Numerical Methods

Partial Differencial equations I

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1 Example problem

Consider as a simple example the heat or diffusion equation posed on the interval $x \in (0,1)$ subject to boundary and initial conditions:

$$\text{PDE:} \qquad \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \tag{1}$$

$$\text{BC:} \qquad T(0,t) = 0 \quad \text{and} \quad T(1,t) = 1, \tag{2}$$

$$\text{IC:} \qquad T(x,0) = x + \sin 4\pi x + 5 \sin 9\pi x. \tag{3}$$

The object is to find a solution to the problem (PDE+BC+IC) for $0 < x < 1$ and $0 < t \leq t_f$ for some final time t_f.

2 Well-Posed Problems

There are three ingredients to a partial differential equation problem:

1. **The equation itself.**
2. **The domain Ω of independent variables on which the partial differential equation is to be satisfied.**
3. **The boundary conditions that the solution must satisfy at the boundary of Ω. (The boundary conditions may be initial conditions if one of the independent variables corresponds to time.)**

The basic problem to be solved in the theory of partial differential equations is the **well-posedness problem:**

*is a partial differential equation together with the specified initial and/or boundary conditions well posed? That is, does a solution **exist** that satisfies the equation within Ω and the prescribed data on the boundary of Ω, is the solution **unique**, and does it depend **continuously** on the prescribed data?*

We view the problem differently and ask what sorts of boundaries and boundary/initial conditions are appropriate for given PDEs in order that the problem be well-posed.

3 Space-time discretization

We consider solutions to the heat equation on a finite interval $x \in (0, \ell)$ subject to Dirichlet boundary conditions and arbitrary (i.e. user specified) initial conditions:

$$\text{PDE:} \qquad \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < \ell, \quad t > 0 \tag{4}$$

$$\text{BC:} \qquad u(0,t) = \gamma_0 \quad \text{and} \quad u(\ell,t) = \gamma_\ell, \quad t > 0 \tag{5}$$

$$\text{IC:} \qquad u(x,0) = u^0(x), \quad 0 \le x \le \ell. \tag{6}$$

Assume the γ's are time-independent. We need a numerical representation for the function $u(x,t)$ and the for operators $\frac{\partial}{\partial t}$ and $\frac{\partial^2}{\partial x^2}$.

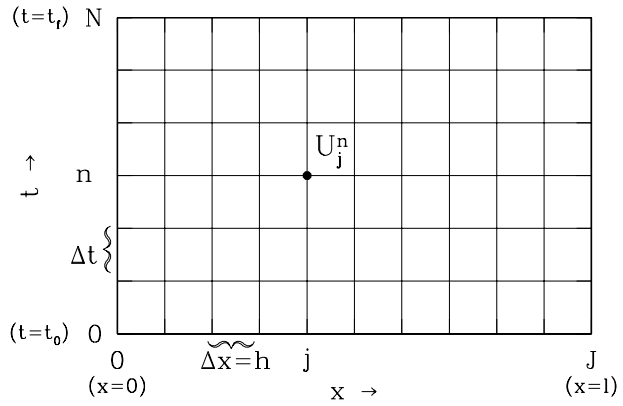
In the simplest case the dependent variable u is represented by values on a uniform grid or lattice in space and time.

- Divide the interval $[0, \ell]$ into J equally spaced intervals of size $\triangle x$ or h (we use these interchangeably). Hence $h = \triangle x = \ell/J$. Only 2 of the three (ℓ, h, J) are independent. There are a total of $J + 1$ grid points labeled x_j. For the uniform grid $x_j = j\triangle x, \;\; j = 0, J$.

- n labels time steps, t_n denotes grid points in the direction, and $\triangle t$ is the time step. When needed, t_0 and t_f will denote the initial and final times and N will denote the total number of time steps. However, usually $t_0 = 0$. Also we frequently need N to represent other quantities and only seldomly we need a notation for the total number of time steps. In the general case: $\triangle t = (t_f - t_0)/N$ and thus $t_n = n\triangle t + t_0$, but we shall usually consider $t_n = n\triangle t$.

- U denotes the numerical approximation to u. U_j^n will denote the numerical solution at time step n and grid point j. If the numerical solution exactly agrees with the true solution, then $U_j^n = u(x_j, t_n)$. One of the goals, though not the only goal, of a numerical scheme is to make

$$\lim_{h, \triangle t \to 0} |U_j^n - u(x_j, t_n)| = 0 \tag{7}$$



4 Explicit Euler scheme

The basic methodology of finite-difference schemes is to approximate the derivatives appearing in the partial differential equation with combinations (differences) of the values on the grid. A variety of different approximations are possible. Here we consider the simplest.

Approximate the time derivative by the *forward difference*:

$$\frac{\partial u}{\partial t}|_{j,n} = \frac{\partial u}{\partial t}(x_j, t_n) \simeq \frac{U_j^{n+1} - U_j^n}{\triangle t} \tag{8}$$

Approximate the space-derivative by the second-order *center difference*:

$$\frac{\partial^2 u}{\partial x^2}|_{j,n} = \frac{\partial^2 u}{\partial x^2}(x_j, t_n) \simeq \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2} \tag{9}$$

With these approximations the heat equation becomes:

$$\frac{U_j^{n+1} - U_j^n}{\triangle t} = \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2} \tag{10}$$

Which can be solved for U_j^{n+1}:

$$U_j^{n+1} = U_j^n + \nu(U_{j-1}^n - 2U_j^n + U_{j+1}^n) \tag{11}$$

where $\nu \equiv \triangle t/h^2$. This is an explicit expression for the U's at the $n+1st$ time step in terms of the U's at the nth time step.

Taking into account the BCs and IC we have the *explicit Euler, or forward Euler, scheme for the heat equation:*

$$\begin{aligned} U_j^0 &= u^0(x_j), \quad 0 \le j \le J \\ U_j^{n+1} &= \begin{cases} \gamma_0, & j = 0 \\ U_j^n + \nu(U_{j-1}^n - 2U_j^n + U_{j+1}^n), & 0 < j < J, \\ \gamma_\ell, & j = J \end{cases} \end{aligned} \tag{12}$$

At each new time step, the dependent variable at each interior grid point and is computed from values at three grid points at the preceding time step.

5 Error Analysis

The analysis of errors in numerical schemes is important for the following reasons:

- It tells us where errors come from and where we should concentrate efforts to reduce errors.
- It allows comparison of different schemes.
- It provides a powerful basis for testing programs.

5.1 Truncation Error

Truncation error is the error in approximating differential operators and PDEs by discrete representations such as finite differences.

Let $\mathcal{L}^A$ be the numerical approximation to a differential operator $\mathcal{L}$ and let $u(x,t)$ be any sufficiently smooth function. The **truncation error** $T(x,t)$ in the numerical approximation $\mathcal{L}^A$ is defined by:

$$\boxed{T(x,t) \equiv \mathcal{L}^A u(x,t) - \mathcal{L}u(x,t)}$$

Example: Define the operator δ_x^2 by

$$\delta_x^2 f(x) = f(x-h) - 2f(x) + f(x+h).$$

The central difference approximation $\mathcal{L}^A = \delta_x^2/h^2$ of the operator $\mathcal{L} = \frac{\partial^2}{\partial x^2}$ gives:

$$T(x,t) = \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2} - \frac{\partial^2 u}{\partial x^2}(x,t) \tag{13}$$

In expression (13) expand $u(x+h,t)$ and $u(x-h,t)$ in Taylor series:

$$\begin{aligned} u(x+h,t) &= u(x,t) + h\frac{\partial u}{\partial x}(x,t) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \dots \\ u(x-h,t) &= u(x,t) - h\frac{\partial u}{\partial x}(x,t) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \dots \end{aligned}$$

giving:

$$T(x,t) = \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(x,t) + \ldots$$

By definition $T(x,t)$ depends on function $u(x,t)$ and this would not seem very useful. However, we are interested in the *scaling* of T with numerical parameters, such as grid spacing.

If $\frac{\partial^4 u}{\partial x^4}(x,t) \neq 0$ (which we can expect generically) then the truncation error goes to zero as h^2 as $h \to 0$ and we write

$$T_h(x,t) = O(h^2) \quad \text{or} \quad T_h = O(h^2).$$

The **order of accuracy** of an approximation to an operator or a PDE is the exponent(s) in leading error term(s). The truncation error in approximating the second derivative with the central difference δ_x^2/h^2 is said to be *second order*.

For a PDE of the form $\mathcal{F}u = 0$ one defines **truncation error** as

$$T(x,t) \equiv \mathcal{F}^A u(x,t) - \mathcal{F}u(x,t)$$

where $\mathcal{F}^A$ is the approximation to the differential equation. While u could be any sufficiently smooth function, it is standard practice to take u to be an exact solution to the PDE $\mathcal{F}u = 0$. Then

$$\boxed{T(x,t) = \mathcal{F}^A u(x,t)}$$

Example: The truncation error for the explicit Euler scheme for the heat equation is

$$\begin{aligned}
T(x,t) &= \frac{\Delta_{+t}u(x,t)}{\triangle t} - \frac{\delta_x^2 u(x,t)}{h^2} \\
&= \frac{u(x,t+\triangle t) - u(x,t)}{\triangle t} - \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2} \\
&= \frac{\partial u}{\partial t}(x,t) - \frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\triangle t}{2}\frac{\partial^2 u}{\partial t^2}(x,t) - \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(x,t) + \ldots \\
&= \frac{\triangle t}{2}\frac{\partial^2 u}{\partial t^2}(x,t) - \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(x,t) + \ldots
\end{aligned}$$

so

$$T_{h,\triangle t}(x,t) = O(\triangle t) + O(h^2)$$

Thus the explicit Euler approximation is first order in $\triangle t$ and second order in h.

It is useful to consider bounds for the truncation error. Using the remainder form of Taylor's theorem:

$$T(x,t) = \frac{\triangle t}{2}\frac{\partial^2 u}{\partial t^2}(x,\eta) - \frac{h^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi,t)$$

where $x - h < \xi < x + h$ and $t < \eta < t + \triangle t$.

If $|\frac{\partial^2 u}{\partial t^2}|$ and $|\frac{\partial^4 u}{\partial x^4}|$ are bounded in the space-time domain of interest $(x,t) \in [0,\ell] \times [0,t_f]$ then

$$|T(x,t)| \leq \frac{\triangle t}{2} M_1 + \frac{h^2}{12} M_2$$

where M_1 and M_2 are bounds for $|\frac{\partial^2 u}{\partial t^2}|$ and $|\frac{\partial^4 u}{\partial x^4}|$ in the domain.

Aside It may be the case that $|\frac{\partial^2 u}{\partial t^2}|$ and/or $|\frac{\partial^4 u}{\partial x^4}|$ are not bounded in the domain. This is easy to arrange if the initial condition does not satisfy the boundary conditions so that necessarily there is a discontinuity at a corner, e.g. $(x,t) = (0,0)$. For the heat equation this is not a fundamental problem because the heat equation smooths solutions and by taking the domain to start at $t = \tau$ for small τ, bounds can be established.

The bound on truncation error can be written as

$$|T(x,t)| \leq \frac{\triangle t}{2}(M_1 + \frac{1}{6\nu} M_2)$$

or as

$$|T(x,t)| \leq \frac{h^2}{2}(\nu M_1 + \frac{1}{6} M_2)$$

From this it can be seen that the truncation error goes to zero with $\triangle t$ or with h for constant ν. Be careful, for $\triangle t \to 0$ with ν constant implies $h \to 0$ and *vice versa* for $h \to 0$ with ν constant. Hence the truncation error goes to zero only for both $\triangle t \to 0$ and $h \to 0$.

Under these conditions, the truncation error in the explicit Euler approximation (12) of the heat equation goes to zero everywhere in the domain as $\triangle t$ and h go to zero. That is, the explicit Euler approximation is **consistent** with the partial differential equation.

Final aside: For the heat equation, because u satisfies the PDE then also $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^4 u}{\partial x^4}$ and therefore

$$T_{h,\triangle t} = \frac{\triangle t}{2}(1 - \frac{1}{6\nu})\frac{\partial^4 u}{\partial x^4} + O(\triangle t^2) + O(h^4)$$

Hence if $\nu = 1/6$, then the truncation error is higher order.

5.2 Discretization Error

The discretization error quantifies the accuracy of solutions (in contrast to the accuracy of the approximation of the equation). It is global in the sense that the error in the solution at time t, in general, depends on errors made in going from the initial condition to the solution at time t.

The **discretization error** e_j^n at a point of the computational grid is defined by:

$$e_j^n \equiv U_j^n - u(x_j, t_n) \tag{14}$$

where U_j^n is an exact solution to the finite difference equations, e.g. (12), and u and U_j^n satisfy the same initial conditions, i.e. $U_j^0 = u(x_j, 0) = u^0(x_j)$.

We are interested in:

$$E^n \equiv \|e_j^n\|_\infty = max_j |e_j^n|$$

which is also referred to as the discretization error.

For the explicit Euler solution of the heat equation (12), we can obtain a bound on the discretization error E^n in terms of a bound on the truncation error.

Let the truncation error at a given grid point to $T_j^n = T(x_j, t_n)$ and assume this to be bounded by $\bar{T}$ on the domain: $|T_j^n| \leq \bar{T}$.

We start with the definition of e_j^{n+1},

$$e_j^{n+1} \quad = \quad U_j^{n+1} - u(x_j, t_{n+1})$$

and work backwards to express e_j^{n+1} in terms of quantities at time n. We use the fact that U_j^{n+1} satisfies (12) exactly and $u(x_j, t_{n+1})$ satisfies (12) up to the truncation error

$$\begin{aligned} e_j^{n+1} &= U_j^{n+1} - u(x_j, t_{n+1}) \\ &= U_j^n + \nu\delta_x^2 U_j^n - u(x_j, t_{n+1}) \\ &= U_j^n + \nu\delta_x^2 U_j^n - \left[u(x_j, t_n) + \nu\delta_x^2 u(x_j, t_n) + \triangle t T_j^n\right] \\ &= e_j^n + \nu\delta_x^2 e_j^n - \triangle t T_j^n \\ &= (1-2\nu)e_j^n + \nu e_{j+1}^n + \nu e_{j-1}^n - \triangle t T_j^n \end{aligned}$$

Then for $\nu \leq 1/2$ the coefficient in front of e_j^n is positive and hence triangle inequality gives

$$|e_j^{n+1}| \quad \leq \quad (1-2\nu)E^n + \nu E^n + \nu E^n + \triangle t|T_j^n| = E^n + \triangle t|T_j^n|$$

Since this holds for all $0 < j < J$ it also holds for the maximum of $|e_j^{n+1}|$ which is E^{n+1}. Hence

$$E^{n+1} \leq E^n + \triangle t\bar{T}.$$

Since U and u satisfy the initial conditions, $E^0 = 0$. Then by induction

$$E^n \leq n\triangle t\bar{T}$$

Or expressed in terms of the final time $t_f = N\triangle t$:

$$E^f \leq t_f\bar{T}. \tag{15}$$

We saw previously that if $|\frac{\partial^2 u}{\partial t^2}|$ and $|\frac{\partial^4 u}{\partial x^4}|$ are bounded throughout the space-time domain, then $\bar{T} \to 0$ as $\triangle t, h \to 0$. Then as long as $\triangle t$ and h are taken to zero such that $\nu = \triangle t/h^2 \leq 1/2$ we have:

$$E^f \to 0$$

i.e. the maximum discretization error at the final time goes to zero. The numerical solution is said to **converge** to the exact solution.

Equation (15) predicts that the error increases with t_f. In practice, this is not always true.

What we can expect, however, is that the dependence of the final (discretization) error on $\triangle t$ and h has the same scaling with $\triangle t$ and h as the truncation error:

$$E^f = |O(\triangle t) + O(h^2)|$$

Note: This is slightly subtle in that the discretization error for one-step is 2nd order in $\triangle t$, i.e.

$$E^1 \leq \triangle t|O(\triangle t) + O(h^2)|$$

For *fixed* final time t_f the number of time steps N necessary to reach t_f increases as $1/\triangle t$ decreases ($N \sim 1/\triangle t$). This cancels the leading $\triangle t$ in the one-step error. Because $N \sim 1/\triangle t$ we cannot consider $E = E^N$ with fixed N but instead we consider a fixed final time and hence the notation E^f.

The scaling of the discretization error with $\triangle t$ and h provides a valuable check on the correctness of a program. We can investigate the final error E^f (at a fixed final time) as a function of $\triangle t$ and h. To make this precise, we need a *refinement path* = $(h_i, \triangle t_i), i = 0, 1, 2, \ldots$ with h_i and $\triangle t_i$ going to zero such that $\nu_i = \triangle t_i/h_i^2 \leq 1/2$. We compute the error E^f at points on the refinement path and verify the scaling of E^f.