Boundary value problems

Sturm-Liouville operator

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u = f(x)\,, \qquad a \leqslant x \leqslant b \tag{1}$$

- 1D heat conduction equation

  $u(x)$ is the temperature

  $w(x) = -p(x)du/dx$ is the heat flux etc
- 1D diffusion equation
- 1D Schrödinger equation

Sturm-Liouville operator

The l.h.s. of (1) with known $p(x)$ and $q(x)$ is a differential operator

$$L[u](x) = -\frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u$$

- Eigenvalue problem

$$L[u](x) = \lambda u(x)$$

- Known r.h.s.:

$$L[u](x) = f(x)$$

A 2nd order differential equation $\Rightarrow$ need to two conditions.

Boundary value problem

2nd order differential equation $\Rightarrow$ need to two conditions.

$$\begin{aligned} &\text{IVP:} \quad u(a) \quad \text{and} \quad u'(a) \\ &\text{BVP:} \quad \underbrace{u(a) = u_a \quad \text{and} \quad u(b) = u_b}_{\text{boundary conditions of the 1st kind}} \end{aligned} \tag{2}$$

Boundary conditions of the 2nd kind: fix the heat flux at a and b

$$\begin{cases} -p(a)u'(a) = w_a \\ -p(b)u'(b) = w_b \end{cases}$$

Recap

Solution of (1) and (2) exists and is unique if:

- $f(x)$ and $q(x)$ are continuous on $[a, b]$
- $p(x) \in C^1[a, b]$
- $p(x) \geqslant p_0 > 0$, $q(x) \geqslant 0$ for $x \in [a, b]$

If $q(x), f(x) \in C^m$ and $p(x) \in C^{m+1}$ on $x \in [a, b]$, then

$$u(x) \in C^{m+2}$$

Recap: Maximum principle

Let $u(x)$ is the solution of

$$L[u] = f(x)\,, \qquad u(a) = u_a\,, \quad u(b) = u_b$$

Suppose that

$$f(x) \leqslant 0\,, \qquad u_a \leqslant 0\,, \quad u_b \leqslant 0$$

Then

$$u(x) \leqslant 0\,, \qquad x \in [a, b]$$

Recap: Maximum principle

Note that any $u(x) \in C^2$ is a solution of a BVP with

$$f(x) = L[u]\,, \qquad u_a = u(a)\,, \quad u_b = u(b)$$

Thus, an alternative formulation of the maximum principle:

If

$$L[u] \leqslant 0\,, \qquad u(a) \leqslant 0\,, \quad u(b) \leqslant 0$$

then

$$u(x) \leqslant 0\,, \qquad x \in [a,b]\,.$$

Maximum principle: the comparison theorem

Let $u(x),\ v(x) \in C^2$ on $x \in [a,b]$. Let

$$L[u] \leqslant L[v]\,, \qquad u(a) \leqslant v(a)\,, \quad u(b) \leqslant v(b)$$

Then

$$u(x) \leqslant v(x)\,, \qquad x \in [a,b]$$

Maximum principle: *a priori* bounds

Let

$$L[u] = f(x)\,, \qquad u(a) = u_a\,, \quad u(b) = u_b$$

Then

$$\max_{[a,b]} |u(x)| \leqslant \max\{|u_a|, |u_b|\} + K \max_{[a,b]} |f(x)|$$

where the *condition number*

$$K = \frac{b-a}{4}\int_a^b \frac{dx}{p(x)}$$

Consider now two BVPs with perturbed boundary values and $f(x)$.

Numeric solutions of two-point BVPs

Shooting method

Given a BVP

$$L[u] = f(x)\,, \qquad u(a) = u_a\,, \quad u(b) = u_b$$

Take an IVP

$$L[u] = f(x)\,, \qquad u(a) = u_a\,, \quad u'(a) = u'_a$$

and solve

$$u(b) - u_b = 0$$

for u'_a.

Finite difference equations (FDE)

Define a mesh ω on $[a, b]$:

$$a = x_0 < x_1 < \cdots < x_N = b$$

A uniform mesh

$$\omega^h = \{x_k \mid x_k = a + hk\,, k = 0 \cdots N\}$$

Internal nodes: $x_k \quad k = 1, \cdots, N-1$

Boundary nodes: x_0 and x_N

Introduce the *mesh* function $y_k \approx u(x_k)$.

Finite difference equations

First, consider $p(x) = 1$:

$$\begin{cases} -u''(x) + q(x)u(x) = f(x) \\ u(a) = u_a \quad u(b) = u_b \end{cases}$$

Approximate the derivatives on a mesh

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + O(h^2)$$

ODE $\to$ FDE

At the *internal nodes* use

$$-\frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + q_k y_k = f_k\,, \qquad 1 \leqslant k \leqslant N-1$$

Boundary nodes: $y_0 = u_a, \quad y_N = u_b$

General case: also approximate the boundary conditions.

Finite difference equations

Tridiagonal linear system

$$\begin{bmatrix} \ddots & \ddots & \\ \ddots & \ddots & \ddots \\ & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \\ y \\ \\ \end{bmatrix} = \begin{bmatrix} \\ f \\ \\ \end{bmatrix}$$

General Thomas algorithm

$$a_k y_{k+1} + b_k y_k + c_k y_{k-1} = f_k h^2$$

Here $a_k = c_k = -1$, $b_k = 2 + h^2 q_k$.

Finite difference equations

Notice that

$$\begin{aligned} &a_k \leqslant 0, \quad c_k < 0, \quad b_k \geqslant 0, \\ &a_k + b_k + c_k \geqslant 0 \end{aligned} \tag{3}$$

The system is diagonally dominant,

$$|b_k| \geqslant |a_k| + |c_k|, \qquad |b_k| > |c_k|,$$

thus

- the solution exists and is unique.
- Thomas algorithm is stable

Properties of finite difference schemes

FD Sturm-Liouville operator

ODE

Differential operator $L[u](x)$

$$L[u] = f(x)$$

with

$$L[u] = \left(-\frac{d^2}{dx^2} + p(x)\right) u(x)$$

FDE

$$\Lambda^h[y] = f^h\,, \qquad x \in \omega^h$$

with

$$\Lambda[y] = -\frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + q_k y_k \tag{4}$$

Maximum principle for FDE

Lemma

Suppose y_k is a solution of

$$a_k y_{k-1} + b_k y_k + c_k y_{k+1} = d_k \,, \qquad k = 1, \cdots, N-1$$
$$y_0 = u_a \qquad y_N = u_b$$

Suppose that a, b, c satisfy Eq. (3):

$$a_k \leqslant 0, \quad c_k < 0, \quad b_k \geqslant 0,$$
$$a_k + b_k + c_k \geqslant 0$$

If $u_a < 0$ and $u_b < 0$ and $d_k < 0$, then

$$y_k < 0 \qquad \text{for all } k$$

Maximum principle for FDE

Proof of the lemma

Suppose that $y_s > 0$ for some internal node s. Then

$$y_s \geqslant y_{s+1}\,, y_{s-1}$$

Therefore

$$a_s y_s \leqslant a_s y_{s-1}\,, \qquad c_s y_s < c_s y_{s-1}$$

Then,

$$\begin{aligned} 0 &\leqslant (a_s + b_s + c_s) y_s \\ &< a_s y_{s-1} + b_s y_s + c_s y_{s+1} = d_s \leqslant 0 \end{aligned}$$

Which is self-contradictory: $0 < 0$.

Maximum principle for FDE

Any mesh function y_k satisfies an FDE with

$$f_k = \Lambda[y_k]\ .$$

For an FDE can prove

- the comparison theorem
- the *a priori* error bound

$$\max_k |y_k| \leqslant \max\{y_0, y_N\} + K\ \max_k |f_k|$$

For (4) $K = l^2/8$.

Approximation + stability = convergence

Stability of an FDE

Let y_k and $\widehat{y}_k$ are solutions of

$$\Lambda[y] = f\,, \qquad y_0 = u_a\,, \quad y_N = u_b$$

$$\Lambda[\widehat{y}] = f + \delta\,, \qquad \widehat{y}_0 = u_a + \epsilon_a\,, \quad \widehat{y}_N = u_b + \epsilon_b$$

Stability

An FDE is *stable* if

$$\max_k |y_k - \widehat{y}_k| \leqslant \max\{\epsilon_a, \epsilon_b\} + K \max_k |\delta_k|$$

Approximation

Let $u(x)$ is the solution of $L[u] = f$. Let y_k is the solution of $\Lambda^h[y] = f^h$.

Define the *residual*, ψ^h, via

$$\Lambda^h[u] = f^h + \psi^h.$$

Approximation

- An FDE $\Lambda^h[y] = f^h$ *approximates* $L[u] = f$ if

$$\max_k |\psi_k| \to 0 \qquad \text{as} \quad h \to 0$$

- An FDE has *degree of approximation* $m > 0$ if

$$\max_k |\psi_k| < \text{const} \times h^m$$

Convergence

Let $u(x)$ is the solution of $L[u] = f$. Let y_k is the solution of $\Lambda^h[y] = f^h$.

Define the *error* of FDE, ε_k,

$$\varepsilon_k = u(x_k) - y_k$$

Convergence

- An FDE *converges* at $h \to 0$ if

$$\max_k |\varepsilon_k| \to 0 \qquad \text{as} \quad h \to 0$$

- An FDE has *degree of convergence* $m > 0$ if

$$\max_k |\varepsilon_k| < \text{const} \times h^m$$

Convergence

Let $q(x)$ and $f(x) \in C^2[a,b]$. FD scheme (4)

- is stable
- approximates $L[u] = f$ with $m = 2$.

Therefore, it converges with the degree $m = 2$:

$$\max_{1 \leqslant k \leqslant N} |u(x_k) - y_k| \leqslant C\, h^2$$

with

$$C = \frac{l^2}{96} \max_{x \in [a,b]} \left| u^{(4)}(x) \right|$$

General Sturm-Liouville operators

Alternative discretizations

Consider a general Sturm-Liouville operator with $p(x) \neq \mathrm{const}$.

Need to approximate $$\frac{d}{dx}\big(p(x)u'(x)\big)$$

Alternative discretizations

Consider a general Sturm-Liouville operator with $p(x) \neq \mathrm{const.}$

Need to approximate $\quad \dfrac{d}{dx}\big(p(x)u'(x)\big)$

First try

$$\big(p(x)u'\big)' = p(x)u''(x) + p'(x)u'(x)$$

$$\Rightarrow \big(p(x)u'\big)' \approx p_k \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + p_k' \frac{y_{k+1} - y_{k-1}}{2h}$$

General Sturm-Liouville operators

This way,

$$-p_k \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} - p'_k \frac{y_{k+1} - y_{k-1}}{2h} + q_k y_k = f_k$$

The system is tridiagonal, with

$$\begin{cases} a_k = -p_k - \frac{h}{2} p'_k \\ b_k = 2p_k + h^2 q_k \\ c_k = -p_k + \frac{h}{2} p'_k \end{cases}$$

The maximum principle, (3), requires that $\quad h \max_k \frac{|p'_k|}{p_k} < 2$

$p(x) \neq \text{const}$, the second try

Need to approximate the flux

$$w(x) = -p(x)\frac{du}{dx}$$

Define $x_{k+\frac{1}{2}} = \frac{1}{2}(x_{k+1} + x_k)$.

Approximate

$$\left.\frac{dw}{dx}\right|_{x=x_k} \approx \frac{w(x_{k+\frac{1}{2}}) - w(x_{k-\frac{1}{2}})}{h}$$

$p(x) \neq \text{const}$, the second try

Furthermore,

$$w(x_{k+\frac{1}{2}}) = -p_{k+\frac{1}{2}} u'(x_{k+\frac{1}{2}}) \approx -p_{k+\frac{1}{2}} \frac{u(x_{k+1}) - u(x_k)}{h}$$

$$w(x_{k-\frac{1}{2}}) = -p_{k-\frac{1}{2}} u'(x_{k-\frac{1}{2}}) \approx -p_{k-\frac{1}{2}} \frac{u(x_k) - u(x_{k-1})}{h}$$

Therefore,

$$w'(x_k) \equiv -\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)\bigg|_{x=x_k}$$

$$\longrightarrow -\frac{1}{h}\left[p_{k+\frac{1}{2}} \frac{y_{k+1} - y_k}{h} - p_{k-\frac{1}{2}} \frac{y_k - y_{k-1}}{h}\right]$$

$p(x) \neq \mathrm{const}$, the second try

The tridiagonal system has

$$\begin{cases} a_k = -p_{k-\frac{1}{2}} \\ c_k = -p_{k+\frac{1}{2}} \\ b_k = p_{k-\frac{1}{2}} + p_{k+\frac{1}{2}} + h^2 q_k \end{cases}$$

which is diagonally dominant irrespective of $p'(x)$.

Can prove that this scheme is stable and converges as $O(h^2)$ for $h \to 0$