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 $x \in \mathbb{R}$, $t \geq 0$, 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

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

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

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

   or

   $$u_x(0,t) = u_x(L,t) = 0, \qquad t \geq 0, \qquad\qquad \text{(insulated boundaries)}$$

2. Wave and Shock Phenomena (hyperbolic).

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

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

   $$u(x,0) = f(x), \ u_t(x,0) = g(x), \quad x \in [0,L], \qquad\qquad \text{(initial displacement and speed)}$$

   $$u(0,t) = a(t), \ u(L,t) = b(t), \qquad t \geq 0, \qquad\qquad \text{(location of string ends)}$$

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

   $$u_{xx}(x) = -f(x), \qquad x \in (0,L), \quad (t \to \infty \text{ in the heat equation})$$

   $$u(0) = A, \ u(L) = B, \qquad\qquad\qquad \text{(boundary conditions)}$$

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

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

The numerical algorithm is implemented as

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

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):

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

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:

$$
\begin{aligned}
u_{xx}(x) &= -f(x), & x \in (0,L), \\
u(0) &= u(L) = 0
\end{aligned}
$$

The numerical method is

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

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.

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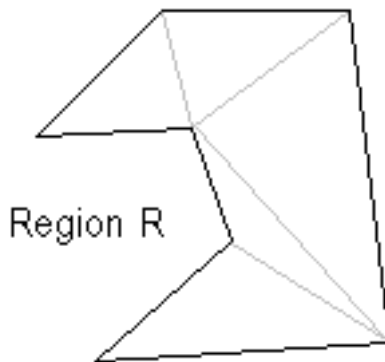
On each triangle approximate the true solution $u(x, y)$ by linear function $v(x, y)$ which interpolates the triangle vertices. That is, $v(x, y)$ is determined by

$$N \bullet (x, y, v) = c,$$
$$N = [(x_2, y_2, v_2) - (x_1, y_1, v_1)] \times [(x_3, y_3, v_3) - (x_1, y_1, v_1)],$$
$$c = N \bullet (x_1, y_1, v_1).$$

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

$$I = \int\int_R u_x^2 + u_y^2 \, dxdy$$

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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

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

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).