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3 Mathematical Models and Numerical Differentiation

3.1 Types of problems

In engineering, the problems can be continuous or discrete. Examples of continuous systems include the response of continuous beam under static or dynamic loads and wave propagation through an elastic media. Lumped mass systems, such as buildings with very stiff and heavy floors relative to the columns can be described by discrete model with good accuracy. Such assumptions drastically reduced the size of the problem compared to a continuous model.

Generally, problems can be classified into 3 broad types:

(a) Equilibrium Problems: state of the system remains constant with time (steady state problems), e.g. statics, steady state flow in fluid.

(b) Eigenvalue Problems: extension of equilibrium problems where critical values of certain parameters need to be determined, e.g. natural frequencies of vibrating structural, mechanical or electrical systems, buckling and stability analyses of structures.

(c) Propagation Problems: determine the subsequent state of a system based on an initial known state, e.g. transient and unsteady state phenomena in heat conduction, vibrations, structural dynamics and stress waves in elastic media.

These problems, when modeled mathematically, are often cast in the form of differential equations. They can be either ordinary or partial differential equations, depending on the number of independent variables involved.

3.2 Ordinary and Partial differential equations

A partial differential equation (PDE) establishes a relationship between an unknown function of *several* variables and its *partial* derivatives.

An ordinary differential equation (ODE) establishes a relationship between an unknown function of a *single* variable and its total derivatives.

Example:
Transverse vibrations of a beam (PDE)

$$\frac{\partial^2}{\partial x^2}\left(EI\,\frac{\partial^2 u(x,t)}{\partial x^2}\right)+m\frac{\partial^2 u(x,t)}{\partial t^2}=0 \quad \text{or} \quad \left(EIu_{xx}\right)_{xx}+mu_{tt}=0 \tag{3.1}$$

where *EI* is the flexural rigidity.

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Dynamic response of a single degree-of-freedom system (ODE)

$$m\frac{d^2u(t)}{dt^2}+ku(t)=f(t) \qquad \text{or} \qquad m\ddot{u}+ku=f(t) \tag{3.2}$$

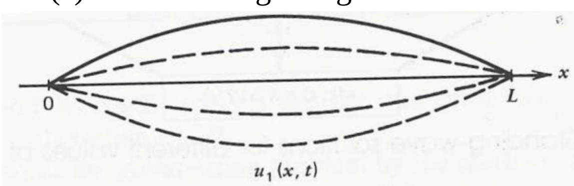
with m = mass, k =stiffness and $f(t)$ = force.

Identify the variable?

3.3 Some PDEs in Engineering

Many natural laws of physics are described by PDE e.g. Newton's equation of motion, Maxwell's equations, Navier-Stokes equations etc. PDE describes physical phenomena by relating space and time derivatives. These derivatives have physical meaning, e.g. velocity, acceleration, flux, current, etc.

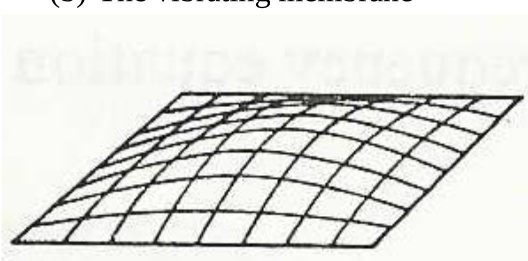
(a) The vibrating string



$$T\frac{\partial^2 u}{\partial x^2}=m\frac{\partial^2 u}{\partial t^2} \tag{3.3}$$

where T is tension on the string.

(b) The vibrating membrane



$$S\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=m\frac{\partial^2 u}{\partial t^2} \tag{3.4}$$

where S is the tension on the membrane.

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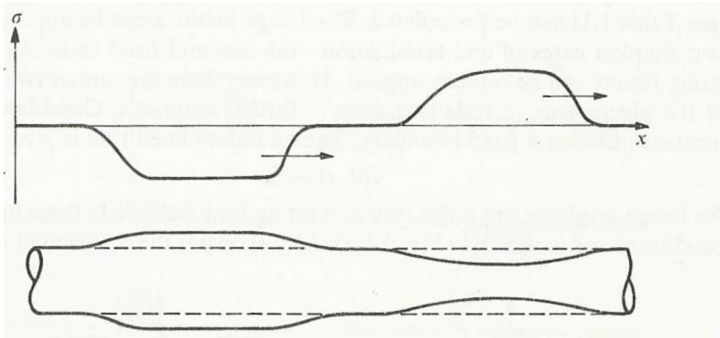
(c) Longitudinal vibrations of a bar

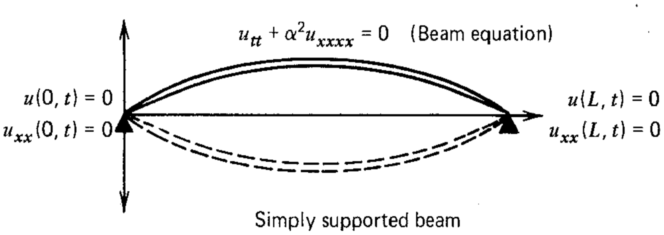


Exaggerated illustration of Poisson expansion and contraction resulting from longitudinal stress pulses.

$$E\frac{\partial^2 u}{\partial x^2} = m\frac{\partial^2 u}{\partial t^2} \tag{3.5}$$

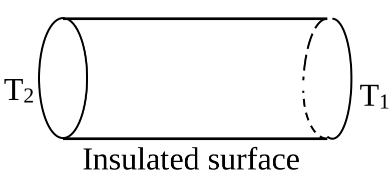
where E is the Young's modulus of the bar.

(d) Transverse vibrations of a beam with flexural rigidity EI



$$\frac{\partial^2}{\partial x^2}\left(EI\frac{\partial^2 u}{\partial x^2}\right) + m\frac{\partial^2 u}{\partial t^2} = 0 \tag{3.6}$$

(e) Heat flow in one dimension



$$\frac{\partial^2 T}{\partial x^2} = \frac{c\rho}{k}\frac{\partial T}{\partial t} \tag{3.7}$$

where c is heat coefficient, k is thermal conductivity and ρ is density.

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(f) Three-dimensional heat equation

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}=\frac{c\rho}{k}\frac{\partial T}{\partial t} \quad \text{or} \quad \nabla^2 T=\frac{c\rho}{k}\frac{\partial T}{\partial t} \tag{3.8}$$

where ∇^2 is the Laplace operator.

(g) Continuity equation (hydrodynamics)

$$\frac{\partial \rho}{\partial t}+\rho\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}\right)=0 \tag{3.9}$$

where ρ is the density of the fluid; u,v,w are the velocities of the fluid in x,y,z direction.

(h) Equation of elasticity

$$\frac{\partial \sigma_x}{\partial x}+\frac{\partial \tau_{yx}}{\partial y}=0 \quad \text{and} \quad \frac{\partial \sigma_y}{\partial y}+\frac{\partial \tau_{xy}}{\partial x}=0 \tag{3.10}$$

One of the techniques used in solving the equation consists of introducing a function $\phi(x,y)$ called *Airy* stress function with the following properties

$$\tau_{xy}=-\frac{\partial^2 \phi}{\partial x \partial y} \quad , \quad \sigma_x=\frac{\partial^2 \phi}{\partial y^2} \quad , \quad \sigma_y=\frac{\partial^2 \phi}{\partial x^2} \tag{3.11}$$

such that

$$\nabla^4 \phi=\left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2 \partial y^2}+\frac{\partial^4}{\partial y^4}\right)\phi=0 \tag{3.12}$$

where (3.12) is a biharmonic (Poisson type) equation.

(i) Bending of an elastic plate

$$\nabla^4 u=\frac{q}{D} \tag{3.13}$$

where *u* is the deflection, *q* is the loading per unit area and *D* is the flexural rigidity.

3.4 Solution methods

(a) *Separation of variables* – reduce PDE in *n* variables to *n* ODEs.

(b) *Integral Transforms* – produces new equations that depend on a different variable and appear in the form of an integral, e.g. Laplace Transforms.

(c) ***Numerical methods*** – solved by iterative methods by changing to system of simultaneous equation or difference equations.

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(d) *Integral equations* – changes PDE into an integral equation and then solved by known techniques, e.g. weighted residues.

(e) *Calculus of variation* – reformulate PDE into a minimization problem, where the minimum of an expression (e.g. total energy) is the solution to the PDE.

(f) *Eigenfunction expansion* – find the solution as an infinite sum of eignfunctions which are obtained by solving the eigenvalue problem corresponding to the original problem.

3.5 General concepts in PDE

3.5.1 Order of a PDE

Defined by the highest derivative in the equation

Examples of second order PDE:

$$\text{Linear:} \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial y} = 0$$

$$\text{Non-linear:} \quad \frac{\partial^2 u}{\partial x^2} + k\left(\frac{\partial u}{\partial y}\right)^3 = 0 \tag{3.14}$$

3.5.2 Linearity of a PDE

First degree in the field variable and its partial derivatives

Examples:

$$\text{Linear:} \quad \frac{\partial F}{\partial x} = \frac{\partial F}{\partial y}$$

$$\text{Non-linear:} \quad \frac{\partial F}{\partial x} = \left(\frac{\partial F}{\partial y}\right)^3 \tag{3.15}$$

How do we test the linearity of PDE?

Consider the equation

$$\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} = 0 \quad or \quad L(u) = 0 \tag{3.16}$$

where $L = \frac{\partial}{\partial x} + y\frac{\partial}{\partial y}$ is an operator.

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If u admits representation $u = \alpha(x, y) + \beta(x, y)$ then it can be shown that

$$L(u) = L(\alpha + \beta) = L(\alpha) + L(\beta) \tag{3.17}$$

If u admits representation $u = c\alpha(x, y)$ then it can be shown that

$$L(u) = L(c\alpha) = cL(\alpha) \tag{3.18}$$

An operator that satisfies both tests implies that the PDE is linear.

On the other hand, consider another PDE

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + u^2 = L^*(u) = 0 \tag{3.19}$$

If u admits representation $u = \alpha(x,t) + \beta(x,t)$ then

$$\begin{aligned} L^*(u) &= \frac{\partial(\alpha+\beta)}{\partial t} - \frac{\partial^2(\alpha+\beta)}{\partial x^2} + (\alpha+\beta)^2 \\ &= \frac{\partial \alpha}{\partial t} - \frac{\partial^2 \alpha}{\partial x^2} + \alpha^2 + \frac{\partial \beta}{\partial t} - \frac{\partial^2 \beta}{\partial x^2} + \beta^2 + 2\alpha\beta \\ &= L^*(\alpha) + L^*(\beta) + 2\alpha\beta \\ &\neq L^*(\alpha) + L^*(\beta) \end{aligned} \tag{3.20}$$

This implies that the PDE is nonlinear.

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3.5.3 Homogeneity of a PDE

Every term in the PDE contains either the field variable *u* or one of its derivatives, i.e. $L(u) = 0$, where *L* is of the form $L\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}, \frac{\partial}{\partial t}\right)$.

Non-homogenous equation can be written in the form $L(u) = f(x, y, t)$ where $f(x, y, t)$ is a non-zero function.

Are the following PDE homogeneous?
(a) $u_{yy} + 3u_y - 4u = 0$
(b) $u_{xy} + u_x + x = 0$
(c) $u_{xx} + 6u_{xy} + 9u_{yy} = 0$

3.5.4 Solution Domain and Boundary

The unknown functions *u* is known as the primary dependent variables and the solution must satisfy the governing differential equation over a particular domain as well as solutions imposed along its boundary.

The domain Ω is therefore defined by its independent variables, e.g. *x, y, t.* The boundary Γ of Ω is the set of points such that in any neighborhood of each of these points, there are points that belong to the domain as well as points that do not. Spatially, Γ is one dimension less than Ω.

A domain is simply connected if any simple closed contour in the domain can be shrunk continuously to a point – the domain consists only of internal points. Otherwise, the domain is multiply connected.

A boundary can be open or closed with respect to one or more of its independent variable. For example, if there is no end time, the boundary is open with respect to *t*. The boundary is closed if it is bounded.

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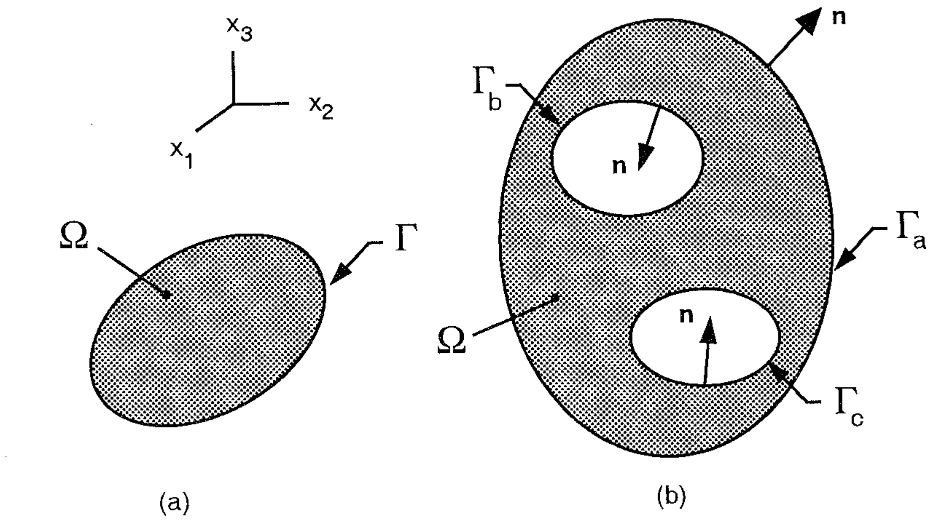


Figure 1.4: Schematic Illustration of a Typical Solution Domain and its Boundary: (a) Simply Connected, (b) Multiply Connected ($\Gamma = \Gamma_a + \Gamma_b + \Gamma_c$)

3.6 Initial and Boundary Conditions

Solution to PDE or ODE has infinite solutions which characterize the physical system. For a specific problem that is being modeled, certain auxiliary conditions must be imposed in the form of *boundary* and/or *initial* conditions.

3.6.1 Boundary conditions (BC)

These conditions must be satisfied at the boundary ***S*** (or also denoted as Γ). The three types of boundary conditions (BC) are

(a) Dirichlet BC: Also known as essential or geometric BC.

If the PDE is of order 2*s*, then equations relating the values of u and its derivatives up to order $s-1$ along ***S*** fall in this class.

E.g. for 2nd order PDE, $s=1 \Rightarrow s-1=0$. Dirichlet BC for the PDE is given by $u = g$ on $\boldsymbol{x} \in \boldsymbol{S}$ (u is zeroth-order) where g is a function prescribed on ***S***.

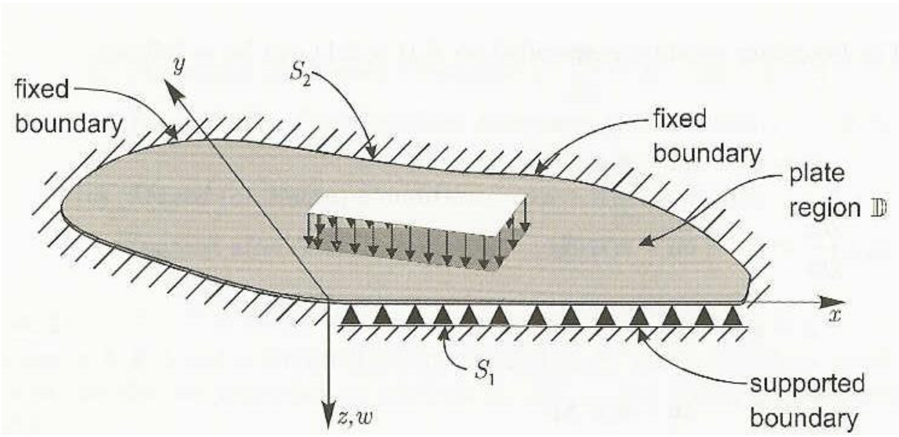
(b) Neumann BC: Also known as non-essential or natural BC.

If the PDE is of order 2*s*, then equations relating to values of derivatives of order *s* to $2s-1$ along ***S*** fall in this class.

E.g. for 2nd order PDE, $s=1$. Neumann BC is $\partial u / \partial n = h$ on $\boldsymbol{x} \in \boldsymbol{S}$ where h is a function prescribed on ***S***.

(c) Mixed (or Robin) Condition: $\lambda u + \mu \, \partial u / \partial n = k$ on $\boldsymbol{x} \in \boldsymbol{S}$ where k, λ and μ are functions prescribed on $\boldsymbol{S}$.

<u>Example</u>



Flexural deflections $w(x,y)$ of an elastic plate of flexural rigidity D and Poison ratio ν subjected to a transverse load $p(x,y)$

$$D\,\nabla^2\nabla^2 w(x,y) = p(x,y) \quad , \quad x \in \mathbf{D} \tag{3.21}$$

where $\mathbf{D}$ is the plate region.

Plate is fixed on part of the boundary and support without transverse movement. Boundary conditions are given by

$$\begin{aligned} w &= 0 \quad , \quad \frac{\partial^2 w}{\partial y^2} + \nu \frac{\partial^2 w}{\partial x^2} = 0 \quad \text{on} \quad x \in S_1 \\ w &= 0 \quad , \quad \frac{\partial w}{\partial n} = 0 \qquad\qquad\quad \text{on} \quad x \in S_2 \end{aligned} \tag{3.22}$$

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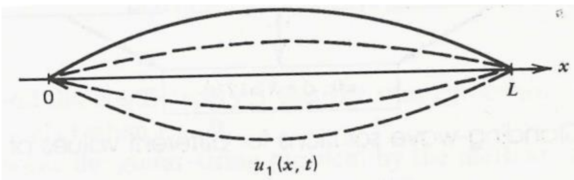
3.6.2 Initial conditions (IC)

These are prescribed conditions that must be satisfied throughout the domain at the instant when the processes described by the PDE commences. The conditions can be a combination of the independent variable and its time derivatives.

Example



Vibrating string

$$\frac{\partial^2 y}{\partial t^2} - c^2 \frac{\partial^2 y}{\partial x^2} = 0 \tag{3.23}$$

BCs $(t \geq 0)$: $y(0,t) = 0$, $y(l,t) = 0$

ICs $(0 \leq x \leq l)$: $y(x,0) = f(x)$, $\dfrac{\partial y(x,0)}{\partial t} = g(x)$

3.6.3 Well-posed problems

Problem is said to be well-posed if

(a) a solution exists
(b) solution is unique
(c) solution depends continuously on the PDE and the IC and BCs (also known as the auxiliary conditions)

E.g. consider a problem of a beam where the BCs are the forces and moments. Then the solution of the displacement is non-unique (but differ by a constant) as the beam is free to move to many different stable positions. But if one end has a displacement BC, e.g. u = 0, then the solution becomes unique.

3.7 Second-order liner PDE in two variables

General form:

$$A\frac{\partial^2 u}{\partial x^2}+B\frac{\partial^2 u}{\partial x\partial y}+C\frac{\partial^2 u}{\partial y^2}+D\frac{\partial u}{\partial x}+E\frac{\partial u}{\partial y}+Fu=G \tag{3.24}$$

$$\Rightarrow Au_{xx}+Bu_{xy}+Cu_{yy}+Du_x+Eu_y+Fu=G$$

3.7.1 Types of second order PDE

There are three basic types of linear 2nd order PDE depending on the quantity B^2-$4AC$.

Parabolic equations: B^2-4AC = 0 (e.g. heat flow and diffusion process).

Hyperbolic equations: B^2-4AC > 0 (e.g. vibrating systems and wave motion).

Elliptic equations: B^2-4AC < 0 (e.g. steady state phenomena).

Example

(a) $u_t = u_{xx}$

The coefficients in (3.24) are given by A = 1, E = -1, B = C = D = F = 0.
Since B^2 - 4AC = 0, it is a parabolic PDE.

(b) $u_{tt} = u_{xx}$

The coefficients in (3.24) are given by A = 1, C = -1, B = D = E = F = 0.
Since B^2 - 4AC = 4, it is a hyperbolic PDE.

(c) $u_{xx} + u_{yy} = 0$

The coefficients in (3.24) are given by A = C = 1, B = D = E = F = 0.
Since B^2 - 4AC = -4, it is a elliptic PDE.

(d) $yu_{xx} + u_{yy} = 0$

The coefficients in (3.24) are given by A = y, C = 1, B = D = E = F = 0.
Since B^2 - 4AC = -4y is a function of y, the PDE can change to parabolic, elliptic or hyperbolic, depending on the domain of interest.

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3.8 Additional notes on PDE classification

3.8.1 Second order Linear PDE in two variables

General form

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g \tag{3.25}$$

If the coefficients *a*, *b*, *c*, *d*, *e* and *f* are constants, then the above is a PDE with constant coefficients.

The characteristics of the solution of Eq (3.25) is, to a large extent, determined by the leading terms in the equation, that is, by the terms containing the derivatives of highest order. This part of the equation (we refer to it as the principal part of the equation) can be written as follows in matrix notation:

$$a\partial_{xx}u + 2b\partial_{xy}u + c\partial_{yy}u = \begin{bmatrix}\partial_x & \partial_y\end{bmatrix}\begin{bmatrix}a & b\\ b & c\end{bmatrix}\begin{bmatrix}\partial_x\\ \partial_y\end{bmatrix}u = [\partial]^T[A][\partial]\,u \tag{3.26}$$

Eq (3.25) can be characterized in terms of the algebraic properties of the matrix [A] in the representation (3.26). In particular, we classify equations of the form (3.26) in terms of the eigenvalues of matrix [A]. This is not the only way in which the classification may be carried out, but it is the one that generalizes most naturally to the case of equations involving more than two independent variables.

Since the matrix [A] is symmetric, its two eigenvalues are both real. In fact, they are the two roots of the equation

$$\left|A - \lambda I\right| = \lambda^2 - (a+c)\lambda - (b^2 - ac) = 0 \tag{3.27}$$

It is not difficult to show that the eigenvalues is controlled by the sign of the discriminant (b^2-ac). That is, the following holds:

(a) $b^2 - ac < 0$, the two roots of (3.27) are of the same sign. In this case we say (3.25)) is of elliptic type.

(b) $b^2 - ac = 0$, one of the two roots of (3.27) is zero and (3.25) is said to be of parabolic type.

(c) $b^2 - ac > 0$, one of the two roots of (3.27) is negative and the other is positive. We say that (3.25) is of hyperbolic type.

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The same analysis can be done in any number of variables, using a bit of linear algebra. Suppose that there are n variables, denoted by x_1, x_2, … x_n, and the equation is

$$\sum_{i,j=1}^{n} a_{ij} u_{x_i x_j} + \sum_{i=1}^{n} e_i u_{x_i} + cu = 0 \tag{3.28}$$

with real constants $a_{ij} = a_{ji}$, e_i and c.

Let $\mathbf{x}=(x_1, x_2, \ldots x_n)$. Consider any linear change of independent variables

$$(\xi_1, \ldots \xi_n) = \boldsymbol{\xi} = \mathbf{B}\boldsymbol{x} \tag{3.29}$$

where $\mathbf{B}$ is an $n\times n$ matrix. That is $\xi_k = \sum_m b_{km} x_m$

Convert to the new variables using the chain rule

$$\frac{\partial}{\partial x_i} = \sum_k \frac{\partial \xi_k}{\partial x_i} \frac{\partial}{\partial \xi_k} \tag{3.30}$$

and

$$u_{x_i x_j} = \Big(\sum_k b_{ki} \frac{\partial}{\partial \xi_k}\Big)\Big(\sum_l b_{lj} \frac{\partial}{\partial \xi_l}\Big) u \tag{3.31}$$

The second order term is converted to

$$\sum_{i,j} a_{ij} u_{x_i x_j} = \sum_{k,l} \Big(\sum_{i,j} b_{ki} a_{ij} b_{lj}\Big) u_{\xi_k \xi_l} \tag{3.32}$$

Note that on the left side u is considered as a function of $\boldsymbol{x}$, whereas on the right side it is considered as a function of $\boldsymbol{\xi}$.

A second order equation in the new variables $\boldsymbol{\xi}$ is thus obtained with the new coefficient matrix given within the parentheses, ie. BAB^T.

The theorem of linear algebra says that for any symmetric real matrix $\mathbf{A}$, there is a rotation $\mathbf{B}$ (an orthogonal matrix with unity determinant) such that $\mathbf{BAB}^T$ is the diagonal matrix

$$\mathbf{BAB}^T = \begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ldots & \\ & & & d_n \end{pmatrix} \tag{3.33}$$

where the real numbers d_1, d_2, … d_n are the eigenvalues of $\mathbf{A}$.

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Definition

For the classification of PDE (3.28), one needs to find the eigenvalues of **A** first.

(a) The PDE (3.28) is elliptic if all the eigenvalues d_1, d_2, …d_n are all positive or all are negative.

(b) The PDE (3.28) is hyperbolic if none of the d_1, d_2, …d_n vanish and one of them has the opposite sign from the (n-1) others.

(c) If none vanish, but at least two of them are positive and at least two are negative, it is called ultra-hyperbolic.

(d) If exactly one of the eigenvalues is zero and all the others have the same sign, the PDE (3.28) is parabolic.

3.8.2 Changing a higher order ODE to a system of lower order ODEs

Consider the transverse vibrations of a beam

$$\frac{\partial^2}{\partial x^2}\left(EI\,\frac{\partial^2 u}{\partial x^2}\right)+m\frac{\partial^2 u}{\partial t^2}=0 \tag{3.34}$$

where EI is the flexural rigidity of the beam.

Let

$$\frac{\partial u}{\partial x}=y_1 \quad , \quad \frac{\partial^2 u}{\partial x^2}=\frac{\partial y_1}{\partial x}=y_2 \quad , \quad \frac{\partial^3 u}{\partial x^3}=\frac{\partial y_2}{\partial x}=y_3 \quad , \quad \frac{\partial u}{\partial t}=y_4 \tag{3.35}$$

such that (3.34) is transformed into

$$EI\,\frac{\partial y_3}{\partial x}+m\frac{\partial y_4}{\partial t}=0 \tag{3.36}$$

From (3.35) and (3.36), the system of equations is given by

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & EI & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \partial u/\partial x \\ \partial y_1/\partial x \\ \partial y_2/\partial x \\ \partial y_3/\partial x \\ \partial y_4/\partial x \end{Bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & m \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} \partial u/\partial t \\ \partial y_1/\partial t \\ \partial y_2/\partial t \\ \partial y_3/\partial t \\ \partial y_4/\partial t \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \\ 0 \\ y_4 \end{Bmatrix} \tag{3.37}$$

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3.8.3 System of first order equations

The general quasi-linear system of n first order partial differential equations in two independent variables has the form

$$\sum_{j=1}^{n} a_{ij} \frac{\partial u_j}{\partial x} + \sum_{j=1}^{n} b_{ij} \frac{\partial u_j}{\partial t} = c_i \quad , \quad i = 1, 2, \dots n \tag{3.38}$$

or in the matrix form

$$\mathbf{A}\mathbf{u}_x + \mathbf{B}\mathbf{u}_t = \mathbf{C} \tag{3.39}$$

A characteristic polynomial is defined by

$$F(\lambda) = |\mathbf{A} - \lambda \mathbf{B}| \tag{3.40}$$

If $F(\lambda)$ has n distinct real zeros (n distinct real roots), we classify the first order system (3.38) as hyperbolic. The system is also called hyperbolic if $F(\lambda)$ has n real zeros and the generalized eigenvalue problem $(\mathbf{A} - \lambda\mathbf{B})\mathbf{u} = 0$ has n linearly independent solutions.

If $F(\lambda)$ has n real zeros but $(\mathbf{A} - \lambda\mathbf{B})\mathbf{u} = 0$ does not have n linearly independent solutions (n real roots but with repeated roots), then the system (3.38)may be classified as parabolic.

If $F(\lambda)$ has no real zeros (imaginary roots), then (3.38) is elliptic.

An exhaustive classification cannot be carried out when $F(\lambda)$ has both real and complex zeros.

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3.9 Numerical differentiation

Approximate numerical methods are often used to solve differential equations, especially with the advancement in computer hardware and software technology. One popular method is the finite difference (FD) method based on the Taylor expansion approximation.

Taylor series expansion of function $f(x)$:

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots \\ \Rightarrow f'(x) &= \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) - \ldots \end{aligned} \tag{3.41}$$

1st order approximation:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h) \tag{3.42}$$

which is the **forward difference approximation** for $f'(x)$ if we ignore the higher order terms. *Assuming* that $f''(x)$ does not change too rapidly, then the truncation error scales with h, which is simply denoted as $O(h)$.

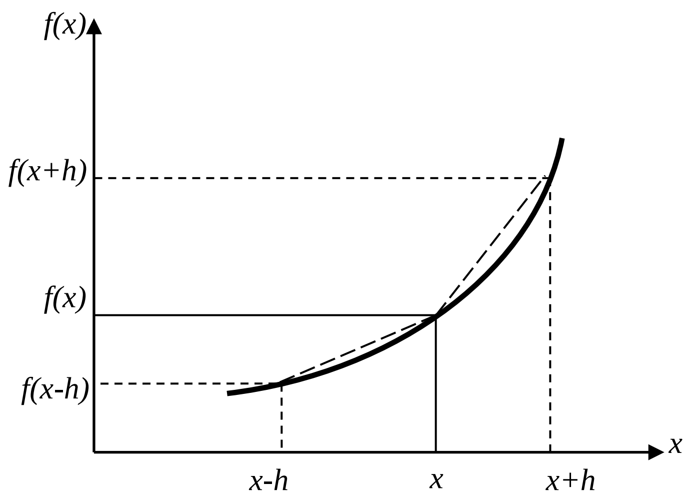

Fig 3.1

Note that it is called 'forward' because the slope at x is approximated using the current point x and forward point $x+h$.

If a backward point *x-h* is used with the current point *x* to approximate *f'(x)*, then (3.42) becomes

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(x) + ...$$
$$\Rightarrow f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2} f''(x) - \frac{h^2}{6} f'''(x) + ... \qquad (3.43)$$

1st order approximation:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h) \qquad (3.44)$$

which is the **backward difference approximation** for $f'(x)$ if we ignore the higher order terms.

Adding (3.41b) and (3.43b) gives

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) - .... \qquad (3.45)$$

1st order approximation:

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] + O(h^2) \qquad (3.46)$$

which is the **central difference approximation** for $f'(x)$ if we ignore the higher order terms.

In this case, the slope at *x* is approximated using the backward point *x-h* and forward point *x+h*, without using the current point *x*. Due to the cancellation of f'' in (3.45), the error is proportional to h^2 rather than h. Hence, the error associated with the central difference approximation reduces more quickly with a decrease in the step size *h*, compared to the other two approximations.

Example: Determine $f'(x)$ at $x = 1$ using the three approximations, given that $f(x) = \tan(x)$.

		% error		
		$h = 0.1$	$h = 0.05$	$h = 0.025$
FDM	$\left[f(1+h) - f(1)\right]/h$	-18.9	-8.5	-4.07
BDM	$\left[f(1) - f(1-h)\right]/h$	13.2	7.1	3.73
CDM	$\left[f(1+h) - f(1-h)\right]/2h$	-2.8	-0.69	-0.17

Note: Exact solution given by $f'(1) = \sec^2(1) = 3.426$. $\text{Error} = (3.426 - \text{approximation})/3.426$.

Observe that the errors associated with FDM and BDM decrease in proportion to *h*. For CDM, the error decreases in proportion to h^2.

Next, we add (3.41a) and (3.43a) to obtain

$$f(x+h) - f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12} f''''(x) + \ldots$$

2nd order approximation:

$$f''(x) = \frac{1}{h^2}\left[f(x+h) - 2f(x) + f(x-h)\right] + O(h^2) \tag{3.47}$$

which is the **central difference approximation** for $f''(x)$ if we ignore the higher order terms.

For ease of presentation below, we write

$$f(x \pm kh) = f_{n\pm k} \tag{3.48}$$

3.10 Higher order derivatives

The higher order derivatives using the backward difference approach are given by

$$\begin{aligned} f_n' &= [f_n - f_{n-1}]/h \\ f_n'' &= [f_n - 2f_{n-1} + f_{n-2}]/h^2 \\ f_n''' &= [f_n - 3f_{n-1} + 3f_{n-2} - f_{n-3}]/h^3 \\ f_n^{iv} &= [f_n - 4f_{n-1} + 6f_{n-2} - 4f_{n-3} + f_{n-4}]/h^4 \end{aligned} \tag{3.49}$$

Similarly, we can derive the higher order derivatives with the forward difference and central difference approaches. The coefficients can be summarized in a tabular form as follows:

Backward Difference

	f_{n-4}	f_{n-3}	f_{n-2}	f_{n-1}	f_n
$h\ f_n'$				-1	1
$h^2 f_n''$			1	-2	1
$h^3 f_n'''$		-1	3	-3	1
$h^4 f_n^{iv}$	1	-4	6	-4	1

Forward difference (3.50)

	f_n	f_{n+1}	f_{n+2}	f_{n+3}	f_{n+4}
$h\ f_n'$	-1	1			
$h^2 f_n''$	1	-2	1		
$h^3 f_n'''$	-1	3	-3	1	
$h^4 f_n^{iv}$	1	-4	6	-4	1

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Central difference

	f_{n-2}	f_{n-1}	f_n	f_{n+1}	f_{n+2}
$h\ f_n'$		-0.5	0	0.5	
$h^2 f_n''$		1	-2	1	
$h^3 f_n'''$	-0.5	1	0	-1	0.5
$h^4 f_n^{iv}$	1	-4	6	-4	1

3.11 Error analysis

Assume that a computer is used to make numerical computations. For a given step *n*, in addition to the truncation error, there is a round-off error due to the precision of the computer.

Consider the central difference approximation given in (3.45), which can be written as

$$f_n' = \frac{1}{2h}\left(f_{n+1} - f_{n-1}\right) + \frac{h^2 f'''(c)}{6} \tag{3.51}$$

where it is assumed that a number c exists in the interval $x-h \le c \le x+h$ such that the truncation error at the current step is given as the last term in (3.51).

For simplicity, consider *n*=0. In a computational calculation,

$$f_0' = \frac{1}{2h}\left(f_1 - f_{-1}\right) + E$$

with the total error E given by

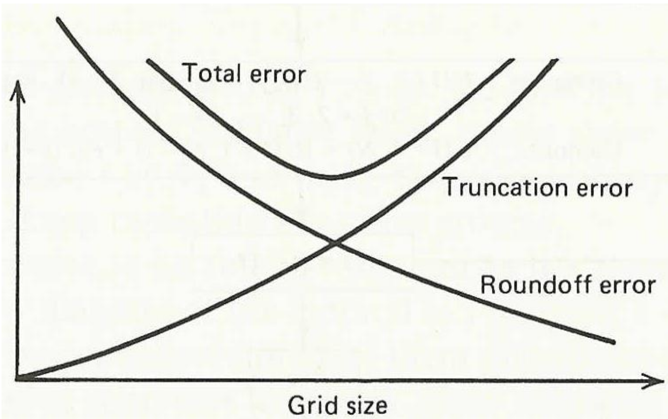
$$\begin{aligned} E &= E_{\text{round}} + E_{\text{trunc}} \\ &= \frac{e_1 - e_{-1}}{2h} + \frac{h^2 f'''(c)}{6} \end{aligned} \tag{3.52}$$

where $e_{\pm 1}$ are the round-off errors at $n = \pm 1$.

Let ε be the maximum round-off error, and f''' be bounded such that $\max_{-1\le h\le 1}\left\{\left|f_h'''\right|\right\} = M$. Then, (3.52) can be expressed as

$$|E| \le \frac{\varepsilon}{h} + \frac{Mh^2}{6} \tag{3.53}$$

Note that as h is reduced, the truncation error decreases, but the round-off error increases. In general. In general, the total error reduces with h, until an optimal value. Beyond this, the total error increases despite using a smaller step-size.



3.12 Stiff differential equations

When the solution to a system of differential equations contains components that change at significantly different rates for a given change in the independent variable, the system is said to be "stiff". When solved with numerical methods, the stepsize h must be extremely small in order to maintain stability.

As an example, consider the following system

$$\mathbf{y}' = \mathbf{A}\mathbf{y} \tag{3.54}$$

A characterization of the stiffness of the system is given by the ratio between the ratio of the largest and smallest (absolute) eigenvalues of $\mathbf{A}$, i.e. $|\lambda_{\max}|/|\lambda_{\min}|$.

For a system with two degrees of freedom, the solution is given by

$$\mathbf{y} = Ae^{\lambda_1 t}\ \mathbf{v}_1 + Be^{\lambda_2 t}\ \mathbf{v}_2 \tag{3.55}$$

where $\mathbf{y} = \begin{bmatrix} y_1 & y_2 \end{bmatrix}^T$, A and B are constants to be determined from the initial conditions, $(\lambda_1\ ,\ \mathbf{v}_1)$ and $(\lambda_2\ ,\ \mathbf{v}_2)$ are the eigenvalues and eigenvectors of matrix $\mathbf{A}$.

Consider $\mathbf{A} = \begin{bmatrix} -0.5005 & -4.995 \\ -0.4995 & -0.5005 \end{bmatrix}$ such that the eigen-solutions are

$$\lambda_1 = -1 \quad , \quad \mathbf{v}_1 = \begin{bmatrix} 1 & 1 \end{bmatrix}^T \quad \text{and} \quad \lambda_2 = -0.001 \quad , \quad \mathbf{v}_2 = \begin{bmatrix} -1 & 1 \end{bmatrix}^T \tag{3.56}$$

For this problem, even if we are interested only in the larger mode, the numerical scheme can be constrained by the much smaller mode, which requires a sufficiently small stepsize to be adopted. This results in a large number of steps over a given interval. Consequently, the methods used to solve stiff problems are generally based on stable techniques.