Numerical Solutions to PDEs

Lecture Notes #20
— Elliptic PDEs and Difference Schemes —
Regularity, Maximum Principle, Boundary Conditions

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   - Introduction
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Introduction

The model equation for Elliptic problems is **Poisson's equation**
(see also: Poisson-Boltzmann)

$$\Delta u = \nabla^2 u = u_{xx} + u_{yy} = f(x,y) \qquad (x,y) \in \Omega$$
$$\alpha u + \beta \nabla u \cdot \mathbf{\bar{n}} = g(x,y) \qquad (x,y) \in \Gamma$$

it describes *e.g.*

- the electrostatic potentials in the presence of charges,
- the electrochemical potential of ions in a diffuse layer,
- the potential energy in gravitational fields,
- the steady-state solution of the heat equation, with sources/sinks in Ω and specified boundary conditions.

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Introduction

Note that in contrast with **hyperbolic** and **parabolic** problems, **elliptic problems are not time-dependent.** The special case $f(x,y) \equiv 0$, *e.g.*

$$\Delta u = 0 \qquad (x,y) \in \Omega$$
$$\alpha u + \beta \nabla u \cdot \mathbf{\bar{n}} = g(x,y) \qquad (x,y) \in \Gamma$$

is known as **Laplace's equation**.

The solutions of Laplace's equation are the *harmonic functions**, which appear in *e.g.* electromagnetism, astronomy, and fluid dynamics; they describe the behavior of electric, gravitational, and fluid potentials. In the study of heat conduction, the Laplace equation is the steady-state sourceless heat equation.

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More Elliptic Problems

The **Helmholtz equation**

$$\nabla^2 u(x,y) + \left[\frac{\omega}{c}\right]^2 u(x,y) = 0,$$

describes *e.g.* the vibrations of a thin plate.
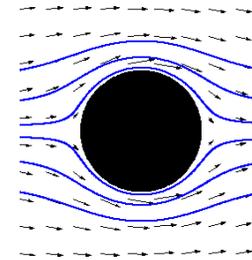
The **Biharmonic equation**

$$\nabla^4 u = \Delta^2 u = u_{xxxx} + 2u_{xxyy} + u_{yyyy} = f(x,y),$$

is used to *e.g.* model the deflections arising in two dimensional rectangular orthotropic symmetric laminate plates.

(Other orthotropic materials/problems: wood, sheet metal, electrical conduction, flow in porous media...)

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More Elliptic Problems

The **steady Stokes equations**

$$\begin{aligned} \nabla^2 u - p_x &= f_1 \\ \nabla^2 v - p_y &= f_2 \\ u_x + v_y &= 0 \end{aligned}$$

describe the steady motion of an incompressible highly viscous fluid.

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Laplace's Equation... and Boundary Conditions

The solutions to Laplace's equation $\nabla^2 u = 0$ are called **harmonic functions**, and the 2D-version of Laplace's equation is strongly connected with **complex analysis**, where the **Cauchy-Riemann equations** for the harmonic function $f(x+iy) = u(x,y) + iv(x,y)$ are

$$u_x - v_y = 0, \qquad u_y + v_x = 0.$$

The common boundary conditions are

$$\textbf{Dirichlet} \qquad u(s) = b_1(s) \quad \text{for } s \in \Gamma_1$$

$$\textbf{Neumann} \qquad \frac{\partial u(s)}{\partial \bar{\mathbf{n}}} = b_2(s) \quad \text{for } s \in \Gamma_2,$$

where $\Gamma_1 \cup \Gamma_2 = \Gamma = \partial\Omega$, is the boundary of Ω.

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Boundary Conditions

If only Neumann conditions are specified, then

$$\iint_\Omega \mathbf{f}\, d\bar{\mathbf{x}} = \iint_\Omega \nabla^2 u\, d\bar{\mathbf{x}} = \int_\Gamma \bar{\mathbf{n}} \cdot \nabla u\, d\bar{\mathbf{s}} = \int_\Gamma \frac{\partial u}{\partial \bar{\mathbf{n}}}\, d\bar{\mathbf{s}} = \int_\Gamma \mathbf{b_2(s)}\, d\bar{\mathbf{s}}$$

If this constraint, the **integrability condition**, is not satisfied, then there are no solutions. — The sources in the region must balance with the heat flux across the boundary, otherwise there can be no steady temperature distribution.

Also note that the solution to $\nabla^2 u = f$, with Neumann boundary conditions on the entire boundary is determined up to an arbitrary constant. — The temperature distribution cannot be determined from the heat fluxes and sources/sinks alone.

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General Definition of Elliptic Equations

Definition

The general (quasi-linear) second-order elliptic equation in two dimensions is an equation that can be written as

$$a(x,y)u_{xx} + 2b(x,y)u_{xy} + c(x,y)u_{yy} + d(x,y,u,u_x,u_y) = f(x,y)$$

where $a, c > 0$ and $b^2 < ac$.

This implies that the quadratic form

$$a(x,y)\xi^2 + 2b(x,y)\xi\eta + c(x,y)\eta^2 > 0, \quad \forall(\xi,\eta) \neq (0,0), \ (x,y) \in \Omega$$

or equivalently that the matrix

$$\begin{bmatrix} a(x,y) & b(x,y) \\ b(x,y) & c(x,y) \end{bmatrix} \quad \text{is positive definite.}$$

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Elliptic Problems — Key Property

Defining Property

The essential property of elliptic problems is that the solutions are more differentiable than the data.

- The solutions to Poisson's equation have two more derivatives than the function f.

- The solutions to the biharmonic equation have four more derivatives than the function f.

- The solutions to Laplace's equation and the Cauchy-Riemann equations are infinitely differentiable.

Ellipticity and Regularity

The property that the solution is smoother (more differentiable) than the data, characterizes an equation or system of equations as elliptic.

The ellipticity of an equation is often expressed in terms of **regularity estimates**; — if P is a differential operator of order $2m$, then the operator is elliptic if there is a constant c_0 such that the symbol of P, denoted by $p(x,\xi)$, defined by

Definition (Symbol of P (without time dependence))

The symbol $p(x,\xi)$ of the differential operator P is defined by

$$P\left(e^{i\xi x}\right) = p(x,\xi)e^{i\xi x}.$$

That is, the symbol is the quantity multiplying the function $e^{i\xi x}$ after operating on this function with the differential operator.

satisfies $|p(x,\xi)| \geq c_0\|\xi\|^{2m}$ for values of $|\xi|$ sufficiently large.

Regularity Estimates for Elliptic Equations   1 of 4

We consider the constant coefficient equation

$$au_{xx} + 2bu_{xy} + cu_{yy} + d_1u_x + d_2u_y + eu = f, \quad (x,y) \in \mathbb{R}^2.$$

The Fourier transform of the solution and the inversion formula are given by

$$\widehat{u}(\xi_1,\xi_2) = \frac{1}{2\pi}\iint_{\mathbb{R}^2} e^{-i(x\xi_1+y\xi_2)}u(x,y)\,dx\,dy$$

$$u(x,y) = \frac{1}{2\pi}\iint_{\mathbb{R}^2} e^{i(x\xi_1+y\xi_2)}\widehat{u}(\xi_1,\xi_2)\,d\xi_1\,d\xi_2.$$

Parseval's relation extends to 2D:

$$\iint_{\mathbb{R}^2}|u(x,y)|^2\,dx\,dy = \iint_{\mathbb{R}^2}|\widehat{u}(\xi_1,\xi_2)|^2\,d\xi_1\,d\xi_2.$$

Regularity Estimates for Elliptic Equations   2 of 4

Further, derivative smoothness estimates also extend:

$$\iint_{\mathbb{R}^2} \left| \frac{\partial^{r+s}}{\partial x^r \partial y^s} u(x,y) \right|^2 dx\, dy = \iint_{\mathbb{R}^2} |\xi_1^r \xi_2^s \widehat{u}(\xi_1,\xi_2)|^2 \ d\xi_1\, d\xi_2$$

$$\leq \iint_{\mathbb{R}^2} (\xi_1^2 + \xi_2^2)^{r+s} |\widehat{u}(\xi_1,\xi_2)|^2 \ d\xi_1\, d\xi_2.$$

We now apply this to the constant coefficient equation, and get

$$(a\xi_1^2 + 2b\xi_1\xi_2 + c\xi_2^2 - id_1\xi_1 - id_2\xi_2 - e)\widehat{u} = -\widehat{f},$$

or

$$\widehat{u}(\xi_1,\xi_2) = \frac{-\widehat{f}(\xi_1,\xi_2)}{(a\xi_1^2 + 2b\xi_1\xi_2 + c\xi_2^2 - id_1\xi_1 - id_2\xi_2 - e)}.$$

Regularity Estimates for Elliptic Equations   3 of 4

Since we are requiring $b^2 < ac$ and $a, c > 0$, we have

$$a\xi_1^2 + 2b\xi_1\xi_2 + c\xi_2^2 \geq c_0(\xi_1^2 + \xi_2^2),$$

for some constant c_0, so that when $|\bar{\xi}|^2 = \xi_1^2 + \xi_2^2 \geq C_0^2$ for some value C_0, we have

$$|a\xi_1^2 + 2b\xi_1\xi_2 + c\xi_2^2 - id_1\xi_1 - id_2\xi_2 - e| \geq c_1(\xi_1^2 + \xi_2^2),$$

and it follows that

$$|\widehat{u}(\xi_1,\xi_2)| \leq C_1 \frac{|\widehat{f}(\xi_1,\xi_2)|}{\xi_1^2 + \xi_2^2}, \quad \xi_1^2 + \xi_2^2 \geq C_0^2.$$

We can now use Parseval's relation and the derivative relation to derive a **regularity estimate** for the derivatives of the solution u...

Regularity Estimates for Elliptic Equations   4 of 4

$$\iint_{\mathbb{R}^2} |\partial_x^{s_1} \partial_y^{s_2} u(x,y)|^2 dx\, dy = \iint_{\mathbb{R}^2} |\xi_1^{s_1} \xi_2^{s_2} \widehat{u}(\xi_1,\xi_2)|^2 d\xi_1\, d\xi_2$$

$$= \iint_{|\bar{\xi}| \leq c_0} |\xi_1^{s_1} \xi_2^{s_2} \widehat{u}(\xi_1,\xi_2)|^2 d\xi_1\, d\xi_2 + \iint_{|\bar{\xi}| > c_0} |\xi_1^{s_1} \xi_2^{s_2} \widehat{u}(\xi_1,\xi_2)|^2 d\xi_1\, d\xi_2$$

$$\leq \iint_{|\bar{\xi}| \leq c_0} |\xi_1^{s_1} \xi_2^{s_2} \widehat{u}(\xi_1,\xi_2)|^2 d\xi_1\, d\xi_2 + C_1^2 \iint_{|\bar{\xi}| > c_0} (\xi_1^2 + \xi_2^2)^{s_1 + s_2 - 2} |\widehat{f}(\xi_1,\xi_2)| d\xi_1\, d\xi_2$$

$$\leq C_0^{2(s_1+s_2)} \iint_{\mathbb{R}^2} |\widehat{u}(\xi_1,\xi_2)|^2 d\xi_1\, d\xi_2 + C_1^2 \iint_{\mathbb{R}^2} (\xi_1^2 + \xi_2^2)^{s_1 + s_2 - 2} |\widehat{f}(\xi_1,\xi_2)| d\xi_1\, d\xi_2.$$

With the following norm-definition

$$\|u\|_s^2 = \sum_{s_1 + s_2 \leq s} \|\partial_x^{s_1} \partial_y^{s_2} u\|^2,$$

the above shows the regularity estimate

$$\|\mathbf{u}\|_{\mathbf{s+2}}^2 \leq \mathbf{C_s}(\|\mathbf{f}\|_{\mathbf{s}}^2 + \|\mathbf{u}\|_{\mathbf{0}}^2), \quad \text{as long as } \exists \text{ solutions } u \in L_2(\mathbb{R}^2).$$

Regularity Estimates: Comments

Similar estimates can be derived for other elliptic equations; the biharmonic, and other fourth-order equations satisfy estimates, which show that the solution has derivatives of order 4 more than the data, *e.g.*

$$\|u\|_{s+4}^2 \leq C_s(\|f\|_s^2 + \|u\|_0^2).$$

Elliptic systems, such as the Stokes equations also satisfy regularity estimates, but the concept of **order** must be generalized.

If the equation $au_{xx} + 2bu_{xy} + cu_{yy} + d_1 u_x + d_2 u_y + eu = f$ holds on a bounded domain $\Omega \subset \mathbb{R}^2$, we can obtain an **interior** estimate on a sub-domain $\Omega_1 \subset \Omega$ whose boundary is contained in Ω:

$$\|u\|_{s+2,\Omega_1}^2 \leq C_s(\Omega, \Omega_1)(\|f\|_{s,\Omega}^2 + \|u\|_{0,\Omega}^2).$$

Second-Order Elliptic Problems: Maximum Principles

Theorem (Maximum Principle)

Let L be a 2nd-order elliptic operator $L\Phi = a\Phi_{xx} + 2b\Phi_{xy} + c\Phi_{yy}$. If a function u satisfies $Lu \geq 0$ in a bounded domain Ω, then the maximum value of u in Ω is attained on the boundary of Ω.

Note that the corresponding minimum principle holds: just change ($\geq$, maximum) $\rightsquigarrow$ ($\leq$, minimum) above.

Theorem

If the elliptic equation

$$au_{xx} + 2bu_{xy} + cu_{yy} + d_1 u_x + d_2 u_y + eu = 0,$$

holds in Ω, with $a, c > 0$ and $e \leq 0$, then the solution $u(x, y)$ cannot have a positive local max. or a negative local min. in the interior of Ω.

Maximum Principle for Laplace's Equation

The physical interpretation of the maximum principle for Laplace's equation (steady-state heat equation with no interior sources/sinks) is that for a steady temperature distribution, both the hottest and the coldest temperatures occur at the boundary of the region.

Harmonic functions (solutions of Laplace's equation, or the Cauchy-Riemann equations) have their maximum and minimum values on the boundary of any domain.

The maximum principle can be used to **prove uniqueness** of the solution to many elliptic equations.
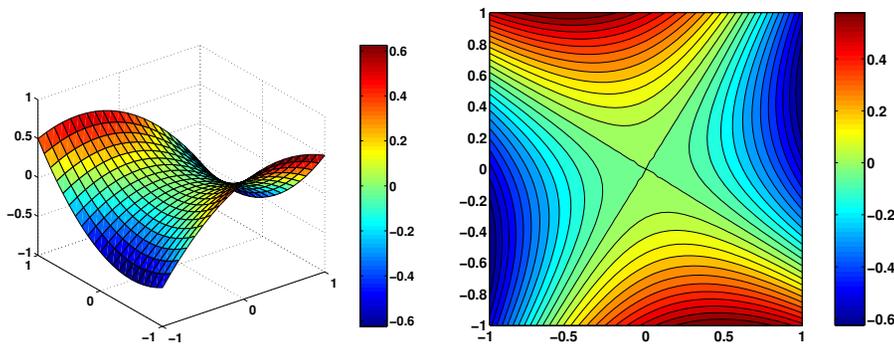
Illustration: Harmonic Function

Figure: The surface and contour plots of the harmonic function $u(x, y) = \frac{1}{2}(-x^2 - xy + y^2)$ on the unit square.

Elliptic Equations: Boundary Conditions

We restrict our discussion to second order equations, and the Dirichlet $u = f$, Neumann $u_{\bar{n}} = g$, and the mixed (Robin) condition

$$\frac{\partial u}{\partial \bar{n}} + \alpha u = b$$

The **existence** and **uniqueness** of the solutions of a general second-order elliptic equation given boundary conditions depend on global constraints, such as the **integrability condition** $\iint_\Omega f \, d\bar{x} = \int_\Gamma b_2(s) \, d\bar{s}$.

For certain equations, *e.g.* Poisson's equation, the existence and uniqueness questions have been answered: with Dirichlet boundary conditions Poisson's equation has a unique solution; and with Neumann BCs there is a unique solution up to an additive constant, if and only if the integrability condition is satisfied.

Boundary Conditions...

If a Dirichlet boundary condition is enforced along a **smooth** part of the boundary, then the normal derivative ($\perp$ to the boundary) at the boundary will be as smooth as the derivative of the boundary data (in the direction of the boundary).

If either the boundary data is discontinuous, or the boundary is non-smooth, we may not be able to control the normal derivative. If the boundary data is discontinuous, then the normal derivative is **unbounded** at discontinuities.

If either Neumann or mixed BCs are enforced along a smooth boundary, then the solution will be differentiable up to the boundary, and the first derivatives will be as well behaved as the boundary data.

Comments about the Examples

The examples on the following slides are meant to illustrate how lack of smoothness at boundaries

— In terms of specified boundary conditions,

— In terms of boundary geometry

impacts the (local) smoothness of the solution in a neighborhood of those points lacking smoothness.

The solutions of elliptic equations will be well behaved near smooth portions of the boundary. At points where the boundary conditions are discontinuous, change type, or the boundary itself is non-smooth, **singularities** in the solution's **derivatives** typically occur.
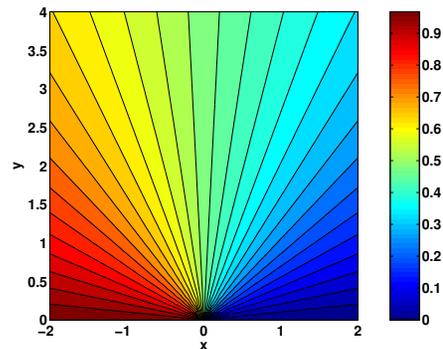
Example #1   Discontinuous Dirichlet BC

Laplace's equation, $(x, y) \in \mathbb{R} \times \mathbb{R}^+$, with BC given along the x-axis

$$u(x, 0) = \begin{cases} 0 & x > 0 \\ 1 & x \le 0 \end{cases}$$

$$u(x, y) = -\frac{1}{\pi} \tan^{-1}\left(\frac{y}{x}\right) = \frac{\theta}{\pi}$$

$$\frac{\partial u(x, y)}{\partial y} = \frac{x}{\pi(x^2 + y^2)}$$

$$u_y(x, 0) = \frac{1}{\pi x}$$

Figure: The normal derivative is well-behaved except at the point $(x, y) = (0, 0)$. Note that $u_y(x, 0)$ is not in L_2 in a neighborhood of the singularity.
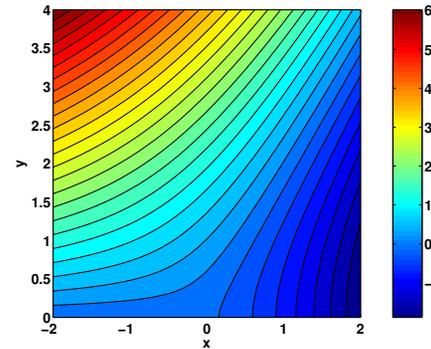
Example #2   Neumann with Non-Smooth "Contact"

Laplace's equation, $(x, y) \in \mathbb{R} \times \mathbb{R}^+$, with BC given along the x-axis

$$\frac{\partial u}{\partial y}(x, 0) = \begin{cases} 0 & x > 0 \\ \sqrt{|x|} & x \le 0 \end{cases}$$

$$u(x, y) = -\frac{2}{3} r^{3/2} \cos\left(\frac{3\theta}{2}\right)$$

$$\left(\frac{\partial u(x, y)}{\partial x}, \frac{\partial u(x, y)}{\partial y}\right) = \left(-r^{1/2} \cos\left(\frac{\theta}{2}\right), r^{1/2} \sin\left(\frac{\theta}{2}\right)\right)$$

$$u_x(x, 0) = -|x|^{1/2} \cos\left(\frac{\theta}{2}\right)$$

Figure: The tangential derivative, u_x, at the boundary has the same smoothness as the specified normal derivative.
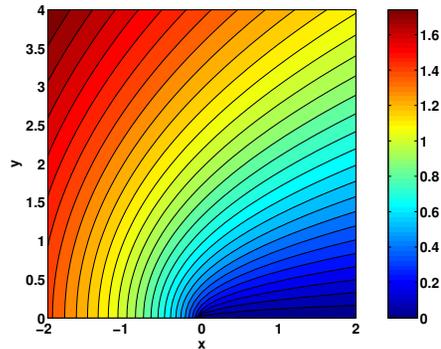
Example #3

Laplace's equation, $(x, y) \in \mathbb{R} \times \mathbb{R}^+$, with BC given along the x-axis

$$\begin{cases} u(x, 0) = 0 & x > 0 \\ u_y(x, 0) = 0 & x \leq 0 \end{cases}$$

$$u(x, y) = r^{1/2} \sin\left(\frac{\theta}{2}\right)$$

$$u_r(r, \theta) = \frac{1}{2} r^{-1/2} \sin\left(\frac{\theta}{2}\right)$$

$$u_{rr}(r, \theta) = -\frac{1}{4} r^{-3/2} \sin\left(\frac{\theta}{2}\right)$$

Figure: Again, u and u_x, u_y are in $L^2(\Omega)$ for any bounded domain Ω, but the second derivatives are not. u is bounded at $(0, 0)$, but no derivatives are.
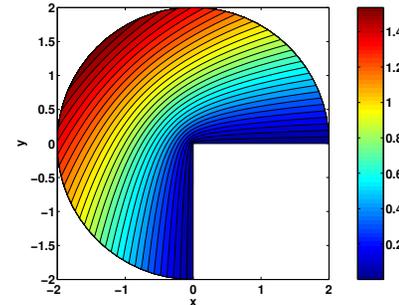
Example #4

Laplace's equation, $(x, y) \in \{(r, \theta) : 0 < r \leq r_0, \, 0 < \theta < 3\pi/2\}$, with BC given along the positive x- and negative y-axes

$$u(x, 0) = 0, \; x > 0; \quad u(0, y) = 0, \; y \leq 0$$

$$u(x, y) = r^{2/3} \sin\left(\frac{2\theta}{3}\right)$$

$$u_r(r, \theta) = \frac{2}{3} r^{-1/3} \sin\left(\frac{2\theta}{3}\right)$$

$$u_{rr}(r, \theta) = -\frac{2}{9} r^{-4/3} \sin\left(\frac{2\theta}{3}\right)$$

Figure: u and u_x, u_y are in $L^2(\Omega)$ for any bounded domain Ω in the upper half-plane whose boundary contains a portion of the real axis around zero. However $u_{xx}, u_{xy}, u_{yy} \notin L^2(\Omega)$ because of the growth at the origin. — The corner, not the data, is the cause of the lack of smoothness in the solution.