Math 6008: Numerical methods for PDEs–Lec 1

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Outline

Outline

Outline

Outline

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1. About this course
2. Introduction to PDEs
3. Basic concepts for PDEs
4. Typical examples
   - The Poisson equations
   - The transport and wave equation
   - The heat equation
5. Classification of second order quasi-linear equations (free reading)
6. Dispersion relation: dispersive and dissipative equations

Outline

Basic Information

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- Teaching Assistant: Weiyi Shao
  - Email: sh_wy1@sjtu.edu.cn;
- References:
  - 路金甫,关治. 偏微分方程数值解法(第3版). 清华大学出版社
  - R. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations, SIAM 2007.
  - Lecture notes by me.

Basic Information

Grading policy:

- Homework (45%). Collected every one or two weeks (depending on the content)
- Quiz (20%). There will be 4-6 quizzes. Each lasts for 10$\sim$15 minutes.
- Project (35%). Numerical Analysis / solving problems.

Content of the course (15 lectures)

- Introduction, basic concepts (week 1–3)
- Finite Difference Method for elliptic equations (week 4–6)
- Finite Difference Method for evolutionary equations (week 7–12)
- Other topics, variational principles and finite element methods; spectral methods (remaining time)

Outline

Definitions

- A differential equation is an equation that relates an unknown function with its derivatives.
- Ordinary Differential Equations, ODE: the unknown function is a one-variable function
- Partial Differential Equations, PDE: the unknown function is a multi-variable function and its partial derivatives are involved.

- $y''(x) - 2y'(x) = 3x$: ODE
- $y'(t) = e^t y$: ODE
- $u_x + u_{yy} = x^2$: PDE
- $u_x(x,y) - 2u_{xx}(x,y) = y^2 u(x,y)$. Formally, this is a PDE but it is intrinsically an ODE because y can be regarded as a parameter.

PDEs may be solved using ODEs

- $u_x(x,y) - 2u_{xx}(x,y) = y^2 u(x,y)$. This is a PDE. However, for each y, define $f(x) = u(x,y)$, one has

$$f'(x) - 2f''(x) = y^2 f(x).$$

  This is an ODE (with constant coefficients) which can be solved.

- $u_t(t,x) + u_x(t,x) = u(t,x)$. If one view this equation along $x(t) = t + x_0$, then

$$\frac{d}{dt} u(t, x(t)) = u(t, x(t))$$

  This is an ODE about $v(t) := u(t, x(t))$.

Outline

Basics

- The order (阶) of a PDE is the largest order of the partial derivatives involved. $u_t(t,x)+u_x(t,x)=0$: first order (一阶方程); $u_{xy}(x,y)+u^2=x^2$ (二阶方程)
- We may collect the terms involving the unknown function u together to rewrite a PDE as
$$L(u,x)=f(x)$$
where $x\in\mathbb{R}^n$ is the variable and $u:\mathbb{R}^n\to\mathbb{R}^p$ is the unknown function.
  - If $L(\cdot,x)$ is a linear operator, meaning $L(c_1u_1+c_2u_2,x)=c_1L(u_1,x)+c_2L(u_2,x)$, then the equation is said to be a linear equation. Otherwise, it is a nonlinear equation.
  - If it is a linear equation and $f\equiv 0$, then it is said to be a linear homogeneous equation.
  - $u_{xx}-2u_{xy}+\frac{1}{2}u_{yy}+3x^2u=e^{-x^2-y^2}$ is linear, nonhomogeneous; $uu_{xx}-2u_{xy}+\frac{1}{2}u_{yy}+3x^2u=e^{-x^2-y^2}$ is nonlinear.
- The linear PDEs can be written as
$$\sum_{\alpha}c_\alpha(x)\partial^\alpha u=f(x)$$
where $\partial^\alpha:=\partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\cdots$.

Evolutionary equations(发展方程)

- In some PDEs, there is a concept of time. This means that for some component of the variable (say x_n), the solution at $x_n = a$ does not depend on the information of the solution for $x_n > a$. That means there is causal relation in the direction of x_n. In this case, we may call x_n the time, and often rewrite as $t := x_n$ and redefine $(x_1, \cdots, x_{n-1})$ to be x.

- Equations with time are called the **evolutionary equations** (发展方程). Typical example include the hyperbolic and parabolic equations, like $u_t + u_x = 0$ and $u_t = u_{xx}$ (where $u = u(t, x)$) as we shall see later.

- Some PDEs do not have the concept of time. Consider the Laplace equation $\partial_{xx} u + \partial_{yy} u = 0$. Even if you call y to be t and get $u_{tt} = -u_{xx}$. This looks like an evolutionary equation, but it is not! The reason is that the solution $u(x, 1)$ depends on the information for $t > 1$. The elliptic equations are typical examples of such PDEs.

definite conditions (定解条件) and system of equations

- The definite conditions are conditions to determine the solutions to a specific PDE so that the solution exists, is unque and the equation can be solved stably with respect to the conditions. Such conditions include the initial conditions/values (初值条件) and boundary conditions (边值条件) for evolutionary equations.

- The problem for solving evolutionary equation with purely initial conditions are called the initial value problem or Cauchy problems (柯西问题).

- For equations without time, the definite conditions are boundary conditions.

- A k-th order system of PDEs is a system consists of m coupled PDEs and the highest order is k. Formally, we can introduce vector-valued functions $\boldsymbol{u} = (u_1, \ldots, u_m)$ so that the k-th order system is a PDE about the vector-valued function $\boldsymbol{u}$.

Wellposedness, notions of solutions

- The problem for solving PDEs with definite conditions is said to be well-posed if the solution exists, is unqiue and stable with repsect to the data in the problem.
- There are several notions of solutions, including classical solutions, strong solutions, weak solutions, mild solutions etc. In our course, we will often talk about classical solutions with enough smoothness.
- In some cases, the solutions can be solved out analytically. However, often, we are not able to find the expressions for the solutions. However, we can prove the existence and uniqueness with the definite conditions for some cases. Moreover, we may also prove the regularity (smoothness) of the solutions.

Outline

Outline

The Laplace operator and Poisson equations

- The Laplace operator in Cartesian coordinates:

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}.$$

  Note that $\nabla = \sum_i \boldsymbol{e}_i \frac{\partial}{\partial x_i}$ so that $\Delta = \nabla \cdot \nabla$. Note that $-\Delta$ is a nonnegative operator in the sense that $\langle u, -\Delta u\rangle = \int |\nabla u|^2 \geq 0$.

- The Poisson equation is given by

$$-\Delta u := -\sum_{i=1}^{n} \partial_{x_i}^2 u = f(x).$$

  If $f = 0$, it is called the **Laplace** equation. A solution of the Laplace equation is called a **harmonic** function.

- The Poisson equation can have variable coefficients

$$-\sum_i \partial_{x_i}(k_i(\boldsymbol{x})\partial_{x_i} u) = f, \quad k_i(x) > 0.$$

A physical example: the membrane problem

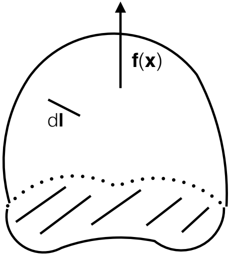

Figure: loaded membrane

- Without load, the membrane is at equilibrium, occupying $\Omega \times \{0\}$ where $\Omega \subset \mathbb{R}^2$.
- The elastic membrane with load $f(x)$ in the z direction per unit area.
- The displacement of the membrane is $u(x)$ under f and we assume $|u| \ll 1$. The membrane is clapped at the boundary so that $u(x \in \partial\Omega) = 0$.

A physical example: the membrane problem

- Consider a small portion of the membrane corresponding to $D \subset \Omega$.
- The load $F = \int_D f(x)dx$.
- The surface tension along the boundary of the membrane. For a small line segment on the membrane, the magnitude of the tension is $\sigma\Delta\ell$ while the direction is tangent to the membrane and perpendicular to $\Delta\ell$.
- The component of the tension in the vertical direction is given by $\sigma\Delta\ell\frac{\partial u}{\partial n}$ (to leading order with $|u| \ll 1$). Hence, the total surface tension acted on the portion of membrane is

$$\int_{\partial D} \sigma \frac{\partial u}{\partial n} ds.$$

  (This relation tells us that the tension density per unit area is $-\kappa ndS$)
- By force balance $\int_D f(x)dx + \int_{\partial D} \sigma\frac{\partial u}{\partial n} ds = 0$ so that

$$-\sigma\Delta u = f, \quad u|_{\partial\Omega} = 0.$$

  [This is closely related to the minimum energy surface]

A physical example: electrostatic problem

- For a point charge, the electric field is given by

$$\vec{E} = \frac{q}{4\pi\varepsilon_0}\frac{\hat{r}}{r^2}.$$

It is relatively easy to see that when $r \neq 0$, $\nabla \cdot \vec{E} = 0$ (in fact, $\nabla \cdot \vec{E} = \frac{q}{\varepsilon_0}\delta(x)$). Hence, for any closed surface enclosing 0, one has

$$\oint_S \vec{E} \cdot n dS = \frac{q}{\varepsilon_0}.$$

- By superposition, if there is a distribution of charges with density ρ (charge per unit volume), one has the Gauss' law (flux of electric field is proportional to the charge enclosed)

$$\oint_S \vec{E} \cdot n dS = \int_V \rho dV / \varepsilon_0.$$

Since $\vec{E} = -\nabla\varphi$ where φ is the charge potential, then

$$-\varepsilon_0 \Delta\varphi = \rho.$$

Suitable boundary conditions for Poisson equation

- Consider the Poisson equation $-\Delta u = f$ in a domain $\Omega \subset \mathbb{R}^n$. On the boundary $\Gamma = \partial\Omega$, we need to specify some boundary conditions to determine the solutions.

- The first type of conditions are the values of u on $\partial\Omega$:

$$u|_{x\in\Gamma} = g(x)$$

  Such conditions are called the Dirichlet boundary conditions.

- A second type of boundary condition is the Neumann boundary conditions

$$\frac{\partial u}{\partial n}|_{x\in\Gamma} = h(x).$$

  Here, $\frac{\partial u}{\partial n} = \nabla u \cdot n$ is the directional derivative along the normal direction.
- Other boundary conditions are possible, like imposing the tangential directional derivatives, the mixture of the Direchlet and Neumann etc.

Some properties of the Poisson equations

- The Poisson equations are usually used for stationary equations (定常问题), like the steady solution of the heat equation below.

- The fundamental solution Φ of the equation $-\Delta u = f(x)$ in $\mathbb{R}^n$ (meaning that $-\Delta\Phi = \delta(x)$) is given by

$$\Phi(x) = \begin{cases} -\frac{1}{2\pi}\log|x| & n = 2 \\ \frac{C_n}{|x|^{n-2}} & n \geq 3. \end{cases}$$

- The unknown function inside a bounded domain U can be *stably* determined by the value on the boundary ∂U and f. Any change on the boundary value affects all the interior values.

- The Poisson equation is a typical example of **elliptic** equations (椭圆方程).

Outline

The transport equation

- The equation
$$u_t + b(t,x)\cdot\nabla u = 0$$
is called the transport equation.

- The solution can be determined by initial conditions given at $t=0$. For bounded domains, we may impose both initial and boundary conditions. The equation can be solved by **characteristics** (特征线) $\dot{x} = b(t,x)$. In fact, for such a trajectory $x(t)$
$$\frac{d}{dt}u(x(t),t) = 0 \Rightarrow u(x(t),t) = u(x_0,0).$$

- The speed of propagation is finite (有限的传播速度). Consequently, the solution at some location at later time only depends on the initial data on some interval.

- The energy $E(u) = \int u^2\,dx$ is stable. In fact,
$$\frac{d}{dt}E(u) = 2\int u(-b\nabla u)\,dx = -\int b\cdot\nabla(u^2)\,dx = \int u^2\nabla\cdot b\,dx \le CE(u).$$

- A typical equation of hyperbolic equations.

Physical interpretation: particle transport

- Consider particle transport by a velocity field v:

$$\dot{x}(t) = v(x(t)).$$

- The mass density (distribution) of the particles satisfies

$$\partial_t \rho + \nabla \cdot (\rho v) = 0.$$

  This is a transport equation.

- If one considers the map $x = x(x_0, t)$ as a function of x_0 and t, then $u(x_0, t) := g(x(x_0, t))$ for any smooth function g, one has

$$\partial_t u - v(x_0) \cdot \nabla_{x_0} u = 0,$$

  which is also a transport equation.

The wave equation

- The equation
$$u_{tt} = a^2 \Delta u + f(x,t)$$
is the **wave equation**.

- One may impose initial conditions. Here, we have second order derivative in time, so one may impose initial conditions for u and u_t at $t = 0$. For bounded domains, one may also impose boundary conditions.

- The speed of propagation is finite. Consequently, the solution at some location at later time only depends on the initial data in some bounded domain (details later).

- The energy $E(u) = \int u_t^2 + |\nabla u|^2\, dx$ is stable.

- The wave equation also has characteristics and is also a typical example of hyperbolic equations.

The wave equation: derivation for string vibration

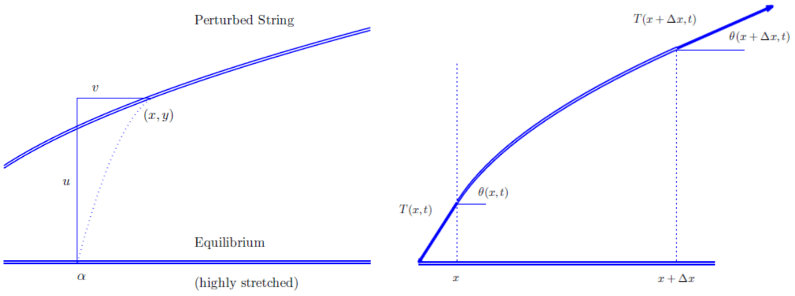

Figure: Vibrating string

- Consider a fully flexible string (no bending).
- The displacement is assumed to be small so that The motion of the point on the string is roughly verticle:

$$y = u(x,t).$$

- The line density ρ (mass per unit length).

The wave equation: derivation for string vibration

- For flexible string, the tension is along the tangential direction, $T = T(x,t)$ with slope $\tan(\theta(x,t)) = \frac{\partial u}{\partial x}$.

- For small amplitude motion, $T(x,t)\cos\theta(x,t) = T(x+\Delta x,t)\cos\theta(x+\Delta x,t)$. Then, $T(x,t) \equiv T_0$ to leading order (the correction is in $O(u^2)$ order, which is small).

- By Newton's law (conservation of momentum):

$$\partial_t(\rho\Delta x\partial_t u) = T_0\sin(\theta(x+\Delta x)) - T_0\sin(\theta(x)) + f_0(x,t)\Delta x$$

  where f_0 is the load.
- Taking $\Delta x \to 0$ and with the approximation $u \ll 1$,

$$\partial_{tt}u = \frac{T_0}{\rho}\partial_{xx}u + \frac{f_0(x,t)}{\rho}$$

D'Alembert formula for 1D

Consider the 1D wave equation

$$\partial_{tt} u - a^2 \partial_{xx} u = f(x,t), \quad u(x,0) = \varphi(x), \quad u_t(x,0) = \psi(x).$$

- The solution is given by the D'Alembert formula (often it refers to the formula with $f = 0$),

$$u(x,t) = \frac{1}{2}[\varphi(x+at) + \varphi(x-at)] + \frac{1}{2a}\int_{x-at}^{x+at} \psi(\xi)d\xi + \frac{1}{2a}\int_0^t d\tau \int_{x-a(t-\tau)}^{x+a(t-\tau)} f(\xi,\tau)d\xi.$$

- Let $f = 0$. Clearly, the solution at (x,t) only depends on the information of the initial data on $[x-at, x+at]$. Hence, this is the **interval of dependence**.
- The above implies that the speed of propagation is finite for wave equation.

Difference between 2D and 3D equations

Consider the homogeneous wave equation $u_{tt} = a^2 \Delta u$ with initial conditions $u(x,0) = \varphi(x), \quad u_t(x,0) = \psi(x)$.

- For 3D, the solution is

$$u(x,t) = \partial_t[\frac{1}{4\pi a^2 t} \iint_{S_{at}(x)} \varphi(y) dS] + \frac{1}{4\pi a^2 t} \iint_{S_{at}(x)} \psi(y) dS.$$

- For 2D, the solution is

$$u(x,t) = \frac{1}{2\pi a} \partial_t [\iint_{D(x,at)} \frac{\varphi(y) dy}{\sqrt{a^2 t^2 - |y-x|^2}}] + \frac{1}{2\pi a} \iint_{D(x,at)} \frac{\psi(y) dy}{\sqrt{a^2 t^2 - |y-x|^2}}$$

- The speed of propagation is still finite and there is also bounded domain of dependence.
- The big difference is that in 3D, the solution only depends on the initial data on the sphere while in 2D, it depends on the initial data on the whole disk $D(x, at)$. In 3D, there is wave front and wave rear (Huygens principle) so that one can hear the sound clearly. In 2D, there is no rear. For creatures in 2D, once the sound is heard, the sound will last forever. (think about waterwave after a stone is dropped into the lake)

Outline

Basics of the heat equation

- The equation
$$\partial_t u = \sum_i \partial_{x_i}(k_i \partial_{x_i} u) + f(x,t)$$
where $k_i(x) > 0$ is called the diffusion equation or the heat equation.

- The heat equation is used to model the *diffusion* effects in nature. The solution can be determined by the initial condition at $t = 0$. If we consider bounded domain, we may also impose both initial condition and boundary conditions.

- Consider the special case $u_t = \Delta u$. The fundamental solution is
$$\Phi(x,t) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x|^2}{4t}\right),$$
which is the solution to the Cauchy problem $\partial_t \Phi = \Delta \Phi, \Phi(x,0) = \delta(x)$.

Interpretation: heat transfer

- The amount of the internal energy transferred from one location to another due to the difference of temperature is the heat (temperature is the averaged kinetic part of internal energy).
- Let u be the distribution of the temperature. By the definition of specific heat (比热容)
$$\delta Q/(m\Delta u) = c.$$
Hence, the heat change in domain D is
$$\int_D c\rho\partial_t u dV.$$
- By Fourier's law, the flow of the heat is given by $q = -k\nabla u$.
- By conservation of energy, for any fixed domain D:
$$\int_D c\rho\partial_t u dV = -\oint_{\partial D} q\cdot n dS + \int_D \rho f_0 dV.$$
- Assuming that c, ρ, k are constants, one has
$$\partial_t u = a^2\Delta u + f.$$

Interpretation: diffusion

- The Brownian motion $W(t)$ can be viewed as the limit of scaled simple random walk. The probability distribution of the particles satisfies the heat equation
$$\partial_t p(x,t) = \frac{1}{2}\Delta p.$$
- The trajectory of a particle is the Brownian motion and not differentiable everywhere. Brownian motion can be used to model the diffusion effects in nature.
- The scales of length and time for typical particles in Brownian motion satisfy $[x]^2 \sim [t]$.

Other properties

- For the general problem $\partial_t u = \Delta u, u(x,0) = u_0(x)$, the solution at $t > 0$ is given by

$$u(x,t) = \Phi(\cdot,t) * u_0 = \int \Phi(x-y,t)u_0(y)\,dy.$$

  From this expression, we find that the solution of u at x for $t > 0$ depends on all $u_0(y)$. That means the speed of propagation for heat equation is infinity! Any perturbation in the space will affect everywhere immediately.

- Energy decreasing. Consider $E(u) = \frac{1}{2}\int u^2\,dx$. Then,

$$\frac{d}{dt}E(u) = \int u\Delta u\,dx = -\int |\nabla u|^2\,dx \le 0.$$

- The heat equation is a typical example of the parabolic equations.

Outline

Classification of 2nd order quasi-linear equations

These equations can be classified into elliptic, hyperbolic, parabolic equations. Read section 2.3 of the book for details and we omit here.

Outline

Linear operator with constant coefficients

- Consider a linear operator L with constant coefficients, given by

$$L = \sum_{\alpha} c_\alpha \partial^\alpha,$$

where c_α does not depend on x. Examples include

$$L = \partial_x, L = \Delta, L = \partial_{xxx}.$$

- For such an opeator, the planer wave $e^{i\xi\cdot x}$ is an eigenfunction of L:

$$L(e^{i\xi\cdot x}) = -i\omega(\xi)e^{i\xi\cdot x}.$$

- Note that a general function can be written as the superposition of such planer waves:

$$f(x) = \int c(\xi)\exp(i\xi\cdot x)\,d\xi =: \int \left[\frac{1}{(2\pi)^d}\hat{f}(\xi)\right]\exp(i\xi\cdot x)\,d\xi.$$

Finding the coefficients $\hat{f}(\xi)$ leads to the **Fourier transform**

$$\hat{f}(\xi) = \int f(x)e^{-i\xi\cdot x}\,dx.$$

Linear evolutionary equations with constant coefficients

- Consider a linear evolutionary equation

$$u_t = Lu,$$

where L is a linear operator with constant coefficients.

- The idea is to decompose u in terms of the eigenfunctions (Fourier modes) and one will obtain the equation for $\hat{u}$:

$$\partial_t \hat{u} = -i\omega(\xi)\hat{u}.$$

Formally, this is obtained by taking Fourier transform on both sides of the equation.

- According to this, one finds that $\hat{u} = c(\xi)\exp(-i\omega(\xi)t)$ so that

$$u = \frac{1}{(2\pi)^d}\int c(\xi)e^{-i\omega(\xi)t}e^{i\xi\cdot x}\,d\xi.$$

The dispersion relation for linear evolutionary equations

- By the formula
$$u = \frac{1}{(2\pi)^d}\int c(\xi)e^{-i\omega(\xi)t}e^{i\xi\cdot x}d\xi,$$
  - The solution is the superposition of different Fourier modes.
  - The properties of the solutions are determined by $\omega(\xi)$ which is called the **dispersion relation**.
  - To find the dispersion relation in practice, one can simply plug in $e^{i(\xi\cdot x-\omega t)}$ into the equation to obtain it.
- The phase velocity is given by $v_p(\xi)=\frac{\omega(\xi)}{\xi}$, which is the velocity for the point that has a specific phase $\phi_0=\xi\cdot x-\omega t$.
- If ω is real, the amplitude of each mode doesn't decay and different mode has different speed, the equation is said to be dispersive (色散的). The equation shows properties of hyperbolic equations.
- If ω is not real and imaginary part is negative, the amplitude decays. The equation is said to be dissipative (耗散的).

Examples

- Consider the heat equation $u_t = a^2 u_{xx}$: $-i\omega = a^2(-\xi^2)$ and $\omega = -ia^2\xi^2$. Hence, for each mode, it evolves like

$$\hat{f}(\omega)\exp(i\xi \cdot x - i\omega t) = \hat{f}(\omega)\exp(i\xi \cdot x - a^2\xi^2 t).$$

  Clearly, the mode decays and the energy of the system is consumed. This is why it is *dissipative*.

- $u_{tt} = a^2 u_{xx}$: $-\omega^2 = a^2(-\xi^2)$ and $\omega = \pm a\xi$. The mode is like

$$\hat{f}(\omega)\exp(i(\xi \cdot x \pm a\xi t)).$$

  Clearly, this is a planar wave.

- Schrodinger equation: $iu_t = -u_{xx}$. $\omega = \xi^2$. Schordinger equation is wave-like and shares properties with hyperbolic equations. Different modes have different speeds. Hence, this is dispersive.

General cases?

- What if the equation is nonlinear? We can't find the dispersion relation. However, if we have a stationary solution, we can linearize the equation around the stationary solution and then do the linear stability analysis.
- What if L depends on x? $e^{ix\xi}$ is not an eigenfunction, but we can fix x and see the local behavior there.