MSc Mathematical Modelling

GM04/MM04 Computational and Simulation Methods

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I am teaching the first part of the course which deals with finite-difference methods. The course was originally designed by Dr N. Ovenden and we follow his ideas with a few modifications here and there. The notes give a brief summary of the topics to be covered in lectures.

The aim of the course is to learn how to formulate a problem involving ordinary differential equations (ODEs) or partial differential equations (PDEs); construct a finite-difference method of solution and test the method for accuracy and stability.

1 Preliminaries.

Order-of-magnitude notation.

We say

$$f(h) = O(h^p) \text{ as } h \to 0 \tag{1.1}$$

if

$$|f(h)| \le Ch^p \tag{1.2}$$

for some constant C. Sometimes this is replaced by a more stringent condition,

$$\lim_{h\to 0} \frac{f(h)}{h^p} = C. \tag{1.3}$$

Equivalence. We say $f(h) \sim h^p$ as $h \to 0$ if

$$\lim_{h\to 0} \frac{f(h)}{h^p} = 1. \tag{1.4}$$

Also,

$$f(h) = o(h^p) \text{ as } h \to 0 \tag{1.5}$$

if

$$\lim_{h\to 0} \frac{f(h)}{h^p} = 0. \tag{1.6}$$

Exercise. Let

$$f(h) = h \sin\left(\frac{1}{h^2}\right). \tag{1.7}$$

Are the following relations correct when $h \to 0$:

$$f(h) = o(1), \qquad f(h) = o(h^{1/2}), \qquad f(h) = O(h), \qquad f(h) \sim h? \tag{1.8}$$

.

Errors.

There are three sources of inaccuracy in numerical methods:
(i) human errors
(ii) truncation errors
(iii) rounding errors

Assuming that human errors can be avoided, truncation errors arise when an infinite process (e.g. series) is replaced by a finite process. For example, let $f(x) = e^x$. Then

$$f(x) = 1 + x + \frac{x^2}{2!} + ... + \frac{x^n}{n!} + ..., \tag{1.9}$$

as a convergent Taylor series.

Suppose we wish to compute $f(0.1) = e^{0.1}$on a calculator which does not have a built-in exponential function. As no exact answer is available, we use approximations.

At small x it seems reasonable to drop very high powers of x and retain only the first few terms in the infinite sum, for example we hope for a fairly good approximation for $f(0.1) = e^{0.1}$ retaining just the first five terms,

$$\bar{f}(0.1) = 1 + 0.1 + \frac{0.1^2}{2!} + \frac{0.1^3}{3!} + \frac{0.1^4}{4!} \approx 1.105, \tag{1.10}$$

where we neglected terms $\frac{0.1^5}{5!}$and smaller.

In our example we can of course evaluate the truncation error which is the difference between the exact and approximate values. It will be, approximately,

$$f(0.1) - \bar{f}(0.1) \approx 10^{-7}. \tag{1.11}$$

Note that, as a rule, estimating the truncation error without knowing the exact answer is quite difficult.

Rounding errors arise when an infinite decimal representation is replaced by a finite decimal fraction. In our example, the approximate value is a periodic decimal,

$$\bar{f}(0.1) = 1.10517083(3). \tag{1.12}$$

If the answer is felt sufficiently accurate with only six decimal places retained, we can use the following approximate value,

$$\hat{f}(0.1) = 1.105171, \tag{1.13}$$

where the usual rounding rule has been applied. The rounding error is

$$\bar{f}(0.1) - \hat{f}(0.1) = -0.00000016(6). \tag{1.14}$$

We have thus computed an approximation, $\hat{f}(0.1)$, with two sources of error, first truncating the infinite Taylor series and then truncating and rounding infinite decimals in the truncated solution. This two-step approximation is typical for numerical methods.

Note that for the total error we have,

$$\text{Total error}=|f(0.1) - \hat{f}(0.1)| = |f(0.1) - \bar{f}(0.1) + \bar{f}(0.1) - \hat{f}(0.1)| \leq \tag{1.15}$$

$$|f(0.1) - \bar{f}(0.1)| + |\bar{f}(0.1) - \hat{f}(0.1)|, \tag{1.16}$$

so

$$\text{Total error} \leq \text{ Truncation error+Rounding error.} \tag{1.17}$$

2 Ordinary differential equations.

An ordinary differential equation (ODE) of order n for a function $y(t)$ can generally be written as

$$\Phi(t, y, \frac{dy}{dt}, \frac{d^2y}{dt^2}, ..., \frac{d^ny}{dt^n}) = 0. \tag{2.1}$$

In applications, the equation is often resolved with respect to the highest derivative,

$$\frac{d^ny}{dt^n} = F(t, y, \frac{dy}{dt}, ..., \frac{d^{n-1}y}{dt^{n-1}}). \tag{2.2}$$

To specify a unique solution, the equation of order n requires n initial and/or boundary conditions, for example

$$y(0) = A_0,\ \frac{dy}{dt}(0) = A_1,\ ...,\ \frac{d^{n-1}y}{dt^{n-1}}(0) = A_{n-1}, \tag{2.3}$$

in the case of initial conditions at $t = 0$ given by constants $A_0, ..., A_{n-1}$. The equation together with the initial conditions forms an initial-value problem.

If boundary conditions are specified at two (or more) different values of t then we can have, for example,

$$y(0) = A_0,\ \frac{dy}{dt}(0) = A_1, \tag{2.4}$$

at $t = 0$ and, in addition,

$$\frac{d^2y}{dt^2}(T) = A_2,\ ...,\ \frac{d^{n-1}y}{dt^{n-1}}(T) = A_{n-1}, \tag{2.5}$$

for some $T > 0$, with the solution required in the interval $0 \leq y \leq T$.

An nth order resolved ODE can be written as a system of n 1st-order differential equations,

$$\frac{dy}{dt} = u_1(t), \tag{2.6}$$

$$\frac{du_1}{dt} = u_2(t), \tag{2.7}$$

$$... \tag{2.8}$$

$$\frac{du_{n-1}}{dt} = F(t, y, u_1, u_2, ..., u_{n-1}), \tag{2.9}$$

or, in vector form,

$$\frac{d\mathbf{Y}}{dt} = \mathbf{G}(t, \mathbf{Y}), \tag{2.10}$$

for the vector $\mathbf{Y} = (y, u_1, u_2, ..., u_{n-1})$, with $\mathbf{G}$ being the vector of the right-hand sides.

Uniqueness and existence theorem. Simply put, the solution of the initial-value problem for a 1st order ODE,

$$\frac{dy}{dt} = F(t, y), \ \ y(t_0) = y_0, \tag{2.11}$$

exists and it is unique if F and $\partial F/\partial y$ are continuous.

In the case of a vector equation, y and F are vectors and $\partial F/\partial y$ is the Jacobian matrix but the requirements remain the same, i.e. continuity of both the right-hand side in the equation and it's 'derivative' with respect to the dependent variable.

Example. Solve

$$\frac{dy}{dt} = y, \ \ y(0) = 1, \tag{2.12}$$

for $t \geq 0$.

Example. Find all continuous solutions of

$$\frac{dy}{dt} = y^{1/2}, \ \ y(0) = 0, \tag{2.13}$$

for $t \geq 0$. Here $y = 0$ is an obvious solution. Are there others? Are they differentiable? Continuously differentiable? Twice differentiable?