

EM425 Assignment #5

Problem Statements

1. (Based on 6.19) Create a user-defined function for linear regression. The signature should be $[a, Er] = \text{LinReg}(x, y)$. In addition to determining the constants a_0 and a_1 for a linear least-squares fit to the data, the function should also calculate the squared residual:

$$Er = \sum_{i=1}^n [y_i - (a_1 x_i + a_0)]^2$$

The input arguments x and y are vectors with the values of the data points. Use the function to find the coefficients for a linear least square fit to the following data and find the error.

x	1	3	4	6	9	12	14
y	2	4	5	6	7	9	11

2. (Based on 6.40) The following are measurements of the rate coefficient, k , for the reaction $\text{CH}_4 + \text{O} \rightarrow \text{CH}_3 + \text{OH}$ at different temperatures T .

T (K)	595	623	761	849	989	1076	1146	1202	1382	1445	1562
$k \times 10^{20}$ (m^3/s)	2.12	3.12	14.4	30.6	80.3	131	186	240	489	604	868

Use the method of least squares to best fit a function of the form $\ln(k) + C + b \ln(T) - \frac{D}{T}$ to the data. Determine the constants C , b and D by curve fitting a linear combination of the functions $f_1(T) = 1$, $f_2(T) = \ln(T)$, and $f_3(T) = \frac{1}{T}$ to the given data. Usually, the rate coefficient is expressed in the form of an Arrhenius equation $k = AT^b e^{-E_a/(RT)}$ where A and b are constants, $R=8.314$ J/mole/K is the universal gas constant, and E_a is the activation energy for the reaction. Having determined C , b , and D , deduce the values of A (m^3/s) and E_a (J/mole) in the Arrhenius expression.

3. (Based on 6.4) The following data is given:

x	0.2	0.5	1	2	3
y	3	2	1.4	1	0.6

By hand, determine the coefficients m and b in the function $y = \frac{1}{mx+b}$ that best fit the data using linear least-squares fit.

$m =$ _____, $b =$ _____

4. (Based on 6.27) The resistance R of a tungsten wire as a function of temperature can be modeled with the equation $R = R_0 [1 + \alpha(T - T_0)]$ where R_0 is the resistance corresponding to temperature T_0 , and α is the temperature coefficient of resistance. Determine R_0 and α such that the equation will best fit the data. Use $T_0 = 20^\circ\text{C}$.

$T (^\circ\text{C})$	20	100	180	260	340	420	500
$R (\Omega)$	500	676	870	1060	1205	1410	1565

5. (Based on 6.30) In a uniaxial tension test, a dog-bone-shaped specimen is pulled in a machine. During the test, the force applied to the specimen, F , and the length of a gage section, L , are measured. The true stress, σ_t , and the true strain, ϵ_t , are defined by:

$$\sigma_t = \frac{F}{A_0} \frac{L}{L_0} \quad \text{and} \quad \epsilon_t = \ln \frac{L}{L_0}$$

Where A_0 and L_0 are the initial cross-sectional area and gage length, respectively. The true stress-strain curve in the region beyond the yield stress is often modeled by:

$$\sigma_t = K \epsilon_t^m$$

The following are values of F and L measured in an experiment. Determine the values of the coefficients K and m that best fit the data. The initial cross-sectional area and gage length are $A_0 = 1.25 \times 10^{-4} \text{ m}^2$, and $L_0 = 0.0125 \text{ m}$. [**Note:** be careful with units.]

$F \text{ (kN)}$	24.6	29.3	31.5	33.3	34.8	35.7	36.6	37.5	38.8	39.6	40.4
$L \text{ (mm)}$	12.58	12.82	12.91	12.95	13.05	13.21	13.35	13.49	14.08	14.21	14.48

Numerical Answers

1. Coefficients:

1.9357

0.6214

Square Residual (error): 1.36429

2. My advice is for the third function just use $1/T$ and not $-1/T$. Let the sign be provided by your curve fit function. Answer: $c_1 = -52.4427$, $c_2 = 2.1216$, $c_3 = -3815.342$ (check your result with a plot of the data and the curve fit)

3. $m = 0.45$, $b = 0.24$

- 4.

$R_o = 505.357$

$\alpha = 0.00441519$

- 5.

$K = 5.49476e+08$

$m = 0.208528$