + xy - ye^x) = 0$$

Part 1 solve the linear problem

If $\lambda = 1$ then we have the original nonlinear equations. If you set $\lambda = 0$ though, you have a simple linear set of equations to solve. Find a solution to those equations for $\lambda = 0$:

This solution represents the solution to the equations when $\lambda = 0$. If we could derive a set of equations for $\frac{dx}{d\lambda}$ and $\frac{dy}{d\lambda}$, then we can treat this linear solution as an initial value, and integrate the ODEs from $\lambda = 0$ to $\lambda = 1$ to find the solution to the nonlinear equations. In what follows, we motivate how to derive those equations.

Part 2 formulate a system of ODEs to solve the nonlinear 3.0.2problem

Next, we consider the equations as

$$f(x,y) = 2 + x + y + \lambda(-x^2 + 8xy + y^3) = 0$$

$$g(x,y) = 1 + 2x - 3y + \lambda(x^2 + xy - ye^x) = 0$$

from calculus, you can show that:

$$\frac{\partial f}{\partial x} \frac{\partial x}{\partial \lambda} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \lambda} = -\frac{\partial f}{\partial \lambda}$$

$$\frac{\partial f}{\partial x}\frac{\partial x}{\partial \lambda} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \lambda} = -\frac{\partial f}{\partial \lambda}$$
$$\frac{\partial g}{\partial x}\frac{\partial x}{\partial \lambda} + \frac{\partial g}{\partial y}\frac{\partial y}{\partial \lambda} = -\frac{\partial g}{\partial \lambda}$$

You can rewrite this in a linear algebra form as:

$$\begin{bmatrix} \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} \frac{\partial g}{\partial y} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial \lambda} \\ \frac{\partial y}{\partial \lambda} \end{bmatrix} = \begin{bmatrix} -\frac{\partial f}{\partial \lambda} \\ -\frac{\partial g}{\partial \lambda} \end{bmatrix}$$
 (2)

The matrix on the left is the Jacobian of F = [f(x, y), g(x, y)].means you can solve for:

$$\begin{bmatrix} \frac{\partial x}{\partial \lambda} \\ \frac{\partial y}{\partial \lambda} \end{bmatrix} = \mathbf{J}^{-1} \begin{bmatrix} -\frac{\partial f}{\partial \lambda} \\ -\frac{\partial g}{\partial \lambda} \end{bmatrix}$$

This last equation defines a set of differential equations that can be integrated from $\lambda = 0$ where we know what (x, y) are, to $\lambda = 1$ which leads to a solution to the original set of nonlinear equations!

Use the last equation to define a function for a system of ODEs, and then integrate the system of ODES from $\lambda = 0$ to $\lambda = 1$ to find the solution to the nonlinear set of equations. The solution is the value of x, y at $\lambda = 1$.

Part 3 Verify the solution you found

Use a method of your choice to verify your solution from Part 2.

3.1 solution solution

```
import autograd.numpy as np
    from autograd import jacobian
    def F(X, L):
4
5
        x, y = X
        f = (2.0 + x + y) + L * (-x**2 + 8 * x * y + y**3)
6
        g = (1.0 + 2.0 * x - 3.0 * y) + L * (x**2 + x * y - y * np.exp(x))
7
        return np.array([f, g])
9
10
    J = jacobian(F)
    J(np.array([-1.4, -0.6]), 0.0)
11
12
13
    dFdL = jacobian(F, 1)
14
15
    x0 = np.linalg.solve([[1., 1.], [2., -3.]], [-2, -1])
    print(x0)
16
17
    def ode(X, L):
18
19
        x, y = X
        j = J(np.array([x, y]), L)
20
        dXdL = np.linalg.inv(j) @ -dFdL(np.array([x, y]), L)
21
22
        return dXdL
23
    from scipy.integrate import odeint
24
25
    lambda_span = np.linspace(0, 1, 1000)
26
27
    X = odeint(ode, x0, lambda_span)
28
29
    xsol, ysol = X[-1]
30
    print('The solution is at x={0:1.3f}, y={1:1.3f}'.format(xsol, ysol))
31
    print(F([xsol, ysol], 1))
        [-1.4 - 0.6] The solution is at x=-1.000, y=0.000 [-1.27841341e-06-1.15929141e-
    06
   from scipy.optimize import fsolve
    fsolve(F, [-1, -0.5], args=(1,))
```

4 ASSIGNED exam3-4 optimization optimization:nori:p2:2

5.09005275e-13])

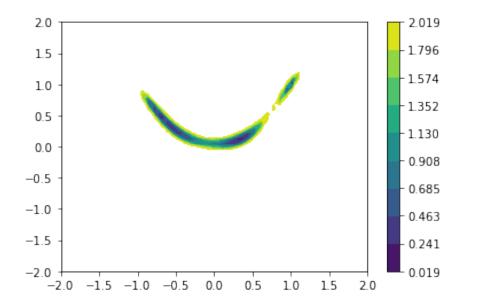
array([-1.0000000e+00,

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The modified Rosenbrock equation:

 $f(x_1,x_2) = 100(x_2-x_1^2)^2 + (6.4(x_2-0.5)^2-x_1-0.6)^2$ has three minima in the range of $-2 < x_1 < 2$ and $-2 < x_2 < 2$. Find these minima and their values. Identify the global minimum.

4.1 solution solution



```
from scipy.optimize import minimize minimize(f, [0.5, 0.5])
```

1

```
fun: 6.140164573341661e-14
  hess_inv: array([[ 0.03267297,  0.01663245],
         [ 0.01663245, 0.01245351]])
       jac: array([ -7.22192585e-07,
                                        9.16138832e-07])
   message: 'Optimization terminated successfully.'
      nfev: 52
       nit: 7
      njev: 13
    status: 0
   success: True
         x: array([ 0.34130744, 0.11649078])
minimize(f, [-0.5, 0.5])
       fun: 0.007415391415502931
  hess_inv: array([[ 0.27910892, -0.36648959],
        [-0.36648959, 0.48612737]])
        jac: array([ -1.37253664e-07, -9.56933945e-08])
   message: 'Optimization terminated successfully.'
      nfev: 68
       nit: 12
      njev: 17
    status: 0
   success: True
         x: array([-0.66369999, 0.44114456])
1 minimize(f, [1, 1])
       fun: 1.2325951644078309e-32
  hess_inv: array([[1, 0],
        [0, 1]])
       jac: array([ 5.97536573e-06,
                                        2.10046770e-06])
   message: 'Optimization terminated successfully.'
      nfev: 4
       nit: 0
      njev: 1
    status: 0
   success: True
         x: array([ 1., 1.])
```

5 ASSIGNED exam3-5 BVP by ODEbvp:ode:john:p3:3

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In this problem we learn a new way to solve a *linear* boundary value problem. The problem of interest is:

$$y'''(x) - x^2y = -x^4$$
 with $y(0) = 0, y'(0) = 0, y(2) = 4$.

This will take some steps, so read the following carefully. Some of these steps will be worked out, and others you will be asked to complete or verify. You do not need to derive these, they are here to guide what you will do.

First, we recall that the general solution of a linear ODE can be written as a linear combination of solutions to the homogeneous equation (where the right hand side is zero) and a particular solution to the non-homogeneous equation (where the right hand side is $-x^4$).

Here are the homogeneous versions and the particular version of the equation above, expressed in *initial value form*. The initial conditions are chosen here to provide three linearly independent functions Y_1, Y_2 , and Y_3 . For Y_p any values can be used since any particular solution will do.

$$Y_1''' - x^2 Y_1 = 0 \text{ with } Y_1(0) = 1, Y_1'(0) = 0, Y_1''(0) = 0$$

$$Y_2''' - x^2 Y_2 = 0 \text{ with } Y_2(0) = 0, Y_2'(0) = 1, Y_2''(0) = 0$$

$$Y_3''' - x^2 Y_3 = 0 \text{ with } Y_3(0) = 0, Y_3'(0) = 0, Y_3''(0) = 1$$

$$Y_p''' - x^2 Y_p = -x^4 \text{ with } Y_p(0) = 0, Y_p'(0) = 0, Y_p''(0) = 0$$

These can be combined to form the general solution to the differential equation.

$$y(x) = C_1 Y_1(x) + C_2 Y_2(x) + C_3 Y_3(x) + Y_p(x)$$

To get towards a solution to the original BVP, we next apply the boundary conditions to find the constants C_i .

$$y(0) = 0 = C_1 + 0 + 0 + 0$$

$$y'(0) = 0 = 0 + C_2 + 0 + 0$$

$$y''(0) = 4 = C_1Y_1(2) + C_2Y_2(2) + C_3Y_3(2) + Y_p(2)$$
 Combined, these lead to:

 $y(x) = \frac{4-Y_p(2)}{Y_3(2)}Y_3(x) + Y_p(x)$ where $Y_p(2)$ means the function Y_p evaluated at x=2 and $Y_3(2)$ means the function Y_3 evaluated at x=2.

That is remarkably the solution to the boundary value problem originally stated, and we can now get Y_3 and Y_p by integrating two ordinary initial

value differential equations!

5.1 Solve for Y_3 and Y_p

Find solutions to these two initial value ODEs over the range of x = 0 to x = 2:

$$Y_3''' - x^2 Y_3 = 0$$
 with $Y_3(0) = 0, Y_3'(0) = 0, Y_3''(0) = 1$
 $Y_p''' - x^2 Y_p = -x^4$ with $Y_p(0) = 0, Y_p'(0) = 0, Y_p''(0) = 0$

5.2 Combine them to get a solution to the BVP

Use your solutions to create the overall solution. $Y_p(2)$ means evaluate $Y_p(x)$ at x = 2. You can do this anyway you want.

$$y(x) = \frac{4 - Y_p(2)}{Y_3(2)} Y_3(x) + Y_p(x)$$

Make a plot of $y(x)$.

7.22888663e-05,

5.3 solution solution

```
xspan = np.linspace(0, 2, 500)
3
    def y3prime(x, Y):
         y3, u3, v3 = Y
4
        y3prime = u3
5
         u3prime=v3
         v3prime = x**2 * y3
7
         return y3prime, u3prime, v3prime
8
9
    from scipy.integrate import solve_ivp
10
11
    y3 = solve_ivp(y3prime, (0, 2), [0, 0, 1], max_step=0.1, dense_output=True)
12
13
    def ypprime(x, Y):
         yp, up, vp = Y
14
         ypprime = up
15
16
         upprime = vp
         \mathtt{vpprime} \ = \ \mathtt{x} * * 2 \ * \ \mathtt{yp} \ - \ \mathtt{x} * * 4
17
18
         return [ypprime, upprime, vpprime]
19
    yp = solve_ivp(ypprime, (0, 2), [0, 0, 0], max_step=0.1, dense_output=True)
20
1
    Y3 = y3.sol(xspan)[0]
    Yp = yp.sol(xspan)[0]
    array([ 0.0000000e+00,
                                            8.03209626e-06,
                                                                      3.21283850e-05,
```

1.28513540e-04,

2.00802406e-04,

```
2.89155464e-04,
                   3.93572714e-04,
                                      5.14054155e-04,
6.50599789e-04,
                  8.03209614e-04,
                                      9.71883631e-04,
1.15662184e-03,
                   1.35742424e-03,
                                      1.57429084e-03,
1.80722163e-03,
                  2.05621661e-03,
                                      2.32127579e-03,
2.60239917e-03,
                  2.89958674e-03,
                                      3.21283851e-03,
3.54215449e-03,
                   3.88753466e-03,
                                      4.24897904e-03,
4.62648762e-03,
                   5.02006041e-03,
                                      5.42969740e-03,
5.85539860e-03,
                  6.29716402e-03,
                                      6.75499366e-03,
7.22888754e-03,
                   7.71884565e-03,
                                      8.22486799e-03,
8.74695458e-03,
                  9.28510542e-03,
                                      9.83932052e-03,
1.04095999e-02,
                   1.09959435e-02,
                                      1.15983515e-02,
1.22168238e-02,
                   1.28513604e-02,
                                      1.35019614e-02,
1.41686268e-02,
                   1.48513566e-02,
                                      1.55501508e-02,
1.62650095e-02,
                   1.69959328e-02,
                                      1.77429205e-02,
1.85059729e-02,
                   1.92850899e-02,
                                      2.00802715e-02,
2.08915179e-02,
                   2.17188290e-02,
                                      2.25622049e-02,
2.34216457e-02,
                  2.42971515e-02,
                                      2.51887224e-02,
2.60963583e-02,
                   2.70200594e-02,
                                      2.79598258e-02,
2.89156575e-02,
                  2.98875547e-02,
                                      3.08755175e-02,
3.18795460e-02,
                   3.28996403e-02,
                                      3.39358005e-02,
3.49880269e-02,
                   3.60563196e-02,
                                      3.71406788e-02,
3.82411045e-02,
                  3.93575971e-02,
                                      4.04901567e-02,
4.16387835e-02,
                   4.28034778e-02,
                                      4.39842397e-02,
4.51810695e-02,
                  4.63939674e-02,
                                      4.76229337e-02,
4.88679686e-02,
                   5.01290726e-02,
                                      5.14062459e-02,
5.26994889e-02,
                   5.40088019e-02,
                                      5.53341852e-02,
5.66756391e-02,
                   5.80331642e-02,
                                      5.94067608e-02,
6.07964294e-02,
                   6.22021704e-02,
                                      6.36239844e-02,
6.50618718e-02,
                  6.65158332e-02,
                                      6.79858692e-02,
6.94719804e-02,
                   7.09741674e-02,
                                      7.24924308e-02,
7.40267713e-02,
                  7.55771896e-02,
                                      7.71436864e-02,
7.87262624e-02,
                  8.03249185e-02,
                                      8.19396553e-02,
8.35704738e-02,
                  8.52173748e-02,
                                      8.68803593e-02,
8.85594282e-02,
                  9.02545826e-02,
                                      9.19658234e-02,
9.36931516e-02,
                  9.54365684e-02,
                                      9.71960749e-02,
9.89716723e-02,
                   1.00763362e-01,
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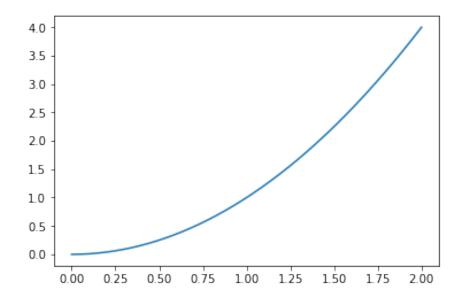
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```

%matplotlib inline

2 import matplotlib.pyplot as plt

plt.plot(xspan, Y)

[<matplotlib.lines.Line2D at 0x1172067f0>]



Here we show the Bcs are satisfied.

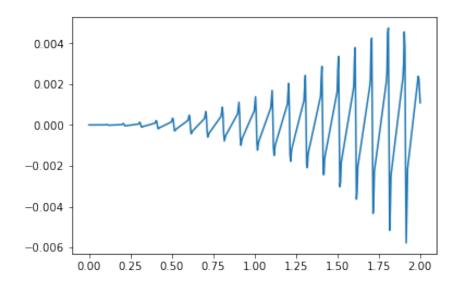
```
1     YP = np.gradient(Y, xspan, edge_order=2)
2     Y[0], YP[0], Y[-1]
```


This is kind of noisy, but small.

```
gf = lambda x: (4 - yp.sol(2)[0]) / y3.sol(2)[0] * y3.sol(x)[0] + yp.sol(x)[0]

from scipy.misc import derivative
    _yp = np.gradient(yf(xspan), xspan, edge_order=2)
    _ypp = np.gradient(_yp, xspan, edge_order=2)
    _yppp = np.gradient(_ypp, xspan, edge_order=2)
    #yppp = [derivative(yf, x, n=3, order=7, dx=1e-6) for x in xspan]
    plt.plot(xspan, _yppp - xspan**2 * yf(xspan) + xspan**4)
```

[<matplotlib.lines.Line2D at 0x117f619b0>]



6 ASSIGNED exam3-6quad:integration:mingjie:p1:2

This is an exam. You must be present in the exam room to get credit for this problem unless you have prior permission from the instructor. You may not talk during the exam except to ask an instructor a question. By turning this in, you agree that this work is your own, and you did not get unauthorized help to complete it or provide unauthorized help to anyone else. You may not modify your exam answer after the due time without permission.

The Γ function is defined by:

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt$$

It is a generalized factorial function. When the arguments to the function are integers, the following relation is true:

$$\Gamma(n+1) = n!$$

Show that this is true for the integers from 1 to 10. You can use the math.factorial function.

```
from math import factorial
factorial(4)
```

24

6.1 solution

solution

```
from math import factorial
    from scipy.integrate import quad
    import numpy as np
    def integrand(t, x):
        return np.exp(-t) * t**(x - 1)
6
8
    def Gamma(x):
        I, err = quad(integrand, 0, np.inf, args=(x, ))
9
10
        return I
11
   for i in range(1, 11):
        print(i, Gamma(i), factorial(i - 1))
13
```

 $1\ 1.00000000000000002\ 1\ 2\ 0.999999999999999\ 1\ 3\ 2.0\ 2\ 4\ 6.0\ 6\ 5\ 24.0\ 24$ $6\ 120.0000000000001\ 120\ 7\ 720.000000000001\ 720\ 8\ 5040.000000000000$ $5040\ 9\ 40320.0\ 40320\ 10\ 362879.999999999$ 362880