

CH2013
Computational Programming and Simulations Lab
Aug-Dec 2021
Problem Sheet #5

Sep 22, 2021

This problem sheet is about linear algebra & curve fitting.

1. Use the 'rand' and 'ones' commands to generate a matrix A (3000x3000) and right hand side vector b(3000x1). Use the 'tic' and 'toc' commands to estimate the time taken to solve $Ax = b$ using three methods:
 - a) Use the \ operator . Let the time taken be designated t1 and the solution x1.
 - b) Find the inverse of A using $\text{inv}(A)$ and get x from this. Time taken is t2 and solution x2.
 - c) Next use the *linsolve* in-built function – time taken is t3 and solution is x3.

Which method worked out better for you? Please note – displaying the matrix or results will take too long so you should suppress that. Also, you may want to re-run the code a few times before concluding anything (can you explain why?)

2. Develop a function “ThomasMethod” (that takes matrix A, vector b, and the size of the matrix A, n, as arguments, and provides the solution vector X as the output). The function should implement the steps in the Thomas Algorithm for a tridiagonal matrix problem. Use the same notations ei, fi, gi that is in the notes to denote the various matrix elements. Use the function in a script file to solve for **X** in the following equation:

$$\begin{bmatrix} 13.422 & 0 & 0 & 0 \\ -13.422 & 12.252 & 0 & 0 \\ 0 & -12.252 & 12.377 & 0 \\ 0 & 0 & -12.377 & 11.797 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix} = \begin{bmatrix} 750.5 \\ 300 \\ 102 \\ 30 \end{bmatrix}$$

I want to check the final values of f1, g1, e2, f2, g2, e3, f3, g3, e4, f4, r1, r2, r3, r4, in addition to the X_i . Use the *timeit* function to estimate the time taken for your function to run. Particularly note the warning in the command window (if any).

3. $A = \begin{bmatrix} 4 & 3 & 7 \\ 1 & 2 & 6 \\ 2 & 0 & 4 \end{bmatrix}$; $b = \begin{bmatrix} 3 \\ 5 \\ 1 \end{bmatrix}$. Solve $Ax = b$ using LU decomposition. Use the **lu** in-built function in MATLAB to first decompose the matrix A. Examine **L** and **U**. Keep in mind that the permutation matrix “**P**” is involved and you have to be careful in how you do the steps after the decomposition. You can use the \ operator to do the forward substitution (to get the **d** vector) and back substitution steps (to get **x**). Estimate the time taken for the entire set of commands (**t_lu**). Note that as this is a v small problem, it may not be very meaningful to use this time for comparisons of performance.

4. The following data is given

Cdata=[0.24; 0.32; 0.70; 1.37; 1.58; 2.04; 2.26; 2.28; 2.39; 2.41]

rdata=[0.3839; 0.3935; 0.911; 1.4975; 1.5735; 1.749; 1.9355; 1.893; 1.970; 1.924]

- a) Perform a polynomial fit to this data. Use a quadratic equation. Report the coefficients as **P1**, **P2** and **P3** (in decreasing order). Find the model-predicted **r** values and report them in a vector “**rmodel1**”. The residual is defined as **rmodel1(i)-rdata(i)** for every data point. Find the residuals for the polynomial fit, and report it in a vector “**residual1**”. Find the total error or distance between the model prediction and the data – label it **err1**. Note that you can just use a “norm” of the vector residual1 to get this.

- b) Actually, a reasonable relationship between C and r can be expressed as

$$r = \frac{AC}{B + C}$$

Use the non-linear least square fit function in MATLAB to find optimal A & B (as *Afinal* and *Bfinal*), the residual (*residual2*), number of iterations (*iterations*), and the function count (*funccount*), starting with an idea that A & B might both have a value of 1.0. Find model predicted r values – in **rmodel2**. Report the total error between **rmodel2** and **rdata** as **err2**.

- c) Create a plot with the original data in symbols and the model predictions from both (a) and (b) **plot(Cdata,rdata,'r+',Cdata,rmodel1,'b-',Cdata,rmodel2,'g-')**. Examine the results and make your own conclusions about them.

WE HAVE REPORTED ALL AS COLUMN VECTORS IN THIS PROBLEM