Overview of the unit. We are concerned with the design and analysis of methods for computing approximations of the solutions of partial differential equations. In essence, the methods considered will replace the original equation, say

$$u_t = F(t, x, y, z, u, u_x, u_y, u_z, \ldots) \qquad \text{(pde)}$$

by a finite system of linear algebraic equations of the form

$$Av = b \qquad \text{(discretisation)}$$

The following questions obviously arise:

(1) How to construct A and b.

(2) How to solve the linear system

(3) How do u and v relate.

The second of these questions is, in principle, completely answered (e.g. use Gaussian elimination!). However, we shall see that v and u only relate well if the order of the matrix A is large, and this fact raises the issue of solving the discrete problem as efficiently as possible.

As one would expect, the answer to the first question depends heavily on the type of the pde, i.e. whether the equation is elliptic, parabolic or hyperbolic. We shall recall in due course the principal properties of the solution for each type. In practice, in order to specify a unique solution, one needs to specify additional conditions that the required solution must satisfy, and the form of these conditions is also an important factor in connection with the first question.

The solution of a typical pde problem is a function, say u, of several variables, say t, x, y, z. In this unit, we shall often think of t as the "time" variable and of x, y and z as the "spatial" variables. Each of the variables take values in some interval of the real line. We shall not aim to construct an approximation of $u(x,y,z,t)$ at every point in the domain of u. Rather, we shall introduce a finite mesh, or grid, of points

$$(x_j, y_k, z_l, t_n), \quad 0 \le j \le J, \quad 0 \le k \le K \quad \text{etc.}$$

and seek approximations of u at those points only, in the first instance. Approximations of u at intermediate points can then be obtained by interpolating between grid points.

Taylor's theorem, interpolation and finite difference

Suppose that a function $u : [a,b]$ is known only at the set of distinct points

$$a \leq x_1, x_2, \dots, x_r \leq b$$

How can one approximate u and its derivatives in $[a,b]$?

To answer this question, we first recall some classical results.

Taylor's theorem Let $u : [a,b] \to \mathbb{R}$ be a function with r continuous derivatives. Let $x_0 \in [a,b]$. Then $\exists\ \xi = \xi(x, x_0) \in [a,b]$ s.t.

$$u(x) = u(x_0) + (x-x_0)u'(x_0) + \dots + \frac{(x-x_0)^{r-1}}{(r-1)!} u^{(r-1)}(x_0)$$

$$+ \frac{(x-x_0)^r}{r!} u^{(r)}(\xi)$$

Lagrange interpolation Given numbers $u_1, u_2, \dots u_r$ and distinct points $x_1, \dots, x_r$ there is one and only one polynomial p_r of degree $< r$ s.t.

$$p_r(x_k) = u_k \quad , \quad 1 \leq k \leq r$$

This polynomial is given explicitly by the formula

$$p_r(x) = u_1 \frac{\prod_{k \neq 1} (x - x_k)}{\prod_{k \neq 1} (x_1 - x_k)} + \dots + u_r \frac{\prod_{k \neq r} (x - x_k)}{\prod_{k \neq r} (x_r - x_k)}$$

Terminology: When $u_k = u(x_k)$, $1 \leq k \leq r$

for some function u, we say that p_r interpolates u at the points $x_1, \dots, x_r$. These points are called the interpolation points. With some abuse of terminology, p_r is sometimes called the interpolant of degree $r-1$ at these points.

Examples and applications

(1) Let $h > 0$ and $x_j \in (a,b)$. Given

$$u(x_j - h), \quad u(x_j) \text{ and } u(x_j + h)$$

find approximations of $u'(x_j)$ and $u''(x_j)$ and discuss their accuracy as $h \to 0$.

We present two methods of solution.

(a) Taylor expansion: let us look for A, B, C s.t.

$E_j := u'(x_j) - A u(x_j - h) - B u(x_j) - C u(x_j + h)$ is smallest in the limit as $h \to 0$

We use

$$u(x_j \pm h) = u(x_j) \pm h u'(x_j) + \frac{h^2}{2} u''(x_j) \pm \frac{h^3}{3!} u'''(x_j) + O(h^4)$$

Then

$$E_j = -u(x_j)\left[A+B+C\right] + u'(x_j)\left[1 + Ah - Ch\right] - \frac{h^2}{2} u''(x_j)\left[A+C\right]$$
$$+ \frac{h^3}{3!} u'''(x_j)\left[A-C\right] + O(h^4)$$

The idea is then to choose A, B, C so as to "knock" as many of the first few coefficients as possible:

$$\left.\begin{aligned} A+B+C &= 0 \\ C-A &= 1/h \\ C+A &= 0 \end{aligned}\right\} \quad C = 1/2h, \; A = -1/2h, \; B = 0$$

Hence

$$\frac{u(x_j+h) - u(x_j-h)}{2h} = u'(x_j) + O(h^2) \text{ as } h \to 0$$

We can do the same in order to find a finite-difference approximation of $u''(x_j)$.

$$E_j := u''(x_j) - A u(x_j - h) - B u(x_j) - C u(x_j + h)$$
$$= -u(x_j)\left[A+B+C\right] + h u'(x_j)\left[A - C\right] + u''(x_j)\left[1 - A\frac{h^2}{2} - C\frac{h^2}{2}\right]$$
$$+ \frac{h^3}{3!} u'''(x_j)\left[A-C\right] + O(h^4)$$

Hence we require

$$\left.\begin{aligned} A+B+C &= 0 \\ A-C &= 0 \\ A+C &= \frac{1}{2h^2} \end{aligned}\right\} \quad A = C = \frac{1}{h^2}, \quad B = -\frac{2}{h^2}$$

o find

$$\frac{2u(x_j) + u(x_j - h)}{} = u''(x_j) + O(h^2)$$

(2) Interpolation: The idea here is to use the function values to construct the interpolating polynomial, and then to use the derivatives of the polynomial as approximations. The quadratic interpolant is

$$p_3(x) = u(x_{j-1})\frac{(x-x_j)(x-x_{j+1})}{(x_{j-1}-x_j)(x_{j-1}-x_{j+1})} + u(x_j)\frac{(x-x_{j-1})(x-x_{j+1})}{(x_j-x_{j-1})(x_j-x_{j+1})}$$

$$+ u(x_{j+1})\frac{(x-x_{j-1})(x-x_j)}{(x_{j+1}-x_{j-1})(x_{j+1}-x_j)}$$

where, for convenience, we have written $x_{j\pm1} = x_j \pm h$. Thus

$$p_3'(x) = u(x_{j-1})\frac{2x-x_j-x_{j+1}}{2h^2} + u(x_j)\frac{2x-x_{j-1}-x_{j+1}}{-h^2} + u(x_{j+1})\frac{2x-x_{j-1}-x_j}{2h^2}$$

$$p_3''(x) = \frac{1}{h^2}\left[u(x_{j-1}) - 2u(x_j) + u(x_{j+1})\right]$$

When we evaluate at x_j, we find the same finite-difference approximations of $u'(x_j)$ and $u''(x_j)$ as we did with the first method.

The interpolation error

Theorem. Let u have r continuous derivatives in the smallest interval containing $x, x_1, \dots, x_r$. Then there exist ξ in that interval s.t.

$$u(x) - p_r(x) = \frac{(x-x_1)\dots(x-x_r)}{r!}\,u^{(r)}(\xi)$$

We can use this result in two ways in order to generate convergent approximations:

(1) Fix r and let the spacing between the interpolation points tend to 0.

This is the essence of the finite-difference approach.

(2) We briefly discuss another approach which is at the basis of spectral methods; it consists of letting $r \to \infty$

Example. Consider the problem of approximating the exponential function in the interval $[0,L]$, using r uniformly spaced points. Then, for $x \in [0,L]$,

$$|u(x) - p_r(x)| = \left|\frac{(x-x_1)\dots(x-x_r)}{r!}\right| e^{\xi}$$

$$\le \frac{L}{(r-1)}\,\frac{1}{r!}\,e^{L}$$

For fixed L, this tends to zero factorially fast

Example. Let now $u(x) = \dfrac{1}{1+a^2x^2}$. Th