

We have found that in order to interpolate data using a cubic spline that tri-diagonal matrices like,

$$\begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & a_3 & b_3 & c_3 & \\ & & & \ddots & \\ & & & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & & a_N & b_N \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_{N-1} \\ r_N \end{pmatrix} \quad (1)$$

need to be solved. We found that with

$$\beta_1 = b_1, \quad \beta_j = b_j - \frac{a_j}{\beta_{j-1}} c_{j-1} \quad j = 2, \dots, N \quad (2)$$

and

$$\rho_1 = r_1, \quad \rho_j = r_j - \frac{a_j}{\beta_{j-1}} \rho_{j-1} \quad j = 2, \dots, N. \quad (3)$$

the solution is given by

$$x_{N-j} = \frac{(\rho_{N-j} - c_{N-j} x_{N-j+1})}{\beta_{N-j}}, \quad j = 1, \dots, N-1 \quad (4)$$

A pseudo code for this is shown below. Translate the pseudo code to **MatLab**. Then discuss how you would this to find cubic splines

```
% Trisolve
%
% Inputs: The coefficients a,b,c and
%         r.h.s. r's
% Outputs: An array containing the solutions
%          to the tridiagonal system
%
% Input the  a, b, c, and r
% Loop 2 to N
%     calculate beta, and rho using
%     Eqs. 2.21 and 2.22
% End Loop
%
% Now back substitute
%
% Loop 1 to N-1
%     find x using Eq. 2.23
% End Loop

Notes: You will have to do the rho(1), beta(1), and
x(N) outside their respective loops. You'll also have
to make sure that no b's = 0. Why?
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Figure 1: Pseudo Code to solve tri-diagonal systems

1 Curve Fitting

Interpolation approximates a function in such a way that the interpolation passes through a known set of points. *Curve fitting* is a procedure that determines the parameters to a function that *best fits* a set of points. This necessarily means that the function will not pass through all the points. What best means and what we mean by parameters are discussed next.

Table 1: Some data which may be linear

x	y	x	y
1	2.5377	11	-11.3500
2	2.6339	12	-8.1651
3	-2.6588	13	-11.3500
4	-0.7378	14	-13.6630
5	-2.4812	15	-14.0850
6	-5.3077	16	-16.2050
7	-5.6336	17	-17.3240
8	-6.0574	18	-16.9100
9	-4.0216	19	-18.1910
10	-6.0306	20	-19.3830

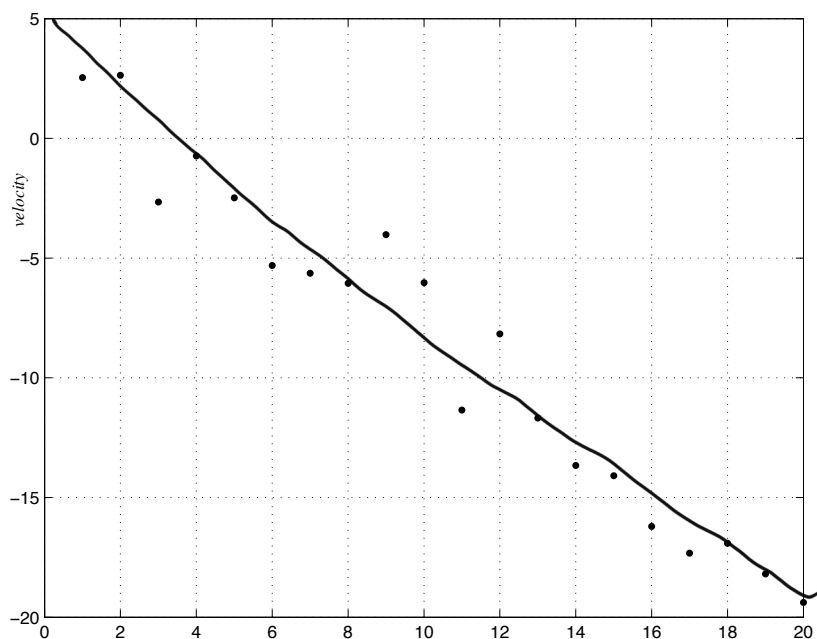


Figure 2: Data perhaps representing a linear function.

- (1) The data from table 1 is plotted in figure 1. Suppose you have reason to believe data should be linear. Sketch some lines that you think best represent the data as a line.

- (2) How might one determine the “best” line through the data

One way to determine the best fit line through some data is to minimize the error between a theoretical line, y_i and the data. If we write the line associated

$$y(x) = y(x; a_1, a_2) = a_1 + a_2x \quad (1)$$

where we are seeking to find a_1, a_2 that give the best line to a particular data set. We do this by minimizing the chi-square function

$$\chi^2(a_1, a_2) = \sum_{i=1}^N \left(\frac{y_i - a_1 - a_2 x_i}{\sigma_i} \right)^2 \quad (2)$$

where the σ_i are the measurement errors and we seek to find the parameters a_1, a_2 .

- (3) Why is the right hand side of Eq. (2) shown as squared?
- (4) In equation (2), what term(s) is one varying in order to find a minimum.
- (5) How does one minimize a function like that given in Eq. (2).
- (6) Translate the pseudo code given in box 2.2.1 in the Course Notes to MatLab.

When we studied interpolation using cubic splines, we found we needed to solve tridiagonal systems of linear equations. In order to *fit* data to higher order polynomials, we'll need to solve general systems of linear equations. We introduce now a method for handling such equations, **LU** factorization.

A general system of equations,

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1N}x_N &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2N}x_N &= b_2 \\ &\vdots \\ a_{N1}x_1 + a_{N2}x_2 + \cdots + a_{NN}x_N &= b_N \end{aligned}$$

can be written in matrix form as

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad (3)$$

where **A** is a matrix containing the coefficients and **b** a vector containing the R.H.S. of the equations.

In **LU** factorization, we try to write the matrix **A** as the product of lower diagonal (**L**) and upper diagonal (**U**) matrices. That is,

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{N1} & a_{N2} & a_{N3} & \cdots & a_{NN} \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{N1} & l_{N2} & l_{N3} & \cdots & l_{NN} \end{pmatrix} \begin{pmatrix} 1 & u_{12} & u_{13} & \cdots & u_{1N} \\ 0 & 1 & u_{23} & \cdots & u_{2N} \\ 0 & 0 & 1 & \cdots & u_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \quad (4)$$

or

$$\mathbf{A} = \mathbf{L}\mathbf{U}$$

where the matrices **L**, **U** are given by the right hand side of Eq. (3).

- (8) If the factorization of a known matrix A by Eq. (3) is possible, we need to find the coefficients, $l_{11}, l_{21}, \dots, u_{12}, u_{13}, \dots$. It turns out this is not too difficult. Let's start with the easiest
- (i) What are l_{j1} in terms of the known a_{ij} .
 - (ii) One down, now find an expression for u_{12}, u_{13}, \dots
 - (iii) Now move to the second column of A and *solve* for unknown l_{2j} .
- (9) Translate the pseudo code given in box 2.2.2 in the Course Notes to **MatLab**.