CS321: Numerical Methods in Comp Mol Bio

Homework 10

Due: Thursday, Nov 17 2005 at the begining of the section

Problem 1

We have seen the protein 1NTF in previous homework.
Create a cubic spline fit to the data from 1NTF.ca and plot it using Matlab's plot3 function.

Problem 2

The matrix

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 4 & 5 & 4 \\ 2 & 1 & 4 \end{pmatrix}$$

can be decomposed using LU decomposition into A=L*U as

$$\begin{pmatrix} 2 & 1 & 1 \\ 4 & 5 & 4 \\ 2 & 1 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 0 & 3 \end{pmatrix} * \begin{pmatrix} 2 & 1 & 1 \\ 0 & 3 & 2 \\ 0 & 0 & 1 \end{pmatrix}$$

Use this to solve the equation Ax=b for

$$b = \begin{pmatrix} 8 \\ 25 \\ 17 \end{pmatrix}$$

Problem 3

Here we will compare a few interpulation techniques we studied in class. Matlab commands
t=-6:1:6
sint=sin(t)
create a vector holding the values of $Sin(x)$ for the integers between -6 and 6.
Use Matlab to create 1) a linear interpulation; 2) a cubic spline interpulation; 3) a polynomial interpulation; fitting the data of sint, evaluated on the points tt=-6:0.1:6.
You might find Matlab functions 'spline', 'interp1', 'polyfit' and 'polyval' useful.
Evaluate the 'goodness' of these interpulation methods by calculating the RMSD of each of these interpulations compared to the actual $Sin(x)$ values along the points of tt.