AM 205: lecture 14

- Last time: Boundary value problems
- Today: Numerical solution of PDEs
A more general approach is to formulate a coupled system of equations for the BVP based on a finite difference approximation.

Suppose we have a grid \( x_i = a + ih, \ i = 0, 1, \ldots, n - 1, \) where \( h = (b - a)/(n - 1) \)

Then our approximation to \( u \in C^2[a, b] \) is represented by a vector \( U \in \mathbb{R}^n \), where \( U_i \approx u(x_i) \)
Recall the ODE:

\[-\alpha u''(x) + \beta u'(x) + \gamma u(x) = f(x), \quad x \in [a, b]\]

Let's develop an approximation for each term in the ODE

For the reaction term \(\gamma u\), we have the pointwise approximation

\(\gamma U_i \approx \gamma u(x_i)\)
Similarly, for the derivative terms:

- Let \( D_2 \in \mathbb{R}^{n \times n} \) denote diff. matrix for the second derivative
- Let \( D_1 \in \mathbb{R}^{n \times n} \) denote diff. matrix for the first derivative

Then \(-\alpha(D_2 U)_i \approx -\alpha u''(x_i)\) and \(\beta(D_1 U)_i \approx \beta u'(x_i)\)

Hence, we obtain \((AU)_i \approx -\alpha u''(x_i) + \beta u'(x_i) + \gamma u(x_i)\), where \(A \in \mathbb{R}^{n \times n}\) is:

\[
A \equiv -\alpha D_2 + \beta D_1 + \gamma I
\]

Similarly, we represent the right hand side by sampling \(f\) at the grid points, hence we introduce \(F \in \mathbb{R}^n\), where \(F_i = f(x_i)\)
Therefore, we obtain the linear\(^1\) system for \(U \in \mathbb{R}^n\):

\[ AU = F \]

Hence, we have converted a linear differential equation into a linear algebraic equation

(Similarly we can convert a nonlinear differential equation into a nonlinear algebraic system)

However, we are not finished yet, need to account for the boundary conditions!

\(^1\)It is linear here since the ODE BVP is linear
Dirichlet boundary conditions: we need to impose $U_0 = c_1$, $U_{n-1} = c_2$

Since we fix $U_0$ and $U_{n-1}$, they are no longer variables: we should eliminate them from our linear system

However, instead of removing rows and columns from $A$, it is slightly simpler from the implementational point of view to:

- “zero out” first row of $A$, then set $A(0, 0) = 1$ and $F_0 = c_1$
- “zero out” last row of $A$, then set $A(n-1, n-1) = 1$ and $F_{n-1} = c_2$
ODE BVPs

We can implement the above strategy for $AU = F$ in Python.

Useful trick\(^2\) for checking your code:

1. choose a solution $u$ that satisfies the BCs
2. substitute into the ODE to get a right-hand side $f$
3. compute the ODE approximation with $f$ from step 2
4. verify that you get the expected convergence rate for the approximation to $u$

e.g. consider $x \in [0, 1]$ and set $u(x) = e^x \sin(2\pi x)$:

$$f(x) \equiv -\alpha u''(x) + \beta u'(x) + \gamma u(x)$$

$$= -\alpha e^x \left[4\pi \cos(2\pi x) + (1 - 4\pi^2) \sin(2\pi x)\right] +$$

$$\beta e^x \left[\sin(2\pi x) + 2\pi \cos(2\pi x)\right] + \gamma e^x \sin(2\pi x)$$

\(^2\)Sometimes called the “method of manufactured solutions”
ODE BVPs

**Python example:** ODE BVP via finite differences

**Convergence results:**

<table>
<thead>
<tr>
<th>$h$</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0e-2</td>
<td>5.07e-3</td>
</tr>
<tr>
<td>1.0e-2</td>
<td>1.26e-3</td>
</tr>
<tr>
<td>5.0e-3</td>
<td>3.17e-4</td>
</tr>
<tr>
<td>2.5e-3</td>
<td>7.92e-5</td>
</tr>
</tbody>
</table>

$O(h^2)$, as expected due to second order differentiation matrices
ODE BVPs: BCs involving derivatives

**Question:** How would we impose the Robin boundary condition \( u'(b) + c_2 u(b) = c_3 \), and preserve the \( O(h^2) \) convergence rate?

**Option 1:** Introduce a “ghost node” at \( x_n = b + h \), this node is involved in both the B.C. and the \((n-1)\text{th}\) matrix row

Employ central difference approx. to \( u'(b) \) to get approx. B.C.:

\[
\frac{U_n - U_{n-2}}{2h} + c_2 U_{n-1} = c_3,
\]

or equivalently

\[
U_n = U_{n-2} - 2hc_2 U_{n-1} + 2hc_3
\]
ODE BVPs: BCs involving derivatives

The \((n-1)^{th}\) equation is

\[-\alpha \frac{U_{n-2} - 2U_{n-1} + U_n}{h^2} + \beta \frac{U_n - U_{n-2}}{2h} + \gamma U_{n-1} = F_{n-1}\]

We can substitute our expression for \(U_n\) into the above equation, and hence eliminate \(U_n\):

\[
\left(-\frac{2\alpha c_3}{h} + \beta c_3\right) - \frac{2\alpha}{h^2} U_{n-2} + \left(\frac{2\alpha}{h^2} (1 + hc_2) - \beta c_2 + \gamma\right) U_{n-1} = F_{n-1}
\]

Set \(F_{n-1} \leftarrow F_{n-1} - \left(-\frac{2\alpha c_3}{h} + \beta c_3\right)\), we get \(n \times n\) system \(AU = F\)

Option 2: Use a one-sided difference formula for \(u'(b)\) in the Robin BC, as in III.2
Partial Differential Equations
As discussed in III.1, it is a natural extension to consider Partial Differential Equations (PDEs)

There are three main classes of PDEs:

<table>
<thead>
<tr>
<th>equation type</th>
<th>prototypical example</th>
<th>equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>hyperbolic</td>
<td>wave equation</td>
<td>$u_{tt} - u_{xx} = 0$</td>
</tr>
<tr>
<td>parabolic</td>
<td>heat equation</td>
<td>$u_t - u_{xx} = f$</td>
</tr>
<tr>
<td>elliptic</td>
<td>Poisson equation</td>
<td>$u_{xx} + u_{yy} = f$</td>
</tr>
</tbody>
</table>

Question: Where do these names come from?

$^3$Notation: $u_x \equiv \frac{\partial u}{\partial x}$, $u_{xy} \equiv \frac{\partial}{\partial y} \left( \frac{\partial u}{\partial x} \right)$
Answer: The names are related to conic sections

General second-order PDEs have the form

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0$$

This “looks like” the quadratic function

$$q(x) = ax^2 + bxy + cy^2 + dx + ey$$
PDEs: Hyperbolic

Wave equation: \( u_{tt} - u_{xx} = 0 \)

Corresponding quadratic function is \( q(x, t) = t^2 - x^2 \)

\( q(x, t) = c \) gives a hyperbola, e.g. for \( c = 0 : 2 : 6 \), we have
PDEs: Parabolic

Heat equation: \( u_t - u_{xx} = 0 \)

Corresponding quadratic function is \( q(x, t) = t - x^2 \)

\( q(x, t) = c \) gives a parabola, e.g. for \( c = 0 : 2 : 6 \), we have
PDEs: Elliptic

Poisson equation: \( u_{xx} + u_{yy} = f \)

Corresponding quadratic function is \( q(x, y) = x^2 + y^2 \)

\( q(x, y) = c \) gives an ellipse, e.g. for \( c = 0 : 2 : 6 \), we have
In general, it is not so easy to classify PDEs using conic section naming

Many problems don’t strictly fit into the classification scheme (e.g. nonlinear, or higher order, or variable coefficient equations)

Nevertheless, the names hyperbolic, parabolic, elliptic are the standard ways of describing PDEs, based on the criteria:

- **Hyperbolic**: time-dependent, conservative physical process, no steady state
- **Parabolic**: time-dependent, dissipative physical process, evolves towards steady state
- **Elliptic**: describes systems at equilibrium/steady-state
Hyperbolic PDEs
We introduced the wave equation $u_{tt} - u_{xx} = 0$ above.

Note that the system of first order PDEs

\[
\begin{align*}
    u_t + v_x & = 0 \\
    v_t + u_x & = 0
\end{align*}
\]

is equivalent to the wave equation, since

\[
    u_{tt} = (u_t)_t = (-v_x)_t = -(v_t)_x = -(-u_x)_x = u_{xx}
\]

(This assumes that $u, v$ are smooth enough for us to switch the order of the partial derivatives)
Hyperbolic PDEs

Hence we shall focus on the so-called linear advection equation

\[ u_t + cu_x = 0 \]

with initial condition \( u(x, 0) = u_0(x), \) and \( c \in \mathbb{R} \)

This equation is representative of hyperbolic PDEs in general.

It’s a first order PDE, hence doesn’t fit our conic section description, but it is:

- time-dependent
- conservative
- not evolving toward steady state

⇒ hyperbolic!
We can see that $u(x, t) = u_0(x - ct)$ satisfies the PDE

Let $z(x, t) \equiv x - ct$, then from the chain rule we have

$$\frac{\partial}{\partial t} u_0(x - ct) + c \frac{\partial}{\partial x} u_0(x - ct) = \frac{\partial}{\partial t} u_0(z(x, t)) + c \frac{\partial}{\partial x} u_0(z(x, t))$$

$$= u'_0(z) \frac{\partial z}{\partial t} + cu'_0(z) \frac{\partial z}{\partial x}$$

$$= -cu'_0(z) + cu'_0(z)$$

$$= 0$$
Hyperbolic PDEs

This tells us that the solution transports (or advects) the initial condition with “speed” $c$

e.g. with $c = 1$ and an initial condition $u_0(x) = e^{-(1-x)^2}$ we have:
Hyperbolic PDEs

We can understand the behavior of hyperbolic PDEs in more detail by considering characteristics.

Characteristics are paths in the $xt$-plane — denoted by $(X(t), t)$ — on which the solution is constant.

For $u_t + cu_x = 0$ we have $X(t) = X_0 + ct$, since

$$\frac{d}{dt} u(X(t), t) = u_t(X(t), t) + u_x(X(t), t) \frac{dX(t)}{dt}$$

$$= u_t(X(t), t) + cu_x(X(t), t)$$

$$= 0$$

\(^4\)Each different choice of $X_0$ gives a distinct characteristic curve.
Hyperbolic PDEs

Hence \( u(X(t), t) = u(X(0), 0) = u_0(X_0) \), i.e. the initial condition is transported along characteristics.

Characteristics have important implications for the direction of flow of information, and for boundary conditions.

Must impose BC at \( x = a \), cannot impose BC at \( x = b \).
Hyperbolic PDEs

Hence \( u(X(t), t) = u(0, X(0)) = u_0(X_0) \), i.e. the initial condition is transported along characteristics

Characteristics have important implications for the direction of flow of information, and for boundary conditions

Must impose BC at \( x = b \), cannot impose BC at \( x = a \)
More generally, if we have a non-zero right-hand side in the PDE, then the situation is a bit more complicated on each characteristic.

Consider \( u_t + cu_x = f(t, x, u(t, x)) \), and \( X(t) = X_0 + ct \)

\[
\frac{d}{dt} u(X(t), t) = u_t(X(t), t) + u_x(X(t), t) \frac{dX(t)}{dt}
\]

\[
= u_t(X(t), t) + cu_x(X(t), t)
\]

\[
= f(t, X(t), u(X(t), t))
\]

In this case, the solution is no longer constant on \((X(t), t)\), but we have reduced a PDE to a set of ODEs, so that:

\[
u(X(t), t) = u_0(X_0) + \int_0^t f(t, X(t), u(X(t), t)) dt
\]
We can also find characteristics for variable coefficient advection

Exercise: Verify that the characteristic curve for \( u_t + c(t, x)u_x = 0 \) is given by

\[
\frac{dX(t)}{dt} = c(X(t), t)
\]

In this case, we have to solve an ODE to obtain the curve \((X(t), t)\) in the \(xt\)-plane
Hyperbolic PDEs: More Complicated Characteristics

*e.g.* for $c(t, x) = x - 1/2$, we get $X(t) = 1/2 + (X_0 - 1/2)e^t$

In this case, the characteristics “bend away” from $x = 1/2$

Characteristics also apply to nonlinear hyperbolic PDEs (*e.g.* Burger’s equation), but this is outside the scope of AM205.
We now consider how to solve $u_t + cu_x = 0$ equation using a finite difference method.

**Question:** Why finite differences? Why not just use characteristics?

**Answer:** Characteristics actually are a viable option for computational methods, and are used in practice. However, characteristic methods can become very complicated in 2D or 3D, or for nonlinear problems.

Finite differences are a much more practical choice in most circumstances.
Hyperbolic PDEs: Numerical Approximation

Advection equation is an Initial Boundary Value Problem (IBVP)

We impose an initial condition, and a boundary condition (only one BC since first order PDE)

A finite difference approximation leads to a grid in the $xt$-plane
The first step in developing a finite difference approximation for the advection equation is to consider the CFL condition\(^5\).

The CFL condition is a necessary condition for the convergence of a finite difference approximation of a hyperbolic problem.

Suppose we discretize \(u_t + cu_x = 0\) in space and time using the explicit (in time) scheme:

\[
\frac{U^n_{j+1} - U^n_j}{\Delta t} + c \frac{U^n_j - U^n_{j-1}}{\Delta x} = 0
\]

Here \(U^n_j \approx u(t_n, x_j)\), where \(t_n = n\Delta t, \ x_j = j\Delta x\).

This can be rewritten as

\[ U_j^{n+1} = U_j^n - \frac{c \Delta t}{\Delta x} (U_j^n - U_{j-1}^n) = (1 - \nu) U_j^n + \nu U_{j-1}^n \]

where

\[ \nu \equiv \frac{c \Delta t}{\Delta x} \]

We can see that \( U_j^{n+1} \) depends only on \( U_j^n \) and \( U_{j-1}^n \)
Definition: Domain of dependence of $U_{j}^{n+1}$ is the set of values that $U_{j}^{n+1}$ depends on.
The domain of dependence of the exact solution $u(t_{n+1}, x_j)$ is determined by the characteristic curve passing through $(t_{n+1}, x_j)$.

CFL Condition:

For a convergent scheme, the domain of dependence of the PDE must lie within the domain of dependence of the numerical method.
The domain of dependence of the exact solution $u(t_{n+1}, x_j)$ is determined by the characteristic curve passing through $(t_{n+1}, x_j)$

CFL Condition:

For a convergent scheme, the domain of dependence of the PDE must lie within the domain of dependence of the numerical method
Suppose the dashed line indicates characteristic passing through \((t_{n+1}, x_j)\), then the scheme below satisfies the CFL condition.
Hyperbolic PDEs: Numerical Approximation

The scheme below does not satisfy the CFL condition
Hyperbolic PDEs: Numerical Approximation

The scheme below does not satisfy the CFL condition (here $c < 0$)
Question: What goes wrong if the CFL condition is violated?
**Answer:** The exact solution \( u(x, t) \) depends on initial value \( u_0(x_0) \), which is outside the numerical method’s domain of dependence.

Therefore, the numerical approx. to \( u(x, t) \) is “insensitive” to the value \( u_0(x_0) \), which means that the method cannot be convergent.
Note that CFL is only a necessary condition for convergence. Its great value is its simplicity: CFL allows us to easily reject F.D. schemes for hyperbolic problems with very little investigation.

For example, for $u_t + cu_x = 0$, the scheme

$$\frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} + c\frac{U_{j}^{n} - U_{j-1}^{n}}{\Delta x} = 0 \quad (*)$$

cannot be convergent if $c < 0$.

**Question:** What small change to $(*)$ would give a better method when $c < 0$?
If $c > 0$, then we require $\nu \equiv \frac{c\Delta t}{\Delta x} \leq 1$ in (\*) for CFL to be satisfied.
As foreshadowed earlier, we should pick our method to reflect the direction of propagation of information.

This motivates the upwind scheme for $u_t + cu_x = 0$

$$U_j^{n+1} = \begin{cases} U_j^n - c \frac{\Delta t}{\Delta x} (U_j^n - U_{j-1}^n), & \text{if } c > 0 \\ U_j^n - c \frac{\Delta t}{\Delta x} (U_{j+1}^n - U_j^n), & \text{if } c < 0 \end{cases}$$

The upwind scheme satisfies CFL condition if $|\nu| \equiv \left| c \frac{\Delta t}{\Delta x} \right| \leq 1$

$\nu$ is often called the CFL number.