Lecture 8

Last time we studied cubic-spline interpolation

Recall $f : [a, b] \to \mathbb{R}$

$a = x_0 < x_1 < x_2 < \cdots < x_n = b$

A cubic spline interpolant $S : [a, b] \to \mathbb{R}$ is a twice continuously differentiable function such that

- $S(x_i) = f(x_i)$ for each i
- S on $[x_i, x_{i+1}]$ is equal to a cubic polynomial $S_i(x)$

subject to 2 boundary condition

1) (free boundary)

$$S''(x_0) = S''(x_n) = 0$$

2) (clampled boundary)

$$S'(x_0) = f'(x_0) \quad \& \quad S'(x_n) = f'(x_n)$$

Last time we proved that a cubic spline interpolant exists for both boundary conditions

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Today we study Numerical integration

Reasons for Numerical integration $\int_a^b f(x)\,dx$

(1) We cannot solve $\int_a^b f(x)\,dx$ exactly

e.g. • $\int_0^1 \sin(x^2)\,dx$

• $\int_0^1 e^{-x^2}\,dx$

• $\int_0^1 \sqrt{1+\cos^4 x}\,dx$

(2) f is not known explicitly. Only values of f at some pts are known

Derivation of Numerical Integration formulae

Let $p_k(x)$ be the function which interpolates $f(x)$ at the points $x_0, x_1, \ldots, x_k$.

We approximate $I(f) = \int_a^b f(x)\,dx$

by $I(p_k) = \int_a^b p_k(x)\,dx$.

$$f(x) = p_k(x) + f[x_0, x_1, \ldots, x_k, x]\,\psi_k(x)$$

where $\psi_k(x) = \prod_{j=0}^{k} (x - x_j)$

Error in our estimate $I(p_k)$ for $I(f)$.

$$E(f) = I(f) - I(p_k) = \int_a^b f[x_0, \ldots x_k, x]\,\psi_k(x)\,dx$$

Simplification of error term

Case 1 :- $\psi_k(x)$ is of one sign on (a,b)

Then by MVT for integrals

$$E(f) = \int_a^b f[x_0, \ldots x_k, x]\, \psi_k(x)\, dx = f[x_0, \ldots, x_k, \xi] \int_a^b \psi_k(x)\, dx$$

If in addition $f(x)$ is $k+1$ times continuously differentiable then

$$(1) \quad \boxed{E(f) = \frac{f^{(k+1)}(\eta)}{(k+1)!} \int_a^b \psi_k(x)\, dx \quad \text{for some } \eta \in (a,b)}$$

Case 2 $\int_a^b \psi_k(x)\, dx = 0.$

We use the identity

$$f[x_0, x_1, \ldots, x_k, x] = f[x_0, x_1, \ldots, x_k, x_{k+1}] + f[x_0, x_1, \ldots, x_{k+1}, x]\,(x - x_{k+1})$$

So

$$E(f) = \int_a^b f[x_0, \dots x_k, x]\, \psi_k(x)\, dx$$

$$= \int_a^b f[x_0, x_1, \dots, x_{k+1}]\, \psi_k(x)\, dx$$

$$+ \int_a^b f[x_0, x_1, \dots, x_{k+1}, x]\,(x - x_{k+1})\,\psi_k(x)\, dx$$

Now $\int_a^b f[x_0, \dots x_{k+1}]\, \psi_k(x)\, dx = f[x_0, \dots x_{k+1}] \int_a^b \psi_k(x)\, dx$

$= 0$

Furthermore $(x - x_{k+1})\,\psi_k(x) = \psi_{k+1}(x) = \prod_{j=0}^{k+1} (x - x_j)$

So $E(f) = \int_a^b f[x_0, \dots, x_{k+1}, x]\, \psi_{k+1}(x)\, dx$

If we can choose x_{k+1} such that

$\psi_{k+1}(x)$ is of one sign on (a, b)

then by MVT of integrals

$$E(f) = f[x_0, x_1, \dots, x_{k+1}, \xi] \int_a^b \psi_{k+1}(x)\, dx$$

If $f(x)$ is $k+2$ times continuously diff

then

(2) $$\boxed{E(f) = \frac{f^{(k+2)}(\eta)}{(k+2)!} \int_a^b \psi_{k+1}(x)\, dx \qquad \eta \in (a, b)}$$

examples

Let $k = 0$

$$P_0(x) = f[x_0] = f(x_0)$$

$$f(x) = f(x_0) + f[x_0, x](x - x_0)$$

$$I = \int_a^b f(x)\,dx = \int_a^b f(x_0)\,dx + \int_a^b f[x_0, x](x - x_0)$$

$$I(P_k) = (b-a) f(x_0)$$

If $x_0 = a$ this approximation becomes

$$I(f) \approx R = (b-a) f(a)$$

$\psi_0(x) = x - a$ has one sign on $[a, b]$

$$E^R = f'(\eta) \int_a^b (x-a)\,dx$$

$$E^R = f'(\eta) \frac{(b-a)^2}{2}$$

$x_0 = \frac{a+b}{2}$ then $\psi_0(x) = x - x_0$

fails to be of one sign.

However $\int_a^b (x - x_0)\,dx = 0$

while $(x - x_0)^2\,dx$ is of one sign

$$\boxed{\begin{aligned} &\text{So } I(f) \approx M = (b-a)\,f(x_0) \\ &\text{"Midpoint rule"} \quad = (b-a) \cdot f\left(\frac{a+b}{2}\right) \end{aligned}}$$

$$E^M = \frac{f''(\eta)}{2} \int_a^b \left(x - \frac{a+b}{2}\right)^2 dx$$

$$= f''(\eta)\,\frac{(b-a)^3}{24} \qquad \eta \in (a,b)$$

Now let

$k = 1$

$$f(x) = f(x_0) + f[x_0, x_1](x - x_0) +$$
$$+ f[x_0, x_1, x]\,\psi_1(x)$$

$$\psi_1(x) = (x - x_0)(x - x_1)$$

$$x_0 = a, \qquad x_1 = b$$

$$\psi_1(x) = (x-a)(x-b) \quad \leq 0 \quad \text{on } [a,b]$$

$$I(f) = \int_a^b \{ f(x_0) + f[a,b](x-a) \}\,dx$$
$$+ \frac{1}{2} f''(\eta) \int_a^b (x-a)(x-b)\,dx$$

$$I(f) \approx T = \frac{1}{2}(b-a)\,[\,f(a) + f(b)\,]$$

Trapezoidal rule.

$$E^T = -\frac{f''(\eta)\,(b-a)^3}{12}$$

$$\eta \in (a, b)$$

Now let $k=2$

$$f(x) = P_2(x) + f[x_0, x_1, x_2, x]\, \psi_2(x)$$

for distinct x_0, x_1, x_2.

$\psi_2(x) = (x-x_0)(x-x_1)(x-x_2)$ is not of one sign on (a,b)

However

$x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b$

$$\int_a^b \psi_2(x)\,dx = \int_a^b (x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,dx$$

$$u = x - \frac{a+b}{2}$$

$$= \int_{-\frac{b-a}{2}}^{\frac{b-a}{2}} \left(u + \frac{b-a}{2}\right) u \cdot \left(u - \frac{b-a}{2}\right) dx$$

$$= 0$$

$x_3 = x_1 = \frac{a+b}{2}$

$$\psi_3(x) = (x-a)\left(x - \frac{a+b}{2}\right)^2 (x-b)$$

is of one sign on (a,b)

$$I(f) = I(P_2) + \frac{1}{4!} f^{(4)}(\eta) \int_a^b \psi_3(x)\,dx$$

One calculates

$$\int_a^b \psi_3(x)\,dx = \int_a^b (x-a)\left(x-\frac{a+b}{2}\right)^2 (x-b)\,dx$$

$$= -\frac{4}{15}\left(\frac{b-a}{2}\right)^5$$

$$\boxed{E^S(f) = -\frac{1}{90} f^{(4)}(\eta)\left(\frac{b-a}{2}\right)^5 \quad \eta \in (a,b)}$$

$$I(f) \simeq I(P_2)$$

$$P_2(x) = f(a) + f[a,b](x-a) + f\left[a,b,\frac{a+b}{2}\right](x-a)(x-b)$$

$$\int_a^b P_2(x)\,dx = f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2} + f\left[a,b,\frac{a+b}{2}\right]\int_a^b (x-a)(x-b)\,dx$$

$$\int_a^b (x-a)(x-b) = -\frac{(b-a)^3}{6}$$

So $\displaystyle\int_a^b P_2(x)\,dx = f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2} - f[a,b,\tfrac{a+b}{2}]\frac{(b-a)^3}{6}$

. $f[a,b](b-a) = f(b) - f(a)$.

, By symmetry of divided diff

$$f[a, b, \tfrac{a+b}{2}] = f[a, \tfrac{a+b}{2}, b]$$

In fact $f[x_0, x_1, \ldots x_n] = f[u_0, u_1, \ldots u_n]$

$x_0, u_1, \ldots u_n = x_0, \ldots x_n$

$f[x_0, \ldots x_n]$ = coeff of x^n in $P_n(x)$

$f[u_0, \ldots u_n]$ = coeff of x^n in $\tilde{P}_n(x)$ (int f at $u_0, u_1, \ldots u_n$)

But $P_n(x) = \tilde{P}_n(x)$.

$$f[a, \tfrac{a+b}{2}, b](b-a)^2$$

$$= \left(f[\tfrac{a+b}{2}, b] - f[a, \tfrac{a+b}{2}] \right)(b-a)$$

$$= \left(\frac{f(b) - f(\frac{a+b}{2})}{\frac{b-a}{2}} - \frac{f(\frac{a+b}{2}) - f(a)}{\frac{b-a}{2}} \right)(b-a)$$

$$= 2\left(f(b) - 2f(\tfrac{a+b}{2}) + f(a) \right)$$

$$I(P_2) = \int_a^b P_2(x)\,dx$$

$$= f(a)(b-a) + \left(f(b) - f(a)\right)\left(\frac{b-a}{2}\right)$$

$$- 2\left(f(b) - 2f\left(\frac{a+b}{2}\right) + f(a)\right) \frac{b-a}{6}$$

$$= \frac{b-a}{6} \left\{ f(a) + 4\, f\left(\frac{a+b}{2}\right) + f(b) \right\}$$

Simpson's rule

i.e. $$\int_a^b f(x)\,dx \approx \frac{b-a}{6} \left\{ f(a) + 4\, f\left(\frac{a+b}{2}\right) + f(b) \right\}$$

$$E^S = -\frac{f^{(4)}(\eta)}{90} \left(\frac{b-a}{2}\right)^5$$

$\underline{\text{Let } k=3}$ "Corrected Trapezoidal rule"

$$f(x) = P_3(x) + f[x_0, x_1, x_2, x_3, x]\,\psi_3(x)$$

$$x_0 = x_1 = a \qquad x_2 = x_3 = b$$

$\psi_3(x) = (x-a)^2 (x-b)^2$ is of one sign on (a,b)

$$E(f) = \frac{1}{4!} f^{(4)}(\eta) \int_a^b (x-a)^2 (x-b)^2 \, dx$$

$$= \frac{f^{(4)}(\eta)\,(b-a)^5}{720}$$

$$P_3[x] = f[a] + f[a,a](x-a) + $$
$$+ f[a,a,b](x-a)^2 +$$
$$+ f[a,a,b,b](x-a)^2 (x-b)$$

$$\int_a^b p_3(x)\,dx = f(a)(b-a) + f[a,a]\frac{(b-a)^2}{2} + f[a,a,b]\frac{(b-a)^3}{3} + f[a,a,b,b]\left\{\frac{(b-a)^4}{4} - \frac{(b-a)^4}{3}\right\}$$

$$f[a,a] = f'(a)$$

$$f[a,a,b] = \frac{\{f[a,b] - f'(a)\}}{b-a}$$

$$f[a,a,b,b] = \frac{f'(b) - 2f[a,b] + f'(a)}{(b-a)^2}$$

$$\int_a^b p_3(x)\,dx = f(a)(b-a) + f'(a)\frac{(b-a)^2}{2} + \{f[a,b] - f'(a)\}\frac{(b-a)^2}{3} - \{f'(b) - 2f[a,b] + f'(a)\}\frac{(b-a)^2}{12}$$

replace $f[a,b]$ by $\dfrac{f(b)-f(a)}{b-a}$

we get

$$I(f) \approx CT = \frac{b-a}{2}\left(f(a)+f(b)\right) + \frac{(b-a)^2}{12}\left(f'(a)-f'(b)\right)$$

"corrected trapezoid rule)

$$E^{CT} = f^{(iv)}(\eta)\,\frac{(b-a)^5}{720}$$

Rectang rule $\quad I \approx (b-a)f(a)$

Midpt rule $\quad I \approx (b-a)\,f\left(\frac{a+b}{2}\right)$

Trapezoidal rule $\quad I \approx \frac{b-a}{2}\left\{f(a)+f(b)\right\}$

Simpsons rule $\quad I \approx \frac{b-a}{6}\left\{f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right\}$

Corr. Trap rule $\quad I \approx \frac{b-a}{2}\left\{f(a)+f(b)\right\}+\frac{(b-a)^2}{12}\left\{f'(a)-f'(b)\right\}$

Example $\int_0^1 \sin(x^2)\,dx$

$\sin 0 = 0$, $\sin(0.5^2) = 0.2474$

$\sin 1 = 0.8415$

Rectangle rule : $1 \cdot f(0) = 0$

Midpt rule = $1 \cdot f\left(\frac{a+b}{2}\right) = 1 \cdot f(0.5)$
$= 0.2474$

Trapezoidal rule

$I \approx \frac{1}{2}(0 + 0.8415) = 0.4208$

Simpson's rule

$I \approx \frac{1}{6}(0 + 4 \times 0.2474 + 0.8415)$
$= \frac{1}{6}(0.9896 + 0.8415)$
$= 0.3052$

corrected Trapezoidal rule

$I \approx T + \frac{1}{12}\{0 - 1.081\} \approx 0.3307$