16 Computation of solutions: introduction

In our study of PDEs we have so far concentrated on deriving solution formulas, thus arriving at ways of finding the solution explicitly. In practice however not all problems are so simple, and may not yield a solution formula. And even if a solution formula can be found, it may not be very revealing about the qualitative behavior of the solution.

In the coming lectures we will reduce the procedure of solving PDEs with auxiliary conditions to a finite number of arithmetic operations, which will allow us to find approximate quantitative solutions of the PDEs. One can then use these approximate solutions to visualize the qualitative behavior of the exact solutions.

There are different methods of reducing PDEs to algebraic equations, from which the numeric solutions are found. We will study the best known method, finite differences, in some detail next.

16.1 Finite differences

The idea of the finite differences method is to replace derivatives by difference quotients. Let us consider a function \( u(x) \) of one variable on the interval \((0, l)\). Choosing a mesh size \( \Delta x \), we would like to approximate the derivatives of \( u \) at the grid points \( j\Delta x \), for \( j = 0, 1, \ldots, J-1 \), by differences of values of \( u \) on the same grid. Recall that the derivative of a function is defined as the limit of a difference quotient,

\[
u'(x) = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x}.
\]

By taking \( \Delta x \) small enough, we can approximate the derivative itself by this quotient.

\[
u'(x) \approx \frac{u(x + \Delta x) - u(x)}{\Delta x}
\]

(1)

Denoting \( u_j = u(j\Delta x) \), we have the following three standard approximations for the first derivative

- **Forward difference**: \( u'(j\Delta x) \approx \frac{u_{j+1} - u_j}{\Delta x} \) \hspace{1cm} (2)
- **Backward difference**: \( u'(j\Delta x) \approx \frac{u_j - u_{j-1}}{\Delta x} \) \hspace{1cm} (3)
- **Centered difference**: \( u'(j\Delta x) \approx \frac{u_{j+1} - u_{j-1}}{2\Delta x} \) \hspace{1cm} (4)

The forward difference approximation (2) is exactly (1) with \( x = j\Delta x \), while the backward difference (3) is the same approximation with \( \Delta x \) replaced by \( -\Delta x \). The centered difference (4), on the other hand, is the average of the forward and backward differences. To estimate the error in the above approximations, we consider the Taylor expansion of \( u(x) \) (assuming \( u \in C^4 \)),

\[
u(x + \Delta x) = u(x) + u'(x)\Delta x + \frac{1}{2} u''(x)(\Delta x)^2 + \frac{1}{6} u'''(x)(\Delta x)^3 + \mathcal{O}(\Delta x)^4,
\]

(5)

where \( \mathcal{O}(\Delta x)^4 \), is used to denote a term of the same order \( (\Delta x)^4 \) in the limit \( \Delta x \to 0 \), i.e. \( \mathcal{O}(\Delta x)^4 / (\Delta x)^4 \) is bounded as \( \Delta x \) approaches zero. Replacing \( \Delta x \) with \( -\Delta x \) in (5), we obtain the following expansion

\[
u(x - \Delta x) = u(x) - u'(x)\Delta x + \frac{1}{2} u''(x)(\Delta x)^2 - \frac{1}{6} u'''(x)(\Delta x)^3 + \mathcal{O}(\Delta x)^4,
\]

(6)

Using (5) and (6), we can compute

\[
\frac{u(x + \Delta x) - u(x)}{\Delta x} = u'(x) + \frac{1}{2} u''(x)\Delta x + \frac{1}{6} u'''(x)(\Delta x)^2 + \mathcal{O}(\Delta x)^3 = u'(x) + \mathcal{O}(\Delta x),
\]
\[
\frac{u(x) - u(x - \Delta x)}{\Delta x} = u'(x) - \frac{1}{2}u''(x)\Delta x + \frac{1}{6}u'''(x)(\Delta x)^2 + \mathcal{O}(\Delta x)^3 = u'(x) + \mathcal{O}(\Delta x),
\]
\[
\frac{u(x + \Delta x) - u(x - \Delta x)}{2\Delta x} = u'(x) + \frac{1}{6}u'''(x)(\Delta x)^2 + \mathcal{O}(\Delta x)^3 = u'(x) + \mathcal{O}(\Delta x)^2.
\]

Thus, the forward and backward difference approximations have an error of order $\Delta x$, while the centered difference approximation has an error of order $(\Delta x)^2$.

Notice that adding (5) and (6) together eliminates $u'(x)$, and we have for the second order derivative
\[
u''(x) = \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2.
\]

From this we get the centered difference approximation for the second derivative,
\[
u''(j\Delta x) \sim \frac{u_{j+1} - 2u_j + u_{j-1}}{(\Delta x)^2}, \tag{7}
\]
which has an error of order $(\Delta x)^2$.

When considering PDEs, one has to account for two (or more) variables. Thus we chose mesh sizes for both variables, and consider a grid for the rectangle $(0, l) \times (0, T)$ with points $(j\Delta x, n\Delta t)$. Then denoting
\[
u^n_j = u(j\Delta x, n\Delta t),
\]
we can approximate the partial derivatives of $u$ with difference quotients of $u$ on the grid. For example the forward difference approximation for $u_t$ is
\[
u_t(j\Delta x, n\Delta t) \sim \frac{u_{j+1}^n - u_j^n}{\Delta t},
\]
while the centered difference approximation for $u_{xx}$ is
\[
u_{xx}(j\Delta x, n\Delta t) \sim \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}.
\]

The errors of the difference approximations of derivatives are called truncation errors, since the approximation arises from truncation of the Taylor series. Using such approximations in a PDE introduces local truncation errors, which are the errors at each step of the approximation. The global truncation error refers to the error in the actual solution arising from the cumulative effect of the local truncation errors. For small mesh sizes $\Delta x, \Delta t$ the truncation errors are small, but they may add up to quite large global errors.

To illustrate how the method of finite differences works for computing the solution of a PDE, we consider the following simple example.

**Example 16.1.** Let us solve the heat equation with the given initial data via finite differences.
\[
\begin{cases}
\nu_t = \nu_{xx}, \\
u(x, 0) = \phi(x).
\end{cases}
\]
Choosing a grid with mesh sizes $\Delta x$ and $\Delta t$, and approximating $u_t$ on the left hand side of the equation by a forward difference, and $u_{xx}$ on the right hand side by a centered difference, we have the difference equation
\[
\frac{u_{j+1}^n - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}. \tag{8}
\]
The truncation error on the left is of order $\Delta t$, while on the right hand side it is of order $(\Delta x)^2$. Choosing a small mesh size $\Delta x$, and taking $\Delta t = s(\Delta x)^2$, (8) will reduce to

$$u_j^{n+1} = s(u_{j+1}^n + u_{j-1}^n) + (1 - 2s)u_j^n. \quad (9)$$

This is a numerical scheme for computing the numerical solution $\{u_j^n\}$, which we call the FTCS scheme (forward time, centered space). Notice that (9) gives the values at the time level $n + 1$ in terms of the values at the previous time level, thus this is an explicit scheme, which can be used to compute the numerical solution at later times from the initial data.

Let us now chose particular values for the relative mesh size $s = (\Delta t)/(\Delta x)^2$, and see what effect the choice of $s$ has on the numerical solution.

$s = 1$. With this choice of $s$ the numerical scheme (9) becomes

$$u_j^{n+1} = u_{j+1}^n - u_j^n + u_{j-1}^n. \quad (10)$$

We take a step function for the initial data $\phi(x)$, which at the grid points $j\Delta x$ is approximated by the values

$$\phi_j : \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad (11)$$

The numerical scheme (10) can be used to “march forward in time”, that is, we take by $u_0^j = \phi_j$ from the initial condition, then compute $u_1^j$ from these values, then $u_2^j$ from the values at the time step 1, and so on. Schematically (10) can be written as the following template

$$\begin{array}{cccc}
* & +1 \bullet & -1 \bullet & +1 \bullet
\end{array}$$

which means that the value at a grid point at a later time denoted by an asterisk can be computed from the values at the bullet points with the given coefficients. Using this template the numerical solution can be computed to be

$$\begin{array}{cccc|cccccccc}
n = 4 & 1 & -4 & 10 & -16 & 19 & -16 & 10 & -4 & 1
n = 3 & 0 & 1 & -3 & 6 & -7 & 6 & -3 & 1 & 0
n = 2 & 0 & 0 & 1 & -2 & 3 & -2 & 1 & 0 & 0
n = 1 & 0 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0
n = 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0
\end{array} \quad (11)$$

Taking into account that we are looking for an approximation to the solution of the heat equation, the above numerical solution appears to be very inaccurate, since the computed values grow in time very fast, while the exact solution of the wave equation decays with time, and can not get larger than the initial data due to the maximum principle. This example shows that although the mesh sizes can be taken to be very small, the numerical scheme can lead to wild numerical solutions.

Let us now try another choice for $s$ in (9).

$s = 1/2$. The numerical scheme and the associated template in this case are

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) \quad \begin{array}{cccc}
& & & \\
* & \frac{1}{2} \bullet & \frac{1}{2} \bullet
\end{array} \quad (12)$$

Using the same initial data (11) as before, we can use the above template to compute the numerical solution.

$$\begin{array}{cccc|cccccccc}
n = 4 & \frac{1}{16} & 0 & \frac{3}{8} & 0 & \frac{5}{8} & 0 & \frac{3}{8} & 0 & \frac{1}{16}
\end{array}$$

Using the same initial data (11) as before, we can use the above template to compute the numerical solution.
While not very accurate, this numerical solution is clearly in the right ballpark, since we see a dissipative behavior, which is expected of solutions of the heat equation.

16.2 Conclusion
We defined the standard difference approximations for the first and second derivatives of a function, and used Taylor’s expansion to estimate the errors in these approximations. Replacing the derivatives in a PDE by these approximations results in a difference equation, which is an algebraic system of equations for the values of the numerical solution at the grid points. Finding the numerical solution through such approximations is the method of finite differences.

We saw an example of the finite differences method applied to the heat equation. For one choice of the mesh sizes we encountered a wild result, while for another the result was qualitatively close to what the expected exact solution should be. In the subsequent lectures we will analyze different numerical schemes, and the conditions that lead to accurate approximations for the solutions.