Due : March 27th, 2012

1. Use the function `linefit` in the NMM toolbox and fit a line to the following data:

x	1	2	4	5
y	1	2	2	3

Calculate the value of the R^2 statistic and decide if this is a good fit or not. Further plot data and the line obtained on one grid using the plot command.

2. The following three files, `cucon1.dat, cucon2.dat, cucon3.dat` have data with measured values of thermal conductivity k versus temperature T for three different samples of copper. The mathematical model for k vs T is widely believed to be

$$k(T) = \frac{1}{\frac{c_1}{T} + c_2 T^2}$$

Let $\gamma(T) = \frac{1}{k(T)}$. Use `fitnorm` and `cuconBasis1` to find the best possible c_1 and c_2 for γ versus T. Suppose we tweak the model to be

$$\gamma(T) = \frac{c_1}{T} + c_2 T^2 + c_3 T,$$

using fitnorm can you find the best possible fit. Compare the above two plots.

3. The function $y = \frac{x}{c_1 x + c_2}$ can be transformed into a linear relationship $z = c_1 w + c_2$ with the change of variable $z = \frac{1}{y}$, $w = \frac{1}{x}$. Write an `xlinxFit` function that calls `linefit` to fit data to $y = \frac{x}{c_1 + c_2 x}$. Test your function by fitting the following sets of data:

x	2.2500	2.5417	2.8333	3.1250	3.4167	3.7083	4.000
y	2.8648	1.936	1.0823	0.8842	0.7677	0.6910	0.6366

x	0.7000	1.0714	1.4429	1.8143	2.1857	2.5571	2.9286	3.3000
y	-0.1714	-0.3673	-0.8243	-3.1096	3.7463	1.4610	1.0039	0.8080

4. Consider the following table:

x	y
0.24	19.9
0.52	28.8
1.93	48.7
3.26	59.0
15.0	106.5

(a) Construct a new table with $\log_{10} x$ and $\log_{10} y$.

(b) Assume that data in your table is close to satistfying

$$\log_{10} y = \alpha \log_{10} x + \beta$$

(c) Construct and solve the normal equations.

(d) Plot the transformed data and the least-square line on the same axes.

(e) Calculate the R^2 statistic. Plot the residual r as function of x.

5. Write a function to fit data to $y = c_1x^5 + c_2x^3 + c_3x + c_4$ without calling `polyfit, fitnorm` or `fitqr`. Your function should take two column vectors `x` and `y` as input and return the coefficient vector. Test your solution with the following data:

x	-3.0000	-1.8571	-0.7143	0.4286	1.5714	2.7143	3.8571	5.0000
y	-4.9262	-4.4720	-3.3136	-2.9396	-2.6697	-1.3906	-0.8669	-3.3823

6. **A QR Algorithm** Let c, s be two real numbers such that $c^2 + s^2 = 1$. For each $1 \leq i < j \leq n$, define the Q_{ij} as the matrix whose entries are given by:

$$q_{kl} = \begin{cases} 1 & \text{if } j \neq k = l \neq i \\ c & \text{if } k = l = j \text{ or } k = l = i \\ -s & \text{if } k = i, l = j \text{ or } k = j, l = i \\ 0 & \text{otherwise} \end{cases}$$

(a) Verify that Q_{ij} is an orthogonal matrix.

(b) Let $x_{n\times 1}$ be given. Find c, s such that $c^2 + s^2 = 1$ and j-th entry of $Q_{ij}x$ is 0 (*Observe that all other row entries except the i-th row remain unchanged*).

(c) Let $n = 2$ and $A_{2\times 2}$ be given a matrix of rank 2. Can you now construct an orthogonal matrix $Q_{2\times 2}$ such that $A = QR$ where $R_{2\times 2}$ is upper triangular.

(d) Let $n = 3$ and $A_{3\times 3}$ be given a matrix of rank 3. Can you now construct an orthogonal matrix $Q_{3\times 3}$ such that $A = QR$ where $R_{3\times 3}$ is upper triangular ?.

(e) Now for any general $A_{m\times n}$ of full column rank, construct an orthogonal matrix $Q_{n\times n}$ such that $A = QR$ where $R_{m\times n}$ matrix whose first n rows form an upper-triangular matrix and the last $m - n$ rows are 0.

CS 2 Computer Science II-Numerical Methods Semester II 2007/08

http://www.isibang.ac.in/~athreya/nm Summary

1. Use the `linefit` function in the NMM Toolbox to obtain a least squares line fit to data and to linearized transformations of $y = c_1e^{c_2x}$ and $y = c_1x^{c_2}$.

2. Use the built-in `polyfit` function to obtain a least squares fit to a polynomial in x. Use the built-in `polyval` function to evaluate the polynomial obtained from `polyfit` at any x.

3. Plot a comparison of a least squares fit and the data used to obtain the fit.

4. Use the `fitnorm` and `fitQR` functions from the NMM Toolbox to obtain least squares fits to linear combinations of arbitrary basis functions.

5. Assign the elements of the matrix `A` of the overdetermined system for a given choice of basis functions. Given this matrix and a vector of y data, obtain the coefficients of the fit by solving the normal equations.

6. Given the matrix of the overdetermined system for the fit, and a vector of y data values, use the \ operator to obtain the coefficients that minimizes $\| r \|_2$ for the overdetermined system.