Finite Difference Methods

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Basic concepts

The basic idea of finite difference methods is to replace derivatives by finite differences. Finite difference methods can be applied on a wide range of problems. However, in order to produce efficient and reliable computational codes, several fundamental questions have to be answered. We now introduce basic concepts by a simple example.

Heat flow through a thin rod can be described by the one-dimensional heat equation

$$\begin{cases} u_t &= \lambda u_{xx} & 0 \le x \le 1, \quad t \ge 0 \\ u(x,0) &= f(x) & \\ u(0,t) &= u(1,t) = 0 & \end{cases} \tag{1}$$

where $\lambda > 0$.

The *solution* of this problem is a function $u = u(x,t)$, which represents the temperature at the point x on the rod at the time t.

The rod has the initial temperature distribution $f(x)$ at time $t = 0$ and has the constant temperature zero at both ends. The value of λ depends on which material the rod is made of.

For every value of t, $u(x,t)$ is a function of x and shows the temperature distribution at the time t. At the beginning, i.e. at $t = 0$, we may have $u(x,0) = f(x) = \sin \pi x + 0.3 \sin 2\pi x - 0.1 \sin 3\pi x$. See Figure 1.

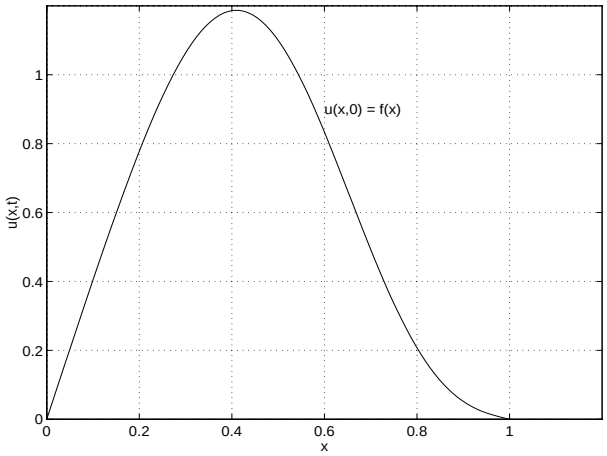

Figure 1: The initial distribution of temperature.

In Figure 2 we have drawn $u(x,t)$ for $t = 0,\ 0.1,\ 0.2,\ 0.3,\ 0.4,\ 0.5$ for the same initial function as above for the case when $\lambda = 0.5$.

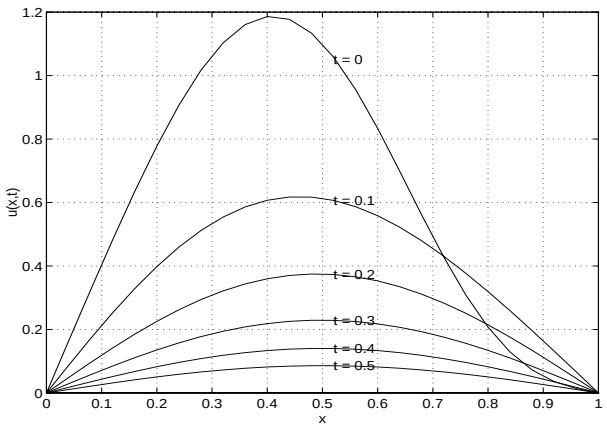

Figure 2: The solution $u(x,t)$ for $t = 0, 0.1, 0.2, 0.3, 0.4,$ and 0.5

In this special case (1) it is relatively easy to write down the solution $u(x,t)$ as a sum of an infinite series which can be computed. This has been done with when producing Figure 2.

However, a PDE-problem can seldom be solved analytically. In most cases we have to rely on numerical methods. Note: In this text we use the standard abbreviation PDE for partial differential equation.

In order to compute the numerical solution a *grid* is introduced. See Figure 3.

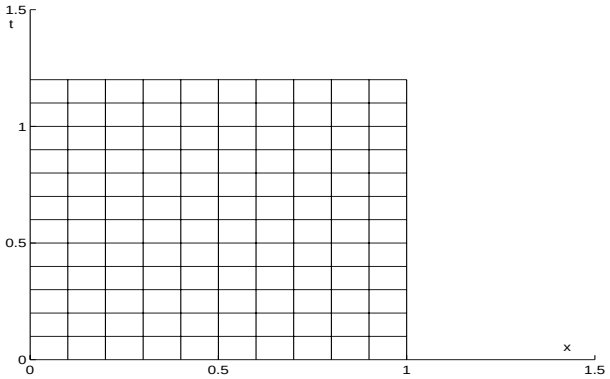

Figure 3: An example of a grid for numerical computations

The following notations are used

Spatial step:	$h = 1/N$	Values of x:	$x_j = j \cdot h,\ j = 0, 1, 2, \ldots, N$
Time step:	k,	Values of t:	$t_n = n \cdot k,\ n = 0, 1, 2, 3, ...$

At the grid point (x_j, t_n) the solution has the value $u(x_j, t_n)$ but this value is not available so we approximate it with u_j^n, i.e. we have

$$u_j^n \approx u(x_j, t_n)$$

The main idea is, as has already been said, that partial derivatives are replaced by finite differences and then the values of u_j^n are computed from the finite difference equations received.

In our example we replace the differential equation $u_t = \lambda u_{xx}$ by the *difference equation*

$$\frac{u_j^{n+1} - u_j^n}{k} = \lambda \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

in each of the interior grid points. It is easy to see that the left hand side approximates u_t. The right hand side corresponds to λu_{xx}.

The values u_j^n can now be computed by the following formulas

$$\begin{cases} u_j^{n+1} = u_j^n + \lambda k/h^2 \cdot (u_{j+1}^n - 2u_j^n + u_{j-1}^n) & j = 1, 2, \ldots, N-1 \\ & n = 0, 1, \ldots \\ u_0^n = u_N^n = 0, & n = 0, 1, \ldots \\ u_j^0 = f(x_j), & j = 0, 1, \ldots, N. \end{cases} \tag{2}$$

The unknowns u_j^n, i.e. the approximations to $u(x, t)$ in the grid points, are computed in the following order

$$u_1^1, u_2^1, \ldots, u_{N-1}^1, \quad u_1^2, u_2^2, \ldots, u_{N-1}^2, \quad \ldots$$

The order is from left to right and from bottom to top in the grid, as illustrated in Figure 4.

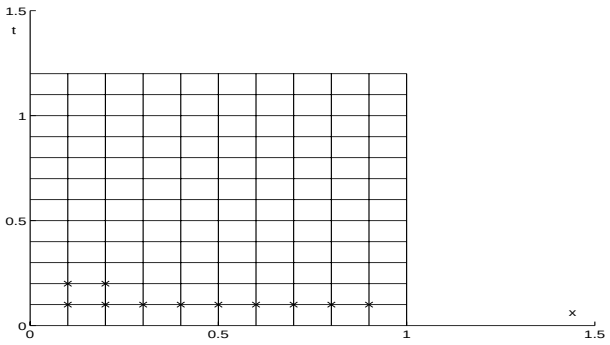

Figure 4: Order of computations

The difference method above is called *Euler's method* or *forward Euler*.

If we replace $u_t = \lambda u_{xx}$ in the grid points by

$$\frac{u_j^{n+1} - u_j^n}{k} = \lambda \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}$$

we get *backward Euler*. The complete formulas are

$$\begin{cases} -\lambda k/h^2 \cdot u_{j+1}^{n+1} + (1 + 2\lambda k/h^2) u_j^{n+1} - \lambda k/h^2 u_{j-1}^{n+1} = u_j^n & j = 1, 2, \ldots, N-1 \\ & n = 1, 2, \ldots \\ u_0^n = u_N^n = 0, & n = 1, 2, \ldots \\ u_j^0 = f(x_j), & j = 0, 1, \ldots, N. \end{cases} \tag{3}$$

Backward Euler is *implicit*. For every time step we have $N-1$ unknowns, u_1^{n+1}, $u_2^{n+1}, \ldots, u_{N-1}^{n+1}$, and $N-1$ equations forming a tridiagonal linear system. Thus, one time step with backward Euler is more expensive than one time step with forward Euler.

If we combine forward Euler and backward Euler, i.e. taking the mean value of these two, we get the *Crank-Nicolson method*.

$$\begin{cases} -\lambda k/(2h^2) \cdot u_{j+1}^{n+1} + (1 + \lambda k/h^2) \cdot u_j^{n+1} - \lambda k/(2h^2) \cdot u_{j-1}^{n+1} & \\ \quad = \lambda k/(2h^2) \cdot u_{j+1}^n + (1 - \lambda k/h^2) \cdot u_j^n + \lambda k/(2h^2) \cdot u_{j-1}^n & j = 1, 2, \ldots, N-1 \\ & n = 1, 2, \ldots \\ u_0^n = u_N^n = 0, & n = 1, 2, \ldots \\ u_j^0 = f(x_j), & j = 0, 1, \ldots, N. \end{cases} \tag{4}$$

This is also an *implicit* method and we have to solve a linear tridiagonal system in every time step.

A finite difference scheme will give useful results only if the computational process is *stable*, i.e. if "errors and perturbations are not amplified" during the computational process. *Stability* is a fundamental concept in numerical analysis. The forward Euler scheme of the one-dimensional heat equation is stable if h and k are chosen such that they satisfy the condition $\lambda k/h^2 \leq 1/2$. This is a hard constraint on k, which has to be of the order h^2. As h must be fairly small to give a good resolution, the time step k has to be very small in order to fulfill the stability condition.

We now give some definitions and a fundamental theorem.

1. A *PDE-problem* consists of a PDE (or a system of PDE:s) and initial and/or boundary conditions. The heat-flow problem (1) is a PDE-problem.

2. A *well-posed PDE-problem* fulfills the following conditions:

   (a) It has a unique solution

   (b) The solution "depends continuously" on initial and boundary data, i.e. small perturbations in these data give only small perturbations in the solution.

   The heat flow problem (1) is a well-posed PDE-problem.

3. The *local truncation error*, Ψ, of a PDE-problem is the difference between the left and right hand members of the difference approximation when applied on the true solution $u(x,t)$ of the PDE-problem. The forward Euler and backward Euler methods have local truncation error $O(k) + O(h^2)$. Thus, *the order of approximation* is $(1,2)$. The Crank-Nicolson method uses symmetric approximations of the derivatives and has order of approximation $(2,2)$.

4. A difference approximation is *consistent* to a PDE-problem if the local truncation error Ψ tends to zero when the step lengths h and k tend to zero.

5. A difference approximation is *convergent* if the solutions of the finite difference equations $u_j^n \to u(x_j, t_n)$. This definition is vague but can of course be formulated in a strict mathematical way.

6. *Lax-Richtmyer's equivalence theorem:* If we have a well-posed PDE-problem and a consistent difference approximation then

$$stability \Leftrightarrow convergence.$$

We need convergence (and in fact *fast* convergence). From Lax-Richtmyer's equivalence theorem we can conclude that examination of the stability is the crucial part when examining convergence.

We present three different ideas of *stability investigation.*

1. *Studies of perturbations*
   Let all initial and boundary values be zero. Then all $u_j^n = 0$ if the PDE is homogeneous. Now, let $u_j^n = \epsilon$ in one grid point and check what happens for a certain combination of h and k. If u_j^n is not increasing with n, then the difference approximation is stable, otherwise unstable.

2. *The Fourier method (the von Neumann method)*
   For every step in time ($t = t_n$) the grid function u_j^n can be represented by a Discrete Fourier Transform (DFT)

   $$u_j^n = \sum \hat{u}_\omega^n e^{i\omega x_j}, \text{ where the integer } \omega \text{ runs between } -r \text{ and } r$$
   $$\text{and where } 2r + 1 = N$$

   This expression is inserted into the difference scheme and the growth of the *Fourier coefficients* is studied. In particular for a one step method we can define the amplification factor $\hat{Q} = \hat{u}_\omega^{n+1}/\hat{u}_\omega^n$. If $\left|\hat{Q}\right| \leq 1$ then the method is stable. This inequality will give the stability condition on h and k. Strictly speaking this method is applicable only for linear problems with constant coefficients and periodic boundary conditions. However, it can be useful also in more general cases giving *necessary* conditions for stability, e.g. if the method is not stable for the case with periodic boundary conditions then it is not stable for any other boundary conditions.

3. *The energy method*
   Here the growth of the *solution* is studied. The norm at time level n is defined by

   $$\|u^n\|^2 = \sum_{j=0}^{N} \left|u_j^n\right|^2 h.$$

   Then the norms $\|u^{n+1}\|^2$ and $\|u^n\|^2$ are compared in order to find out if the perturbations will grow or not.