Numerical Methods for Partial Differential Equations

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Second-order linear partial differential equations arise naturally in modeling physical phenomena. They are characterized as parabolic, hyperbolic, or elliptic. Let $x \in \mathbb{R}$, $t \ge 0$, and $u = u(x,t) \in \mathbb{R}$ in the following examples.

1. Heat Transfer, Population Dynamics (parabolic).

Diffusion of heat u(x,t) in a rod of length L and with heat source f(x) is modeled by

$$u_t(x,t)=u_{xx}(x,t)+f(x), \qquad x\in (0,L),\ t>0, \quad \text{(from conservation laws)}$$

$$u(x,0)=g(x), \qquad x\in [0,L], \qquad \text{(initial heat distribution)}$$

$$u(0,t)=a(t),\ u(L,t)=b(t), \quad t\geq 0, \qquad \text{(temperature known at boundaries)}$$
 or
$$u_x(0,t)=u_x(L,t)=0, \qquad t\geq 0, \qquad \text{(insulated boundaries)}$$

2. Wave and Shock Phenomena (hyperbolic).

Displacement u(x,t) of an elastic string is modeled by

$$u_{tt}(x,t) = u_{xx}(x,t),$$
 $x \in (0,L), t > 0,$ (from conservation laws)
 $u(x,0) = f(x), u_t(x,0) = g(x), x \in [0,L],$ (initial displacement and speed)
 $u(0,t) = a(t), u(L,t) = b(t),$ $t \ge 0,$ (location of string ends)

3. Steady-State Heat Flow, Potential Theory (elliptic).

Steady-state distribution of heat u(x) in a bar of length L with heat source f(x) is modeled by

$$u_{xx}(x) = -f(x),$$
 $x \in (0, L),$ $(t \to \infty \text{ in the heat equation})$
 $u(0) = A, \ u(L) = B,$ (boundary conditions)

1 Numerical Solution by Finite Differences

1.1 Heat Equation

Consider the heat equation with no source and constant temperature at the rod ends:

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

 $u(x,0) = g(x), \quad x \in [0,L],$
 $u(0,t) = u(L,t) = 0, \quad t \ge 0.$

Numerical solution is as follows:

• Select m+1 spatial locations uniformly sampled as

$$x_i = i\Delta x, \ 0 \le i \le m, \ \Delta x = L/m.$$

• Select temporal samples as

$$t_j = j\Delta t, \ j \ge 0, \ \Delta t > 0.$$

• The estimates of temperature are

$$u_i^{(j)} \doteq u(x_i, t_j), \ 0 \le i \le m, \ j \ge 0.$$

• The sampled initial temperature is

$$g_i = g(x_i), \ 0 \le i \le m.$$

• Approximate time derivative by forward difference

$$u_t(x,t) \doteq \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t}.$$

Approximate spatial derivatives by central difference

$$u_{xx}(x,t) \doteq \frac{u(x+\Delta x,t) - 2u(x,t) + u(x-\Delta x,t)}{(\Delta x)^2}.$$

Replace in heat equation to obtain

$$\frac{u_i^{(j+1)} - u_i^{(j)}}{\Delta t} = \frac{u_{i+1}^{(j)} - 2u_i^{(j)} + u_{i-1}^{(j)}}{(\Delta x)^2}.$$

• The boundary conditions are

$$u_0^{(j)} = u_m^{(j)} = 0, \quad j \ge 0.$$

The numerical algorithm is implemented as

$$\begin{aligned} u_i^{(0)} &= g_i, & 0 \le i \le m \\ u_0^{(j)} &= u_m^{(j)} = 0, & j \ge 0 \\ u_i^{(j+1)} &= u_i^{(j)} + \frac{\Delta t}{(\Delta x)^2} \left(u_{i+1}^{(j)} - 2u_i^{(j)} + u_{i-1}^{(j)} \right), & 1 \le i \le m-1, \ j \ge 0. \end{aligned}$$

For this to be *stable*, you need $\Delta t < (\Delta x)^2/2$.

An alternate scheme is Crank-Nicholson method

$$u_i^{(j+1)} = u_i^{(j)} + \frac{\Delta t}{(\Delta x)^2} \left(\frac{u_{i+1}^{(j)} - 2u_i^{(j)} + u_{i-1}^{(j)}}{2} + \frac{u_{i+1}^{(j+1)} - 2u_i^{(j+1)} + u_{i-1}^{(j+1)}}{2} \right).$$

Method is stable for all $\Delta t > 0$, but is harder to solve since $u_i^{(j+1)}$ is implicitly defined.

1.2 Wave Equation

Consider the wave equation where the string ends are clamped (no displacement):

$$u_{tt}(x,t) = u_{xx}(x,t),$$
 $x \in (0,L), t > 0,$
 $u(x,0) = f(x), u_t(x,0) = g(x), x \in [0,L],$
 $u(0,t) = u(L,t) = 0,$ $t > 0.$

Using similar notation as in heat equation, and using centralized differences both in space and time, the numerical method is

$$\begin{aligned} u_i^{(0)} &= f_i, & 0 \leq i \leq m \\ u_i^{(1)} &= u_i^{(0)} + (\Delta t) g_i, & 0 \leq i \leq m \\ u_0^{(j)} &= u_m^{(j)} = 0, & j \geq 0 \\ \frac{u_i^{(j+1)} - 2u_i^{(j)} + u_i^{(j-1)}}{(\Delta t)^2} &= \frac{u_{i+1}^{(j)} - 2u_i^{(j)} + u_{i-1}^{(j)}}{(\Delta x)^2}, & 1 \leq i \leq m-1, \ j \geq 1. \end{aligned}$$

The method is stable when $\Delta t < \Delta h$. If right-hand side is modified as in Crank-Nicholson, then method is stable for all $\Delta t > 0$.

1.3 Potential Equation

Consider steady-state heat flow for the constant temperature boundary problem:

$$u_{xx}(x) = -f(x), \quad x \in (0, L),$$

 $u(0) = u(L) = 0$

The numerical method is

$$u_0 = 0, \ u_m = 0,$$

 $\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} = -f_i, \quad 1 \le i \le m-1$

Define the $(m-1) \times 1$ vectors $u = [u_i]$ where $1 \le i \le m-1$ and $b = [-(\Delta x)^2 f_i]$. This vector is the unknown in a linear system

$$Au = b$$

where A is tridiagonal with main diagonal -2 and sub- and super-diagonals 1. Such systems are solved robustly in O(m) time.

2 Extension to Higher Dimensions

Consider u(x, y, t) for two dimensional problem. The heat equation is

$$u_t = u_{xx} + u_{yy},$$

the wave equation is

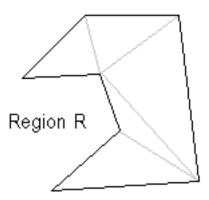
$$u_{tt} = u_{xx} + u_{yy},$$

and the potential equation is

$$u_{xx} + u_{yy} = f(x, y).$$

If domain for (x, y) is a rectangle, then discretizations such as in the one dimensional problems extend easily.

If domain is not rectangular, then use *finite elements*. For example, consider $u_{xx} + u_{yy} = 0$ where R is nonrectangular. Let u(x,y) be specified on ∂R (boundary of R). Decompose region R into triangles.



On each triangle approximate the true solution u(x,y) by linear function v(x,y) which interpolates the triangle vertices. That is, v(x,y) is determined by

$$N \bullet (x, y, v) = c,$$

$$N = [(x_2, y_2, v_2) - (x_1, y_1, v_1)] \times [(x_3, y_3, v_3) - (x_1, y_1, v_1)],$$

$$c = N \bullet (x_1, y_1, v_1).$$

The boundary v_i are known, but the interior v_i must be determined.

Solving the potential equation on R is equivalent to finding function u which minimizes

$$I = \int \int_{R} u_x^2 + u_y^2 \, dx dy$$

subject to the boundary conditions. Define \tilde{I} to be the approximate integral where u is replaced by v. For triangle T, let $v_T(x,y) = \alpha_T x + \beta_T y + \gamma_T$. Then

$$\tilde{I} = \sum_{T} \left(\alpha_T^2 + \beta_T^2 \right) \operatorname{area}(T).$$

Since α_T and β_T are linear in the interior v_i , \tilde{I} is quadratic in v_i . Minimizing a quadratic function can be done by solving a linear system (set derivatives equal to zero) or by conjugate gradient method (equivalent to solving the linear system, but uses root finding techniques).