Chapter 25 Sturm-Liouville problem (II)

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Reference: [1] Veerle Ledoux, Study of Special Algorithms for solving Sturm-Liouville and Schrodinger Equations.

[2] 王信華教授, chapter 8, lecture note of Ordinary Differential equation

Prufer method

Sturm-Liouville Dirichlet eigenvalue problem: $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0$

Scaled Prufer transformation

$$\begin{cases} y=\frac{1}{\sqrt{S}}\rho\sin\theta \\ z=py'=\sqrt{S}\rho\cos\theta \end{cases}$$

where $S(x;E)>0$: scaling function

Simple Prufer transformation

$$\begin{cases} y=\rho\sin\theta \\ z=py'=\rho\cos\theta \end{cases}$$

$$\frac{d\theta}{dx}=\frac{S}{p}\cos^2\theta+\frac{Ew-q}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta$$

$$\frac{2}{\rho}\frac{d\rho}{dx}=\left(\frac{S}{p}-\frac{Ew-q}{S}\right)\sin 2\theta-\frac{S'}{S}\cos 2\theta$$

$\xrightarrow{S=1}$

$$\frac{d\theta}{dx}=\frac{1}{p}\cos^2\theta+(Ew-q)\sin^2\theta$$

$$\frac{1}{\rho}\frac{d\rho}{dx}=\left(\frac{1}{p}-(Ew-q)\right)\sin\theta\cos\theta$$

So far we have shown that Sturm-Liouville Dirichlet problem has following properties

1. Eigenvalues are real and simple, ordered as $E_0<E_1<E_2<\cdots$
2. Eigen-functions are orthogonal in $L^2([0,a],w)$ with inner-product $\langle\phi|\psi\rangle_W \triangleq \int_0^a \phi^*(x)\psi(x)w(x)dx$
3. Eigen-functions are real and twice differentiable

Moreover we have implemented (Scaled) Prufer equation $\frac{d\theta}{dx}=\frac{S}{p}\cos^2\theta+\frac{Ew-q}{S}\sin^2\theta+\frac{S'}{S}\sin\theta\cos\theta$

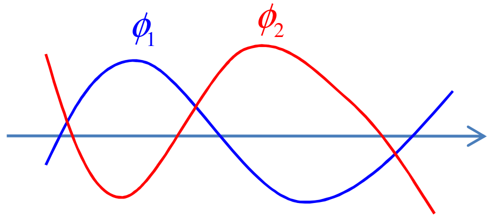
with Forward Euler Method (not stable, but it can be used so far)

Sturm's Comparison [1]

Theorem (Sturm's first Comparison theorem): let $(\phi_1, E_1), (\phi_2, E_2)$ be eigen-pair of Sturm-Liouville problem.

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)\,y = Ew(x)\,y$$

suppose $E_2 > E_1$, then ϕ_2 is more oscillatory than ϕ_1 . Precisely speaking



Between any consecutive two zeros of ϕ_1 , there is at least one zero of ϕ_2

Theorem (Sturm's second Comparison theorem): let $(\phi_1, E_1), (\phi_2, E_2)$ be solutions of Sturm-Liouville problem.

$$-\frac{d}{dx}\left(p_1(x)\frac{d\phi_1}{dx}\right)=\left(E_1 w(x)-q_1(x)\right)\phi_1$$

$$-\frac{d}{dx}\left(p_2(x)\frac{d\phi_2}{dx}\right)=\left(E_2 w(x)-q_2(x)\right)\phi_2$$

suppose $p_2(x) \le p_1(x)$ and $\left(E_1 w(x)-q_1(x)\right) < \left(E_2 w(x)-q_2(x)\right)$ on $[a,b]$

(1) $\theta_1(a) \le \theta_2(a) \;\Rightarrow\; \theta_1(x) \le \theta_2(x)$

(2) Between any consecutive two zeros of ϕ_1 , there is at least one zero of ϕ_2

<proof of (1)>

$$-\frac{d}{dx}\left(p_1(x)\frac{d\phi_1}{dx}\right)=\left(E_1 w(x)-q_1(x)\right)\phi_1$$

$$-\frac{d}{dx}\left(p_2(x)\frac{d\phi_2}{dx}\right)=\left(E_2 w(x)-q_2(x)\right)\phi_2$$

Simple Prufer →

$$\frac{d\theta_1}{dx}=\frac{1}{p_1}\cos^2\theta_1+\left(E_1 w-q_1\right)\sin^2\theta_1$$

$$\frac{d\theta_2}{dx}=\frac{1}{p_2}\cos^2\theta_2+\left(E_2 w-q_2\right)\sin^2\theta_2$$

Sturm's Comparison [2]

First we consider $\theta_1(a)=\theta_2(a)=\theta_0$

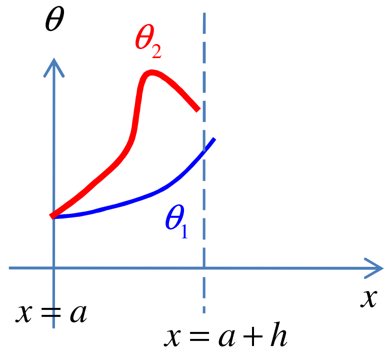
$$\frac{d\theta_1}{dx}=\frac{1}{p_1}\cos^2\theta_1+(E_1w-q_1)\sin^2\theta_1\equiv F(x,\theta_1) \qquad \frac{d\theta_2}{dx}=\frac{1}{p_2}\cos^2\theta_2+(E_2w-q_2)\sin^2\theta_2\equiv G(x,\theta_2)$$

$$\theta_1(a)=\theta_0 \qquad \theta_2(a)=\theta_0$$

suppose $p_2(x)\le p_1(x)$ and $(E_1w(x)-q_1(x))<(E_2w(x)-q_2(x))$ on $[a,b]$

1

$$\left\{\begin{array}{l}\theta_1(a)=\theta_2(a)=\theta_0\\ p_2(a)\le p_1(a)\\ (E_1w(a)-q_1(a))<(E_2w(a)-q_2(a))\end{array}\right. \longrightarrow F(a,\theta_1(a))<G(a,\theta_2(a))$$



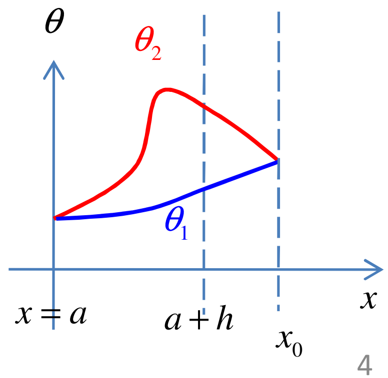
continuity of ***F, G***

$$\longrightarrow F(x,\theta_1(x))<G(x,\theta_2(x)) \quad \forall x\in[a,a+\delta]$$

$$\longrightarrow \frac{d\theta_1}{dx}(x)<\frac{d\theta_2}{dx}(x) \quad \forall x\in[a,a+\delta] \xrightarrow{\theta_1(a)=\theta_2(a)=\theta_0} \theta_1(x)<\theta_2(x) \quad \forall x\in(a,a+\delta]$$

2 Suppose $\theta_1(x_0)=\theta_2(x_0),\ x_0>a+h$, then

$$\left\{\begin{array}{l}\theta_1(x_0)=\theta_2(x_0)\\ p_2(x_0)\le p_1(x_0)\\ (E_1w(x_0)-q_1(x_0))<(E_2w(x_0)-q_2(x_0))\end{array}\right. \longrightarrow F(x_0,\theta_1(x_0))<G(x_0,\theta_2(x_0))$$



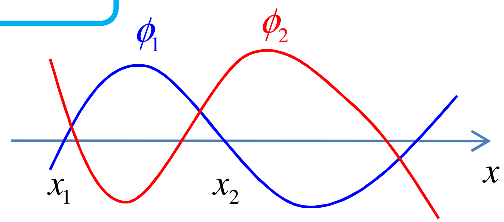
$$\longrightarrow \theta_1(x)<\theta_2(x) \quad \forall x\in(a+h,a+h+\delta]$$

Sturm's Comparison [3]

1 and 2 $\longrightarrow$ $\theta_1(a)=\theta_2(a) \Rightarrow \theta_1(x)\le\theta_2(x)$

Question: How to deal with the case $\theta_1(a)<\theta_2(a)$

<proof of (2)> Between any consecutive two zeros of ϕ_1, there is at least one zero of ϕ_2



Suppose ϕ_1 has consecutive zeros at x_1, x_2

Without loss of generality, we assume $\phi_1(x)>0$ on (x_1,x_2)

Moreover $\phi_2(x_1)\neq 0$, we may assume $\phi_2(x)>0$ on $[x_1,x_1+\delta)$

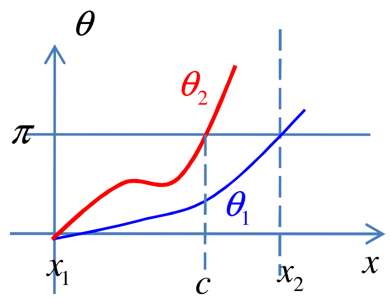
1 $\phi_1(x)=0,\ \dfrac{d}{dx}\phi_1(x_1)>0$ $\longrightarrow$ $\theta_1(x_1)=\tan^{-1}\left(\dfrac{\phi_1(x_1)}{p(x_1)\phi_1'(x_1)}\right)=0$ and $\theta_1(x)>0$ on $(x_1,x_1+\delta)$

2 $\phi_2(x)>0$ on $[x_1,x_1+\delta)$ $\longrightarrow$ $\theta_2(x_1)=\tan^{-1}\left(\dfrac{\phi_2(x_1)}{p(x_1)\phi_2'(x_1)}\right)=\gamma<\pi$ $\begin{cases}0<\gamma<\dfrac{\pi}{2} & \text{if } \phi_2'(x_1)>0\\ \dfrac{\pi}{2}<\gamma<\pi & \text{if } \phi_2'(x_1)<0\end{cases}$

Apply result of (1), set $a=x_1, b=x_2$, then

$$\theta_1(x_1)=\theta_2(x_1) \Rightarrow \theta_1(x)<\theta_2(x)$$

$$\theta_1(x_2)=\pi \xrightarrow{\theta_1(x)<\theta_2(x)} \theta_2(c)=\pi \xrightarrow{y=\rho\sin\theta} \phi_2(c)=0$$



Pitfall [1]

Recall Sturm-Liouville Dirichlet eigenvalue problem: $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0$

1. Eigenvalues are real and simple, ordered as $E_0 < E_1 < E_2 < \cdots$

   Question: How about asymptotic behavior of eigenvalue, say $\lim_{n\to\infty} E_n = \infty$ or $\lim_{n\to\infty} E_n = \alpha$

2. Eigen-functions are orthogonal in $L^2([0,a],w)$ with inner-product $\langle \phi | \psi \rangle_W \triangleq \int_0^a \phi^*(x)\psi(x)w(x)\,dx$

   Question: are eigen-functions complete in $L^2([0,a],w)$

   $\longleftrightarrow$ $\{(E_n,\psi_n): n=1,2,3\cdots\}$ is eigen-pair of $-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y,\quad y(0)=y(a)=0$

   $$cl(sp\{\psi_n\}) = cl\{f = \text{finite combination of } \psi_n\} = L^2([0,a],w)$$

   $\longleftrightarrow$ $\forall f \in L^2([0,a],w) \xrightarrow{?} \lim_{n\to\infty}\sum_{k=1}^{n}\langle \psi_n, f\rangle \psi_n = f$

3. Eigen-functions are real and twice differentiable

The more important question is

Question: is operator $L=\frac{1}{w(x)}\left\{-\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)+q(x)\right\}$ diagonalizable in $L^2([0,a],w)$

Pitfall [2]

Question: How about asymptotic behavior of eigenvalue, say $\lim_{n\to\infty} E_n = \infty$ or $\lim_{n\to\infty} E_n = \alpha$

General Sturm-Liouville problem

$$-\frac{d}{dx}\left(p(x)\frac{d\phi_2}{dx}\right)+q(x)\phi_2 = Ew(x)\phi_2$$
$$\phi_2(0)=0$$

$$\frac{d\theta_2}{dx}=\frac{1}{p}\cos^2\theta_2+(Ew-q)\sin^2\theta_2$$
$$\theta_2(0)=0$$

$$p_M = \max\{p(x): x\in[0,a]\}>0$$
$$q_M = \max\{q(x): x\in[0,a]\}$$
$$w_m = \min\{w(x): x\in[0,a]\}>0$$

$\longrightarrow$

Model problem

$$-p_M\frac{d^2\phi_1}{dx^2}+q_M\phi_1 = Ew_m\phi_1$$
$$\phi_1(0)=0$$

$$\frac{d\theta_1}{dx}=\frac{1}{p_M}\cos^2\theta_1+(Ew_m-q_m)\sin^2\theta_1$$
$$\theta_1(0)=0$$

Sturm's second Comparison theorem

(1) $\theta_1(0)\le\theta_2(0) \Rightarrow \theta_1(x)\le\theta_2(x)$

(2) Between any consecutive two zeros of ϕ_1, there is at least one zero of ϕ_2

Hook's Law: $\dfrac{d^2\phi_1}{dx^2}+k^2\phi_1=0,\quad k=\sqrt{\dfrac{Ew_m-q_M}{p_M}}$, require $Ew_m>q_M$ $\longrightarrow$ solution: $\phi_1(x)=\sin kx$

$\phi_1(0)=0$

Zeros of solution is $x_m=\dfrac{m\pi}{k}$ with space $\Delta x = x_m - x_{m-1}=\dfrac{\pi}{k}\searrow$ as $E\nearrow$

Exercise: Between any consecutive two zeros of ϕ_1, there is at least one zero of ϕ_2 shows $\lim_{n\to\infty}E_n=\infty$

Pitfall [3]

Question: are eigen-functions complete in $L^2([0,a],w)$

General Sturm-Liouville problem

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=Ew(x)y$$
$$y(0)=y(a)=0$$

$p=1,\ q=0,\ w=1,\ a=\pi$ →

Model problem

$$-\frac{d^2y}{dx^2}=Ey$$
$$y(0)=y(\pi)=0$$

Question : solution of modal problem is $\psi_k=\sin(kx),\ \ k=1,2,3,\cdots$

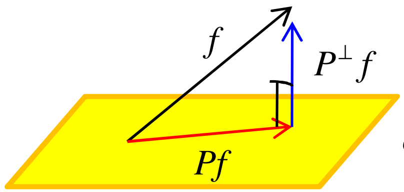
Is such eigenspace $\{\psi_k \mid k=1,2,3,\cdots\}$ complete in $L^2([0,\pi])$

Consider space $L^2([-\pi,\pi])=\left\{f:[-\pi,\pi]\to R \mid \int_{-\pi}^{\pi}|f|^2\,dx<\infty\right\}$ with inner-product $\langle f \mid g\rangle=\int_{-\pi}^{\pi}\overline{f}\cdot g\,dx$

1 $\{\varphi_k\equiv e^{ikx} \mid k=\cdots,-3,-2,-1,0,1,2,3,\cdots\}$ is orthogonal in $L^2([-\pi,\pi])$

$$\langle\varphi_k \mid \varphi_m\rangle=\int_{-\pi}^{\pi}e^{-ikx}\cdot e^{imx}dx=\begin{cases}2\pi & \text{if } k=m\\ 0 & \text{if } k\neq m\end{cases}$$

2 $cl\left(sp\{\varphi_k\equiv e^{ikx} \mid k\in\mathbb{Z}\}\right)\subseteq L^2([-\pi,\pi])$ is a closed subspace



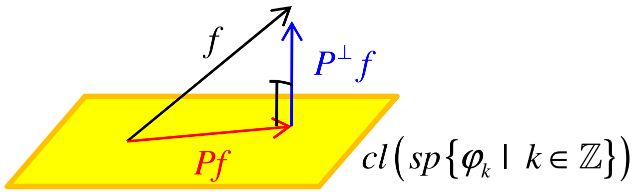
$cl\left(sp\{\varphi_k \mid k\in\mathbb{Z}\}\right)$

decomposition $f=Pf+P^{\perp}f$ is unique

where $Pf\in cl\left(sp\{\varphi_k \mid k\in\mathbb{Z}\}\right)$

$P^{\perp}f\perp cl\left(sp\{\varphi_k \mid k\in\mathbb{Z}\}\right)$

Pitfall [4]



Informally, $Pf = \sum_{k=1}^{\infty} c_k \varphi_k$ for some $\{c_k\}_{k=1}^{\infty}$ to be determined

$$P^{\perp} f = f - Pf \perp cl\left(sp\{\varphi_k \mid k \in \mathbb{Z}\}\right)$$

$$P^{\perp} f \perp cl\left(sp\{\varphi_k \mid k \in \mathbb{Z}\}\right) \longrightarrow P^{\perp} f \perp \varphi_k \quad \forall k \in \mathbb{Z} \longrightarrow \left\langle \varphi_k \mid P^{\perp} f \right\rangle = 0 \quad \forall k \in \mathbb{Z}$$

$$\xrightarrow{P^{\perp} f = f - Pf} \left\langle \varphi_k \mid f \right\rangle = \left\langle \varphi_k \mid Pf \right\rangle \quad \forall k \in \mathbb{Z} \longrightarrow \left\langle \varphi_k \mid f \right\rangle = \sum_{m=1}^{\infty} c_m \left\langle \varphi_k \mid \varphi_m \right\rangle \quad \forall k \in \mathbb{Z}$$

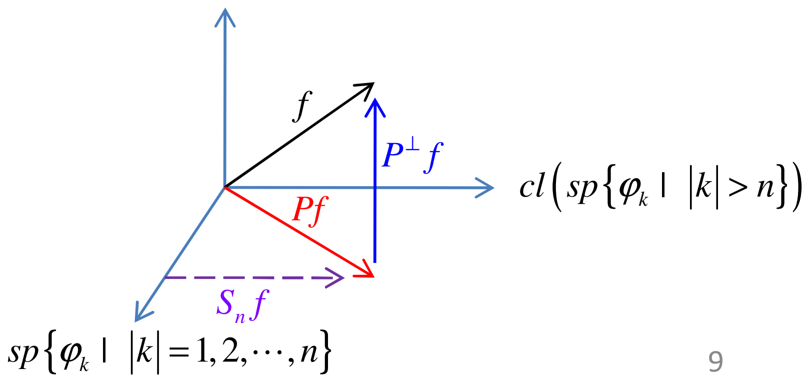
$$\xrightarrow{\left\langle \varphi_k \mid \varphi_m \right\rangle = \begin{cases} 2\pi & \text{if } k = m \\ 0 & \text{if } k \neq m \end{cases}} c_k = \frac{1}{2\pi} \left\langle \varphi_k \mid f \right\rangle \quad \forall k \in \mathbb{Z}$$

Formally speaking, when we write $Pf = \sum_{k=1}^{\infty} c_k \varphi_k$, in mathematical sense we construct partial sum $S_n f = \sum_{k=-n}^{n} c_k \varphi_k$

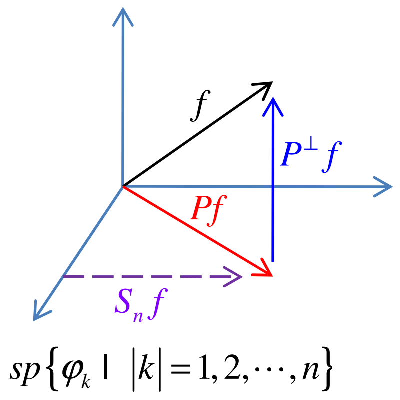
such that $S_n f \to Pf$ in ***L2*** sense.

$$\longleftrightarrow \quad S_n f \to Pf \quad \text{in} \quad L^2\left([-\pi, \pi]\right)$$

$$\longleftrightarrow \quad \lim_{n \to \infty} \left\| Pf - S_n f \right\|_{L^2} = \lim_{n \to \infty} \sqrt{\int_{-\pi}^{\pi} \left| Pf - S_n f \right|^2 dx} = 0$$



Pitfall [5]



$$\begin{cases} M_n \equiv sp\{\varphi_k \mid |k| = 1, 2, \cdots, n\} \\ N_n \equiv cl\left(sp\{\varphi_k \mid |k| > n\}\right) \\ M_\infty \equiv cl\left(sp\{\varphi_k \mid k \in \mathbb{Z}\}\right) \end{cases} \longrightarrow L^2([-\pi, \pi]) = M_n \oplus N_n \oplus M_\infty^C$$

$$f = S_n f + (Pf - S_n f) + P^{\perp} f$$

$f \to L^2([-\pi,\pi])$, $S_n f \to M_n$, $(Pf - S_n f) \to N_n$, $P^{\perp} f \to M_\infty^C$

$$\begin{matrix} S_n f \perp (Pf - S_n f) \\ S_n f \perp P^{\perp} f \end{matrix} \longrightarrow S_n f \perp f - S_n f = (Pf - S_n f) + P^{\perp} f \longrightarrow \langle \varphi_k \mid f - S_n f \rangle = 0 \quad \forall |k| \le n$$

$$\longrightarrow \langle \varphi_k \mid f \rangle = \langle \varphi_k \mid S_n f \rangle \quad \forall |k| \le n \longrightarrow c_k = \frac{1}{2\pi} \langle \varphi_k \mid f \rangle \quad \forall |k| \le n$$

Exercise: $S_n f = \sum_{k=-n}^{n} c_k \varphi_k, \; c_k = \frac{1}{2\pi} \langle \varphi_k \mid f \rangle \quad \forall |k| \le n$ is the solution of $\min \left\{ \left\| f - \sum_{k=1}^{n} c_k \varphi_k \right\|_{L^2}^2 : \{c_k\}_{k=1}^{n} \in R^n \right\}$

Pitfall [6]

$$S_n f = \sum_{k=-n}^{n} c_k \varphi_k,\quad c_k = \frac{1}{2\pi}\langle \varphi_k \mid f \rangle \quad \forall |k| \le n \quad \longrightarrow \quad S_n f = c_0 + \sum_{k=1}^{n} c_k e^{ikx} + c_{-k} e^{-ikx}$$

$$\longrightarrow \quad S_n f = c_0 + \sum_{k=1}^{n} c_k \left(\cos kx + \sqrt{-1}\sin kx\right) + c_{-k}\left(\cos kx - \sqrt{-1}\sin kx\right)$$

$$\longrightarrow \quad S_n f = c_0 + \sum_{k=1}^{n} (c_k + c_{-k})\cos kx + \sqrt{-1}\,(c_k - c_{-k})\sin kx$$

$$\longrightarrow \quad S_n f \equiv \frac{1}{2}a_0 + \sum_{k=1}^{n} a_k \cos kx + b_k \sin kx$$

where

$$\left\langle \frac{1}{2} \mid \cos kx \right\rangle = 0$$

$$\left\langle \frac{1}{2} \mid \sin kx \right\rangle = 0$$

$$\langle \sin mx \mid \cos kx \rangle = 0, \quad m \ne k$$

and

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f dx$$

$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f \cos kx dx$$

$$b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f \sin kx dx$$

Theorem: trigonometric basis is complete in $L^2([-\pi,\pi])$

$$\longleftrightarrow \quad cl\left(sp\{\varphi_k \equiv e^{ikx} \mid k \in \mathbb{Z}\}\right) = L^2([-\pi,\pi])$$

$$\longleftrightarrow \quad L^2([-\pi,\pi]) = M_n \oplus N_n \oplus M_\infty^C \qquad M_n \equiv sp\{\varphi_k \mid |k| = 1,2,\cdots,n\} \quad N_n \equiv cl\left(sp\{\varphi_k \mid |k| > n\}\right)$$

$\longleftrightarrow \quad S_n f \to f$ in ***L2*** sense, where $S_n f \equiv \frac{1}{2}a_0 + \sum_{k=1}^{n} a_k \cos kx + b_k \sin kx$

Pitfall [7]

Exercise: we have shown $cl\left(sp\left\{\varphi_k \equiv e^{ikx} \mid k \in \mathbb{Z}\right\}\right) = cl\left(sp\left\{1, \cos kx, \sin kx : k = 1, 2, \cdots\right\}\right) = L^2\left([-\pi, \pi]\right)$

$$S_n f \equiv \frac{1}{2} a_0 + \sum_{k=1}^{n} a_k \cos kx + b_k \sin kx \to f \in L^2\left([-\pi, \pi]\right)$$

where $a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f dx,\quad a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f \cos kx dx$: Fourier cosine coefficient

$b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} f \sin kx dx$: Fourier sine coefficient

We abbreviate ***f*** as $f \sim \lim_{n\to\infty} S_n f = \frac{1}{2} a_0 + \sum_{k=1}^{\infty} a_k \cos kx + b_k \sin kx$

1. If function ***f*** is even, say $f(x) = f(-x)$, then $f \sim \frac{1}{2} a_0 + \sum_{k=1}^{\infty} a_k \cos kx,\quad a_k = \frac{2}{\pi}\int_0^{\pi} f \cos kx dx$

2. If function ***f*** is odd, say $f(x) = -f(-x)$, then $f \sim \sum_{k=1}^{\infty} b_k \sin kx,\quad b_k = \frac{2}{\pi}\int_0^{\pi} f \sin kx dx$

Modal problem $\begin{aligned} -\frac{d^2 y}{dx^2} &= Ey \\ y(0) = y(\pi) &= 0 \end{aligned}$ has eigen-pair $\left(E_k = k^2, \psi_k = \sin(kx)\right),\quad k = 1, 2, 3, \cdots$

From above exercise, for any $f \in L^2\left([0, \pi]\right)$, we can do odd extension $f_{odd}(x) = \begin{cases} f(x) & \text{if } x > 0 \\ -f(-x) & \text{if } x < 0 \end{cases} \in L^2\left([-\pi, \pi]\right)$

then $f \sim \sum_{k=1}^{\infty} b_k \sin kx$. Hence $cl\left(sp\left\{\psi_k = \sin(kx) : k = 1, 2, \cdots\right\}\right) = L^2\left([0, \pi]\right)$

Question: How about if we do even extension $f_{even}(x) = \begin{cases} f(x) & \text{if } x > 0 \\ f(-x) & \text{if } x < 0 \end{cases} \in L^2\left([-\pi, \pi]\right)$

Pitfall [8]

Question: is operator $L = \frac{1}{w(x)}\left\{ -\frac{d}{dx}\left(p(x)\frac{d}{dx} \right) + q(x) \right\}$ diagonalizable in $L^2([0,a],w)$

From Prufer transformation, we can show $L\psi_k = E_k\psi_k$, $\psi_k(0) = \psi_k(a) = 0$ and

1. Eigenvalues are real and simple, ordered as $E_0 < E_1 < E_2 < \cdots$, $\lim_{k\to\infty} E_k = \infty$
2. Eigen-functions are orthogonal in $L^2([0,a],w)$ with inner-product $\langle \phi | \psi \rangle_W \triangleq \int_0^a \phi^*(x)\psi(x)w(x)dx$

Define domain of operator L with Dirichlet boundary condition as $D(L) = \left\{ f \in L^2([0,a],w) : f(0) = f(a) = 0 \right\}$

Clearly we have $cl(sp\{\psi_k : k = 1,2,\cdots\}) \subseteq D(L)$,but we can not say L is diagonalizable in $D(L)$

Finite dimensional matrix computation

Jordan form: $A\begin{pmatrix} u & v \end{pmatrix} = \begin{pmatrix} u & v \end{pmatrix}\begin{pmatrix} 2 & 1 \\ & 2 \end{pmatrix}$

$Au = 2u \Rightarrow u$: eigenvector

$Av = 2v + u \Rightarrow v$: generalized eigenvector

infinite dimensional functional analysis

$L\psi_k = E_k\psi_k$, $\psi_k(0) = \psi_k(a) = 0$ $\longrightarrow$ ψ_k : eigenfunction

$L\phi = E_k\phi + \psi_k$, $\phi(0) = \phi(a) = 0$ $\longrightarrow$ ϕ : generalized eigenfunction

Question: does such ϕ : generalized eigenfunction exists?

Idea: if we can show that $cl(sp\{\psi_k : k = 1,2,\cdots\}) = D(L)$, then even such ϕ exists, $\phi \notin D(L)$, why?

Then operator ***L*** is diagonalizable in $D(L)$

Scaled Prufer Transformation [1]

Scaled Prufer transformation

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)\,y=Ew(x)\,y$$

$$\begin{cases} y=\dfrac{1}{\sqrt{S}}\rho\sin\theta \\ z=py'=\sqrt{S}\rho\cos\theta \end{cases} \qquad S(x;E)>0$$

$$\frac{d\theta}{dx}=\frac{1}{2}\left[\left(\frac{S}{p}+\frac{Ew-q}{S}\right)+\left(\frac{S}{p}-\frac{Ew-q}{S}\right)\cos 2\theta+\frac{S'}{S}\sin 2\theta\right]$$

$$=A(x)+B(x)\cos 2\theta+C(x)\sin 2\theta$$

Time-independent Schrodinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x)$$

$$\psi(0)=\psi(\pi)=0$$

$$\frac{d\theta}{dx}=\frac{1}{2}\left[\left(2S+\frac{E-V}{S}\right)+\left(2S-\frac{E-V}{S}\right)\cos 2\theta+\frac{S'}{S}\sin 2\theta\right]$$

$$\theta(0;E)=0$$

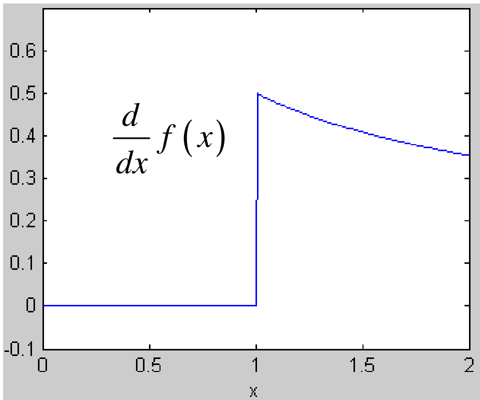
Suppose we choose $S(x)=\frac{1}{\sqrt{2}}\begin{cases}1 & \text{if } E-V(x)\le 1\\ \sqrt{E-V(x)} & \text{if } E-V(x)>1\end{cases}=\frac{1}{\sqrt{2}}f\left(E-V(x)\right)$ where $f(x)=\begin{cases}1 & \text{if } x\le 1\\ \sqrt{x} & \text{if } x>1\end{cases}$

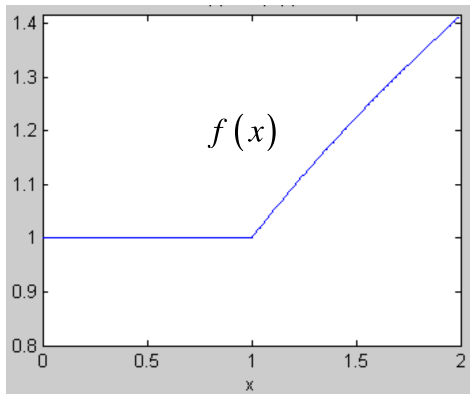
Question: function ***f*** is continuous but not differentiable at ***x = 1.*** How can we obtain $\frac{df}{dx}$

$$\frac{d}{dx}f(x)=\begin{cases}0 & \text{if } x<1\\ \dfrac{1}{2\sqrt{x}} & \text{if } x>1\end{cases}$$

$$\frac{df}{dx}(1^-)=0,\quad \frac{df}{dx}(1^+)=\frac{1}{2}$$

$\frac{df}{dx}$ has jump discontinuity at $x=1$





Scaled Prufer Transformation [2]

Observation: $f(x)=\begin{cases}1 & \text{if } x\le 1\\ \sqrt{x} & \text{if } x>1\end{cases}$ and $\frac{d}{dx}f(x)=\begin{cases}0 & \text{if } x<1\\ \frac{1}{2\sqrt{x}} & \text{if } x>1\end{cases}$ $\frac{df}{dx}(1)$ does not exist, we ignore it.

Then fundamental Theorem of Calculus also holds, say $f(x)=1+\int_0^x \frac{df}{dx}(s)\,ds$

1 $0<x<1,\ \frac{df}{dx}(x)=0$, fundamental Theorem of Calculus holds, $f(x)=f(0)+\int_0^x \frac{df}{dx}(s)\,ds=1,\ \ 0<x<1$

2 $f(1^-)=1$ —— ***f*** is continuous ——> $f(1^+)=f(1^-)=1$

3 $1<x,\ \frac{df}{dx}(x)=\frac{1}{2\sqrt{x}}$, fundamental Theorem of Calculus holds, $f(x)=f(1^+)+\int_1^x \frac{df}{dx}(s)\,ds=1+\int_1^x \frac{1}{2\sqrt{s}}\,ds=\sqrt{x},\ \ 1<x$

Question: although fundamental theorem of calculus holds for function ***f*** , but if $\frac{df}{dx}$ is given,

How can we find ***f(x)*** numerically and have better accuracy?

Reason to discussion of fundamental theorem of calculus:

$$\frac{d\theta}{dx}=\frac{1}{2}\left[\left(2S+\frac{E-V}{S}\right)+\left(2S-\frac{E-V}{S}\right)\cos 2\theta+\frac{S'}{S}\sin 2\theta\right] \longrightarrow \theta(x)=\theta(0)+\int_0^x \frac{d\theta}{ds}(s,\theta(s))\,ds$$

$\frac{d\theta}{dx}$ depends on ***S(x)***, accuracy of $\theta(x)$ is equivalent to accuracy of obtaining ***S(x)***

$$S(x)=\frac{1}{\sqrt{2}}f(E-V(x)),\quad f(x)=\begin{cases}1 & \text{if } x\le 1\\ \sqrt{x} & \text{if } x>1\end{cases}$$

Numerical integration [1]

$$f(x) = f_0 + x f_0^{(1)} + \frac{x^2}{2} f_0^{(2)} + \frac{x^3}{3!} f_0^{(3)} + \frac{x^4}{4!} f_0^{(4)} + O\left(x^5\right), \quad f_0 = f(0), \quad f_0^{(k)} = f^{(k)}(0)$$

↓ Ignore odd power since it does not contribute to integral

$$\int_{-h}^{h} f dx = \int_{-h}^{h} \left[f_0 + \frac{x^2}{2} f_0^{(2)} + \frac{x^4}{4!} f_0^{(4)} + O\left(x^6\right) \right] dx = 2h f_0 + \frac{h^3}{3} f_0^{(2)} + O\left(h^5\right)$$

$$f(h) = f_0 + h f_0^{(1)} + \frac{h^2}{2} f_0^{(2)} + \frac{h^3}{3!} f_0^{(3)} + \frac{h^4}{4!} f_0^{(4)} + O\left(h^5\right)$$

$$+\quad f(-h) = f_0 - h f_0^{(1)} + \frac{h^2}{2} f_0^{(2)} - \frac{h^3}{3!} f_0^{(3)} + \frac{h^4}{4!} f_0^{(4)} - O\left(h^5\right)$$

$$f(h) + f(-h) = 2 f_0 + h^2 f_0^{(2)} + O\left(h^4\right)$$

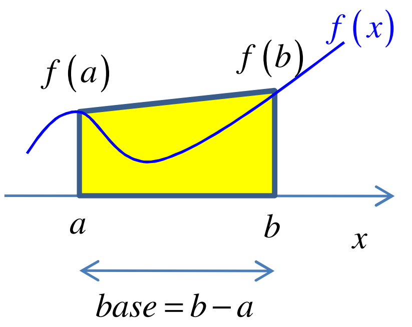
$$\int_{-h}^{h} f dx = \frac{2h}{2} \left[f(h) + f(-h) \right] - \frac{2}{3} \frac{(2h)^3}{8} f_0^{(2)} + O\left(h^5\right)$$

↓ general form

$$\int_{a}^{b} f dx = \frac{b-a}{2} \left[f(a) + f(b) \right] - \frac{1}{12} (b-a)^3 f^{(2)}(c)$$

↓

Trapzoid rule (梯形法)

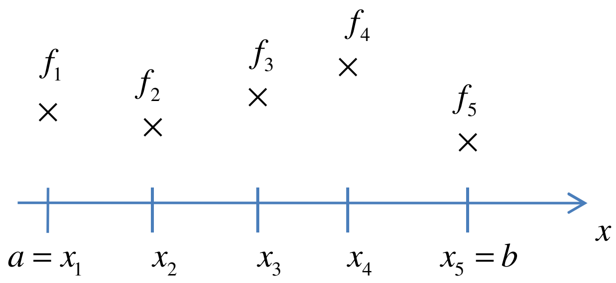


Numerical integration [2]

Example: given a partition $a = x_1 < x_2 < x_3 < x_4 < x_5 = b$

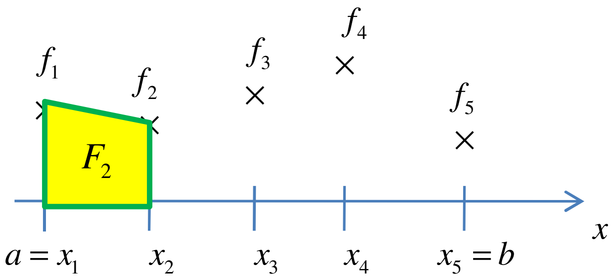
and grid function $f_k = f(x_k), k = 1,2,3,4,5$

We use Trapezoid rule to find $F(x) = \int_a^x f(t)\,dt$

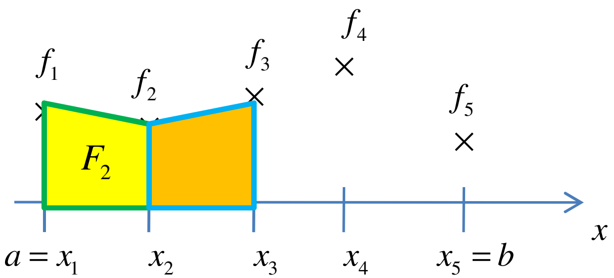


1. $F_1 = F(x_1) = 0$

2. $F_2 = F(x_2) = \dfrac{x_2 - x_1}{2}(f_1 + f_2)$



3. $F_3 = F_2 + \dfrac{x_3 - x_2}{2}(f_2 + f_3)$



Exercise 1: let $f(x) = \cos x, \quad a = 0, \quad b = 1$

Try number of grids = 10, 20, 40, 80, 160, compute $F(x) = \int_a^x f\,dt$

and measure maximum error $\max\left\{ \left| F(x_k) - \sin x_k \right| \right\}$

Plot error versus grid number, what is order of accuracy ?

Exercise 2: let $f(x) = \begin{cases} 0 & \text{if } x < 1 \\ \dfrac{1}{2\sqrt{x}} & \text{if } x > 1 \end{cases} \quad a = 0, \quad b = 2$

1. If x = 1 is in the grid partition, what is order of accuracy

2. If x = 1 is NOT in the grid partition, what is order of accuracy

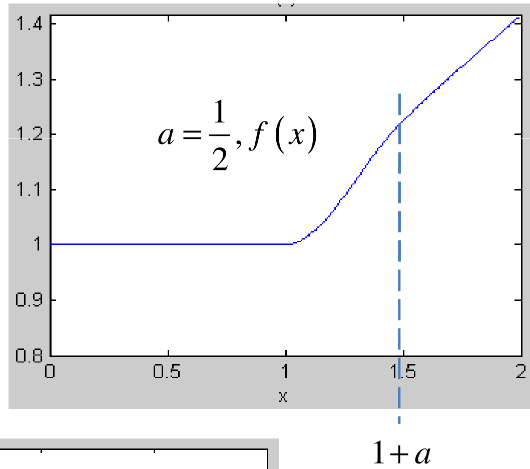
Scaled Prufer Transformation [3]

Question: can we modify function ***f*** slightly such that it is continuously differentiable , say

$$f(x)=\begin{cases}1 & \text{if } x\le 1\\ p\left(\dfrac{x-1}{a}\right) & \text{if } 1<x<1+a\\ \sqrt{x} & \text{if } x\ge 1+a\end{cases} \quad \text{and} \quad f'(x)=\begin{cases}0 & \text{if } x\le 1\\ \dfrac{1}{a}p'\left(\dfrac{x-1}{a}\right) & \text{if } 1<x<1+a\\ \dfrac{1}{2\sqrt{x}} & \text{if } x\ge 1+a\end{cases}$$

where $p(z)=a_0+a_1z+a_2z^2+a_3z^3$ is polynomial of degree 3, a_0,a_1,a_2,a_3 are chosen such that $f\in C^1$

<sol> $f\in C^1$ is achieved by following 4 conditions



1 $f(1^-)=f(1^+) \longrightarrow 1=p(0) \longrightarrow 1=a_0$

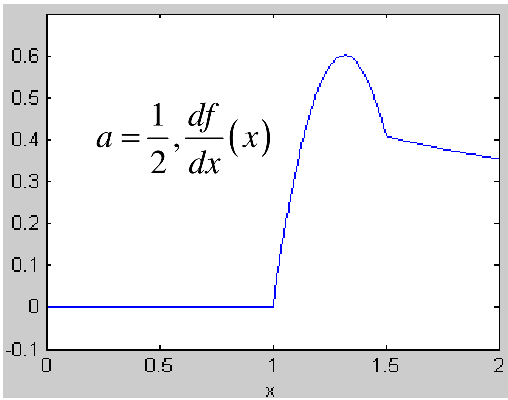
2 $f'(1^-)=f'(1^+) \longrightarrow 0=\frac{1}{a}p'(0) \longrightarrow 0=a_1$

3 $f(1+a^-)=f(1+a^+) \longrightarrow \sqrt{1+a}=p(1) \longrightarrow \sqrt{1+a}=1+a_2+a_3$

4 $f'(1+a^-)=f'(1+a^+)$

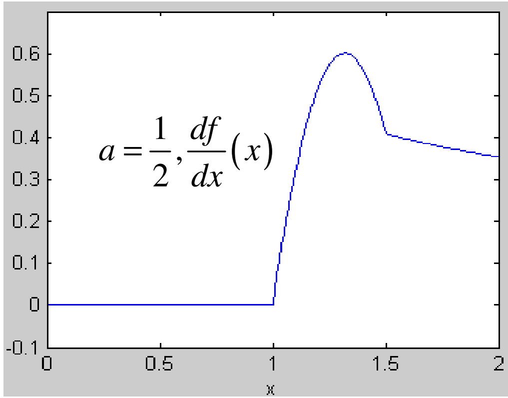
$$\frac{1}{2\sqrt{1+a}}=\frac{1}{a}p'(1) \longrightarrow \frac{a}{2\sqrt{1+a}}=2a_2+3a_3$$

$$p(z)=1+a_2z^2+a_3z^3 \quad \text{where} \quad \begin{pmatrix}a_2\\ a_3\end{pmatrix}=\begin{pmatrix}3 & -1\\ -2 & 1\end{pmatrix}\begin{pmatrix}\sqrt{1+a}-1\\ \dfrac{a}{2\sqrt{1+a}}\end{pmatrix}$$



Scaled Prufer Transformation [4]

$$f(x)=\begin{cases}1 & \text{if } x\le 1\\ p\left(\dfrac{x-1}{a}\right) & \text{if } 1<x<1+a\\ \sqrt{x} & \text{if } x\ge 1+a\end{cases}$$ and $$f'(x)=\begin{cases}0 & \text{if } x\le 1\\ \dfrac{1}{a}p'\left(\dfrac{x-1}{a}\right) & \text{if } 1<x<1+a\\ \dfrac{1}{2\sqrt{x}} & \text{if } x\ge 1+a\end{cases}$$



$f(x)\in C^1$ but $\dfrac{d^2 f}{dx^2}$ has jump discontinuity at $x=1,1+a$

Exercise 3: try to construct $f(x)\in C^2$

$$f(x)=\begin{cases}1 & \text{if } x\le 1\\ p\left(\dfrac{x-1}{a}\right) & \text{if } 1<x<1+a\\ \sqrt{x} & \text{if } x\ge 1+a\end{cases}$$ where $p(z)=a_0+a_1z+a_2z^2+a_3z^3+a_4z^4+a_5z^5$ is polynomial of degree 5

1 use Symbolic toolbox to determine coefficients $a_0,\ a_1,\ a_2,\ a_3,\ a_4,\ a_5$

2 plot $f(x),\ \dfrac{d}{dx}f(x),\ \dfrac{d^2}{dx^2}f(x)$

3 use Trapezoid method to compute $f(x)=1+\int_0^x \dfrac{df}{dx}(t)\,dt$,what is order of accuracy ?

Review Finite Difference Method

Model problem:

$$-\frac{d^2\psi}{dx^2}(x) = k^2\psi(x), \quad \psi(0)=\psi(\pi)=0$$

solution is $\psi_k(x) = \sin(kx), \quad k = 1,2,3\cdots$

FDM $\longrightarrow$

$$-D_h^2\psi(x_j) = \lambda\psi(x_j) \quad \text{for} \quad j=1,2,\cdots,n, \quad h=\frac{\pi}{n+1}$$

eigen-pair:

$$\vec{\psi} = \left\{\sin(kx_j) : j = 0,1,2,\cdots,n,n+1, k\in\mathbb{N}\right\}$$

$$\lambda_k = \frac{4\sin^2(kh/2)}{h^2} \equiv k_{num}^2$$

$$\Delta k = |k - k_{num}| = \frac{|\cos(c_k)|}{24}k^3h^2 = O(k^3h^2)$$

Question: why does error of eigenvalue increase as wave number *k* increases? $\Delta k \propto k^3$

$$-\frac{d^2\psi}{dx^2}(x) = k^2\psi(x) \xrightarrow{D_h^2 f(x) = f^{(2)}(x) + \frac{h^2}{12}f^{(4)}(x) + O(h^4)} -D_h^2\psi(x) + \frac{h^2}{12}\psi^{(4)}(x) \simeq k^2\psi(x)$$

Substitute $\psi(x) = \sin(kx)$, $\psi^{(4)}(x_j) = k^4\psi(x_j)$ $\longrightarrow$

$$k_{num}^2 + \frac{h^2k^4}{12} \simeq k^2 \longrightarrow k_{num} \simeq k\sqrt{1-\frac{h^2k^2}{12}} \simeq k\left[1-\frac{1}{2}\frac{h^2k^2}{12} + O(h^4k^4)\right] \simeq k - \frac{h^2k^3}{24}$$

Exercise 4: find analytic solution of $-\frac{d^2\psi}{dx^2} + V\psi(x) = E\psi(x), \quad \psi(0)=\psi(\pi)=0$ where

$$V(x) = \begin{cases} -1 & \frac{\pi}{4} < x < \frac{3\pi}{4} \\ 0 & \text{otherwise} \end{cases}$$

Then use FDM to solve $-D_h^2\psi(x_j) + V(x_j)\psi(x_j) = E_{num}\psi(x_j), \quad \psi(0)=\psi(\pi)=0$

What is order of accuracy? measure $|E_{num} - E|$