Curtin University

Advanced Numerical Analysis

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Boundary Value Problems

1 Classification of PDEs

2 Boundary and Initial Conditions

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Classification of PDEs

Modelling of most real world problems in science and engineering usually leads to a BVP:

A differential equation (or a set of differential equations)

Subject to certain initial and boundary conditions.

In this lecture, we focus on the following topics

1. Classification of partial differential equations (P.D.Es).
2. Classification of boundary conditions (B.C.).
3. An overview of methods for solving boundary value problems (B.V.P.).

Example

The transient temperature field in a bounded domain Ω with convection boundary $\partial\Omega$ can be modelled by

$$\rho c \frac{\partial T}{\partial t} = k\nabla^2 T + Q(x) \quad \forall \mathbf{x} \in \Omega, \quad t \in [0, T] \tag{1}$$

subject to

$$\begin{aligned} \rho c \frac{\partial T}{\partial t} &= k\nabla^2 T + Q(x) \quad \forall \mathbf{x} \in \Omega, \quad t \in [0, T] && (2) \\ k\frac{\partial T}{\partial n}(\mathbf{x}) &= -h(T - T_\infty) \quad \forall \mathbf{x} \in \partial\Omega, \quad t \in [0, T] && (3) \\ T(0, \mathbf{x}) &= T_0(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega, && (4) \end{aligned}$$

where $Q(\mathbf{x})$ is heat source and ρ, c, k and h are constants.

Definition 1 A 1st order partial differential equation

$$Lu \;=\; a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} + c = 0$$

is said to be

- Linear if $a = a(x, y), b = b(x, y)$, and c constant
- Quasi-linear if if these coefficients depend in addition on the unknown u;
- Non-linear if if these coefficients depend further on the derivatives of the unknown u.

Let $\quad \mathbf{s} = \frac{1}{\sqrt{a^2+b^2}} \begin{bmatrix} a \\ b \end{bmatrix}$ be the unit vector

then the above PDE can be expressed as

$$\mathbf{s} \cdot \nabla u + d = 0,$$

with $d = c/\sqrt{a^2 + b^2}$.

Characteristic curves

The curves, starting from an initial curve I_0, and with a slope,

$$\frac{dy}{dx} = \frac{b}{a},$$

are called characteristic curves. A point on these curves is reckoned by the curvilinear abscissa σ,

$$(d\sigma)^2 = (dx)^2 + (dy)^2.$$

Typically, σ is set to 0 on the initial curve I_0. Then

$$\mathbf{s} = \begin{bmatrix} dx/d\sigma \\ dy/d\sigma \end{bmatrix}$$

and the PDE becomes an ordinary differential equation (ODE) for $u(\sigma)$:

$$\frac{\partial u}{\partial x}\frac{\partial x}{\partial \sigma} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \sigma} + d = \frac{\partial u}{\partial \sigma} + d$$

For a system of 1st order PDEs,

$$L \cdot \mathbf{u} = \mathbf{a} \cdot \frac{\partial \mathbf{u}}{\partial t} + \mathbf{b} \cdot \frac{\partial \mathbf{u}}{\partial x} + \mathbf{c} = 0$$

or

$$\lambda \cdot L \cdot \mathbf{u} = \mathbf{p} \cdot \frac{d\mathbf{u}}{d\sigma} + r = 0$$

The vector λ appears to be a left eigenvector of the matrix $\mathbf{a}\frac{\partial x}{\partial t} - \mathbf{b}$, namely

$$\lambda \cdot (\mathbf{a}\frac{\partial x}{\partial t} - \mathbf{b}) \;=\; 0.$$

$$with \quad \frac{\lambda \cdot \mathbf{a}}{dt} \;=\; \frac{\lambda \cdot \mathbf{b}}{dx} = \frac{\mathbf{p}}{d\sigma}.$$

For the eigenvector not to vanish, the associate coefficient matrix should be singular,

$$det(\mathbf{a}\frac{\partial x}{\partial t} - \mathbf{b}) = 0$$

Classification of 1st order linear PDEs

The system of 1st order PDEs is said to be

$$\begin{cases} \textit{elliptic,} & \text{if the number of real eigenvalues is 0 ;} \\ \textit{hyperbolic} & \text{if the eigenvalues are real and distinct,} \\ & \text{or if the eigenvalues are real} \\ & \quad \text{and the system is not defective;} \\ \textit{parabolic,} & \text{if the eigenvalues are real, but the system is defective;} \end{cases}$$

Let us recall that a system of size n is said non defective if its eigenvectors generate $\Re^n$, i.e., the algebraic and geometric multiplicities of each eigenvector are identical.

Definition 2 A 2nd order partial differential equation for the unknowm $u(x, y)$ is said to be

- Linear if it is a linear equation of the unknown function and its derivatives,

$$au_{xx} + bu_{yy} + cu_x + du = Q;$$

- Quasi-linear if all the highest derivative terms are linear but some of the lower order derivatives are non-linear,

$$au_{xx} + bu_x^2 = f(x, y, u);$$

- Non-linear if the equation is neither linear nor quasi-linear,

$$u_{xx} + 2u_{xy}^2 + bu = Q(x, y).$$

Most partial differential equations arising from real world problems are second order and thus we will focus only on second order equations.

The general form of the second order quasi-linear partial differential equation is

$$au_{xx} + bu_{xy} + cu_{yy} + h(x, y, u, u_x, u_y) = 0,$$

which can be classified into three categories according to the value of $b^2 - 4ac$,

- elliptic : $b^2 - 4ac < 0$
- parabolic : $b^2 - 4ac = 0$
- hyperbolic : $b^2 - 4ac > 0$

Limiting Cases

Example

1) The poisson equation

$$\nabla^2 u = \sigma$$

is elliptic ($a = c = 1, b = 0$);

2) The diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

is parabolic ($a = 1, b = c = 0$);

3) The wave equation

$$\frac{\partial^2 u}{\partial t^2} = \alpha^2 \frac{\partial^2 u}{\partial x^2}$$

Example

4) Convection-Diffusion

$$\frac{\partial u}{\partial t} + U \cdot \nabla u = \kappa \nabla^2 u + f,$$

where $\nabla \equiv (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$, $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z,}$
$U,\ \kappa > 0,\ f$ are given functions of (x, y, z).
It is a Scalar, Linear, Parabolic equation.

If a,b and c are functions of x, y and u, the equation may change its type from one region to the other in the computation domain

Example

The following partial differential equation

$$(1 - M^2(x,y))\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0$$

may change its type from one sub-domain to the other. It can be classified as

1) elliptic equation if $M(x,y) < 1$;
2) parabolic equation if $M(x,y) = 1$;
3) hyperbolic equation if $M(x,y) > 1$.

Boundary and initial conditions

If we do not distinguish between time and space as independent variables, an initial condition can also be regarded as a boundary condition.

For real world problems, usually, we know the value of the unknown function and/or its derivatives on part of the boundary $\partial\Omega$.

As the solution must satisfy the boundary conditions, we have to solve the partial differential equation in Ω subject to the boundary conditions on $\partial\Omega$.

Boundary conditions

Boundary conditions are usually of the following types:

- Dirichlet type (also called essential boundary condition in FEM)
  eg. $u = \hat{u}$ on $\partial\Omega$
- Neumann type (natural boundary condition)
  eg. $\frac{\partial u}{\partial n} = \hat{\sigma}$ on $\partial\Omega$
- Robin type (mixed or general boundary condition)
  eg. $\alpha \frac{\partial u}{\partial n} + ku = f,\ \alpha \neq 0,\ k \neq 0$, on $\partial\Omega$

Boundary value problems are classified based on the type of partial differential equations and the type of boundary conditions.

For example, a boundary value problem defined by an elliptic equation and a Neumann boundary condition is called a Neumann elliptic problem.

Methods of Solution

In general, a BVP of an unknown function u can be written as

$$L(u) = f(\mathbf{x}) \quad \texttt{in } \Omega \tag{5}$$

$$B(u) = g(\mathbf{x}) \quad \texttt{on } \partial\Omega \tag{6}$$

where $f(\mathbf{x})$ and $g(\mathbf{x})$ are known functions, L denotes a linear or nonlinear differential operator and B is a boundary operator.
To solve a BVP is to find the unknown function u that satisfies the differential equation in Ω and the boundary conditions on $\partial\Omega$. There are many alternative approaches available for solving linear and nonlinear BVPs, ranging from completely analytical to completely numerical.

The following approaches deserve attention:

Direct Integration (yielding exact solutions)

- Separation of variables;
- Similarity solutions;
- Fourier and Laplace transformations;

Approximate Solution Methods

- Perturbation, Power series, Probability schemes (Monte Carlo);
- The method of characteristics for hyperbolic equations;
- Finite difference technique;
- Ritz method;
- Boundary element method;
- Finite element method.

Remarks

1) Only for very simple problems, it is possible to obtain an exact solution by direct integration of the differential equations.
2) The Power series method is powerful, but since the method requires generation of a coefficient for each term in the series, it is relatively tedious.
3) The perturbation method is applicable primarily when the nonlinear terms in the equation are small in relation to the linear terms.
4) The probability schemes(Monte Carlo Method) are used for obtaining a statistical estimate of a desired quantity random sampling.
5) With the advent of high-speed computers, it appears that the three currently outstanding methods for obtaining approximate solutions of high accuracy are the FDM, FEM and BEM.

Model Equation/Applications

Example

$$\frac{\partial u}{\partial t} + U \cdot \nabla u = \kappa \nabla^2 u + f,$$

If u is

- Temperature $\longrightarrow$ Heat Transfer
- Pollutant Concentration $\longrightarrow$ Coastal Engineering
- Probability Distribution $\longrightarrow$ Statistical Mechanics
- Price of an Option $\longrightarrow$ Financial Engineering

Fourier Analysis

Definition

Let $g(x)$ be an "arbitrary" periodic real function with period 2π

$$g(x) = \sum_{k=-\infty}^{\infty} g_k e^{ikx}$$

- $\int_0^{2\pi} e^{ikx} e^{-ik'x} dx = 2\pi\delta_{kk'}$ $\quad(orthogonality)$
- $g_k = \frac{1}{2\pi} \int_0^{2\pi} g(x) e^{-ikx}\, dx$

Rate at which $|g_k| \to 0$ for k large determines smoothness.

Fourier Analysis/Differentiation

$$u(x) = \sum_{k=-\infty}^{\infty} u_k e^{ikx} \quad or \quad u(x,t) = \sum_{k=-\infty}^{\infty} u_k(t) e^{ikx}$$

- $\frac{\partial^n u}{\partial x^n} = \sum_{k=-\infty}^{\infty} (ik)^n u_k e^{ikx} \quad \frac{\partial u}{\partial t} = \sum_{k=-\infty}^{\infty} \frac{du_k}{dt} e^{ikx}$
- $n = 2m \longrightarrow (ik)^n = (-1)^m k^{2m} \quad (real)$
- $n = 2m - 1 \longrightarrow (ik)^n = -i(-1)^m k^{2m-1} \quad (imaginary)$

Fourier Analysis-Poisson Equation

Example

$$-u_{xx} = f(x) \quad x \in (0,\ 2\pi)$$

with

$$u(0) = u(2\pi),\ u_x(0) = u_x(2\pi)$$

and

$$\int_0^{2\pi} u\, dx = 0,\ \int_0^{2\pi} f(x) dx = 0$$

Let $u = \sum_{k=-\infty}^{\infty} u_k e^{ikx}, \qquad f = \sum_{k=-\infty}^{\infty} f_k e^{ikx} \ (f_0 = 0)$

We obtain $-u_{xx} = \sum_{k=-\infty}^{\infty} k^2 u_k e^{ikx}$

$$\Longrightarrow u_k = \frac{f_k}{k^2} \ (u_0 = 0)$$

Fourier Analysis-Heat Equation

Example

$$u_t \;=\; \kappa u_{xx} \quad x \in (0,\ 2\pi)$$

with

$$u(0,t) = u(2\pi,t), \quad u_x(0,t) = u_x(2\pi,t),$$

and

$$u(x,0) = u^0(x) = \sum_{k=-\infty}^{\infty} u_k^0 e^{ikx},$$

Let $\quad u = \sum_{k=-\infty}^{\infty} u_k(t) e^{ikx}$

We obtain $\quad u_t = \sum_{k=-\infty}^{\infty} \frac{du_k}{dt} e^{ikx} \quad u_{xx} = \sum_{k=-\infty}^{\infty} -k^2 u_k e^{ikx}$

$$\frac{du_k}{dt} = -\kappa k^2 u_k$$

As $\frac{du_k}{dt} = -\kappa k^2 u_k,$

and $u_k(t = 0) = u_k^0$

$$\rightarrow u_k(t) = u_k^0 e^{-\kappa k^2 t}$$

Thus,

$$u(x, t) = \sum_{k=-\infty}^{\infty} u_k^0 e^{-\kappa k^2 t} e^{ikx}$$

- exponential decay of initial condition (dissipation)
- higher decay for "higher modes" (larger k) $\equiv$ smoothness

Fourier Analysis-Wave Equation

Example

$$u_t + \alpha u_x \;=\; 0 \quad x \in (0,\ 2\pi)$$

with

$$u(0,t) = u(2\pi, t),$$

and

$$u(x,0) = u^0(x) = \sum_{k=-\infty}^{\infty} u_k^0 e^{ikx},$$

Let $\quad u = \sum_{k=-\infty}^{\infty} u_k(t) e^{ikx}$

We obtain $\quad u_t = \sum_{k=-\infty}^{\infty} \frac{du_k}{dt} e^{ikx} \quad u_x = \sum_{k=-\infty}^{\infty} iku_k e^{ikx}$

$$\frac{du_k}{dt} = -i\alpha k u_k$$

As $\quad \frac{du_k}{dt} = -i\alpha k u_k,$

and $\quad u_k(0) = u_k^0$

$$\rightarrow u_k(t) = u_k^0 e^{-i\alpha k t}$$

Thus, $\quad u(x,t) = \sum_{k=-\infty}^{\infty} u_k^0 e^{-i\alpha k t} e^{ikx}$

$$= \sum_{k=-\infty}^{\infty} u_k^0 e^{ik(x-\alpha t)} = u^0(x - \alpha t)$$

- no decay, propagation with wave speed $c = \alpha$
- no dispersion (c constant) $\equiv$ invariant shape

Fourier Analysis-General Equation

Example

$$u_t = \frac{\partial^n u}{\partial x^n} \quad x \in (0,\ 2\pi)$$

with

$$u(0, t) = u(2\pi, t),$$

$$u_x(0, t) = u_x(2\pi, t),$$

$$u_x^{(n-1)}(0, t) = u_x^{(n-1)}(2\pi, t),$$

$$u(x, 0) = u^0(x)$$

Let $\quad u = \sum_{k=-\infty}^{\infty} u_k(t) e^{ikx}$

We obtain $\quad u_t = \sum_{k=-\infty}^{\infty} \frac{du_k}{dt} e^{ikx} \quad u_x^{(n)} = \sum_{k=-\infty}^{\infty} (ik)^n u_k e^{ikx}$

$$\frac{du_k}{dt} = \mu u_k, \quad \mu = (ik)^n$$

$$\begin{cases} \text{n=1}, \ \mu = ik & \text{Propagation, } c = -\mu/ik = -1 \text{ (no Dispersion);} \\ \text{n=2}, \ \mu = -k^2, & \text{Decay;} \\ \text{n=3}, \ \mu = -ik^3 & \text{Propagation, } c = k^2 \text{ (and Dispersion);} \\ \text{n=4}, \ \mu = k^4 & \text{Growth } (-u_{xxxx} \text{ much faster Decay than } u_{xx}. \end{cases}$$

Fourier Analysis-Eigenvalue Problem

Example

$$u_{xx} + \lambda u \;=\; 0 \quad x \in (0,\, 2\pi)$$

with

$$u(0) = u(2\pi),$$

$$u_x(0) = u_x(2\pi)$$

Need to determine non-trivial pairs ($u^n(x),\ \lambda^n$)

It can be easily verify that the eigenvalues are

$$\lambda^n = n^2 \;\; for \;\; n = 1, 2, 3, \ldots$$

The eigenvectors associated with λ^n are

$$u_1^n(x) = e^{inx}, \; u_2^n(x) = e^{-inx}, \;\; for \;\; n = 1, 2, 3, \ldots$$

Eigenmodes $\equiv$ Fourier modes

Eigenvalue Formal Extension

Eigenvalues determine temporal evolution of the associated time-dependent problem. Higher λ gives higher decay/frequency (more oscillations)

Let $\quad \frac{\partial u}{\partial t} = Lu, \;\; for \;\; x \in (0,\ 2\pi)$

with homogeneous BC $\quad u(x, y, t) = \sum_{n=0}^{\infty} a_n(t) u^n(x, y)$

$(u^n,\ \lambda^n)$ solution of $Lu - \lambda u = 0$

$$Lu = \sum_{n=0}^{\infty} \lambda^n a_n u^n$$

$$\frac{\partial u}{\partial t} = \sum_{n=0}^{\infty} \frac{da_n}{dt} u^n, \quad \frac{da_n}{dt} = \lambda^n a_n$$

$$\Longrightarrow a_n(t) = a_n^0 e^{\lambda^n t}$$

$$u(x, y, t) = \sum_{n=0}^{\infty} a_n^0 e^{\lambda^n t} u^n(x, y)$$

Exercises

Q1. Classify the following 2nd order PDEs:

1. $3u_{xx} + 2u_{xy} + 5u_{yy} + 2u_y = 0$
2. $c^2 u_{tt} - u_{xx} = 0$
3. $u_t - u_{xx} = 0$
4. $e^{2x} u_{xx} + 2e^{x+y} u_{xy} + e^{2y} u_{yy} = 0$

Q2. Find the Fourier series solution to the heat equation of a rod of length L using the heat equation:

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2}$$

where $u(0, t) = u(L, t) = 0$ and $u(x, 0) = f(x)$.

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