Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.
- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.
- Include the source code of your program. Comment your program properly.
- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.
- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.
- Try to evaluate the reliabilty and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.
- Try to give an interpretation of you results in your answers to the problems.
- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.
- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.

Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats. As programming language we prefer that you choose between C/C++ and Fortran90/95. You could also use Java or Python as programming languages. Matlab/Maple/Mathematica/IDL are not allowed as programming languages for the handins, but you can use them to check your results where possible. The following prescription should be followed when preparing the report:

- Use Classfronter to hand in your projects, log in at blyant.uio.no and choose 'fellesrom fys3150 og fys4150'. Thereafter you will see an icon to the left with 'hand in' or 'innlevering'. Click on that icon and go to the given project. There you can load up the files within the deadline.

- Upload **only** the report file and the source code file(s) you have developed. The report file should include all of your discussions and a list of the codes you have developed. Do not include library files which are available at the course homepage, unless you have made specific changes to them.

- Comments from us on your projects, approval or not, corrections to be made etc can be found under your Classfronter domain and are only visible to you and the teachers of the course.

Finally, we do prefer that you work two and two together. Optimal working groups consist of 2-3 students. You can then hand in a common report.

Project 1, deadline 19 september 12pm (midnight)

The aim of this project is to get familiar with various matrix operations, from dynamic memory allocation to the usage of programs in the library package of the course. For Fortran users memory handling and most matrix and vector operations are included in the ANSI standard of Fortran 90/95. For C++ user however, there are three possible options

1. Make your own functions for dynamic memory allocation of a vector and a matrix. Use then the library package lib.cpp with its header file lib.hpp for obtaining LU-decomposed matrices, solve linear equations etc.

2. Use the library package lib.cpp with its header file lib.hpp which includes a function `matrix` for dynamic memory allocation. This program package includes all the other functions discussed during the lectures for solving systems of linear equations, obatining the determinant, getting the inverse etc.

3. Finally, we provide on the web-page of the course a library package which uses Blitz++'s classes for array handling. You could then, since Blitz++ is installed on all machines at the lab, use these classes for handling arrays.

Your program, whether it is written in C++ or Fortran 90/95, should include dynamic memory handling of matrices and vectors.

(a) Consider the linear system of equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= w_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= w_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= w_3. \end{aligned}$$

This can be written in matrix form as

$$\mathbf{Ax} = \mathbf{w}.$$

Use the included programs for LU decomposition to solve the system of equations

$$\begin{aligned} -x_1 + x_2 - 4x_3 &= 0 \\ 2x_1 + 2x_2 &= 1 \\ 3x_1 + 3x_2 + 2x_3 &= \tfrac{1}{2}. \end{aligned}$$

Use first standard Gaussian elimination and compute the result analytically. Compare thereafter your analytical results with the numerical ones obtained using the LU programs in the program library.

(b) Consider now the 4×4 linear system of equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 &= w_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4 &= w_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + a_{34}x_4 &= w_3 \\ a_{41}x_1 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 &= w_4. \end{aligned}$$

with

$$\begin{aligned} x_1 + 2x_3 + x_4 &= 2 \\ 4x_1 - 9x_2 + 2x_3 + x_4 &= 14 \\ 8x_1 + 16x_2 + 6x_3 + 5x_4 &= -3 \\ 2x_1 + 3x_2 + 2x_3 + x_4 &= 0. \end{aligned}$$

Use again standard Gaussian elimination and compute the result analytically. Compare thereafter your analytical results with the numerical ones obtained using the programs in the program library.

(c) If the matrix A is real, symmetric and positive definite, then it has a unique factorization (called Cholesky factorization)

$$A = LU = LL^T$$

where L^T is the upper matrix, implying that

$$L^T_{ij} = L_{ji}.$$

The algorithm for the Cholesky decomposition is a special case of the general LU-decomposition algorithm. The algorithm of this decomposition is as follows

- Calculate the diagonal element L_{ii} by setting up a loop for $i = 0$ to $i = n-1$ (C++ indexing of matrices and vectors)

$$L_{ii} = \left(A_{ii} - \sum_{k=0}^{i-1} L_{ik}^2 \right)^{1/2} . \tag{1}$$

- within the loop over i, introduce a new loop which goes from $j = i+1$ to $n-1$ and calculate

$$L_{ji} = \frac{1}{L_{ii}} \left(A_{ij} - \sum_{k=0}^{i-1} L_{ik} l_{jk} \right) . \tag{2}$$

For the Cholesky algorithm we have always that $L_{ii} > 0$ and the problem with exceedingly large matrix elements does not appear and hence there is no need for pivoting. Write a function which performs the Cholesky decomposition. Test your program against the standard LU decomposition by using the matrix

$$\mathbf{A} = \begin{pmatrix} 6 & 3 & 2 \\ 3 & 2 & 1 \\ 2 & 1 & 1 \end{pmatrix} \tag{3}$$

(d) Finally, use the Cholesky method to solve

$$\begin{aligned} 0.05x_1 + 0.07x_2 + 0.06x_3 + 0.05x_4 &= 0.23 \\ 0.07x_1 + 0.10x_2 + 0.08x_3 + 0.07x_4 &= 0.32 \\ 0.06x_1 + 0.08x_2 + 0.10x_3 + 0.09x_4 &= 0.33 \\ 0.05x_1 + 0.07x_2 + 0.09x_3 + 0.10x_4 &= 0.31 \end{aligned}$$

You can also use the LU codes for linear equations to check the results.