Coding Exercise - Mohamadhossein Faramarzi - Dec, 6th

First we explain our approach to solve the problem. The reference of our solution is the paper "Deconvolution of Serum Cortisol Levels by Using Compressed Sensing" written by Dr. Rose Faghih in 2014. We explain our step by step approach to deconvolve the cortisol concentration of blood (sampled from serum) based on the u(t) signal which is an abstraction of the hormone pulses that result in cortisol secretion. Based on this problem we want to optimize values of θ_1 and θ_2 which based on the paper represent the infusion rate of cortisol from the adrenal glands into the blood and the clearance rate of cortisol by the liver.

1) First we use the model based on a stochastic differential equation (SDE) that describes diurnal cortisol patterns.

$$\frac{dx_1(t)}{dt} = -\theta_1 x_1(t) + u(t) \text{ (Adrenal Glands)}$$

$$\frac{dx_2(t)}{dt} = \theta_1 x_1(t) - \theta_2 x_2(t)$$
 (Serum)

Discretize equation for programming perspective:

$$x_{1}(t + \Delta t) = x_{1}(t) + \Delta t \cdot (\theta_{1}x_{2}(t) + u(t))$$

$$x_{2}(t + \Delta t) = x_{2}(t) + \Delta t \cdot (\theta_{1}x_{2}(t) - \theta_{1}x_{2}(t))$$

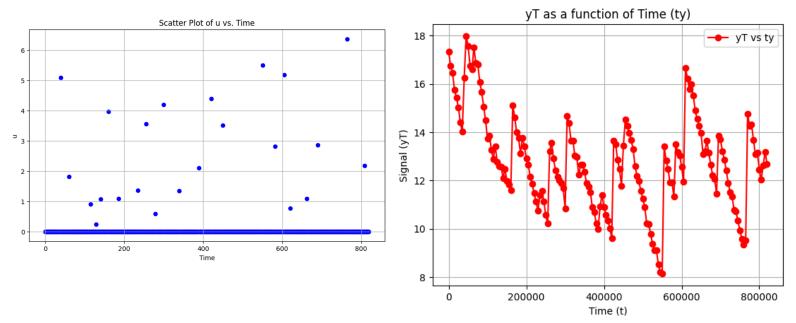
When we have the impulse response y(t) and the input u(t), we should assume that $x_1(t)$ follows the dynamics dictated by the first-order differential equation, starting from an initial condition (typically $x_1(0)=0$), and then we use it for the second equation to find x2. Then based on this we can estimate y but for the best estimation accuracy we need to optimize θ_1 and θ_2 which is our problem for this coding exercise. Then we have to define an objective function which the most simple option is the "L" function which measures the square error between the model's predicted output and the actual observed data.

$$\mathsf{L}(heta_1, heta_2) = \sum_{i=1}^N \left(y_i - \hat{y}_i(heta_1, heta_2)
ight)^2$$

We define an initial guess for the parameters $\theta 1$ and $\theta 2$ and then apply the **L-BFGS-B** algorithm to minimize the objective function. The bounds on the parameters are set to ensure that they remain positive as we assumed both $\theta 1$ and $\theta 2$ be positive.

Then we can pass the calculated $\theta 1$ and $\theta 2$ after optimization to let the differential model estimate the "y" using these parameters.

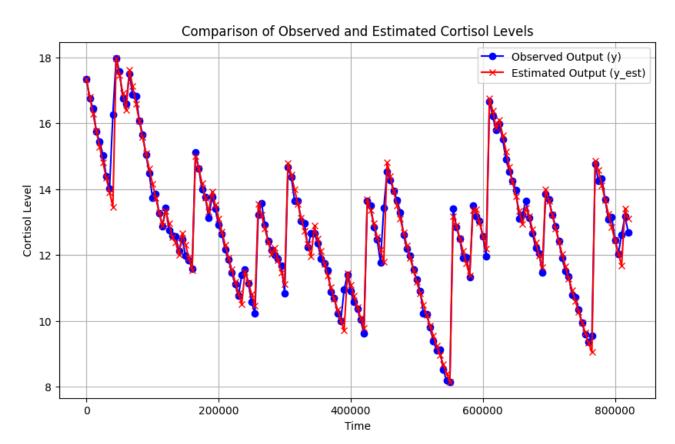
Here are the inputs we have from the data set. We plot them to observe them in a visual way:



Now based on the approach we explained we try to estimate the y by optimizing theta1 and theta2. Here is a table of measured parameters of our model:

The parameter	θ1	θ2	L function final value	R2 of estimation
Value	0.5942	0.0063	18.5143	0.972

And here is the final result - The code with descriptions are attached



Laoding Dataset

```
from google.colab import drive
drive.mount('/content/drive')
→ Mounted at /content/drive
import scipy.io as sio
Data = sio.loadmat(mat_file_path,squeeze_me=True)
print(Data.keys())
u=Data['u']
tu=Data['tu']
y=Data['y']
ty=Data['ty']

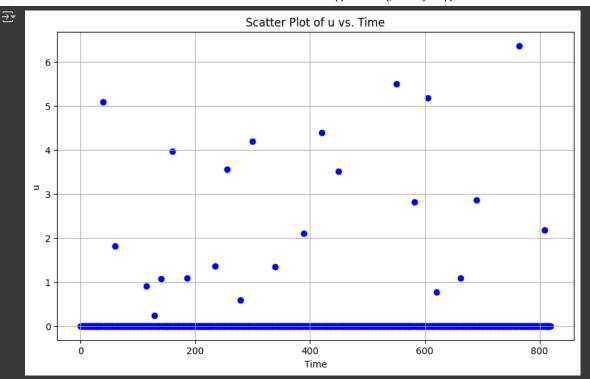
    dict_keys(['__header__', '__version__', '__globals__', 'u', 'tu', 'ty', 'y'])

print(u.shape)
print(tu.shape)
print(y.shape)
print(ty.shape)
   (820,)
    (820,)
   (165,)
   (165,)
```

Plot Inputs

```
import matplotlib.pyplot as plt

uT = u.transpose()
tus=tu/1000;
# scatter plot u
plt.figure(figsize=(10, 6))
plt.scatter(tus, uT, marker='o', color='b', label='u')
plt.xlabel('Time')
plt.ylabel('u')
plt.ylabel('u')
plt.title('Scatter Plot of u vs. Time')
plt.grid(True)
plt.show()
```

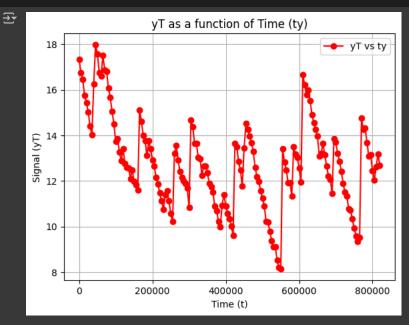


```
ty_s = ty / 1000
yT = y.transpose()
plt.plot(ty, yT, marker='o', linestyle='-', color='r')

plt.xlabel('Time (t)')
plt.ylabel('Signal (yT)')
plt.title('yT as a function of Time (ty)')

plt.grid(True)
plt.legend(['yT vs ty'])

# Display the plot
plt.show()
```



Deconvolution Problem

In this part we have defined a midel baased on the stochastic differential equation model of diurnal cortisol patterns. (Deconvolution of Serum Cortisol Levels by Using Compressed Sensing, 2014, Rose T. Faghih)

```
# Modeling of cortisol concentration of Adrenal Glands (x1) and cortisol concentration of Serum (x2)
import numpy as np
# DIfferential equation (1) - Adrenal Glands
def DEQ1(u, theta1):
    x1 = np.zeros(len(u))
    for t, u_t in enumerate(u):
            x1[t + 1] = x1[t] - theta1 * x1[t] + u_t
    return x1
# DIfferential equation (2) - Serum
def DEQ2(y, x1, theta1, theta2):
 x2=np.zeros(len(x1)) # Changed: Initialize with the same size as x1
 x2[0] = y[0] # Set initial condition
  for t in range(1, len(x1)): # Changed: Updated range to avoid index error
    x2[t] = x2[t - 1] + (theta1 * x1[t - 1]) - (theta2 * x2[t - 1]) # Update x2
  return x2
# Estimation of Observed serum cortisol level based on model output (x2)
def Estimation(x2, ty, tu):
 y_est = np.interp(ty, tu, x2)
 return y_est
```

Then we have to face an optimization problem. Every Optimization problem needs an objective function to do the optimization by minimizing that function. In our problem:

- A) What variables we want to optimize? 01 and 02
- B) What is our objective function? Least square error between Original y and estimated

```
def objective(OptimizedParameters, u, y, tu, ty):
    theta1 = OptimizedParameters[0]
    theta2 = OptimizedParameters[1]
    x1 = DEQ1(u, theta1)
    X2 = DEQ2(y, x1, theta1, theta2)
    y_est = Estimation(X2, ty, tu)
    return np.sum(np.power(y - y_est, 2))

# Initial values for Theta1 and Theta2
initial_guess = [0.1, 0.05]
# Using L-BFGS-B Minimizing method
result = minimize(objective, initial_guess, args=(u, y, tu, ty), method='L-BFGS-B', bounds=[(1e-6, None)])

theta1_est, theta2_est = result.x
objective((theta1_est, theta2_est), u, y, tu, ty)

18.51430247414958
```

Based on the optimization process the final value of theta1 is 0.5943 and final value of theta2 is 0.0063

```
from scipy.optimize import minimize

# Example using L-BFGS-B with bounds
result = minimize(objective, initial_guess, args=(u, y, tu, ty), method='L-BFGS-B', bounds=[(1e-6, None), (1e-6, None)])

theta1_est, theta2_est = result.x
print(f'Estimated theta1: {theta1_est:.4f}')
print(f'Estimated theta2: {theta2_est:.4f}')
```

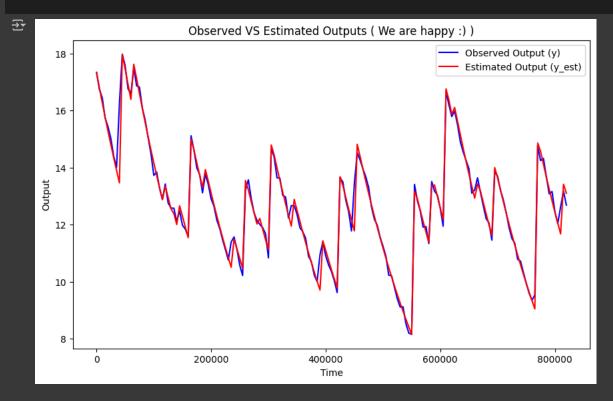
```
Estimated theta1: 0.5943
Estimated theta2: 0.0063
```

Now we want to see what we have done! We pass the optimized parameters thata1 and theta2 to the differential models we defined before. Then we can find an estimated y that shows how well we have done the estimation

```
X1Final= DEQ1(u, theta1_est)
X2Final = DEQ2(y, X1Final, theta1_est, theta2_est)
y_est = Estimation(X2Final, ty, tu)
```

Comparing original y with estimated y which shows good estimation. Nice!

```
plt.figure(figsize=(10, 6))
plt.plot(ty, y, label='Observed Output (y)', color='b')
plt.plot(ty, y_est, label='Estimated Output (y_est)', color='r')
plt.xlabel('Time')
plt.ylabel('Output')
plt.title('Observed VS Estimated Outputs ( We are happy :) )')
plt.legend()
plt.show()
```



And here is the R2 values

```
from sklearn.metrics import r2_score

# Calculate R-squared
r2 = r2_score(y, y_est)
print(f'R-squared: {r2}')
```

Least square Optmiziation method

₹ R-squared: 0.9719941149367466

We Solved the problem with another optimization approach, which did not show a considerable difference. Both results and parameter values are similar to those before.

```
import numpy as np
```

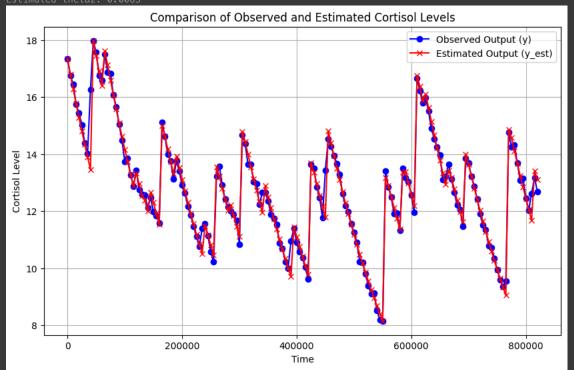
```
from scipy optimize import least_squares
import matplotlib.pyplot as plt
def DEQ1(u, theta1):
    x1 = np.zeros(len(u))
    for t, u_t in enumerate(u):
           x1[t + 1] = x1[t] - theta1 * x1[t] + u_t
    return x1
def DEQ2(y, x1, theta1, theta2):
  x2=np.zeros(len(x1))
  x2[0] = y[0]
  for t in range(1, len(x1)):
    x2[t] = x2[t - 1] + (theta1 * x1[t - 1]) - (theta2 * x2[t - 1])
  return x2
def Estimation(x2, ty, tu):
  y_est = np.interp(ty, tu, x2)
  return y_est
def residuals(params, u, y, tu, ty):
    theta1, theta2 = params
    if theta1 <= 0 or theta2 <= 0:</pre>
        return np.inf * np.ones_like(y)
    x1 = DEQ1(u, theta1)
    x2 = DEQ2(y, x1, theta1, theta2)
    y_est = Estimation(x2, ty, tu)
    return y - y_est
def jacobian(params, u, y, tu, ty):
    epsilon = 1e-8
    J = []
    for i in range(len(params)):
        params_eps = np.array(params)
        params_eps[i] += epsilon
        res1 = residuals(params_eps, u, y, tu, ty)
        res0 = residuals(params, u, y, tu, ty)
        J.append((res1 - res0) / epsilon)
    return np.array(J).T
initial\_guess = [0.1, 0.05]
# Define bounds for theta1 and theta2
lower_bounds = [1e-6, 1e-6]
upper_bounds = [np.inf, np.inf]
result = least_squares(
    residuals,
    initial_guess,
    args=(u, y, tu, ty),
    bounds=(lower_bounds, upper_bounds),
    method='trf'
    loss='linear',
    verbose=2
theta1_est, theta2_est = result.x
print(f'Estimated theta1: {theta1_est:.4f}')
print(f'Estimated theta2: {theta2_est:.4f}')
# Compute estimated output
x1_{est} = DEQ1(u, theta1_{est})
x2_est = DEQ2(y, x1_est, theta1_est, theta2_est)
y_est = Estimation(x2_est, ty, tu)
plt.figure(figsize=(10, 6))
plt.plot(ty, y, label='Observed Output (y)', marker='o', color='b')
             v est. label='Estimated Output (v est)'. marker='x'.
```

 $\overline{\pm}$

```
plt.xlabel('Time')
plt.ylabel('Cortisol Level')
plt.title('Comparison of Observed and Estimated Cortisol Levels')
plt.legend()
plt.grid(True)
plt.show()
```

<u>-</u>	Iteration	Total nfev	Cost	Cost reduction	Step norm	Optimality
			1.0037e+04			3.35e+03
			1.1887e+03	8.85e+03	1.18e-01	5.04e+03
			1.5233e+01	1.17e+03	1.52e-01	4.01e+02
			9.4463e+00	5.79e+00	1.15e-01	6.65e+00
			9.2760e+00	1.70e-01	6.93e-02	1.06e+00
			9.2589e+00	1.71e-02	3.11e-02	2.27e-01
			9.2573e+00	1.56e-03	1.10e-02	6.25e-02
			9.2572e+00	1.37e-04	3.43e-03	1.80e-02
			9.2572e+00	1.20e-05	1.03e-03	2 . 92e-02
		10	9.2572e+00	1.04e-06	3.05e-04	1.25e-02
	10	11	9.2572e+00	9.03e-08	8.99e-05	4.02e-03
	`ftol` terminat	ion condition i	c caticfied			

Function evaluations 11, initial cost 1.0037e+04, final cost 9.2572e+00, first-order optimality 4.02e-03. Estimated theta1: 0.5942 Estimated theta2: 0.0063



from sklearn.metrics import r2_score

Calculate R-squared $r2 = r2 \ score(v. \ v \ est)$