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Chapter 5: Differential equations

1. Partial differential equations
2. Ordinary differential equations
3. Nonhomogeneous equations
4. Self-adjoint ODEs

Differential equations

Partial differential equations (PDE): two or more variables
Ordinary differential equations (ODE): one variables

Linear operation:

$$\frac{\partial\left(a\varphi(x,y)+b\psi(x,y)\right)}{\partial x}=a\frac{\partial\varphi(x,y)}{\partial x}+b\frac{\partial\psi(x,y)}{\partial x}$$

In general, $L\left(a\varphi+b\psi\right)=aL(\varphi)+bL(\psi)$

Examples:

Laplace equation $\nabla^2\psi=0$

Poisson equation $\nabla^2\psi=-\rho/\varepsilon_0$

Diffusion equation $\nabla^2\psi=\frac{1}{a^2}\frac{\partial\psi}{\partial t}$

Time-dependent wave equation

$$\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi=0$$

Helmholtz (wave) equation $\nabla^2\psi\pm k^2\psi=0$

Schrodinger (wave) equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=i\hbar\frac{\partial}{\partial t}\psi \qquad -\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi$$

Classes of PDE

Solving PDEs

1. By transform
2. Separation of variables
3. Numerical methods

Linear operator:

$$L = a\frac{\partial^2}{\partial x^2} + 2b\frac{\partial^2}{\partial x\partial y} + c\frac{\partial^2}{\partial y^2} + d\frac{\partial}{\partial x} + e\frac{\partial}{\partial y} + f$$

Let $x, y \Rightarrow \xi = \xi(x,y), \eta = \eta(x,y)$

Characteristic equation:

$$a\left(\frac{\partial \xi}{\partial x}\right)^2 + 2b\left(\frac{\partial \xi}{\partial x}\right)\left(\frac{\partial \eta}{\partial y}\right) + c\left(\frac{\partial \eta}{\partial y}\right)^2 = 0$$

1. Elliptic: $D = ac - b^2 > 0$ two solutions complex conjugate
2. Parabolic: $D = ac - b^2 = 0$ one solution
3. Hyperbolic: $D = ac - b^2 < 0$ two independent solutions

Characteristics

Assuming d=e=f=0 for simplicity

$$L = a\frac{\partial^2}{\partial x^2} + 2b\frac{\partial^2}{\partial x \partial y} + c\frac{\partial^2}{\partial y^2}$$

Look for the solution

$$\psi = F(\xi), \xi = \xi(t,x)$$

$$\frac{\partial \psi}{\partial x} = \frac{\partial \xi}{\partial x}\frac{dF}{d\xi}, \frac{\partial \psi}{\partial t} = \frac{\partial \xi}{\partial t}\frac{dF}{d\xi} \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = \frac{\partial^2 \xi}{\partial x^2}\frac{dF}{d\xi} + \left(\frac{\partial \xi}{\partial x}\right)^2 \frac{d^2 F}{d\xi^2}$$

$$\frac{\partial^2 \psi}{\partial x \partial t} = \frac{\partial^2 \xi}{\partial x \partial t}\frac{dF}{d\xi} + \frac{\partial \xi}{\partial x}\frac{\partial \xi}{\partial t}\frac{d^2 F}{d\xi^2}, \quad \frac{\partial^2 \psi}{\partial t^2} = \frac{\partial^2 \xi}{\partial t^2}\frac{dF}{d\xi} + \left(\frac{\partial \xi}{\partial t}\right)^2 \frac{d^2 F}{d\xi^2}$$

For the linear $\xi = \alpha x + \beta t$

$$\frac{\partial^2 \psi}{\partial x^2} = \alpha^2 \frac{d^2 F}{d\xi^2}, \quad \frac{\partial^2 \psi}{\partial x \partial t} = \alpha\beta \frac{d^2 F}{d\xi^2}, \quad \frac{\partial^2 \psi}{\partial t^2} = \beta^2 \frac{d^2 F}{d\xi^2}$$

PDE becomes:

$$\left(a\alpha^2 + 2b\alpha\beta + c\beta^2\right)\frac{d^2 F}{d\xi^2} = 0$$

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Solutions of PDE

Characteristic equation:

$$a\alpha^2 + 2b\alpha\beta + c\beta^2 = 0 \qquad r_{1,2} = \frac{1}{c}\left[-b \pm \left(b^2 - ac\right)^{1/2}\right]$$

1. Elliptic: $D = ac - b^2 > 0$ two solutions complex conjugate
2. Parabolic: $D = ac - b^2 = 0$ one solution
3. Hyperbolic: $D = ac - b^2 < 0$ two independent solutions

Solutions:

$$D \neq 0: \ \psi(x,t) = F(\xi_1) + G(\xi_2), \quad \xi_{1,2} = x + r_{1,2}t$$

$$D = 0: \ \psi(x,t) = F\left(x - \frac{b}{c}t\right) + \psi_0(x,t)G\left(x - \frac{b}{c}t\right), \quad \psi_0 = x, \text{or } \psi_0 = t$$

Examples:

Hyperbolic: $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\psi = 0$

$$\left(\frac{\partial \xi}{\partial t}\right)^2 - c^2\left(\frac{\partial \xi}{\partial x}\right)^2 = 0 \qquad \psi(x,t) = F(\xi_1) + G(\xi_2), \quad \xi_{1,2} = x \pm ct$$

Elliptic: $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi = 0$

$$\psi(x,t) = F(\xi_1) + G(\xi_2), \quad \xi_{1,2} = x \pm iy$$

ODE

First order ODE:

$$\frac{dy}{dx} = f(x, y) = -\frac{P(x, y)}{Q(x, y)}$$

Separable variables:

$$\frac{dy}{dx} = f(x, y) = -\frac{P(x)}{Q(y)} \Rightarrow \int_{x_0}^{x} P(x)dx + \int_{y_0}^{y} Q(y)dy = 0$$

Exact differential equations:

$$P(x, y)dx + Q(x, y)dy = 0$$

$$P(x, y) = \frac{\partial \varphi}{\partial x}, \quad Q(x, y) = \frac{\partial \varphi}{\partial y}, \quad \frac{\partial P(x, y)}{\partial y} = \frac{\partial Q(x, y)}{\partial x} \Rightarrow \varphi(x, y) = C$$

Linear first-order ODEs:

$$\frac{dy}{dx} + p(x)y = q(x) \qquad y(x) = \exp\left[-\int^{x} p(t)dt\right]\left\{\int^{x} \exp\left[\int^{x} p(t)dt\right] q(s)ds + C\right\}$$

$$ex. \quad L\frac{dI(t)}{dt} + RI(t) = V(t)$$

Separation of variables

Helmholtz equation in Cartesian coordinates:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+k^2\psi=0$$

Look for the solution:

$$\psi(x,y,z)=X(x)Y(y)Z(z)$$

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2}=-l^2,\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=-m^2,\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=-n^2,k^2=l^2+m^2+n^2$$

$$\Psi=\sum_{l,m,n}a_{lmn}\psi_{lmn},\quad \psi_{lmn}=X_l(x)Y_m(y)Z_n(z)$$

Spherical polar coordinates:

$$\frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\varphi^2}\right]+k^2\psi=0$$

$$\psi(r,\theta,\varphi)=R(r)\Theta(\theta)\Phi(\varphi)$$

$$\psi_{Qm}(r,\theta,\varphi)=\sum_{Q,m}R_Q(r)\Theta_{Qm}(\theta)\Phi_m(\varphi)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+k^2R-\frac{QR}{r^2}=0,\quad \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{\sin^2\theta}\Theta+Q\Theta=0,\quad \frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}$$

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Linear 2nd order ODE

Homogeneous:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)y=0$$

Nonhomogeneous:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)y=F(x)$$

solutions:

$$y(x)=c_1y_1(x)+c_2y_2(x)+y_p(x)$$

particular solution from F(x)

Linear independence of solutions:

$$\sum_\lambda k_\lambda\varphi_\lambda=0,\ \sum_\lambda k_\lambda\varphi'_\lambda=0,\ldots\ \sum_\lambda k_\lambda\varphi_\lambda^{(m)}=0$$

Wronskian:

$$W=\begin{vmatrix}\varphi_1 & \varphi_2 & \cdots & \varphi_n\\ \varphi'_1 & \varphi'_2 & \cdots & \varphi'_n\\ \cdots & \cdots & \cdots & \cdots\\ \varphi_1^{(n-1)} & \varphi_2^{(n-1)} & \cdots & \varphi_n^{(n-1)}\end{vmatrix}$$

Ex. Solutions of linear oscillator

$$y''+\omega^2y=0$$

$$\varphi_1=\sin(\omega x),\varphi_2=\cos(\omega x)$$

The 2nd solution

Homogeneous:

$$y'' + P(x)y' + Q(x)y = 0$$

Differentiating W:

$$W' = -P(x)W$$

$$\Rightarrow W(x) = W(a)\exp\left[-\int_a^x P(x_1)dx_1\right]$$

Wronskian:

$$W = \begin{vmatrix} y_1 & y_2 \\ y_1' & y_2' \end{vmatrix} = y_1 y_2' - y_1' y_2$$

$$W = y_1^2 \frac{d}{dx}\left(\frac{y_2}{y_1}\right)$$

$$\frac{d}{dx}\left(\frac{y_2}{y_1}\right) = W(a)\frac{\exp\left[-\int_a^{x_2} P(x_1)dx_1\right]}{y_1^2}$$

The 2nd solution:

$$y_2(x) = y_1(x)\int^x \frac{\exp\left[-\int^{x_2} P(x_1)dx_1\right]}{y_1^2(x_2)} dx_2, W(a) = 1$$

Ex. Solutions of Chebyshev equation

$$\left(1 - x^2\right)y'' - xy' + n^2 y = 0$$

$$y_1(x) = x \text{ for n} = 1, \varphi_2 = ?$$

$$\varphi_2 = -\sqrt{1 - x^2}$$

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Green's function

Homogeneous:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)y=0$$

$\longleftrightarrow$

Nonhomogeneous:

$$\frac{d^2y}{dx^2}+P(x)\frac{dy}{dx}+Q(x)y=F(x)$$

Solutions:

$$y(x)=c_1y_1(x)+c_2y_2(x)+y_p(x)$$

Green's function:

A solution to Poisson's equation with a point source

$$\nabla^2 G=-\delta(\mathbf{r}_1-\mathbf{r}_2)$$

Poisson's equation

$$\nabla^2\psi=-\frac{\rho}{\varepsilon_0}$$

Green's theorem

$$\int\left(\psi\nabla^2 G-G\nabla^2\psi\right)d\tau_2=\int\left(\psi\nabla G-G\nabla\psi\right)\cdot d\sigma=0$$

$$\Rightarrow\int\psi\nabla^2 G\,d\tau_2=\int G\nabla^2\psi\,d\tau_2$$

$\Longrightarrow$

$$\psi(\mathbf{r}_1)=\frac{1}{\varepsilon_0}\int G(\mathbf{r}_1,\mathbf{r}_2)\rho(\mathbf{r}_2)d\tau_2$$

Source and potential:

$$G(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{4\pi|\mathbf{r}_1-\mathbf{r}_2|}\qquad\psi(\mathbf{r}_1)=\frac{1}{4\pi\varepsilon_0}\int\frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|}d\tau_2$$

Ex. Electrostatic potential

$$\psi=\frac{1}{4\pi\varepsilon_0}\sum_i\frac{q_i}{r_i}\rightarrow\frac{1}{4\pi\varepsilon_0}\int\frac{\rho(\mathbf{r})}{r}d\tau$$

General 2nd order linear nonhomogeneous differential equation

$$Ly(\mathbf{r}_1)=-f(\mathbf{r}_1)\qquad LG(\mathbf{r}_1,\mathbf{r}_2)=-\delta(\mathbf{r}_1-\mathbf{r}_2)\qquad y(\mathbf{r}_1)=\int G(\mathbf{r}_1,\mathbf{r}_2)f(\mathbf{r}_2)d\tau_2$$

Green's function

Examples:

	Laplace ∇^2	Helmholtz $\nabla^2 + k^2$	Modified Helmholtz $\nabla^2 - k^2$
3 D space $G(\mathbf{r}_1, \mathbf{r}_2)$	$\frac{1}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$	$\frac{\exp(ik\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$	$\frac{\exp(-k\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}$

<u>Quantum scattering:</u>

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$\nabla^2\psi(\mathbf{r}) + k^2\psi(\mathbf{r}) = -\left[-\frac{2m}{\hbar^2}V(\mathbf{r})\right]\psi(\mathbf{r}), \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}} + f_k(\theta,\varphi)\frac{e^{ikr}}{r}$$

no scattering outgoing scattered

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}} - \int \frac{2m}{\hbar^2}V(\mathbf{r}_2)\psi(\mathbf{r}_2)G(\mathbf{r}_1,\mathbf{r}_2)d^3r_2$$

The solution:

$$\psi(\mathbf{r}_1) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}_1} - \int \frac{2m}{\hbar^2}V(\mathbf{r}_2)\psi(\mathbf{r}_2)\frac{\exp(ik\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}d^3r_2$$

Neumann series:

0-th order $\psi_0(\mathbf{r}_1) = e^{i\mathbf{k}_0\cdot\mathbf{r}_1}$

1st order $\psi(\mathbf{r}_1) \sim e^{i\mathbf{k}_0\cdot\mathbf{r}_1} - \int \frac{2m}{\hbar^2}V(\mathbf{r}_2)e^{i\mathbf{k}_0\cdot\mathbf{r}_2}\frac{\exp(ik\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert)}{4\pi\lvert\mathbf{r}_1 - \mathbf{r}_2\rvert}d^3r_2$

~~Vector~~ Function space

The collection of ~~vectors~~ functions forms ~~vector~~ function space. And it has the following properties:

1. Vector function equality
   1. **A**=**B** => $A_i=B_i$
2. Addition
   1. Associativity (**A**+**B**)+**C**=**A**+(**B**+**C**)
   2. Commutativity **A+B=B+A**
   3. Distributivity a*(**A+B**)=a*A+a*B; (a+b)*A=a*A+a*B
3. Scalar multiplication
   1. Compatibility a*(b*A)=(a*b)*A
   2. Identity element 1*A=A
4. Negative of a ~~vector~~ function (inverse element)
   A+(-**A**)=0
5. Null ~~vector~~ function (identity element of addition)
   A+0=**A** for any **A**

Inner product

$$\langle f | g \rangle = \int_a^b f^*(x) g(x) w(x) dx$$

Adjoint operator

Adjoint:

L, M are operators in the function space V, $\forall u, v \in V$

$$(v, Lu) = (Mv, u) \quad \text{i.e.} \int_a^b v^* Lu dx = \int_a^b (Mv)^* L dx$$

Self-adjoint: $(v, Lu) = (Lv, u)$

Ex.

$$L = \frac{d}{dx}, \quad y(a) = y(b), y = u, v$$

$$\int_a^b v^* \frac{du}{dx} dx = v^* u\Big|_a^b - \int_a^b \frac{dv^*}{dx} u dx$$

$$L = i\frac{d}{dx}, \quad y(a) = y(b), y = u, v$$

$$\int_a^b v^* \left(i\frac{du}{dx} \right) dx = v^* u\Big|_a^b + \int_a^b \left(i\frac{dv}{dx} \right)^* u dx$$

Properties for self-adjoint operators:

1. Eigenvalules are real
2. Eigenfunctions are orthogonal
3. Eigenfunctions form a complete set

Strum-Liouville ODEs

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S-L equation:

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right]+\left[\lambda\rho(x)-q(x)\right]y=0$$

$p(x), q(x), \rho(x)$ are real functions.

Transformed:

$$L=-\frac{d}{dx}\left[p(x)\frac{d}{dx}\right]+q(x) \qquad \langle y_1|y_2\rangle=\int_a^b y_1^*(x)y_2(x)\rho(x)dx$$

$$Ly=\lambda\rho(x)y$$

$$L'=-\frac{d}{dx}\left[\varphi(x)\frac{d}{dx}\right]+\psi(x) \qquad \langle u_1|u_2\rangle=\int_a^b u_1^*(x)u_2(x)dx$$

$$u(x)=\sqrt{\rho(x)}y(x)$$

$$\varphi(x)=\frac{p(x)}{\rho(x)},\quad \psi(x)=-\frac{1}{\sqrt{\rho(x)}}\frac{d}{dx}\left[p(x)\frac{d}{dx}\frac{1}{\sqrt{\rho(x)}}\right]+\frac{q(x)}{\rho(x)}$$

$$L'u(x)=\lambda u(x)$$

Theorem:

$$u_1^*L'u_2-(L'u_1)^*u_2=-\frac{d}{dx}\left[\varphi(x)\left(u_1^*\frac{du_2}{dx}-u_2\frac{du_1^*}{dx}\right)\right]$$

$$u_1^*L'u_2-(L'u_1)^*u_2=y_1^*Ly_2-(Ly_1)^*y_2 \implies y_1^*Ly_2-(Ly_1)^*y_2=-\frac{d}{dx}\left[p(x)\left(y_1^*\frac{dy_2}{dx}-y_2\frac{dy_1^*}{dx}\right)\right]$$

Theorem:

L is self-adjoint under the boundary condition: $p(x)\left(y_1^*\frac{dy_2}{dx}-y_2\frac{dy_1^*}{dx}\right)\Big|_a^b=0$

Homework

- Chap 9:

  9.2.11, 9.6.11, 9.6.13, 9.6.25, 9.6.26
- Chap 10:

  10.1.6, 10.1.8, 10.2.8, 10.2.10