Numerical Solutions for Partial Differential Equations

S. DELAHAIES

February 14, 2012

1 Preliminaries

1.1 Taylor theorem

Theorem 1.1 (Taylor formula in 1D) *Let $n \geq 0$ be an integer and f a function from $\mathbb{R}$ to $\mathbb{R}$ which is n times continuously differentiable on the closed interval $[a, b]$ and $n+1$ times differentiable on the open interval (a, b), then for $x \in (a, b)$ and $x + h \in (a, b)$ we have*

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2!} + \cdots + f^{(n)}\frac{h^n}{n!} + R(x), \tag{1}$$

where the remainder term $R(x)$ is such that $R(x) = O(x^{n+1})$. The right hand side of (1) is called the Taylor expansion of order n of f at x.

Definition 1.2 (Banach-Landau notation) *...*

Example 1.3 *Find the Taylor expansion of order 3 of the function $x \mapsto \cos x$ at $\pi/2$ and find a bound for the remainder term.*

Theorem 1.4 (Taylor formula in 2D) *Let $n \geq 0$ be an integer and f a function from $\mathbb{R}^2$ to R which is $n+1$ times continuously differentiable with respect to all its variables on the open set $(a, b) \times (c, d)$, then for $(x, y) \in (a, b) \times (c, d)$ and $(x + \Delta x, y + \Delta y) \in (a, b) \times (c, d)$ we have*

$$f(x+\Delta x, y+\Delta y) = f(x, y) + \sum_{k=1}^{n} \frac{1}{n!}\left[\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y}\right]^n f_{|(x,y)} + R(x, y), \tag{2}$$

where the remainder term $R(x, y)$ is such that $R(x, y) = O(x^{n+1}, y^{n+1})$. The right hand side of (2) is called the Taylor expansion of order n of f at (x, y).

Example 1.5 *Find the Taylor expansion of order 1 of the function $(x, y) \mapsto \mathrm{e}^y \cos x$ at $(0, 2)$ and find a bound for the remainder term.*

1.2 PDE background

Let (E) be the following second order PDE

$$\underbrace{au_{xx} + bu_{xy} + cu_{yy}}_{\text{principal linear part (2nd order)}} \quad + f(x, y, u, u_x, u_y) = 0. \tag{3}$$

The PDE is :

- elliptic if $b^2 - 4ac < 0$,
- parabolic if $b^2 - 4ac = 0$,
- hyperbolic if $b^2 - 4ac > 0$.

Example 1.6

- *Poisson equation* $u_{xx} + u_{yy} = f(x, y)$ *: elliptic,*
- *Heat equation* $u_t = \kappa u_{xx},\ \kappa > 0$ *: parabolic,*
- *wave equation* $u_{tt} = u_{xx},\ u_t = u_x,\ u_t = -u_x$ *: hyperbolic.*

2 Finite differences

2.1 Discretization

Let $\mathcal{E}$ be the following "model" 2nd order partial differential equation (PDE)

$$F\left(x^1, \ldots, x^n, u(x^1, \ldots, x^n), \ldots, \frac{\partial u}{\partial x^i}, \ldots, \frac{\partial^2 u}{\partial x^i \partial x^j}\right) = 0, \tag{4}$$

for a function u on a domain $\Omega \in \mathbb{R}^n$. Using numerical methods to find an approximate solution U on the domain Ω consists in :

- discretizing the domain Ω,
- defining an approximate equation E.
- considering an approximate solution U on the discretized domain,
- characterizing the accuracy of the approximate solution U.

We consider a smooth solution u depending on n variables $x^1, \ldots, x^n$ on a rectangular domain $[a_1, b_1] \times \cdots \times [a_n, b_n]$. We discretize the domain into a set of $m_1 \ldots ...m_n$ points (nodes) $\{x^1_{k_1}, \ldots, x^n_{k_n}\}$ given by

$$\left\{ \begin{array}{ccc} x^1_{k_1} & = & a_1 + k_1 \Delta x^1,\ k_1 = 1..m_1 \\ & ... & \\ x^n_{k_n} & = & a_n + k_n \Delta x^n,\ k_n = 1..m_n \end{array} \right. \tag{5}$$

where $\Delta x^i = (b_i - a_i)/m_i$. The set $\{x^1_{k_1}, \ldots, x^n_{k_n}\}_{k_1,\ldots,k_n}$ is called a mesh or a grid, $(\Delta x^i)_i$ defines the mesh spacing. For simplicity a point $(x^1_{k_1}, \ldots, x^n_{k_n})$ will be denoted by $(k_1, \ldots, k_n)$. Let

$$u_{k_1,\ldots,k_n} = u(x^1_{k_1}, \ldots, x^n_{k_n}) \tag{6}$$

be the exact solution at the mesh point $(k_1, \ldots, k_n)$, and

$$U_{k_1,\ldots,k_n} = u_{k_1,\ldots,k_n} \tag{7}$$

be the approximate solution at that mesh point.

2.2 Finite differences

Let $u(x)$ be a smooth function from a real interval (a,b) to $\mathbb{R}$. The Taylor series expansion for $u(x)$ at $x^* \in (a,b)$ can be written as

$$u(x^*+h) = u(x^*) + u_x\Big|_{x^*} h + u_{xx}\Big|_{x^*} \frac{h^2}{2!} + u_{xxx}\Big|_{x^*} \frac{h^3}{3!} + \ldots, \tag{8}$$

or

$$u(x^*-h) = u(x^*) - u_x\Big|_{x^*} h + u_{xx}\Big|_{x^*} \frac{h^2}{2!} - u_{xxx}\Big|_{x^*} \frac{h^3}{3!} + \ldots, \tag{9}$$

from which we can write

$$u_x\Big|_{x^*} = \frac{u(x^*+h) - u(x^*)}{h} - u_{xx}\Big|_{x^*} \frac{h}{2!} - u_{xxx}\Big|_{x^*} \frac{h^2}{3!} - \ldots, \tag{10}$$

$$u_x\Big|_{x^*} = \frac{u(x^*) - u(x^*-h)}{h} + u_{xx}\Big|_{x^*} \frac{h}{2!} - u_{xxx}\Big|_{x^*} \frac{h^2}{3!} + \ldots. \tag{11}$$

We can then consider two approximations to the first derivative of u at x^*, given by

$$u_x\Big|_{x^*} \approx \frac{u(x^*+h) - u(x^*)}{h} \tag{12}$$

$$u_x\Big|_{x^*} = \frac{u(x^*) - u(x^*-h)}{h}. \tag{13}$$

Both approximations introduce an error E_{x^*}. This error is characterised by the first (and largest) term in the truncated series, it is given by

$$E_{x^*} = \pm \frac{h}{2} u_{xx}\Big|_{x^*} = O(h),$$

The error (or the approximation) is then said to be of order h or 1 (that is the degree of h). Adding (10) and (11) and solving for u_x, we see that

$$u_x\Big|_{x^*} \approx \frac{u(x^*+h) - u(x^*-h)}{2h}, \tag{14}$$

and the first truncated term is given by

$$E_{x^*} = \frac{h^2}{6} u_{xxx}\Big|_{x^*} = O(h^2),$$

thus of order 2. Substracting (11) from (10) and solving for u_{xx} we see that

$$u_{xx}\Big|_{x^*} \approx \frac{u(x^*+h) - 2u(x^*) + u(x^*-h)}{h^2}, \tag{15}$$

and the first truncated term is given by

$$E_{x^*} = \frac{h^2}{12} u_{xxxx}\Big|_{x^*} = O(h^2),$$

thus of order 2.

Consider a discretization of the variable x into a grid x_i of the form $x_i = a + i\Delta x$, and an approximation U_i of u at the mesh point i. Equations (12), (13), (14) and (15) give the following approximations for u_x and u_{xx} :

$$u_x\Big|_{x_i} \approx \frac{U_{i+1} - U_i}{\Delta x}, \tag{16}$$

$$u_x\Big|_{x_i} \approx \frac{U_i - U_{i-1}}{\Delta x}. \tag{17}$$

$$u_x\Big|_{x_i} \approx \frac{U_{i+1} - U_{i-1}}{2\Delta x}, \tag{18}$$

$$u_{xx}\Big|_{x_i} \approx \frac{U_{i+1} - 2U_i + U_{i-1}}{\Delta x^2}. \tag{19}$$

Let us introduce the following notation and terminology

- the *forward* difference operator F_x:

$$F_x U_i = U_{i+1} - U_i,$$

- the *backward* difference operator :

$$B_x U_i = U_i - U_{i-1},$$

- the *1st order central* difference operator :

$$D_x U_i = U_{i+1} - U_{i-1},$$

- the *2nd order central* difference operator :

$$\delta_x^2 U_i = U_{i+1} - 2U_i + U_{i-1}.$$

In terms of these operators u_x can be approximated by $\frac{F_x U_i}{\Delta x}$, $\frac{B_x U_i}{\Delta x}$ and $\frac{D_x U_i}{2\Delta x}$ at the mesh point x_i, and u_{xx} at x_i can be approximated by $\frac{\delta_x^2 U_i}{2\Delta x}$ at that point.

So far we considered a function u of a single variable x, we now consider u as a smooth function of 2 variables $u = u(x, y)$ on a rectangular domain $\Omega = [a_1, b_1] \times [a_2, b_2]$. Let $x_i, y_{j_{i,j}}$ be a mesh discretizing Ω such that

$$x_i = a_1 + i\Delta x \ , \ y_j = a_2 + j\Delta y,$$

and let $U_{i,j}$ be an approximation of u at the mesh point (x_i, y_j), that is

$$U_{i,j} \approx u_{i,j} = u(x_i, y_j).$$

Using a forward difference operator we obtain the 1st order approximation for u_x and u_y at (i, j) given by

$$u_x\Big|_{(i,j)} \approx \frac{U_{i+1,j} - U_{i,j}}{\Delta x} \quad \text{and} \quad u_y\Big|_{(i,j)} \approx \frac{U_{i,j+1} - U_{i,j}}{\Delta y} \ ,$$

and a 2nd order central difference operator gives the approximation for $u_x x$ and $u_y y$ at (i,j) given by

$$u_{xx}\Big|_{(i,j)} \approx \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{\Delta x^2} \quad \text{and} \quad u_{yy}\Big|_{(i,j)} \approx \frac{U_{i,j+1} + 2U_{i,j} - U_{i,j-1}}{\Delta y^2}.$$

We now need to find an approximation for the mixed derivative u_{xy}. We have

$$\begin{aligned}
u_{xy}\Big|_{i,j} &= \frac{\partial}{\partial x}\left[\frac{\partial u}{\partial y}\right]\Big|_{i,j} \\
&= \frac{1}{2\Delta x}\left[\frac{\partial u}{\partial y}\Big|_{i+1,j} - \frac{\partial u}{\partial y}\Big|_{i-1,j}\right] + O(\Delta x^2) \\
&= \frac{1}{2\Delta x}\left[\frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y} + \frac{\Delta y^2}{3!}u_{yyy}\Big|_{i+1,j} + \dots \right. \\
&\qquad \left. + \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y} - \frac{\Delta y^2}{3!}u_{yyy}\Big|_{i-1,j} + \dots\right] + O(\Delta x^2) \\
&= \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{2\Delta x \Delta y} + O(\Delta x^2, \Delta y^2)
\end{aligned}$$

then we obtain the following approximation of order (2,2) for u_{xy} at (i,j)

$$u_{xy}\Big|_{i,j} = \frac{U_{i+1,j+1} - U_{i+1,j-1} - U_{i-1,j+1} + U_{i-1,j-1}}{2\Delta x \Delta y} \tag{20}$$

3 Parabolic equations

We consider the model equation of heat diffusion in one spatial dimension, ie

$$u_t = u_{xx}, \quad x \in (0,1), \quad t > 0, \tag{21}$$

with Dirichlet boundary conditions

$$u(0,t) = a(t) \tag{22}$$
$$u(1,t) = b(t) \tag{23}$$

and initial condition

$$u(x,0) = f(x). \tag{24}$$

We will use this canonical example to illustrate different approximation schemes and to introduce the concepts of consistency, convergence and stability of the methods.

3.1 discretization

We start with the discretization of the domain $[0,1] \times \mathbb{R}^+$. We divide the spatial domain in N regular blocks so that $\Delta x = 1/N$ and we choose a time step Δt, then the grid is formed of points (x_i, t_j) with

$$\begin{aligned}
x_i &= i\Delta x\ , i = 1, \dots, N, \\
t_j &= j\Delta t\ , j \in \mathbb{N}.
\end{aligned}$$

We replace u by an approximation U such that

$$U_{i,j} \approx u_{i,j} = u(x_i, t_j).$$

We now need to discretize equation (21). We use a foward time central space (FTCS) scheme (also called Euler scheme) that is

$$u_t\Big|_{i,j} \approx \frac{F_t U_{i,j}}{\Delta t} \quad , \quad u_{xx}\Big|_{i,j} \approx \frac{\delta_x^2 U_{i,j}}{\Delta x^2}.$$

therefore our approximation to the PDE becomes

$$\frac{U_{i,j+1} - U_{i,j}}{\Delta t} = \frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{\Delta x^2}. \tag{25}$$

The above expression can be rearranged in the form

$$U_{i,j+1} = rU_{i+1,j} + (1 - 2r)U_{i,j} + rU_{i-1,j}, \tag{26}$$

where $r = \Delta t / \Delta x^2$ is called the mesh ratio. Equation (26) applies to all interior points, that is for $i = 1, \ldots, N-1$ and $j > 0$. The boundary conditions give

$$U_{0,j} = a(t_j) \quad , \quad U_{N,j} = b(t_j), \tag{27}$$

and initial condition gives

$$U_{i,0} = f(x_i). \tag{28}$$

Then (27), (28) together with equation (26) provides us with a recursion relation to calculate an approximate solution to (21) for all t_j, $j \geq 0$. The FTCS sheme is said to be *explicit* for we only need values of U at earlier times to calculate the value of U at the present time. Moreover it is a *one step* scheme for it only requires the values of U at the previous time step.

Algorithm :

1. Choose N and r and find Δx and Δt.
2. Use the initial conditions to find $U_{i,0}$, $i = 0, \ldots, N$.
3. Use equation (26) to calculate $U_{i,j+1}$ from $U_{:,j}$ for all $i = 1, \ldots, N-1$, and use the boundary conditions to calculate $U_{0,j+1}$ and $U_{1,j+1}$.
4. Set $j = j + 1$ and repeat 3. and 4. until the desired time is reached.

Example 3.1 *Use the FTCS scheme with $N = 4$ and $r = 0.4$ to calculate an approximate solution to*

$$u_t = u_{xx}, \quad x \in (0, 1), \quad t > 0, \tag{29}$$

with boundary conditions

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

and initial condition

$$u(x, 0) = \sin \pi x,$$

up to time t=1/20.

We use the algorithm described above:

1. $\Delta x = 1/N = 1/4$ and since $r = \Delta t/\Delta x^2$ then $\Delta t = r\Delta x^2 = 0.4(1/4)^2 = 1/40$. We need to find the solution up to $t = 1/20$ this require $(1/20)/(1/40)$ steps, that is 2 steps.we need to calculate the values of U at each of the mesh points.

2. We calculate $U_{i,0}$, $i = 0, \dots, 4$, using the initial condition:

$$\begin{aligned} U_{0,0} &= \sin \pi 0 = 0, \\ U_{1,0} &= \sin 0.25\pi = 1/\sqrt{2}, \\ U_{2,0} &= \sin 0.5\pi = 1, \\ U_{3,0} &= \sin 0.75\pi = 1/\sqrt{2}, \\ U_{4,0} &= \sin \pi = 0. \end{aligned}$$

3. We calculate the values of U for the interior points using the FTCS scheme:

$$U_{i,j+1} = rU_{i+1,j} + (1-2r)U_{i,j} + rU_{i-1,j},$$

for $i = 1, \dots, 3$ and $j = 1, 2$. We have (!!)

$$\begin{aligned} U_{0,1} &= 0 \quad \text{from boundary condition} \\ U_{1,1} &= rU_{2,0} + (1-2r)U_{1,0} + rU_{0,0} \\ &= (0.4)(0) + (1-0.8)(1/\sqrt{2}) + (0.4)(1) \\ &= 0.5414 \quad \text{to 4 decimals} \\ U_{2,1} &= rU_{3,0} + (1-2r)U_{2,0} + rU_{1,0} \\ &= (0.4)(1/\sqrt{2}) + (1-0.8)(1) + (0.4)(1/\sqrt{2}) \\ &= 0.7656 \quad \text{to 4 decimals} \\ U_{3,1} &= rU_{4,0} + (1-2r)U_{3,0} + rU_{2,0} \\ &= (0.4)(1) + (1-0.8)(1/\sqrt{2}) + (0.4)(0) \\ &= 0.5414 \quad \text{to 4 decimals} \\ U_{4,1} &= 0 \quad \text{from boundary condition.} \end{aligned}$$

We set $j = j + 1 = 2$ and we repeat the calculation

$$\begin{aligned} U_{0,2} &= 0 \quad \text{from boundary condition} \\ U_{1,2} &= rU_{2,1} + (1-2r)U_{1,1} + rU_{0,1} \\ &= (0.4)(0) + (1-0.8)(0.5414) + (0.4)(0,7656) \\ &= 0.4145 \quad \text{to 4 decimals} \\ U_{2,2} &= rU_{3,1} + (1-2r)U_{2,1} + rU_{1,1} \\ &= (0.4)(0.5414) + (1-0.8)(0.7656) + (0.4)(0.5414) \\ &= 0.5862 \quad \text{to 4 decimals} \\ U_{3,2} &= rU_{4,1} + (1-2r)U_{3,1} + rU_{2,1} \\ &= 0.4145 \quad \text{to 4 decimals} \\ U_{4,2} &= 0 \quad \text{from boundary condition.} \end{aligned}$$

3.2 Local truncation error

In the previous section we derived a method for finding an approximate solution to the heat diffusion equation $u_t = u_{xx}$, how accurate is this approximate solution? We can characterize the accuracy of the approximate solution using the notion of local truncation error.

Definition 3.2 (Local truncation error)
Let $\mathcal{L}$ be a differential operator such that $\mathcal{L}u = 0$, ie u is a solution, and let $\mathcal{L}_\Delta$ be an approximating difference operator to $\mathcal{L}$. The local truncation error (LTE) is given by $\mathcal{L}_\Delta u$.

Definition 3.3 (Order of an approximation, consistency)
The order of an approximation is given by the order of the leading term of the LTE. That is, if the leading term is of order $O(\Delta x^{\,p}, \Delta t^{\,q})$ then the method is said to be of order p in space and of order q in time.

A method is called consistent with the PDE if LTE $\to 0$ as $\Delta x \to 0$ and $\Delta t \to 0$.

Note that consistency requires that the order (p, q) satisfies $p > 0$ and $q > 0$.

Example 3.4 *Find the LTE for the FTCS scheme for the heat diffusion equation.*

The heat diffusion equation is $u_t = u_{xx}$, it can be writen as $\mathcal{L}u = 0$ where $\mathcal{L}$ is the differential operator given by

$$\mathcal{L} = \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}. \tag{30}$$

The FTCS approximate differential operator is given by

$$\mathcal{L}_\Delta = \frac{F_t}{\Delta t} - \frac{\delta_x^2}{\Delta x^{\,2}}, \tag{31}$$

then the LTE is $\mathcal{L}_\Delta u$ where u is a solution of $\mathcal{L}u = 0$. We have

$$\mathcal{L}_\Delta u = \frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} - \frac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{\Delta x^{\,2}},$$

and we use Taylor's theorem to simplify this expression:

$$\begin{aligned}\frac{F_t u}{\Delta t} &= \frac{1}{\Delta t}\left[u(x,t) + u_t \Delta t + \frac{\Delta t^{\,2}}{2!}u_{tt} + \frac{\Delta t^{\,3}}{3!}u_{ttt} + O(\Delta t^{\,4}) - u(x,t)\right] \\ &= u_t + \frac{\Delta t}{2!}u_{tt} + \frac{\Delta t^{\,2}}{3!}u_{ttt} + O(\Delta t^{\,3})\end{aligned}$$

and

$$\begin{aligned}\frac{\delta_x^2 u}{\Delta x^{\,2}} = \frac{1}{\Delta x^{\,2}}\Bigg[&u(x,t) + u_x \Delta x + \frac{\Delta x^{\,2}}{2!}u_{xx} + \frac{\Delta x^{\,3}}{3!}u_{xxx} + \frac{\Delta x^{\,4}}{4!}u_{4x} + \frac{\Delta x^{\,5}}{5!}u_{5x} \\ &+ O(\Delta t^{\,6}) - 2u(x,t) + u(x,t) - u_x \Delta x + \frac{\Delta x^{\,2}}{2!}u_{xx} - \frac{\Delta x^{\,3}}{3!}u_{xxx} \\ &+ \frac{\Delta x^{\,4}}{4!}u_{4x} - \frac{\Delta x^{\,5}}{5!}u_{5x} + O(\Delta t^{\,6})\Bigg] \\ = u_{xx} + \frac{\Delta x^{\,2}}{12}u_{4x} + O(\Delta x^{\,4})&\end{aligned}$$

therefore we have

$$\mathcal{L}_\Delta u = u_t + \frac{\Delta t}{2!} u_{tt} + \frac{\Delta t^2}{3!} u_{ttt} + O(\Delta t^3) - \left(u_{xx} + \frac{\Delta x^2}{12} u_{4x} + O(\Delta x^4) \right).$$

Since $u_t - u_{xx} = 0$ and then $u_{tt} - u_{xxxx} = 0$, the LTE becomes

$$\mathcal{L}_\Delta u = \left(\frac{\Delta t}{2} - \frac{\Delta x^2}{12} \right) u_{tt} + \frac{\Delta t^2}{6} u_{ttt} + O(\Delta t^3) + O(\Delta x^4).$$

Therefore the FTCS scheme is 1st order in time and 2nd order in space. Note that for $\Delta t = (1/6)\Delta x^2$ then the scheme becomes 2nd order in time and 4th order in space.