Numerical Solutions to PDEs

Lecture Notes #2 — Finite Difference Schemes

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Outline

Three Main Types of PDEs

A second order PDE in two independent variables (x, y) takes the form

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g$$

The coefficients a, b, c, d, e, f, and g are here (for now) assumed to be functions of (x, y) only, so the equation is **linear**.

Through a **change of variables**

$$\xi = \xi(x, y), \quad \eta = \eta(x, y)$$

it is possible to transform the PDE above to one of the three **canonical forms** (here the "..." terms hide (potentially) complicated expressions including u and its first derivatives): —

$$u_{\xi\xi} - u_{\eta\eta} + \cdots = 0,$$
$$u_{\xi\xi} + \cdots = 0,$$
$$u_{\xi\xi} + u_{\eta\eta} + \cdots = 0.$$

Three Main Types of PDEs

It can be shown that the coefficients for the second order term (a, b and c) in the PDE

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g$$

determine what canonical form the equation can be reduced to

Canonical Form	Condition	Type
$u_{\xi\xi} - u_{\eta\eta} + \cdots = 0,$	$b^2 - ac > 0$	**Hyperbolic**
$u_{\xi\xi} + \cdots = 0,$	$b^2 - ac = 0$	**Elliptic**
$u_{\xi\xi} + u_{\eta\eta} + \cdots = 0,$	$b^2 - ac < 0$	**Parabolic**

Examples:
The Wave Equation is hyperbolic, the Heat Equation is parabolic, and Laplace's equation is elliptic.

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Three Main Types of PDEs

Rough characterizations:

- **Hyperbolic equations** have "wave-like" propagating solutions; where information propagates in space with finite speeds.
- **Parabolic equations** have "diffusion-like" solutions; where information gets "smoothed out" over time – the propagation speed may be infinite.
- **Elliptic equations** have no sense of "time evolution" and tend to show up in electrostatics, continuum mechanics, and as sub-problems in computational fluid dynamics.
- Many physical problems have multiple behaviors: imagine an oil-spill spreading out (diffusing) as it is being propagated by ocean currents.

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Hyperbolic PDEs

We begin with an overview of Hyperbolic PDEs; from the simplest model equation, to hyperbolic systems, and equations with variable coefficients.

We introduce the central concepts

- **convergence**,
- **consistency**, and
- **stability**

for finite difference schemes.

These three concepts are related by the **Lax-Richtmyer Theorem**.

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Full Wave Equation $\rightsquigarrow$ One-way Wave Equation

The full wave equation yields solutions propagating both ways; by formally "factoring" the differential operator

$$\left(\partial_t^2 - a^2\partial_x^2\right) u = \left(\partial_t - a\partial_x\right)\left(\partial_t + a\partial_x\right) u \equiv \left(\partial_t + a\partial_x\right)\left(\partial_t - a\partial_x\right) u = 0,$$

it is clear that solutions to either

$$\left(\partial_t - a\partial_x\right) u = 0, \quad \text{or} \quad \left(\partial_t + a\partial_x\right) u = 0,$$

are solutions to the original equation.

These are known as **advection equations** describing a physical transport mechanism (with propagation speed a LengthUnits/TimeUnits).

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Advection: Prototype Hyperbolic PDE

The simplest prototype for Hyperbolic PDEs is the **one-way wave equation**

$$u_t(t,x) + a u_x(t,x) = 0,$$

where a is a constant, $t \in \mathbb{R}^+$ represents time, and $x \in \mathbb{R}$ the spatial location. The initial state, $u(0,x)$, must be specified.

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The One-Way Wave Equation

Once the **initial value** $u(0,x) = u_0(x)$ is specified, the **unique solution** to the one-way wave equation for $t > 0$ is given by

$$u(t,x) = u_0(x - at).$$

The solution at time t is just a shift of the initial value, $u_0(x)$. When $a > 0$ it is a shift to the right and when $a < 0$ it is a shift to the left.

The solution depends only on the value of $\xi = x - at$. These lines in the (t,x)-plane are called **characteristics**, and

$$\text{units}(a) = \text{units}(x)/\text{units}(t) = \textbf{length}/\textbf{time},$$

hence a is the **propagation speed**.

This is typical for Hyperbolic Equations: **The solution propagates with finite speed along characteristics.**

The One-Way Wave Equation

We note that the exact solution

$$u(t,x) = u_0(x - at),$$

requires no differentiability of u (or u_0), whereas the equation

$$u_t + au_x = 0,$$

appears to only make sense if u is differentiable.

This picture shows a volume with low pressure near the rear of the aircraft at high subsonic airspeeds (transonic speed regime). [U.S. Navy photo By PHAN(AW) Jonathan D. Chandler]

Hyperbolic equations feature solutions that are discontinuous (worse than non-differentiable); *e.g.* the **sonic boom** produced by an aircraft exceeding the speed of sound (Mach-1, or $\approx$ 750 miles per hour at sea level) is an example of this phenomena. The discontinuity creates a **shock wave**.

Devising numerical schemes which allow for discontinuous solutions requires "a bit" of ingenuity.

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A More General Hyperbolic Equation

$$\begin{aligned} u_t + au_x + bu &= f(t,x), \quad t > 0 \\ u(0,x) &= u_0(x) \end{aligned}$$

Where a and b are constants. We can introduce the following change of variables (and its inverse):

$$\begin{cases} \tau = t \\ \xi = x - at, \end{cases} \qquad \begin{cases} t = \tau \\ x = \xi + a\tau \end{cases}$$

With $\tilde{u}(\tau,\xi) = u(t,x)$, we can transform the PDE to an ODE along the characteristics:

$$\tilde{u}_\tau = -b\tilde{u} + f(\tau, \xi + a\tau).$$

A More General Hyperbolic Equation

The exact solution is given by

$$\tilde{u}(\tau, \xi) = u_0(\xi) e^{-b\tau} + \int_0^{\tau} f(\sigma, \xi + a\sigma) e^{-b(\tau-\sigma)}\, d\sigma,$$

which expressed in the original variables is

$$u(t, x) = u_0(x - at) e^{-bt} + \int_0^{t} f(s, x - a(t-s)) e^{-b(t-s)}\, ds.$$

With some work this method can be extended to nonlinear equations of the form

$$u_t + u_x = f(t, x, u), \quad \textbf{Note: } f \text{ depends on } u$$

From a numerical point of view, the key thing to note is that the solution evolves with **finite speed along the characteristics.**

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Systems of Hyperbolic Equations

Now consider systems of hyperbolic equations with constant coefficients in one space dimension; $\bar{\mathbf{u}}$ is now a d-dimensional vector (containing various quantities, *e.g.* density (ρ), pressure (p), velocity (v), energy (E), and momentum (ρv) of a fluid or gas).

Definition (Hyperbolic System)

A system of the form

$$\bar{\mathbf{u}}_t + A\bar{\mathbf{u}}_x + B\bar{\mathbf{u}} = F(t,x)$$

is hyperbolic if the matrix A is diagonalizable with real eigenvalues.

Systems of Hyperbolic Equations: Diagonalizablity

The matrix A is **diagonalizable**, if there exists a non-singular matrix P such that

$$PAP^{-1} = \mathrm{diag}(\lambda_1, \dots, \lambda_d) = \Lambda,$$

is a diagonal matrix. The eigenvalues $\lambda_1, \dots, \lambda_d$ are the **characteristic speeds** of the system.

In the easiest case, $B = 0$, we get

$$\bar{\mathbf{w}}_t + \Lambda \bar{\mathbf{w}}_x = PF(t,x) = \tilde{F}(t,x)$$

under the change of variables $\bar{\mathbf{w}} = P\bar{\mathbf{u}}$. This is a reduction to d independent scalar hyperbolic equations.

When $B \neq 0$, the resulting system is coupled, but only in undifferentiated terms. The lower order term $B\bar{\mathbf{u}}$ causes growth, decay, or oscillations in the solution but **does not** alter the primary feature of solutions propagating along characteristics.

(Silly) Example: Hyperbolic System

$$\begin{bmatrix} u \\ v \end{bmatrix}_t + \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}_x = 0$$

with $u(0,x) = 1$ if $|x| \leq 1$, and 0 otherwise; and $v(0,x) = 0$.

The eigenvalues are $\lambda = \{3, 1\}$, and without too much difficulty ($P = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$) we can find the solution

$$\begin{aligned} u(t,x) &= \frac{1}{2}\Big[u_0(x-3t) + u_0(x-t)\Big], \\ v(t,x) &= \frac{1}{2}\Big[u_0(x-3t) - u_0(x-t)\Big]. \end{aligned}$$

(Silly) Example: Hyperbolic System

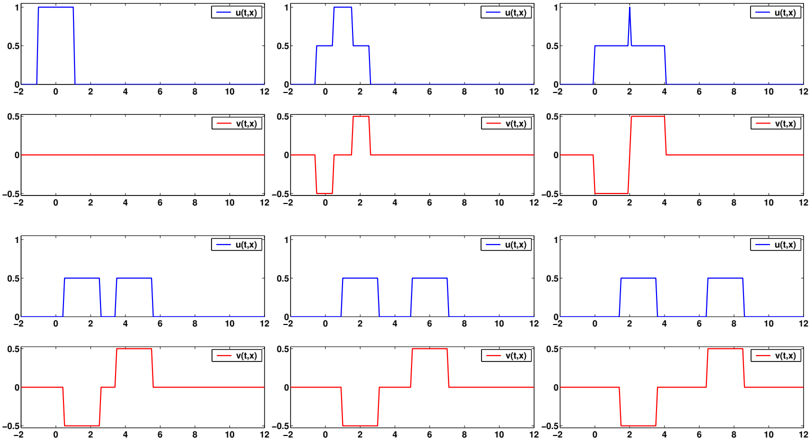

Figure: The solution at times $t = 0, 1/2, 1, 3/2, 2, 5/2$. (∃ Movie)

Hyperbolic Equations with Variable Coefficients

What happens when the propagation speed is variable, *e.g.*

$$u_t + a(t,x)u_x = 0\,?$$

In this example the solution is constant along characteristics, but the characteristics are not straight lines. Here, we get an ODE for the x-coordinate

$$\frac{dx}{d\tau} = a(\tau, x), \quad x(0) = \xi.$$

If, *e.g.* $a(\tau, x) = x$, then $x(\tau) = \xi e^{\tau}$ (so that $\xi = xe^{-t}$), and we get

$$u(t,x) = \tilde{u}(\tau, \xi) = u_0(\xi) = u_0(xe^{-t}).$$

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Hyperbolic Systems with Variable Coefficients

We can extend the definition of hyperbolicity to systems:

Definition (Hyperbolic System)

A system of the form

$$\bar{\mathbf{u}}_t + A(t,x)\bar{\mathbf{u}}_x + B(t,x)\bar{\mathbf{u}} = F(t,x)$$

is hyperbolic if there exists a matrix function $P(t,x)$ such that

$$P(t,x)A(t,x)P^{-1}(t,x) = \mathrm{diag}(\lambda_1(t,x),\ldots,\lambda_d(t,x)) = \Lambda(t,x)$$

is diagonal with real eigenvalues and the matrix norms of $P(t,x)$ and $P^{-1}(t,x)$ are bounded in x and t for $x \in \mathbb{R}$, $t \geq 0$.

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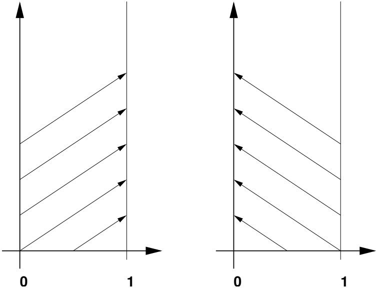
Boundary Conditions

We now consider solving a hyperbolic equations on finite intervals, *e.g.* $0 \leq x \leq 1$.

First, consider the simple equation

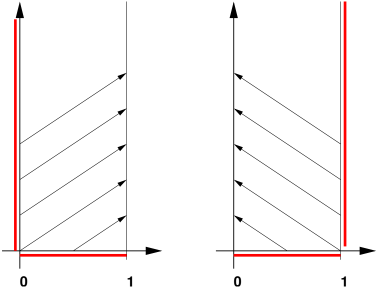
$$u_t + au_x = 0, \quad 0 \leq x \leq 1, \; t \geq 0,$$

If a is positive then the information propagates to the right and if a is negative it propagates to the left.



Boundary Conditions

When $a > 0$, in addition to the initial value $u(0,x)$ $0 \leq x \leq 1$, we must also specify the boundary value $u(t,0)$ for all $t > 0$, and when $a < 0$ we must specify $u(t,1)$ for $t > 0$.



The problem of determining a solution when both initial and boundary data are present is known as an **Initial-Boundary Value Problem** (IBVP).

IBVP for Systems

Consider the hyperbolic system (assume $a > 0$, $b > 0$)

$$\begin{bmatrix} u \\ v \end{bmatrix}_t + \begin{bmatrix} a & b \\ b & a \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}_x = 0$$

on the interval $0 \leq x \leq 1$. The characteristic speeds are $(a+b)$ and $(a-b)$, so that with $w = u + v$, and $z = u - v$

$$\begin{bmatrix} w \\ z \end{bmatrix}_t + \begin{bmatrix} a+b & \\ & a-b \end{bmatrix} \begin{bmatrix} w \\ z \end{bmatrix}_x = 0$$

If $b < a$, then both characteristic speeds are positive, but when $b > a$, we get one positive and one negative speed.

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IBVP for Systems

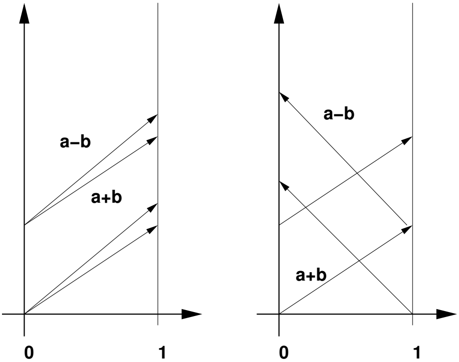


Figure: Illustration of Hyperbolic propagation; in the left panel $b < a$, so both characteristics propagate to the right. In the right panel $b > a$, so the characteristics propagate in opposite directions.

IBVP for Systems

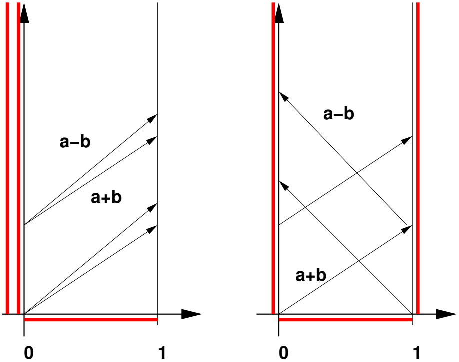


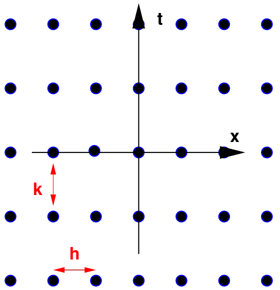
Figure: In order for the IBVPs to be **well-posed** we must (LEFT) specify the initial condition and two boundary conditions at $x = 0$; and (RIGHT) the initial condition, a boundary condition at $x = 0$, and a boundary condition at $x = 1$. Note that the specified boundary conditions must be linearly independent from the outgoing (leaving the domain) characteristic.

Introduction to Finite Difference Schemes

Let

$$G(k,h) = \{(t_n, x_m) = (n \cdot k, m \cdot h) \; : \; n, m \in \mathbb{Z}\}$$

be a grid on $\mathbb{R}^2$:



We are interested in small values of h, and k (sometimes denoted by Δx, and Δt; or δx, and δt.)

Introduction to Finite Difference Schemes

The basic idea is to replace derivatives by finite difference approximations, *e.g.* the time derivative at the point (t_n, x_m) can be represented as

$$\frac{\partial u}{\partial t}(t_n, x_m) \approx \begin{cases} \dfrac{u(t_n + k, x_m) - u(t_n, x_m)}{k} \\ \dfrac{u(t_n + k, x_m) - u(t_n - k, x_m)}{2k} \end{cases}$$

These are valid approximation since, for differentiable functions u

$$\frac{\partial u}{\partial t}(t_n, x_m) = \begin{cases} \displaystyle\lim_{\epsilon \to 0} \frac{u(t_n + \epsilon, x_m) - u(t_n, x_m)}{\epsilon} \\ \displaystyle\lim_{\epsilon \to 0} \frac{u(t_n + \epsilon, x_m) - u(t_n - \epsilon, x_m)}{2\epsilon} \end{cases}$$

We frequently use the notation $v_m^n = u(t_n, x_m)$.

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Introduction to Finite Difference Schemes

Applying these ideas to $u_t + au_x = 0$ we can write down a number of finite difference approximations at (t_n, x_m), *e.g.*

$$\frac{v_m^{n+1} - v_m^n}{k} + a\frac{v_{m+1}^n - v_m^n}{h} = 0 \qquad \text{Forward-Time-Forward-Space}$$

$$\frac{v_m^{n+1} - v_m^n}{k} + a\frac{v_m^n - v_{m-1}^n}{h} = 0 \qquad \text{Forward-Time-Backward-Space}$$

$$\frac{v_m^{n+1} - v_m^n}{k} + a\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0 \qquad \text{Forward-Time-Central-Space}$$

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} + a\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0 \qquad \text{Central-Time-Central-Space, } \textbf{leapfrog}$$

It is quite easy to derive these schemes (see *e.g.* polynomial approximation in `Math 541`) and/or to see that they may be viable approximations.

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Introduction to Finite Difference Schemes

The main difficulty of finite difference schemes is the analysis required to determine if they are **useful approximations**. Indeed, some of the schemes on the previous slide are useless.

The schemes presented so far can all be written expressing v_m^{n+1} as linear combinations of v_μ^ν at previous time-levels $\nu \in \{n-1,\, n\}$. The Forward-Time-Forward-Space scheme can be written as

$$v_m^{n+1} = (1 + a\lambda)v_m^n - a\lambda v_{m+1}^n$$

where $\lambda = k/h$ is the ratio of the time- and space- discretization. This scheme is a **one-step scheme** since it only involves information from one previous time-level.

The leapfrog scheme is a two-step (multi-step) scheme.

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Example: Leapfrog Solutions

(At time T=2)

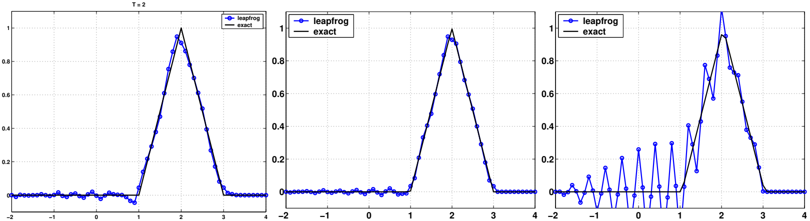

Figure: Solutions for the leapfrog scheme with $\lambda = \{0.8,\ 0.95,\ 1.02\}$ for the equation $u_t + u_x = 0$ with initial condition

$$u_0(x) = \begin{cases} 1 - |x| & \text{if } |x| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

and boundary condition

$$u(t, -2) = 0.$$

Clearly something "strange" happens when we let $\lambda > 1$. We introduce the discussion on convergence, consistency, and stability next time. ($\exists$ Movie)

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Leapfrog Simulation — Final Error

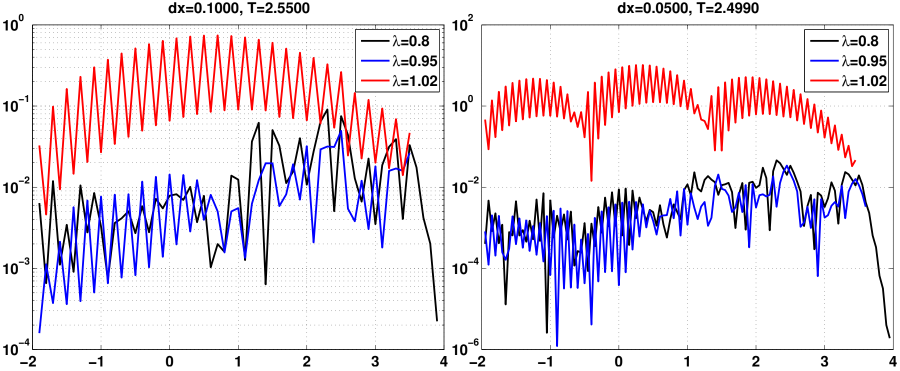

Figure: We notice that the errors shrink with the size of dx when $\lambda < 1$, but grow when $\lambda > 1$.

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