

```
In [ ]: import numpy as np
import matplotlib.pyplot as plt
```

Question 1

Linearized least squares problem with exponential growth model

Part a

```
In [ ]: from numpy import log, exp

# Establish data vectors
t = np.arange(1,11, dtype=np.float64).T
y = np.array([6.2, 9.5, 12.3, 13.9, 14.6, 13.5, 13.3, 12.7, 12.4, 11.9]).T

# Define (linearized) least squares vectors
A = np.column_stack((np.ones(10, dtype=np.float64), t))
b_ = log(y) - log(t)

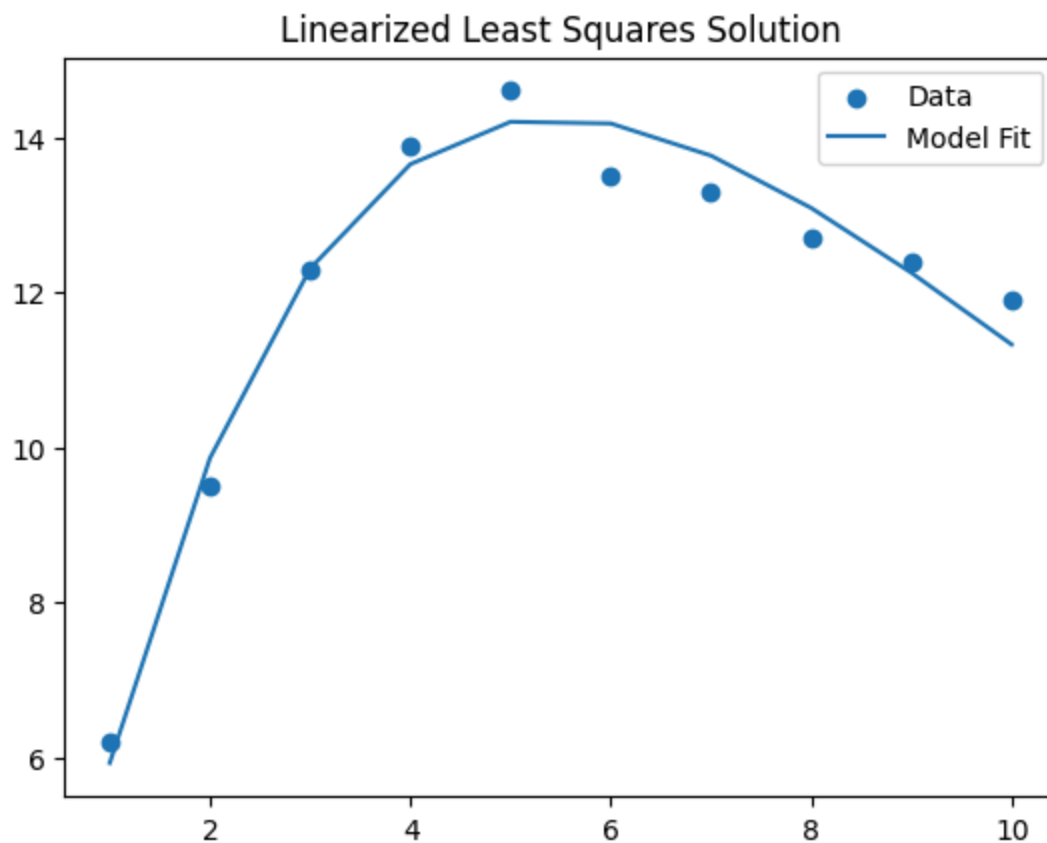
# Solve linearized least squares
c_ = np.linalg.solve(A.T @ A, A.T @ b_.T)
c = c_.copy()
c[0] = exp(c[0]) # Convert linearized solution to original form

print(f"c1: {round(c[0],3)}, c2: {round(c[1],3)}")

# Use fitted model to obtain predictions
y_pred = c[0]*t*exp(c[1]*t)

plt.scatter(t,y, label='Data')
plt.plot(t,y_pred, label='Model Fit')
plt.legend()
plt.title('Linearized Least Squares Solution')
plt.show()

c1: 7.122, c2: -0.184
```



Part b

To approximate the max, we will take very small steps between 4 and 7 using our model.

```
In [ ]: t_ = np.linspace(4,7,1000)
vals = c[0]*t_*exp(c[1]*t_)
time_index_of_max = np.argmax(vals)

print(f"Approximate max dose: {round(np.max(vals),3)}")
```

Approximate max dose: 14.251

Part c

We seek the approximate time for the drug to reach half of its initial (maximum dose), which in our case is $14.25/2 = 7.125$:

$$7.125 = c_1 * \bar{t} * e^{c_2 * \bar{t}}$$

where c_1 and c_2 are known from above. We can reduce this expression to

$$\ln(7.125) - \ln(c_1) - \ln(\bar{t}) - c_2 * \bar{t} = 0$$

```
In [ ]: from scipy.optimize import fsolve
f = lambda t: log(7.125) - log(c[0]) - log(t) - c[1]*t

# We set x0 = 10 to avoid the solution to this equation at
# 1.3 that corresponds to a time before the max dose is reached
total_half_life = fsolve(f, 10)[0]

half_life_from_peak = total_half_life - t_[time_index_of_max]
```

```
print(f"The half-life is approximately {round(half_life_from_peak,2)} hours")
```

The half-life is approximately 9.13 hours

Part d

We seek to estimate the time that the drug is within therapeutic levels (4 - 15 ng/ml). We must find the time between when it first hits 4 and when it later returns to 4 since we estimate it never passes 15. We use a similar equation to above:

$$\ln(4) - \ln(c_1) - \ln(\bar{t}) - c_2 * \bar{t} = 0$$

First, we set x0 (for the root finder) to be 0 to find the first time it passes 4, then we will set it to some later time that will be closer to the second time it hits 4.

```
In [ ]: f = lambda t: log(4) - log(c[0]) - log(t) - c[1]*t

first_hit = fsolve(f,1)[0]
second_hit = fsolve(f,10)[0]

active_time = second_hit - first_hit

print(f"Active time: {round(active_time,3)} hours")
```

Active time: 18.584 hours

Question 2

Use of "manual" Gram-Schmidt to produce an orthogonal basis that spans the same set as a given list of vectors

Part a

```
In [ ]: def proj(u,w):
    "Project w onto u"
    if np.all(u == 0):
        return 0
    return (np.dot(w, u) / np.dot(u, u)) * u

def gram_schmidt(w):
    [m,n] = w.shape
    u = np.zeros_like(w)

    # For all columns
    for j in range(n):
        # Initialize the orthogonal column
        u[:,j] = w[:,j].copy()
        # Subtract the projection of each previous column
        for i in range(j):
            u[:,j] -= proj(u[:,i], w[:,j])

    return u

w1 = np.array([1., -1., 1., -1.]
```

```
w2 = np.array([1., 1., 3., -1.])
w3 = np.array([-3., 7., 1., 3.])

u = gram_schmidt(np.column_stack([w1,w2,w3]))
print(u.round(3))
```

```
[[ 1.  0.  0.]
 [-1.  2.  0.]
 [ 1.  2.  0.]
 [-1.  0.  0.]]
```

The last vector is zero since the given vectors, w_1, w_2, w_3 are linearly dependent.

Part b

To check if the resulting vectors are in fact orthogonal, we see if the dot product of all three equals zero.

```
In [ ]: print(np.dot(u[:,0], u[:,1]))
print(np.dot(u[:,0], u[:,2]))
print(np.dot(u[:,1], u[:,2]))

0.0
0.0
0.0
```

Typically we expect $u^T u$ to be a diagonal matrix, but since the vectors are not linearly independent, we don't get this exactly and there is one zero on the diagonal. Also, the diagonal entries are not 1 since we did not normalize.

```
In [ ]: print(u.T @ u)

[[4. 0. 0.]
 [0. 8. 0.]
 [0. 0. 0.]]
```

Question 3

Comparison of Classical vs Modified Gram-Schmidt for QR factorization

Classical Gram-Schmidt

```
In [ ]: def classic_gram_schmidt(A):
    [m,n] = A.shape
    Q = np.zeros((m,n), dtype=np.float64)
    R = np.zeros((n,n), dtype=np.float64)

    # Classical Gram-Schmidt algorithm
    for j in range(n):
        # Initialize orthogonal vector
        y = A[:,j]
        # Subtract projection of previous vectors
        for i in range(j):
            R[i,j] = Q[:,i].T @ A[:,j]
            y -= R[i,j] * Q[:,i]
        # Set diagonal component of R and obtain normalized
        # orthogonal vector
        R[j,j] = np.linalg.norm(y)
```

```

    Q[:,j] = y / R[j,j]

    return Q, R

```

Modified Gram-Schmidt

```

In [ ]: def modified_gram_schmidt(A):
        [m,n] = A.shape
        Q = np.zeros((m,n), dtype=np.float64)
        R = np.zeros((n,n), dtype=np.float64)

        # Modified Gram-Schmidt algorithm
        for j in range(n):
            y = A[:,j]
            for i in range(j):
                R[i,j] = Q[:,i].T @ y # Here we instead subtract projection of the most recent
                y -= R[i,j] * Q[:,i]
            R[j,j] = np.linalg.norm(y)
            Q[:,j] = y / R[j,j]

        return Q, R

```

```

In [ ]: delta = 10e-10

w1 = np.array([1., delta, delta/2, delta/3])
w2 = np.array([1., delta/2, delta/3, delta/4])
w3 = np.array([1., delta/3, delta/4, delta/5])

A = np.column_stack([w1,w2,w3])

Q_classic = classic_gram_schmidt(A)[0]
Q_modified = modified_gram_schmidt(A)[0]

```

If Q is in fact perfectly orthogonal, we expect $Q^T * Q$ to yield to identity matrix, but we suspect it will not be exact since we used such small values.

```

In [ ]: # Check accuracy
print(f"Q^T * Q (classic):\n {Q_classic.T @ Q_classic}")
print('')
print(f"Q^T * Q (modified):\n {Q_modified.T @ Q_modified}")

Q^T * Q (classic):
[[ 1.00000000e+00 -1.14527425e-09 -2.20872348e-10]
 [-1.14527425e-09  1.00000000e+00 -2.49475840e-15]
 [-2.20872348e-10 -2.49475840e-15  1.00000000e+00]]

Q^T * Q (modified):
[[ 1.00000000e+00 -2.63539188e-27  3.72078702e-27]
 [-2.63539188e-27  1.00000000e+00 -2.45460252e-17]
 [ 3.72078702e-27 -2.45460252e-17  1.00000000e+00]]

```

We see significantly more accuracy from modified Gram-Schmidt.

Question 4

QR factorization to solve least squares

```

In [ ]: def full_QR(A):
        # Pad matrix A to add identity to extra k = m-n columns

```

```

[m,n] = A.shape
A_ = np.eye(m, dtype=np.float64)
A_[:, :n] = A

Q, R_ = modified_gram_schmidt(A_)

# R is mxm but we only want nxn part
R = R_[:, :n].copy()

return Q, R

w1 = np.array([1., -1., 1., 1.])
w2 = np.array([4., 1., 1., 0.])
A = np.column_stack((w1, w2))

print(A)
Q, R_hat = full_QR(A)

```

```

[[ 1.  4.]
 [-1.  1.]
 [ 1.  1.]
 [ 1.  0.]]

```

To solve least squares, we solve $\hat{R}x = \hat{d}$, where \hat{R} is the upper $n \times n$ block of R from QR, and \hat{d} is the first n entries from $d = Q^T b$

```

In [ ]: # Define important vectors
b = np.array([3, 1, 1, -3])
d = Q.T @ b
n = R_hat.shape[0]
d_hat = d[:n].copy() # We only want the first n components

x = np.linalg.solve(R_hat, d_hat) # Solve Rx=d
y_pred = A @ x
x

```

```

Out[ ]: array([-1.,  1.])

```

Question 5

5.9) $A \in \mathbb{R}^{(n \times n)}$

A is orthogonal \Rightarrow its columns are pairwise orthogonal

$$A^T A = I \quad \Rightarrow \quad \begin{bmatrix} -q_1^T- \\ -q_2^T- \\ \vdots \\ -q_n^T- \end{bmatrix} \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \dots & q_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix}$$

we can see

$$\begin{array}{ccccccc} q_1^T q_1 = 1 & q_1^T q_2 = 0 & \dots & q_1^T q_n = 0 \\ q_2^T q_1 = 0 & q_2^T q_2 = 1 & \dots & q_2^T q_n = 0 \\ \vdots & \vdots & & \vdots \\ q_n^T q_1 = 0 & \dots & \dots & q_n^T q_n = 1 \end{array}$$

Hence, we can say that the columns of A are pairwise orthogonal unit vectors

A has pairwise orthogonal columns \Rightarrow A is orthogonal

If A has this property,

$$\begin{array}{ccccccc} q_1^T q_1 = 1 & q_1^T q_2 = 0 & \dots & q_1^T q_n = 0 \\ \vdots & \vdots & & \vdots \\ q_n^T q_1 = 0 & \dots & \dots & q_n^T q_n = 1 \end{array}$$

This is equivalent to

$$\begin{bmatrix} -q_1^T \\ -q_2^T \\ \vdots \\ -q_n^T \end{bmatrix} \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \dots & q_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix}$$

Which can be expressed as $A^T A = I$

We can also transpose both sides: $AA^T = I^T = I$

Hence, we have that A is orthogonal

b) Let $A, B \in \mathbb{R}^{(n \times n)}$ and A, B are orthogonal

$$\text{Thus, we have } A^T A = A A^T = I \\ B^T B = B B^T = I$$

We seek to prove $AB = C$

$$\Rightarrow C^T C = I$$

$$\Rightarrow (AB)^T AB$$

$$\Rightarrow B^T \underbrace{A^T A}_I B$$

$$= \underbrace{B^T B}_I$$

$$= I$$

C) By definition, every subspace contains a basis. Thus

$\exists u_1, \dots, u_n \in \mathbb{R}^n$ s.t. $\{u_1, \dots, u_n\}$ spans an arbitrary, non-empty subspace U of \mathbb{R}^n

Since they form a basis, u_1, \dots, u_n are linearly independent. Also, the dimension of the basis set is less than or equal to \mathbb{R}^n . Hence, we can use Gram-Schmidt, which guarantees $q_1, \dots, q_n \in \mathbb{R}^n$ that span the same set as $\{u_1, \dots, u_n\}$ and are mutually orthogonal.

Hence, we have shown that every non-empty subset of \mathbb{R}^n has an orthogonal basis

Question 6

6. a) False

When you apply a non-linear transformation to the model, distortion occurs in the sense that you are no longer minimizing the euclidean norm of the "original" residuals. While this certainly introduces bias, this bias can sometimes be favorable since it can lead to a better fit.

b) True

this is true b/c $Q^T Q = I$

c) False

\hat{R} is an upper triangular $(n \times n)$ matrix

d) True

$$\underset{n \times n}{A} = \underset{n \times n}{Q} \underset{n \times n}{R}$$

Question 7

7. a)

i) Increase the order of the linear model

Suppose we suspect there is a parabolic relationship between X and Y . Then we can change our underlying model from linear to second order:

$$y = a + bx \Rightarrow y = a + bx + cx^2$$

This idea can be extended to higher orders (more coefficient and x^3, x^4, \dots) or w/ a multi-variate input where some or all of the inputs have higher order terms. This method retains linearity since it is a linear combination of the coefficients

ii) Linearization of suspected non-linear model

Suppose we suspect some data have the form $y = c_1 e^{c_2 t}$. We can fit this model using OLS if we linearize the model first:

$$\ln y = \ln c_1 + c_2 \cdot t$$

$$y^{\bullet} = c_1^{\bullet} + c_2 \cdot t$$

We fit y^{\bullet} to c_1^{\bullet}, c_2 using OLS then

transform back:

$$c_1 = e^{c_1^0}$$

$$y = c_1 e^{c_2 \cdot t}$$

$$b) \quad y_1 = w_1 \quad q_1 = \frac{y_1}{\|y_1\|}$$

$$y_2 = w_2 - q_1^T (q_1, w_2) \quad q_2 = \frac{y_2}{\|y_2\|}$$

$$y_3 = w_3 - q_1^T (q_1, w_3) - q_2^T (q_2, w_3) \quad q_3 = \frac{y_3}{\|y_3\|}$$

c) Suppose we have A, Q, R

Our goal is to minimize $\|Ax - b\|$

We will use $A = QR$ and $QQ^T = I \Rightarrow b = QQ^T b$

$$\min_x \|Ax - b\| = \min_x \|QRx - QQ^T b\| = \min_x \|Q(Rx - Q^T b)\|$$

Since we minimize across x , we can drop the common Q

$$\min \|Rx - Q^T b\| \quad \text{let } d = Q^T b$$

If we examine the residuals

$$\begin{bmatrix} e_1 \\ \vdots \\ e_n \\ e_{n+1} \\ \vdots \\ e_m \end{bmatrix} = \begin{bmatrix} r_{11} & \dots & r_{1n} \\ & r_{22} & \dots \\ & & \ddots & \ddots \\ & & & r_{nn} \\ 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} - \begin{bmatrix} d_1 \\ \vdots \\ d_n \\ d_{n+1} \\ \vdots \\ d_m \end{bmatrix}$$

We notice that our choice of x does not impact the lower block of e (e_{n+1}, \dots, e_m).

However, the correct choice of x allows the top block to be 0:

$$\hat{R} = R^{(n \times n)} \quad \hat{d} = [d_1, \dots, d_n]$$

$$\hat{R}x = \hat{d}$$

since \hat{R} is upper triangular, it is invertible

$$x = \hat{R}^{-1} \hat{d}$$

this is the least squares solution