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PDEs, part 1

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Mathematical Models, Analysis and Simulation
Fall semester, 2010

Partial differential equations

The solution depends on several variables, and the equation contains partial derivatives with respect to these variables.
Example:

$$au_{xx} + bu_{xy} + cu_{yy} = 0, \quad u = u(x, y).$$

There are three main classes of well-posed PDEs.

1. Parabolic ($b^2 - 4ac = 0$).
2. Elliptic ($b^2 - 4ac < 0$).
3. Hyperbolic ($b^2 - 4ac > 0$).

Partial differential equations

1. Parabolic PDEs
   - *Model equation:* $u_t = u_{xx}$. Heat equation or diffusion equation.
   - *Phenomena:* Diffusion, "smearing". Time dependent, goes to steady state (without forcing).
   - *Physics:* Heat conduction, diffusion processes.
2. Elliptic PDEs
   - *Model equation:* $\Delta u = u_{xx} + u_{yy} = f(x, y)$. (Poisson's equation, or with $f = 0$, Laplace's equation).
   - *Phenomena:* Equilibrium. Stationary ($t \to \infty$ in parabolic).
   - *Physics:* Electric potential, potential flow, structural mechanics.
3. Hyperbolic PDEs
   - *Model equation:* $u_{tt} = u_{xx}$ (wave equation) and $u_t = u_x$ (transport or advection equation).
   - *Phenomena:* Transport. Wave propagation. (time dependent, but no steady state).
   - *Physics:* Electromagnetic, acoustic, elastic waves.

Well posedness for PDEs

A PDE (together with the boundary conditions given) is well posed if

1. A solution exists.
2. The solution is unique.
3. The solution depend continuously on the data.

Problems that are not well-posed are called ill-posed.
The examples we have given here, are all well posed.
Other examples:

- "Backward" heat equation, $t \to -t$, $\Rightarrow u_t = -u_{xx}$. Going from a smooth solution to a highly peaked one. Very sensitive to initial data. Not well posed.
- Boundary conditions are important:

$$u_t = u_x, \quad u(0) = u(1) = 0, \quad u(x, 0) \neq 0.$$

  Not well posed.

Complications

Our initial examples of PDEs models idealized situations. The reality is often more complicated, even if the most important phenomena are captured by the model equations.
Examples:

- Higher dimension. $u_t = u_{xx} \Rightarrow u_t = \Delta u \qquad u = u(x, y, z, t)$.
- Variable coefficients. $u_{tt} = u_{xx} \Rightarrow u_{tt} = c(x)^2 u_{xx}$.
- System of equations. $u_t = u_x \Rightarrow \bar{u}_t = A\bar{u}_x, \quad \bar{u} \in \mathbb{R}^n$.
- Non-linearities. $u_t = u_x \Rightarrow \bar{u}_t = f(u)_x, \quad (u_t = f'(u)u_x)$.
- Lower order terms. $-u_{xx} = f(x) \Rightarrow -u_{xx} + u = f(x)$.
- Source terms. $u_t = u_{xx} \Rightarrow u_t = u_{xx} + f(x)$.
- Combinations from all of the above.

Important PDE

Example: Navier-Stokes equations for incompressible viscous flow.

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} = \nu \Delta \mathbf{u} - \nabla p + f$$
$$\nabla \cdot \mathbf{u} = 0,$$

u velocity, p pressure, ν kinematic viscosity ($\nu = \mu/\rho$, μ dynamic viscosity, ρ density.)
Very much used PDE, central to the field of fluid mechanics. But: very difficult to analyze, and also often to solve numerically (depending on parameters, geometry, and if additional physics is added.).

Well-posedness has **not been proven** in 3D.
(One million USD to anyone who proves (or dis-proves) this!
`http://www.claymath.org/millennium/`)

Solving PDEs extremely useful for modeling and understanding different physical processes. Usually too complicated to solve analytically. Very important to be able to do so numerically. Want robustness and accuracy!

Elliptic equations

Strang, Chapter 3.
Model equation: The *Poisson equation* in a domain $\Omega \subset \mathbb{R}^d$.

$$\begin{aligned} \Delta u &= f(\mathbf{x}) \quad \mathbf{x} \in \Omega \\ u(\mathbf{x}) &= g(\mathbf{x}) \quad \mathbf{x} \in \partial\Omega \end{aligned}$$

Model for equilibrium problems, not time-dependent.
This problem is well-posed, it has a unique stable solution (if f and $\partial\Omega$ "nice enough".

If $f \equiv 0$, we have *Laplace's equation*.
Solutions to Laplace's equation are called harmonic functions.

Examples of applications: Electrostatics, steady fluid flow, analytic functions, ...

Poisson's equation with Neumann boundary conditions

When we set the value of u at the boundary, we have Dirichlet boundary conditions. With Neumann boundary conditions,

$$\Delta u = f(\mathbf{x}) \quad \mathbf{x} \in \Omega, \qquad \frac{\partial u(\mathbf{x})}{\partial n} = h(\mathbf{x}) \quad \mathbf{x} \in \partial\Omega,$$

we need to impose an additional condition to ensure that a solution exists, and also in this case the solution is only determined up to a constant. We need (follows from the divergence theorem)

$$\int_{\partial\Omega} h(\mathbf{x})dS = \int_{\Omega} f(\mathbf{x})d\mathbf{x}.$$

Laplace's equation

Solutions to Laplace's equation are called harmonic functions.

Maximum principle: Let Ω be a connected open bounded set in $\mathbb{R}^d$, $d = 2$ or 3. Let $u(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$ be a harmonic function in Ω that is continuous on $\bar{\Omega} = \Omega \cup \partial\Omega$. *Then the maximum and minimum values of u are attained on $\partial\Omega$ and nowhere inside (unless $u \equiv$ constant).*

The maximum principle can e.g. be used to prove uniqueness to the Poisson problem with Dirichlet boundary conditions.

Translation invariance: The Laplacian is invariant under all rigid motions in space, i.e any combination of translations and rotations. We have

$$\Delta u = u_{xx} + u_{yy} + u_{zz} = u_{x'x'} + u_{y'y'} + u_{z'z'} = \Delta' u.$$

(To show, use that any rotation in 3D is given by $\mathbf{x}' = \mathbf{B}\mathbf{x}$, where $\mathbf{B}$ is an orthogonal matrix).

Well known theorems/identities

1. The divergence (Gauss) theorem:

$$\int_\Omega \nabla \cdot \mathbf{f} \, d\mathbf{x} = \int_{\partial\Omega} \mathbf{f} \cdot \mathbf{n} \, dS,$$

where $\partial\Omega$ is a closed surface, $\mathbf{f}$ a vector valued function, and $\mathbf{n}$ outward unit normal.

2. Green's first identity (G1) ($\frac{\partial u}{\partial n} = \mathbf{n} \cdot \nabla u$):

$$\int_{\partial\Omega} v \frac{\partial u}{\partial n} \, dS = \int_\Omega \nabla v \cdot \nabla u \, d\mathbf{x} + \int_\Omega v \Delta u \, d\mathbf{x}$$

3. Green's second identity (G2):

$$\int_\Omega (u\Delta v - v\Delta u) \, d\mathbf{x} = \int_{\partial\Omega} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right) dS$$

where $\frac{\partial u}{\partial n} = \mathbf{n} \cdot \nabla u$. (Use (G1) for u, v, then for v, u, subtract).

Representation formula

This formula represents any harmonic function as an integral over the boundary.
if $\Delta u = 0$ in Ω, then

$$u(\mathbf{x}_0) = \frac{1}{4\pi} \int_{\partial\Omega} \left(-u(\mathbf{x}) \frac{\partial}{\partial n} \frac{1}{|\mathbf{x} - \mathbf{x}_0|} + \frac{1}{|\mathbf{x} - \mathbf{x}_0|} \frac{\partial u}{\partial n} \right) dS, \quad \mathbf{x}_0 \in \Omega.$$

If you know the values of u at the boundary, you can hence compute the value of u anywhere inside the domain.

- Special case of (G2) with the choice of $v(\mathbf{x}) = (-4\pi|\mathbf{x} - \mathbf{x}_0|)^{-1}$.
- RHS agrees with RHS of (G2).
- We have assumed $\Delta u = 0$, and $\Delta v = 0$ for $\mathbf{x} \neq \mathbf{x}_0$ (Check it!).
- Simply inserting $\Delta u = 0$, and $\Delta v = 0$ into LHS of (G2) yields 0.

Where does the left side of this formula come from? [notes]

Fundamental solution

- The fundamental solution, or "free space" Green's function for Laplace's equation obeys the equation:

$$\Delta G = -\delta(\mathbf{x} - \mathbf{x}_0).$$

- This means that for any volume V that encloses $\mathbf{x}_0$: $\int_V \Delta G \, d\mathbf{x} = -1$.
- A simple way to find G is based on the fact that the Laplace equation is invariant under rotation, i.e. G function of $|\mathbf{x} - \mathbf{x}_0|$ only. The result is (notes):

$$G(\mathbf{x} - \mathbf{x}_0) = \frac{1}{4\pi|\mathbf{x} - \mathbf{x}_0|}.$$

Note: this is for $\mathbb{R}^3$, the Green's function in $\mathbb{R}^2$ has a logarithmic singularity.

Hence, the $v(\mathbf{x})$ used to obtain the representation formula was this fundamental solution. (Modulo a sign).

Analytic solutions by separation of variables

In some simple geometries, Laplace's equation can be solved by the technique of separation of variables. Examples:

- In a square: Separation in x and y.
- In a circle. Write Laplace's equation in polar coordinates, separate in r and θ.

(See Strang, not only Sec 3.4, but also Sec 4.1).

Separation of variables and the Poisson formula for a circle

$$\begin{aligned} \Delta u &= 0 \qquad \text{for } x^2 + y^2 < a \\ u &= h(\theta) \quad \text{for } x^2 + y^2 = a \end{aligned}$$

Solution - see notes.
Plugging in the expression of the Fourier coefficients into the Fourier series, one is actually able to sum this explicitly, using the formula for a geometric series:

$$\sum_{n=1}^{\infty} \rho^n = \frac{\rho}{1-\rho} \text{ as applied to } \sum_{n=1}^{\infty} \left(\frac{r}{a}\right)^n e^{in\alpha}$$

The result is the Poisson formula:

$$u(r,\theta) = \frac{(a^2 - r^2)}{2\pi} \int_0^{2\pi} \frac{h(\phi)}{a^2 - 2ar\cos(\theta - \phi) + r^2} \, d\phi$$

Finite differences

Assume we want to solve Poisson's equation in a rectangle, $[0, L_x] \times [0, L_y]$.

1. Define a computational grid with points $(x_i, y_j) = (i\Delta x, j\Delta x)$, $0 \leq i \leq N+1$, $0 \leq i \leq M+1$. (Assume that dimensions of domain such that we can have the same grid size in both directions).
2. Replace the Laplacian with divided differences. Second order approximation yields the "five point formula". Difference equations for all internal grid points.
3. Discretize the boundary conditions.
4. Order the unknowns in a vector, and collect the equations to express the system as a linear system of equations on matrix form,

   $$\mathbf{Au} = \mathbf{b},$$

   where $\mathbf{A}$ is a sparse matrix with five non-zero diagonals.
5. Solve the linear system of equations to obtain your approximative solution.

Notes for details.

Analysis of this finite difference method

- Define the local truncation error as the residual of the exact solution inserted into the finite difference equation.
- Taylor expansion yields $\tau_{kl} = O(\Delta x^2)$.
- We say that the method is *consistent* if $|\tau|_\infty \to 0$ when $\Delta x \to 0$, and of order p if $|\tau|_\infty = O(\Delta x^p)$.
- The five point formula is second order accurate.

- Numerical solution vector $\mathbf{u}$ solution to $\mathbf{Au} = \mathbf{b}$.
- Exact solution vector $\tilde{\mathbf{u}}$ solution to $\mathbf{A}\tilde{\mathbf{u}} = \mathbf{b} + (\Delta x)^2\bar{\tau}$, where $\bar{\tau}$ vector of truncation errors.
- The error $\mathbf{e} = \tilde{\mathbf{u}} - \mathbf{u}$ is a solution to $\mathbf{Ae} = (\Delta x)^2\bar{\tau}$, and hence $\mathbf{e} = (\Delta x)^2\mathbf{A}^{-1}\bar{\tau}$.
- $\|\mathbf{e}\| \leq (\Delta x)^2\|\mathbf{A}^{-1}\|\|\bar{\tau}\| \leq C_1(\Delta x)^4\|\mathbf{A}^{-1}\|$.
- Can show that $\|\mathbf{A}^{-1}\| < C_2/(\Delta x)^2$. (Eigenvalues of $\mathbf{A}$ explicitly known. Using that for a symmetric matrix, $\|\mathbf{A}^{-1}\| = \rho(A^{-1}) = 1/\lambda_{min}$, where λ_{min} is the smallest eigenvalue of $\mathbf{A}$.)
- Hence, $\|\mathbf{e}\| \leq C(\Delta x)^2$.

Finite element methods

Consider the one-dimensional elliptic problem (boundary value problem)

$$-\frac{d}{dx}a(x)\frac{du}{dx} + b(x)u = f(x) \quad x \in (0,1)$$
$$u(0) = u(1) = 0,$$

with $a(x) > 0$, $b(x) \geq 0$ in $[0,1]$.
Multiply by a test function $v \in C^1$ and integrate. Integration by parts and use of BCs yield the weak form:

$$B(u,v) = \langle f, v\rangle$$

where $B(u,v)$ is the bilinear form $B(u,v) = \int_0^1 (au_x v_x + b\ uv)\ dx$, and the L^2 inner product $\langle f, v\rangle = \int_0^1 fv\ dx$.
The solutions to the "strong" and the "weak" form are equivalent, if $B(u,v) = \langle f, v\rangle$ for all $v \in H_0^1(0,1)$, where the "Sobolev space" $H_0^1(0,1)$ is defined as

$$H_0^1(0,1) := \{v | \int_0^1 (v^2 + (v')^2)dx < \infty, v(0) = v(1) = 0\}.$$

Notes for details.

Minimization

If we have symmetry such that $B(u,v) = B(v,u)$, then the weak formulation is equivalent to the minimization problem

> Find $u \in H_0^1$ such that $J(u) = \min_{v \in H_0^1} J(v)$, where
> $J(v) = \frac{1}{2}B(v,v) - \langle f, v\rangle$.

In equilibrium, the energy of the system attains a minimum, and this is the solution that we are after. In our example, with $a = 1$ and $b = 0$,

$$J(v) = \int_0^1 \frac{1}{2}(v')^2 - fv\ dx.$$

Galerkin's method

Based on the weak form (or variational form) of the equation.

1. Approximate $H_0^1(0,1)$ by a finite dimensional subspace $V_m \subset H_0^1$.
2. Exchange H_0^1 by V_m in the weak formulation and solve

   $$\text{Find } \tilde{u} \in V_m \text{ s.t. } B(\tilde{u}, v_m) = \langle f, v_m \rangle \quad \forall v_m \in V_m.$$

   Yields a solution $\tilde{u}$ that approximates the exact solution u.
3. Assume that V_m is m-dimensional and let $\varphi_1, \varphi_2, \ldots, \varphi_m$ be linearly independent basis functions for V_m, i.e.

   $$V_m = span\{\varphi_1, \varphi_2, \ldots, \varphi_m\}$$

   In FEM, basis functions φ_i normally local piecewise polynomial functions. In spectral methods, one works with trigonometric polynomials.
4. Let $\tilde{u}(x) = \sum_{j=1}^{m} u_j \varphi_j(x)$ and pick an arbitrary function in V_m, $v_m(x) = \sum_{j=1}^{m} \bar{v}_j \varphi_j(x) \in V_m$. Plug in and use the fact that the equation should hold for all $v_m \in V_m$. This yields

   $$\mathbf{Au} = \mathbf{b},$$

   where $(\mathbf{A})_{ij} = B(\varphi_i, \varphi_j)$ and $b_i = \langle f, \varphi_i \rangle$.

Galerkin's method, contd.

- The residual of the Galerkin solution is orthogonal to all of V_m.
- One can show that is the original problem is elliptic, then **A** is symmetric and positive definite and the system $\mathbf{Au} = \mathbf{b}$ has a unique solution.
- If the basis functions φ_j have compact support, we will have $a_{ij} = B(\varphi_i, \varphi_j) = 0$ for many combinations i, j, when the supports do not overlap. See example with linear hat-fcns: tri-diagonal **A** for this 1D problem. Trigonometric functions are not local, give full matrix.

FEM in 2D.

Consider Poisson's equation

$$\begin{aligned} -\Delta u &= f \quad \mathbf{x} \in \Omega \\ u &= 0 \quad \mathbf{x} \in \partial\Omega \end{aligned}$$

The weak form is $B(u, v) = \langle f, v \rangle \; \forall v \in H_0^1$ with

$$\begin{aligned} B(u, v) &= \int_\Omega \nabla u \cdot \nabla v \, d\mathbf{x} \\ \langle f, v \rangle &= \int_\Omega fv \, d\mathbf{x} \end{aligned}$$

Introduce a triangulation of Ω, wtih nodes $\{\mathbf{x}_j\}$.
As basis functions for approximate space V_m, use "tent" or "pyramid" functions instead of hat functions. Still piecewise linear, but now bilinear. (Of course, can use higher order piecewise polynomials for higher order accuracy).

Remarks on FEM

- Easier to handle complex geometries as compared to Finite Difference methods. Need to triangulate domain (2D) or define tetrahedras 3D. Once this is done, the framework is in place.
- Theory for FEM/Galerkin is identical in higher dimensions. Offers tools for error estimation.
- Spatial adaptivity based on error estimation is relatively simple. (Smaller triangles where derivatives of solution large, and more sophisticated versions thereof, depending on computed quantity of interest.)