Finite difference methods are schemes for approximating the solution to an ODE or PDE, at a discrete set of grid points. We begin by studying schemes for the reaction-diffusion equation and the convection-diffusion equation in one dimension (both ODEs) and then discuss finite differences for the one-dimensional heat equation (a PDE).

5.1. The Reaction-Diffusion Equation

Consider the following problem. Find $u(x)$ satisfying

$$-\frac{d^2u(x)}{dx^2} + r(x)\,u(x) = f(x), \qquad 0 < x < 1,$$

together with the boundary conditions

$$u(0) = 0, \qquad u(1) = 0.$$

The coefficient $r(x)$ is called the reaction coefficient. It controls the strength of the reaction and hence, the size of the reaction term compared to the diffusion term. We will assume that $r(x)$ and $f(x)$ are real-valued functions and a unique solution exists. When working with approximation schemes, it is useful to find examples with exact solutions, to investigate the accuracy of the approximation.

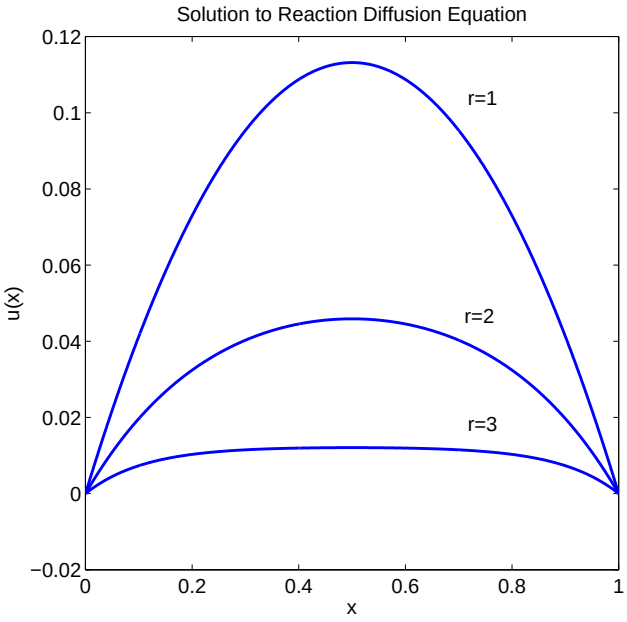

Figure 1: The exact solution to the reaction-diffusion equation when $r = 1, 2, 3$ and $f = 1$.

Example. Suppose $r(x) = 0$ and $f(x) = 1$. Clearly, the exact solution is $u(x) = \frac{1}{2}(x - x^2)$.

Example. Suppose $r(x) = \omega^2$ and $f(x) = 1$. The exact solution (see Figure 1) is

$$u(x) = \frac{1}{\omega^2} - \frac{e^{\omega x} + e^{\omega(1-x)}}{\omega^2(1 + e^{\omega})}.$$

To approximate $u(x)$ we apply the following steps.

1. Set up a grid of uniformly spaced points on the interval $[0,1]$ (the interval on the x-axis on which we want to solve the ODE). If we divide $[0,1]$ into N sub-intervals of width $h = 1/N$, there are $N+1$ grids points x_j with

$$x_0 = 0, \quad x_1 = h, \quad x_2 = 2h, \quad \ldots, \quad x_N = Nh = 1.$$

2. Write down the differential equation at each grid point. We have

$$-\frac{d^2u(x_j)}{dx^2} + r(x_j)\,u(x_j) = f(x_j), \qquad j = 1, 2, \ldots, N-1,$$

and the boundary conditions give

$$u(x_0) = 0, \qquad u(x_N) = 0.$$

3. Approximate the derivatives by **finite difference formulae.**

4. Solve the resulting set of $N-1$ algebraic equations for approximate values $U_j \approx u(x_j)$.

There are lots of possibilities in step 3. We will consider only a 'centred' finite difference scheme.

Definition: Centred Difference. The centred difference δu of $u(x)$ at $x = x_j$ is defined as

$$\delta u(x_j) = u\left(x_j + \frac{h}{2}\right) - u\left(x_j - \frac{h}{2}\right).$$

Applying the above definition twice (exercise) gives the second centred difference

$$\delta^2 u(x_j) = \delta\left(\delta u(x_j)\right) = u(x_{j+1}) - 2u(x_j) + u(x_{j-1}).$$

Notice that if we divide by the distance between the x-values where u is evaluated, then we can use the centred difference $\delta u(x_j)$ to approximate the first derivative. That is

$$\frac{1}{h}\delta u(x_j) = \frac{u\left(x_j + \frac{h}{2}\right) - u\left(x_j - \frac{h}{2}\right)}{h} \approx \frac{du(x_j)}{dx}.$$

Since the second derivative is the first derivative of the first derivative, we also have

$$\frac{1}{h^2}\delta^2 u(x_j) \approx \frac{d^2u(x_j)}{dx^2}.$$

If we make this approximation in the equations written in step 2, then the solution is no longer $u(x_j)$ but an approximate value $U_j \approx u(x_j)$. We have

$$-\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + r_j\,U_j = f_j, \qquad j = 1, 2, \ldots N-1,$$

where we have also used the short-hand notation $r_j = r(x_j), f_j = f(x_j)$. At the boundaries, there is no need to make an approximation, because we already know the solution there so

$$U_0 = u(x_0) = 0, \qquad U_N = u(x_N) = 0.$$

Rearranging the finite difference equations gives

$$-\frac{1}{h^2}U_{j-1} + \left(\frac{2}{h^2} + r_j\right)U_j - \frac{1}{h^2}U_{j+1} = f_j, \qquad j = 1, 2, \ldots, N-1.$$

This is the centred finite difference scheme for the reaction-diffusion equation. We can write the $N-1$ equations for the approximations U_j as a matrix problem

$$\begin{pmatrix} b_1 & c & & & & \\ a & b_2 & c & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & c \\ & & & & a & b_{N-1} \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ \vdots \\ \vdots \\ U_{N-1} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ \vdots \\ f_{N-1} \end{pmatrix},$$

where

$$a = -\frac{1}{h^2}, \qquad b_j = \frac{2}{h^2} + r_j, \quad c = -\frac{1}{h^2}.$$

So, we have to solve a tridiagonal system of equations to obtain approximate values $U_1, \ldots, U_{N-1}$. See the **handout on centred finite differences for the reaction-diffusion equation** for some examples and details about how to solve this system in MATLAB.

The above centred finite difference equations were derived from the approximation for the second derivative

$$\frac{1}{h^2}\delta^2 u(x_j) \approx \frac{d^2u(x_j)}{dx^2}.$$

Is this a good approximation? First, we consider the following Taylor series expansions about x_j

$$u(x_{j+1}) = u(x_j + h) = u(x_j) + hu'(x_j) + \frac{h^2}{2}u''(x_j) + \frac{h^3}{6}u'''(x_j) + \frac{h^4}{24}u^{(4)}(x_j) + \ldots$$

and

$$u(x_{j-1}) = u(x_j - h) = u(x_j) - hu'(x_j) + \frac{h^2}{2}u''(x_j) - \frac{h^3}{6}u'''(x_j) + \frac{h^4}{24}u(4)(x_j) - \ldots.$$

Substituting these into the approximation for the second derivative gives

$$\begin{aligned} \frac{1}{h^2}\delta^2 u(x_j) &= \frac{u(x_j + h) - 2u(x_j) + u(x_j - h)}{h^2} \\ &= \frac{d^2u(x_j)}{dx^2} + \frac{h^2}{12}\frac{d^4u(x_j)}{dx^4} + \text{ terms with higher powers of } h. \end{aligned}$$

Hence, the error in approximating the true second derivative at x_j is

$$\frac{1}{h^2}\delta^2 u(x_j) - \frac{d^2u(x_j)}{dx^2} = \frac{h^2}{12}\frac{d^4u(x_j)}{dx^4} + \text{ terms with higher powers of } h.$$

What about the error in approximating the solution $u(x_j)$ by U_j?

Definition: Global error. The global error in $u(x_j)$ at $x = x_j$ is

$$e_j = u(x_j) - U_j.$$

Definition: Convergence. A finite difference scheme converges if

$$\max_{0\leq j\leq N} \mid e_j \mid \to 0, \qquad \text{as} \qquad N \to \infty.$$

The experiments on the **handout on centred finite differences for the reaction-diffusion equation** show that the centred scheme does converge for the test problems considered. In general, if we don't know the exact solution, then we can't study the global error. We need a way to the quantify error in our approximation that doesn't require the exact solution.

Definition: Truncation error. The truncation error T_j at x_j is the remainder when the exact solution $u(x_j)$ is substituted into the finite difference scheme.

The centred finite difference scheme applied to the reaction-diffusion equation gives

$$-\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} + r_j\, U_j = f_j, \qquad j = 1, 2, \ldots N-1,$$

so substituting $u(x_j)$ for the approximate value U_j and finding the remainder (when we subtract the right-hand side from the left-hand side) gives

$$T_j = -\left(\frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2}\right) + r_j u(x_j) - f_j, \qquad j = 1, 2, \ldots N-1.$$

Now, we also know that $u(x_j)$ satisfies the differential equation so

$$0 = -\frac{d^2u(x_j)}{dx^2} + r_j u(x_j) - f_j, \qquad j = 1, 2, \ldots N-1.$$

Subtracting these gives

$$T_j = \frac{d^2u(x_j)}{dx^2} - \frac{1}{h^2}\left(u(x_{i+1}) - 2u(x_j) + u(x_j - 1)\right).$$

Hence, the truncation error T_j is the error in approximating the second derivative by the centred finite difference. Using the Taylor series calculation above, we have

$$T_j = -\frac{h^2}{12}\frac{d^4u(x_j)}{dx^4} + \text{ terms with higher powers of } h.$$

Definition: Order. The order of a finite difference method is the lowest power of h occurring in T_j.

The centred scheme for the reaction-diffusion equation is second-order.

5.2. The Convection-Diffusion Equation

Consider the following problem. Find $u(x)$ satisfying

$$-\frac{d^2u(x)}{dx^2} + w\,\frac{du(x)}{dx} = f(x), \qquad 0 < x < 1,$$

together with the boundary conditions

$$u(0) = \alpha, \qquad u(1) = \beta.$$

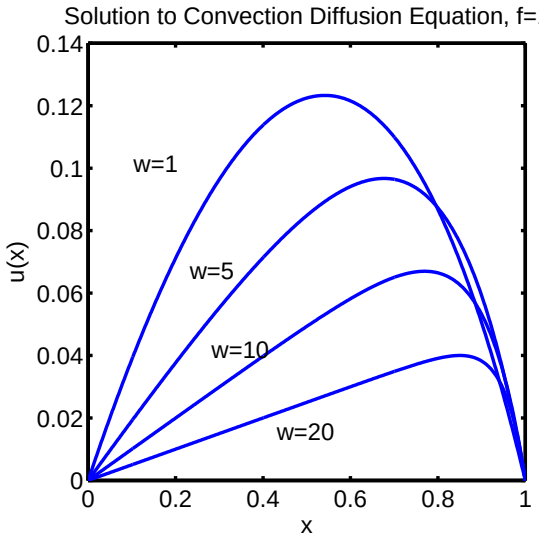

Figure 2: The exact solution to the convection-diffusion equation when $f = 1$ and we have zero boundary conditions.

The coefficient w is called the convection coefficient and we will assume this is a constant. The exact solution in the case of zero boundary conditions is shown in Figure 2.

Notice that there are two derivatives in this equation. We need finite difference approximations for both the second derivative and the first derivative. On Exercise Sheet 7, you are asked to investigate two different schemes. Details of numerical experiments performed in MATLAB are given on the **handout on finite differences for the convection-diffusion problem**.

Centred Finite Differences

The centred method uses the same centred approximation to the second derivative that we used for the reaction-diffusion equation. That is,

$$\frac{d^2u(x_j)}{dx^2} \approx \frac{1}{h^2}\delta^2 u(x_j), \qquad j = 1, 2, \ldots, N-1.$$

In addition, we use a centred approximation for the first derivative given by

$$\frac{du(x_j)}{dx} \approx \frac{u(x_j + h) - u(x_j - h)}{2h} = \frac{u(x_{j+1}) - u(x_{j-1})}{2h}.$$

Combining these approximations, the resulting finite difference equations are

$$-\left(\frac{U_{j+1} - 2U_j + U_{j-1}}{h^2}\right) + w\left(\frac{U_{j+1} - U_{j-1}}{2h}\right) = f_j, \qquad j = 1, 2, \ldots, N-1,$$

and, using the boundary conditions, we have $U_0 = \alpha$, $U_N = \beta$. Again, we have to solve a system of $N-1$ algebraic equations to find $U_1, \ldots, U_{N-1}$. The numerical experiments performed on the handout reveal that there is a problem with this scheme. There are non-physical oscillations in the approximation. The scheme is **unstable**. The scheme is stable only when

$$\frac{|w|h}{2} \leq 1.$$

(You can test this out yourself by doing the numerical experiments on the handout and varying w and h). This means that when w is large, h has to be very small to get a stable solution. The smaller h is, the more equations we have to solve and the more expensive the method becomes.

Upwind Finite Differences

Alternatively, we can keep the centred approximation to the second derivative, as before, but use an 'improved' approximation for the first derivative. The so-called upwind approximation is

$$\frac{du(x_j)}{dx} \approx \frac{u(x_j) - u(x_j - h)}{h} = \frac{u(x_j) - u(x_{j-1})}{h}.$$

The resulting finite difference scheme is stable. There are no restrictions no h. However, for the same value of h, the method is less accurate (see Exercise Sheet 7 and the experiments on the **handout on finite differences for the convection-diffusion problem**).

5.3. The One-Dimensional Heat Equation

Consider the following problem. Find $u(x,t)$ satisfying the one-dimensional heat equation,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < 1, \quad t > 0,$$

together with the boundary conditions

$$u(0,t) = 0, \qquad u(1,t) = 0,$$

and the initial condition

$$u(x,0) = u_0(x).$$

We already know that the exact solution can be expressed as an infinite series, using the method of separation of variables. However, an infinite series is not useful for practical purposes. For instance, if we want to know the value of u at some particular value of x and t, then it is not possible to use the infinite series. (We can never add up infinitely many quantities). We could truncate the series after a few terms and use the truncated series as an approximation. Alternatively, we can use finite difference schemes.

We follow the same steps as for ODEs but to start off, we need a grid in space and time (a space-time grid). The easiest thing is to think about space in the horizontal direction and time t running in the vertical direction. Since $0 < x < 1$, we may use N intervals of length $h = 1/N$ in the x-direction, and label the x-values as

$$x_0 = 0, \quad x_1 = h, \quad \ldots, \quad x_j = jh, \quad x_N = 1.$$

In the t-direction, we'll use intervals of size k, with t-values

$$t_0 = 0, \quad t_1 = k, \quad \ldots, \quad t_m = mh, \quad \ldots.$$

Note that there is no upper limit on the time variable t. We just keep taking steps until we reach the value of t where we want to approximate the solution. We now have two discretisation parameters: h (the spacing in the x-direction) and k (the spacing in the t-direction).

Let U_j^m denote our approximation to $u(x_j, t_m)$. Starting from the known initial values

$$U_j^0 = u(x_j, t_0) = u(x_j, 0) = u_0(x_j), \qquad j = 0, 1, \ldots, N,$$

we compute approximations sequentially at each time step. We briefly look at two finite difference schemes: the explicit method and the implicit method.

Explicit Scheme

The heat equation has two derivatives and we need to approximate both of them, at the grid points (x_j, t_m). For the 'explicit' scheme, we replace the time derivative with a 'first forward difference' and the space derivative with a 'second centred difference'. That is

$$\frac{\partial^2 u(x_j,t_m)}{\partial x^2} \approx \frac{u(x_{j+1},t_m) - 2u(x_j,t_m) + u(x_{j-1},t_m)}{h^2}$$

and

$$\frac{\partial u(x_j,t_m)}{\partial t} \approx \frac{u(x_j,t_{m+1}) - u(x_j,t_m)}{k}.$$

Notice that to approximate the partial derivative with respect to t, we keep the value of x constant and only take a difference over distinct t values, and similarly for the partial derivative with respect to x.

If we write down the heat equation at the point (x_j, t_m) and replace the derivatives with the above approximations, and then replace the exact values $u(x_j, t_m)$ with approximate ones, we obtain the finite difference equations

$$\frac{U_j^{m+1} - U_j^m}{k} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \qquad j = 1, \ldots, N-1, \quad m = 0, 1, \ldots$$

or, writing $\nu = \frac{k}{h^2}$, we can rearrange to give

$$U_j^{m+1} = U_j^m + \nu\left(U_{j+1}^m - 2U_j^m + U_{j-1}^m\right), \qquad j = 1, \ldots, N-1, \quad m = 0, 1, \ldots,$$

with

$$U_0^m = 0, \quad U_N^m = 0, \qquad m = 0, 1, 2, \ldots,$$

(from the boundary conditions) and

$$U_j^0 = u_0(x_j), \qquad j = 0, 1, \ldots, N,$$

(from the initial condition).

The above scheme is called 'explicit' because new values at time level $m+1$ can be computed from the old values at time level m directly. We start from the initial values U_j^0, $j = 0, 1, \ldots, N$ (which are given) and then compute the values U_j^1 at time $t_1 = k$, then at $t_2 = k$, etc. In matrix notation, at step $m+1$, we have to compute

$$\begin{pmatrix} U_1^{m+1} \\ U_2^{m+1} \\ \vdots \\ \vdots \\ \vdots \\ U_{N-1}^{m+1} \end{pmatrix} = \begin{bmatrix} 1-2\nu & \nu & 0 & 0 & \ldots & 0 \\ \nu & 1-2\nu & \nu & 0 & \ldots & 0 \\ 0 & \nu & 1-2\nu & \nu & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \nu & 1-2\nu & \nu \\ 0 & 0 & 0 & 0 & \nu & 1-2\nu \end{bmatrix} \begin{pmatrix} U_1^m \\ U_2^m \\ \vdots \\ \vdots \\ \vdots \\ U_{N-1}^m \end{pmatrix}, \quad m = 0, 1, 2, \ldots$$

At step $m+1$, we know the vector on the right. To compute the vector on the left, all we have to do is a matrix-vector product. No linear system of equations needs to be solved. More details about this computation, and how to do experiments in MATLAB are given on the **handout on the explicit finite difference scheme for the heat equation**.

Example. On the handout, results of two experiments are reported. The initial condition is chosen as

$$u_0(x) = \begin{cases} 2x & 0 \le x \le 1/2 \\ 2 - 2x & 1/2 \le x \le 1 \end{cases}.$$

The explicit finite difference scheme is applied in two different ways. First, we set $h = 1/20$ (so, choose $N = 20$ intervals in space) and $k = 0.0012$. In this case, we have $\nu = k/h^2 = 0.48$. The finite difference approximation seems to be a good one, at each time step (see the pictures on the handout). Now, if we repeat the experiment but choose $k = 0.0013$ (and keep $h = 1/20$) then the approximation has non-physical oscillations and the approximation is terrible! As time progresses, these oscillations only get worse. In this second case, we have $\nu = k/h^2 = 0.52$.

The message from this experiment is that we need to choose h and k very carefully. These parameters have to be compatible. It can be shown that the explicit scheme is **unstable** whenever $\nu > 1/2$. See Exercise Sheet 8 for a further investigation of this issue. To analyse the explicit method properly, we'll need to investigate the error. Again, we must distinguish between global error and truncation error (which can be analysed, even if we don't know the exact solution).

Definition: Global error. The global error in $u(x_j, t_m)$ at the point (x_j, t_m) is

$$e_j^m = u(x_j, t_m) - U_j^m.$$

Definition: Truncation error. The truncation error T_j^m at a point (x_j, t_m) is the remainder when the exact solution is substituted into the approximation scheme.

So, for the explicit scheme,

$$T_j^m = \frac{u(x_j, t_{m+1}) - u(x_j, t_m)}{k} - \left(\frac{u(x_j, t_m) - 2u(x_j, t_m) + u(x_{j-1}, t_m)}{h^2} \right).$$

If we expand the terms $u(x_j, t_{m+1}), u(x_{j+1}, t_m)$ and $u(x_{j-1}, t_m)$ about (x_j, t_m) using Taylor series (in 2 variables now), we find that:

$$T_j^m = \frac{k}{2} \frac{\partial^2 u(x_j, t_m)}{\partial t^2} - \frac{h^2}{12} \frac{\partial^4 u(x_j, t_m)}{\partial x^4} + \text{ terms with higher powers of } h \text{ and } k.$$

So, the scheme is first order in time and second order in space. See Exercise Sheet 8.

Implicit Scheme

The restriction that $\nu < 1/2$ for the explicit scheme means that we need $k \le \frac{1}{2}h^2$. This poses a restriction on the time step and the method becomes expensive for small h. We can improve stability, however, by changing the approximation used for the time derivative.

The 'implicit' finite difference scheme for the heat equation uses the same centred approximation for the space derivative as before

$$\frac{\partial^2 u(x_j, t_m)}{\partial x^2} \approx \frac{u(x_{j+1}, t_m) - 2u(x_j, t_m) + u(x_{j-1}, t_m)}{h^2}$$

and a 'backward' difference approximation for the time derivative

$$\frac{\partial u(x_j, t_m)}{\partial t} \approx \frac{u(x_j, t_m) - u(x_j, t_{m-1})}{k}.$$

If we write down the heat equation at the point (x_j, t_m) and replace the derivatives with the above approximations, and then replace the exact values $u(x_j, t_m)$ with approximate ones, we obtain the finite difference equations

$$\frac{U_j^m - U_j^{m-1}}{k} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{h^2}, \qquad j = 1, \ldots, N-1, \quad m = 1, 2, \ldots$$

or, writing $\nu = \frac{k}{h^2}$, and relabelling $m-1$ as m we can rearrange to give

$$U_{j+1}^m = -\nu U_{j-1}^{m+1} + (1+2\nu)\, U_j^{m+1} - \nu U_{j+1}^{m+1}, \qquad j = 1, \ldots, N-1, \quad m = 0, 1, \ldots,$$

with

$$U_0^m = 0, \quad U_N^m = 0, \qquad m = 0, 1, 2, \ldots,$$

(from the boundary conditions) and

$$U_j^0 = u_0(x_j), \qquad j = 0, 1, \ldots, N,$$

(from the initial condition).

This time, we do need to solve a linear system of equations to compute the approximation at the next time level. At step $m+1$ we have to solve:

$$\begin{bmatrix} 1+2\nu & -\nu & 0 & 0 & \ldots & 0 \\ -\nu & 1+2\nu & -\nu & 0 & \ldots & 0 \\ 0 & -\nu & 1+2\nu & -\nu & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & -\nu & 1+2\nu & -\nu \\ 0 & 0 & 0 & 0 & -\nu & 1+2\nu \end{bmatrix} \begin{pmatrix} U_1^{m+1} \\ U_2^{m+1} \\ \vdots \\ \vdots \\ \vdots \\ U_{N-1}^{m+1} \end{pmatrix} = \begin{pmatrix} U_1^m \\ U_2^m \\ \vdots \\ \vdots \\ \vdots \\ U_{N-1}^m \end{pmatrix}, \quad m = 0, 1, 2, \ldots$$

The implicit scheme converges for all values of $\nu > 0$. There is no restriction on how we choose k and h (for stability). On the **handout on the implicit finite difference scheme for the heat equation**, the same experiment that was conducted with the explicit scheme is repeated. No oscillations are now observed when we choose $\nu = 0.52$.