COMPUTATIONAL PDE LECTURE 2

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1. Outline of today

- Derive Poisson's equation in 3D using divergence theorem.
- Begin discussion of second order elliptic boundary value problems (BVP) in 1D
  - Green's function

2. Derivation of Poisson's Equation from Electrostatics

Here, we derive Poisson's equation in 3D using divergence theorem. The key takeaway from this section is the use of divergence theorem for PDEs. Divergence theorem is a critical tool that we will use throughout the course.

We first begin with two facts from electrostatics:

- Let $\rho : \mathbb{R}^3 \to \mathbb{R}$ be a charge density. We also consider $\Omega \subset \mathbb{R}^3$ to be an open, bounded, and simply connected domain. *Gauss's Law* is an experimental law that states that the electric field $\mathbf{e} : \mathbb{R}^3 \to \mathbb{R}^3$ that is produced by ρ must satisfy

$$\int_{\partial\Omega} \mathbf{e}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS = \int_{\Omega} \underbrace{\frac{\rho(\mathbf{x})}{\varepsilon_0}}_{=:f(\mathbf{x})} d\mathbf{x} \tag{1}$$

  where
  - $\partial\Omega$ denotes the boundary of Ω, which we will assume is smooth.
  - $\mathbf{n} : \partial\Omega \to \mathbb{R}^3$ is the outward unit normal vector of $\partial\Omega$
  - ε_0 is the electric permitivity of free space
- An electrostatic field $\mathbf{e} : \mathbb{R}^3 \to \mathbb{R}^3$ is conservative. A fact that follows from $\mathbf{e}$ being conservative is there exists a potential $u : \mathbb{R}^3 \to \mathbb{R}$ such that $\nabla u = \mathbf{e}$.

Remark 2.1 (vector notation)**.** Bold face $\mathbf{x}$ denotes a vector $\mathbf{x} = (x, y, z)$ and boldface $\mathbf{v} = (v_1, v_2, v_3)$.

Remark 2.2 (volume and surface integrals)**.** The integral $\int_\Omega f(\mathbf{x})d\mathbf{x}$ can be written in more familiar multivariable calculus language as

$$\int_\Omega f(\mathbf{x})d\mathbf{x} = \iiint_\Omega f(x, y, z)dxdydz,$$

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and a surface integral $\int_{\partial\Omega} f(\mathbf{x})dS$ can be written in more familiar multivariable calculus language as

$$\int_{\partial\Omega} f(\mathbf{x})dS = \oiint_{\partial\Omega} f(x,y,z)dS,$$

To derive Poisson's equation, we need another tool, which is the divergence theorem. We first define divergence below.

Definition 2.1 (divergence)**.** The divergence of $\mathbf{v} = (v_1, v_2, v_3)$ is

$$\operatorname{div} \mathbf{v}(\mathbf{x}) = \nabla \cdot \mathbf{v}(\mathbf{x}) = \frac{\partial}{\partial x} v_1(\mathbf{x}) + \frac{\partial}{\partial y} v_2(\mathbf{x}) + \frac{\partial}{\partial z} v_3(\mathbf{x}) \tag{2}$$

If $\mathbf{v} : \mathbb{R}^2 \to \mathbb{R}^2$ is a 2D vector field, then the divergence is

$$\operatorname{div} \mathbf{v}(\mathbf{x}) = \nabla \cdot \mathbf{v}(\mathbf{x}) = \frac{\partial}{\partial x} v_1(\mathbf{x}) + \frac{\partial}{\partial y} v_2(\mathbf{x}).$$

Theorem 2.1 (divergence theorem)**.** Let $\Omega \subset \mathbb{R}^3$ be an open, bounded domain with smooth boundary, and let $\mathbf{n} : \partial\Omega \to \mathbb{R}^3$ be the outward unit normal of Ω. Then for any continuously differentiable vector field $\mathbf{v} : \overline{\Omega} \to \mathbb{R}^3$, we have

$$\int_{\Omega} \operatorname{div} \mathbf{v}(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} \mathbf{v}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS \tag{3}$$

Remark 2.3 (divergence theorem with dimension 1 and 2)**.** The divergence theorem in 2D is

$$\int_{\Omega} \operatorname{div} \mathbf{v}(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} \mathbf{v}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds$$

where $\int_{\partial\Omega} \mathbf{v}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) ds$ is the path integral over the curve $\partial\Omega$. The divergence theorem in 1D is

$$\int_a^b \frac{dv}{dx}(x) dx = v(b) - v(a), \tag{4}$$

which is the Fundamental Theorem of Calculus.

We return to the derivation and now combine the divergence theorem (3) with Gauss's law (1) to obtain

$$\int_{\Omega} \operatorname{div} \mathbf{e}(\mathbf{x}) d\mathbf{x} = \int_{\Omega} f(\mathbf{x}) d\mathbf{x}.$$

We substitute $\mathbf{e} = \nabla u$ (since $\mathbf{e}$ is conservative) in the above equation to obtain

$$\int_{\Omega} \operatorname{div} \nabla u(\mathbf{x}) d\mathbf{x} = \int_{\Omega} f(\mathbf{x}) d\mathbf{x}.$$

Using the definition of divergence (2), we have

$$\operatorname{div} \nabla u(\mathbf{x}) = \frac{\partial}{\partial x}\frac{\partial}{\partial x}u(\mathbf{x}) + \frac{\partial}{\partial y}\frac{\partial}{\partial y}u(\mathbf{x}) + \frac{\partial}{\partial z}\frac{\partial}{\partial z}u(\mathbf{x}) = u_{xx}(\mathbf{x}) + u_{yy}(\mathbf{x}) + u_{zz}(\mathbf{x})$$

Definition 2.2 (Laplacian of u)**.** We often denote

$$\Delta u(\mathbf{x}) = u_{xx}(\mathbf{x}) + u_{yy}(\mathbf{x}) + u_{zz}(\mathbf{x})$$

and call Δu the Laplacian of u.

We finally insert $\Delta u(\mathbf{x}) = \operatorname{div} \nabla u(\mathbf{x})$ into the above equation to obtain

$$\int_\Omega \Delta u(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) d\mathbf{x}.$$

Note that Ω has been an arbitrary domain with smooth boundary. In particular, we can take $\Omega = B_r(\mathbf{x}_0)$ to be a ball of radius r centered at x_0. Dividing both sides of the above equation by the volume of $B_r(\mathbf{x}_0)$, which is $\frac{4}{3}\pi r^3$, we have

$$\frac{1}{\frac{4}{3}\pi r^3}\int_{B_r(\mathbf{x}_0)} \Delta u(\mathbf{x}) d\mathbf{x} = \frac{1}{\frac{4}{3}\pi r^3}\int_{B_r(\mathbf{x}_0)} f(\mathbf{x}) d\mathbf{x}.$$

Taking the limit as $r \to 0$ of both sides yields

$$\Delta u(\mathbf{x}_0) = f(\mathbf{x}_0),$$

which is Poisson's equation.

Exercise 2.1 (optional)**.** Prove the following for a continuous function $f : \mathbb{R}^3 \to \mathbb{R}$:

$$\lim_{r\to 0} \frac{1}{\frac{4}{3}\pi r^3}\int_{B_r(\mathbf{x}_0)} f(\mathbf{x}) d\mathbf{x} = f(\mathbf{x}_0).$$

3. Elliptic Boundary Value Problems in 1D

We'll focus on properties of Poisson's equation and similar problems in 1 dimension and use

$$\begin{cases} -u''(x) = f(x) & \text{for } x \in (0,1), \\ u(0) = u(1) = 0 \end{cases} \tag{5}$$

as the example. Note that we are enforcing

$$u(0) = u(1) = 0$$

rather than enforcing the initial conditions

$$u(0) = u_0 \text{ and } u'(0) = v_0.$$

The condition $u(0) = u(1) = 0$ is known as a **boundary condition**. The combination of a PDE and boundary conditions is called a **boundary value problem (BVP)** . There are different types of boundary conditions.

- Dirichlet boundary conditions: We set $u(0) = u_l$ and $u(1) = u_r$
- Neumann boundary conditions: We set $u'(0) = g_l$ and $u'(1) = g_r$
- Robin boundary conditions: We set $\alpha u(0) + \beta u'(0) = b_l$ and $\gamma u(1) + \delta u'(1) = b_r$

We may also mix these boundary conditions. For example, we may have Dirichlet on the left and Neumann on the right. The particular boundary conditions we are studying are also called **homogenous** boundary conditions, which means $u \equiv 0$ satisfies the boundary condition. A PDE is called homogenous if $u \equiv 0$ solves the PDE. The differential equation $-u'' = f$ is homogenous if and only if $f(x) = 0$ for all $x \in (0, 1)$.

A boundary value problem will translate better to PDEs in higher dimensions.

Remark 3.1. The minus sign in front of u'' is a common convention.

3.1. **Constructing Solutions: Green's Functions.** This discussion follows Chapter 2.1 of the textbook.

We will now actually construct an exact solution to (5) of the form

$$u(x) = \int_0^1 G(x, y) f(y) dy,$$

where G is known as a **Green's function**. If we can find such a function G, then this gives a very general way of constructing solutions to (5) for any f.

We'll construct G by reverse engineering. Suppose u is a twice continuously differentiable solution of (5). First we apply Fundamental Theorem of Calculus (4) to u to get

$$u(x) = u(0) + \int_0^x u'(y) dy = \int_0^x u'(y) dy.$$

Note that we used $u(0) = 0$ from (5). Applying Fundamental Theorem of Calculus (4) again to $u'(y) = u'(0) + \int_0^y u''(s) ds$, we have

$$u(x) = \int_0^x \left[u'(0) + \int_0^y u''(s) ds \right] dy = xu'(0) + \int_0^x \int_0^y u''(s) ds dy$$

Note that we now have u'' in the above expression for u. Using the differential equation $-u''(x) = f(x)$ in (5), we write

$$u(x) = xu'(0) - \int_0^x \int_0^y f(s) ds dy.$$

To simplify the next step, we write define

$$F(y) := \int_0^y f(s)ds,$$

and simplify the expression for u:

$$u(x) = xu'(0) - \int_0^x F(y)dy. \tag{6}$$

Note that $u(0) = 0$. In order to proceed to simplify the farthest right term of (6), we'll need integration by parts.

Lemma 3.1 (integration by parts)**.** Let $u, v : [a, b] \to \mathbb{R}$ be continuously differentiable on (a, b), then

$$\int_a^b w'(x)v(x)dx = w(b)v(b) - w(a)v(a) - \int_a^b w(x)v'(x)dx \tag{7}$$

Exercise 3.1. Prove integration by parts using Fundamental Theorem of Calculus (4) and the product rule: $(wv)'(x) = w'(x)v(x) + w(x)v'(x)$.

We now apply (7) to the farthest right term of (6) with $v(y) = F(y)$ and $w(y) = y$, $a = 0$ and $b = x$ to get

$$\int_0^x F(y)dy = \int_0^x F(y) \cdot 1dy = xF(x) - \cancelto{0}{0 \cdot F(0)} - \int_0^x yF'(y)dy$$

We then use the definition of $F(y) = \int_0^y f(s)ds$ to get $F'(y) = f(y)$ and

$$\int_0^x F(y)dy = x\int_0^x f(s)ds - \int_0^x yf(y)dy = \int_0^x (x-y)f(y)dy$$

Thus (6) becomes

$$u(x) = xu'(0) - \int_0^x (x-y)f(y)dy. \tag{8}$$

Substituting $x = 1$ into (8) and using the boundary condition $u(1) = 0$, we have

$$0 = u'(0) - \int_0^1 (1-y)f(y)dy.$$

Hence $u'(0) = \int_0^1 (1-y)f(y)dy$ and (8) simplifies to

$$u(x) = x\int_0^1 (1-y)f(y)dy - \int_0^x (x-y)f(y)dy$$

Note that

$$\int_0^x (x-y)f(y)dy = \int_0^x (x-y)f(y)dy + \int_x^1 0 \cdot f(y)dy = \int_0^1 \max\{(x-y), 0\}f(y)dy,$$

so the u may be expressed as

$$u(x) = \int_0^1 \left[x(1-y) - \max\{(x-y), 0\}\right] f(y)dy.$$

Hence, we may write the solution u as:

$$u(x) = \int_0^1 G(x,y)f(y)dy, \tag{9}$$

where

$$G(x,y) = \left[x(1-y) - \max\{(x-y), 0\}\right] = \begin{cases} x(1-y), & y > x \\ y(1-x) & y \leq x \end{cases}.$$

This derivation is reverse engineering. Next class, we will show that the formula (9) is a an actual solution to (5).