Numerieke methoden in de natuurwetenschappen

Ex. 3b: Cubic spline interpolation. Numerical solution by use of the NAG library

Suppose we have a set of datapoints $\{(x_0, f(x_0)),(x_1, f(x_1)), (x_n, f(x_n))\}$ can be interpolated by use of a piecewise polynomial approximation. The most common method is the cubic spline interpolation. The method is described in Sect. 3.4 of the book Numerical analysis by Burden and Faires. Given n points, n cubic polinomials S_j (j=0,1,.. n-1)of the form

$$S_j = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$$

are constructed by imposing the conditions b-f given in the book. As shown there, the problem of determining the coefficients of the polynomials S_j is reduced to finding the solutions of the system of linear equations of the form A**y**=**b** given by eq. 3.22.

Consider now the exercise 5 of the set 3.4 of the same book. The purpose is to construct a free cubic spline for the function cos(π x) by using the numerical values at 5 points, x=0., 0.25,0.5,0.75, 1. Write a program to construct the matrix A and the vector **b**. Solve the problem by use of a subroutine chosen within the NAG library and compare the cubic spline to the original function cos(x).

The NAG library is a collection of ready-to-use subroutines which can be called from a f77, f90 or C program. It is useful to learn using them. The first step is to identify the appropriate subroutine, the second to understand which is the required input and where the output is given. A list of the avalaible subroutines can be found by invoking nagdtext or by looking at the manuals on paper which can be found in the computer room of mathematics on the second floor. A description of how to use them can be found at:

http://www.sci.kun.nl/cncz/software/local/html/nag.html.

In short, you have to give the path by typing:

setenv LD_LIBRARY_PATH /usr/lib:/usr/ccs/lib:/usr/local/lib

and compile with the options:

f90 myprog.f90 -lnag -lF77

or (hopefully, let me know if it works)

CC myprog.c -lnag -lF77 -lM77 -lsunmath -lm -lc

The -lF77 option is needed because the NAG library is written in F77.