Mathematics 471 Problem Set 5

Due Thursday, April 26, 2001

By submitting a paper for this assignment you declare that you are not submitting any unattributed work of any other person.

Hand in all analytical work that contributes to your solution. Submit printed copies of all programs (except those provided with the textbook), output tables, and graphs. (Use the `diary` feature to get printed output from MATLAB sessions.) Be sure to

(a) Include explanatory comments in all programs, and make informative labels for all tables and graphs.

(b) Edit output to make it compact and easy to read.

1. Consider **Problem k** for $k = 3, 4, 5, \ldots$: compute the slope and intercept of the line $y = mx + b$ that best fits the data

x	y
$666 \times 10^k - 1$	-1
666×10^k	0
$666 \times 10^k + 1$	1

in the least squares sense. The correct solution is $m = 1$, $b = -666 \times 10^k$.

Using the least squares fitting capability of any software system (except MATLAB and *Mathematica*) or calculator you choose, solve this problem for $k = 3, 4, 5, \ldots$ until the system fails, and report the following:

(a) What software system or calculator did you use?

(b) Does the documentation indicate what algorithm is used for solving linear least squares problems? Does it warn of possible ill-conditioning and how to detect it?

(c) What is the smallest k for which the system failed to solve the problem?

(d) Did the system detect the failure? If so, what diagnostic information did it provide?

2. Retrieve the M-file `MalateEqs.m` from the `Examples` directory in the class web site, together with auxiliary M-files `X0.m`, `eqlbrm.m` and `eqljac.m`. These files solve the equilibrium equations for the malate-NADP-magnesium complex in the previous assignment. The solution, combined with other experimental data, will be used to determine certain parameters governing the reactions.

In the laboratory, the experimenter adds a measured amount of Malate to a prepared solution of NADP and manganese chloride, $MnCl_2$. Then spectrographic equipment measures the "reaction velocity," the rate at which the manganese-malate metal-enzyme complex is formed.

The concentration $S =$ [Malate.Mn] of the metal-enzyme complex grows at a rate determined by the *Michaelis-Menten* equation,

$$\frac{dS}{dt} = \frac{\lambda S}{K_m + S}. \tag{1}$$

and the experimenter wants to know the values of parameters λ and K.

If we write V for $\frac{dS}{dt}$ (the velocity) in (1) we see that $1/V$ is a linear function of $1/S$:

$$\frac{1}{V} = \frac{1}{\lambda} + \left(\frac{K_m}{\lambda}\right)\frac{1}{S}. \tag{2}$$

This means that you can estimate the constants λ and K_m by fitting a straight line to the graph of $1/V$ versus $1/S$ obtained from the experimental data. Biochemists call this double reciprocal plot a "Lineweaver-Burke diagram". This is your task in the present assignment.

The measured values of V are shown in the table below along with the input values of the three reactants.

1-1: $a_3 = 100$		1-2: $a_3 = 200$		1-3: $a_3 = 400$	
a_1	V	a_1	V	a_1	V
31.25	0.8912	15.0	0.8855	15.0	2.1732
62.5	1.709	31.25	2.9116	31.25	4.3547
125.0	4.975	62.5	4.2913	62.5	5.2662
187.5	5.722	125.0	5.7062	125.0	6.6334
250.0	6.1119	250.0	7.0891	250.0	7.9120
500.0	6.9423	500.0	7.6272	500.0	8.3868

The equilibrium concentration S is computed from equilibrium concentrations of free malate and manganese (calculated in the previous assignment) by

$$S = [\text{Malate.Mn}] = c\epsilon^{-1}xz \tag{3}$$

Make a table of $1/V$ versus $1/S$ for each pair of columns (corresponding to a set value of a_3) in the table above. Then find the slope m and intercept b of the best-fitting straight line

$$\frac{1}{V} = b + m\frac{1}{S}$$

for the six points in each table. Then use m and b to calculate the Michaelis-Menten coefficients λ and K_m in (2).

3. The following table shows the refractive index μ for fused quartz glass measured as a function of the wavelength of light λ in microns:

λ	0.35	0.40	0.45	0.50	0.55	0.65	0.70	0.80	0.90
$\mu(\lambda)$	1.477	1.470	1.466	1.462	1.459	1.457	1.455	1.453	1.452

(These data may be retrieved from the course web site, in the `Examples` directory, file `quartz_refr.dat`.)

Perform a least squares fit of the index of refraction data by polynomials of degrees 2 through 7. Plot each fit as a solid curve, and plot the data as discrete points along with the curve. Do any of these fits appear satisfactory? (You may also want to check the residuals to help decide.)

Finally, fit a curve of the form

$$\mu = c_1 + \frac{c_2}{\lambda} + \frac{c_3}{\lambda^2}$$

to the data and compare this fit to the least-squares polynomials.