763315A ATK II – NUMERICAL MODELLING

Exam 4.5.2007

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Answer five (5) questions!

1. a) Explain briefly, with the aid of examples, what the following *Mathematica* concepts mean:
      - the difference between direct and delayed substitution (the difference between the operators `=` and `:=`)
      - list
      - rule

   b) What do the following *Mathematica* functions do? What are their arguments?
      - `Table`
      - `Reduce`
      - `Simplify`

2. How do you carry out the following tasks in *Mathematica*?
   - solve the differential equation $y''(x)+xy'(x) = 2y(x)$ with the boundary conditions $y(0) = 1$ and $y'(0) = 0$
   - solve the equation $\tan x = x$
   - define the function $f(x) = e^x \ln x \cos^2 x$ and plot it on the given interval $a < x < b$
   - calculate (i) the total differential of g and (ii) the partial derivatives $\frac{\partial g}{\partial x}$ ja $\frac{\partial^2 g}{\partial z^2}$, when $g(x, y, z) = 2^{\cos x} y^9 + e^z \sin y$
   - execute *Mathematica* commands written in a file named `program.m`, located in the folder `C:\ATK2`
   - construct the matrix
     $$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$
     calculate its inverse matrix M^{-1} and check the result by calculating the matrix products MM^{-1} and $M^{-1}M$

3. What does interpolation mean in general? How can you do it in *Mathematica*?

TURN!

4. Explain at least two ways of implementing loop structures in *Mathematica*. Using one of these ways, write a program which calculates the first ten Fibonacci numbers. The Fibonacci numbers $x_0, x_1, \ldots$ are defined by the following recursion relation:

$$\begin{cases} x_0 = 0 \\ x_1 = 1 \\ x_n = x_{n-1} + x_{n-2}, \text{ when } n \geq 2. \end{cases}$$

5. Consider the Schrödinger equation

$$-y''(r) - \frac{2}{r} y(r) = E y(r).$$

   It is a differential equation with an eigenvalue. When it is solved, one obtains the eigenvalue E and the corresponding eigenfunction $y(r)$. In quantum mechanics this equation describes a Hydrogen atom, E is the energy of the electron and from the eigenfunction y one can calculate the probability density associated with the electron. Suppose that the asymptotic behavior of the function y near the origin and at infinity is known. These boundary conditions determine the values of E for which the corresponding function y is a satisfactory solution, i.e. (i) y is continuous and (ii) y' is continuous. Explain in detail the algorithm for solving this equation. You don't have to write a *Mathematica* program.

6. Consider the Schrödinger equation for the harmonic oscillator:

$$-y''(r) + \frac{1}{2} r^2 y(r) = E y(r), \qquad 0 < r < a.$$

   By approximating the derivatives with finite differences, the above equation can be transformed into a set of linear equations for the variables $y(r_i)$, where $\{r_i \mid i = 1, \ldots n\}$ is a set of points from the interval $[0, a]$. This set of equations can be written in matrix form as $MY = EY$, where $Y = (y(r_1), \ldots, y(r_n))^T$. Explain *in detail*, how you form this matrix equation, starting from the above differential equation. Derive the formulas with which you approximate the derivatives. Also, explain how to solve the equation $MY = EY$ in *Mathematica*.