Lecture 5

Last time we ~~studied~~ learnt cubic spline Interpolation and some methods to compute $\int_a^b f(x)\,dx$ numerically

Rectangle rule

$$\int_a^b f(x)\,dx \approx f(a)(b-a)$$

Midpoint rule

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

Trapezoidal rule

$$\int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)\left(f(a)+f(b)\right)$$

Simpsons' rule

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

Corrected Trapezoidal rule

$$\int_a^b f(x)\,dx \cong \frac{b-a}{2}\left[f(a)+f(b)\right] + \frac{(b-a)^2}{12}\left[f(a)+f(b)\right]$$

Example

$$I = \int_0^1 \sin x\,dx = -\cos x\Big|_0^1 = 4.597\ E-1$$

1. Rectangle rule

$$Ans = f(a)(b-a) = 0$$

2. Midpoint rule

$$Ans = \sin(0.5) = 4.794\ E-1$$

3. Trapezoidal Rule

$$Ans = 4.207\ E-1$$

4. Simpsons rule

$$Ans = 4.599\ E-1$$

5. Corrected Trapezoidal rule.

$$Ans \approx 4.590\ E-1$$

It is important to keep track of the errors involved

Always $\int_a^b f(x)\,dx$ = Approximation + error

$$E_R = \frac{f'(\eta)(b-a)^2}{2} \qquad \eta \in [a,b]$$

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

$$E_T = -\frac{f''(\eta)(b-a)^3}{12} \qquad \eta \in (a,b)$$

$$E_S = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{iv}(\eta) \qquad \eta \in (a,b)$$

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

Thus if

f is a linear polynomial then

$$f''(x) = 0$$

So $E_M = \frac{f''(\eta)\,(b-a)^3}{24} = 0$

Thus midpoint rule is exact

Ily $E_T = -\frac{f''(\eta)\,(b-a)^3}{12} = 0$

If f is a cubic polynomial then

$$f^{iv}(x) \equiv 0$$

So $E_S = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{iv}(\eta) = 0$

So Simpson's rule is exact if

$f(x)$ is a polynomial of degree ≤ 3.

Basic idea for deriving the formulas

$P_n(x)$ interpolates $f(x)$ on

$x_0, x_1, \ldots, x_n \in [a, b]$

Exact $\int_a^b f(x)\,dx$

approximate $\int_a^b P_n(x)\,dx$

$$f(x) = P_n(x) + f[x_0, x_1, \ldots, x_n, x]\,\psi_n(x)$$

$$\psi_n(x) = \prod_{i=0}^{n} (x - x_i)$$

$$\text{ERROR} = \int_a^b f[x_0, x_1, \ldots, x_n, x]\,\psi_n(x)\,dx$$

Today we write $P_n(x)$ in Lagrange form

$$P_n(x) = \sum_{i=0}^{n} f(x_i)\, l_i(x)$$

$$l_i(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)}{(x_i - x_k)}$$

$$\int_a^b P_n(x)\,dx = \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)\,dx$$

Set $C_i = \int_a^b l_i(x)\,dx$

So $\int_a^b P_n(x)\,dx = f(x_0)C_0 + f(x_1)C_1 + \cdots + f(x_n)C_n$

Does $\exists$ choice of $x_0, x_1, \ldots, x_n$ such that the error is small?

We want the formula to give exact answer when $f(x)$ is a polynomial of degree $\leq 2n+1$

$\{$ $2n+2$ parameters $f(x_0), C_0, f(x_1), C_1, \ldots, f(x_n), C_n \}$

Suppose we want to determine c_0, c_1, x_0, x_1 so that the integration

$$\int_{-1}^{1} f(x)\,dx = c_0 f(x_0) + c_1 f(x_1)$$

gives exact answers whenever $f(x)$ is a polynomial of degree $\leq 2(2)-1 = 3$

i.e when $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$

Since $\int_{-1}^{1} f(x)\,dx = a_0 \int_{-1}^{1} 1\,dx + a_1 \int_{-1}^{1} x\,dx$

$$+ a_2 \int_{-1}^{1} x^2\,dx + a_2 \int_{-1}^{1} x^3\,dx$$

This is equivalent of showing that the formula gives exact answers for $f(x) = 1, x, x^2, x^3$.

So we get the following equations

1. $c_0 \cdot 1 + c_1 1 = \int_{-1}^{1} 1\,dx = 2$

2. $c_0 x_0 + c_1 x_1 = \int_{-1}^{1} x\,dx = 0$

3. $c_0 x_0^2 + c_1 x_1^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}$

4. $c_0 x_0^3 + c_1 x_1^3 = \int_{-1}^{1} x^3\,dx = 0$

If we solve this system we get

$c_0 = 1$ $\quad$ $c_1 = 1$

$x_0 = -\frac{\sqrt{3}}{3}$ $\quad$ $x_1 = \frac{\sqrt{3}}{3}$

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

This formula produces exact answer for every polynomial of degree ≤ 3.

Example

$$I = \int_0^1 \sin x \, dx$$

$$x = \frac{t+1}{2}$$

$$I = \int_{-1}^{1} \frac{1}{2} \sin\left(\frac{t+1}{2}\right) dt$$

$$\simeq \frac{1}{2} \sin\left(\frac{\frac{-\sqrt{3}}{3}+1}{2}\right) + \frac{1}{2} \sin\left(\frac{\frac{\sqrt{3}}{3}+1}{2}\right)$$

$$\simeq 4.596 \; E-1$$

Correct answer = $4.597 \; E-1$

Note the error of Simpson's rule and this rule is the same.
But this rule only has two function evaluations while Simpson's rule has three function evaluations.

In the interval $[-1, 1]$ there exists a choice of nodes $x_0, x_1, \ldots, x_n$ such that error is quite small

Note $$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(b + \frac{b-a}{2}(t-1)\right) \frac{b-a}{2}\,dt$$

Thus it is enough to solve the problem for the interval $[-1, 1]$.

This solution is called Gaussian quadrature

$x_0, x_1, \ldots, x_n$ will be roots of "Legendre polynomials".

Introduction to Legendre's polynomials

$\{Q_0, Q_1, Q_2, \ldots, Q_n, Q_{n+1}, \ldots\}$ is the set of Legendre polynomial.

- $Q_0(x) = 1$
- $Q_n(x)$ is monic and has degree n
- $\int_{-1}^{1} P(x) Q_n(x)\, dx = 0$ whenever $P(x)$ is a polynomial of degree $< n$

$$Q_1(x) = x$$

$$Q_2(x) = x^2 - \frac{1}{3}$$

$$Q_3(x) = x^3 - \frac{3}{5}x$$

$$Q_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{25}.$$

Important property of Legendre polynomials

$Q_n(x)$ has n distinct roots in $(-1,1)$

Furthermore the roots are symmetric w.r.t the origin

Notation

$x_0, x_1, \ldots, x_n$ zeros of $Q_{n+1}(x)$

$$C_i = \int_{-1}^{1} \left(\prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \right) dx$$

$i = 0, 1, \ldots, n$

Theorem Let $P(x)$ be a polynomial of degree $\leq 2n+1$.

Then

$$\int_{-1}^{1} P(x)\,dx = \sum_{i=0}^{n} f(x_i) C_i$$

Proof :-

Case 1 $\deg P(x) \leq n$

$$P(x) = f(x_0)\, l_0(x) + f(x_1)\, l_1(x) + \cdots + f(x_n)\, l_n(x)$$

(exactly)

[why ?]

$$\int_{-1}^{1} P(x)\,dx = f(x_0)\int_{-1}^{1} l_0(x)\,dx + f(x_1)\int_{-1}^{1} l_1(x)\,dx + \cdots + f(x_n)\int_{-1}^{1} l_n(x)\,dx$$

Note that $c_i = \int_{-1}^{1} l_i(x)\,dx \qquad i = 0, 1, \ldots, n$

Thus $\int_{-1}^{1} P(x)\,dx = \sum_{i=0}^{n} f(x_i)\, c_i$

Case 2 $n+1 \leq \deg P(x) \leq 2n+1$

we divide $P(x)$ by $Q_{n+1}(x)$

$$P(x) = h(x)\, Q_{n+1}(x) + r(x)$$

Note that $\deg h(x) \leq n$

Also degree $r(x) \leq n$ or $r(x) = 0$

$$P(x) = h(x)\, Q_{n+1}(x) + r(x)$$

$$P(x_i) = 0 + r(x_i)$$

$$= r(x_i)$$

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} h(x)\, Q_{n+1}(x)\,dx + \int_{-1}^{1} r(x)\,dx$$

$$= \int_{-1}^{1} r(x)\,dx \qquad \left[\text{by property of Legendre polynomials}\right]$$

$$\sum_{i=0}^{n} P(x_i) C_i = \sum_{i=0}^{n} r(x_i) C_i$$

$$= \int_{-1}^{1} r(x)\,dx \qquad \text{By case 1}$$

$$= \int_{-1}^{1} P(x)\,dx$$

Legendre polynomials are known

Roots are also known

c_i are computed to a high degree of precision

$$Q_1(x) = x \qquad x_0 = 0$$

$$Q_2(x) = x^2 - \frac{1}{3} \qquad x_0 = \frac{-1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}$$

$$c_0 = 1, \quad c_1 = 1$$

$$Q_3(x) = x^3 - \frac{3}{5}x$$

$$x_0 = -\sqrt{\frac{3}{5}} = -0.7746$$

$$x_1 = 0$$

$$x_2 = \sqrt{\frac{3}{5}} = 0.7746$$

$$c_0 = 0.5556$$

$$c_1 = 0.8889$$

$$c_2 = 0.5556$$

Example

1. Approximate $\int_{-1}^{1} e^x \cos x \, dx$

using Gaussian Quadrature of order 2 and 3

Ans Order 2

$$\int_{-1}^{1} e^x \cos x \, dx \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

$$= 0.4704 + 1.493$$

$$= 1.963$$

exact answer = 1.933 (correct upto 4 sig digits)

Gaussian of order 3

$$\int_{-1}^{1} e^x \cos x \, dx \approx f(-0.7746) \times 0.5556 + f(0) \times 0.8889 + f(0.7746) \times 0.5556$$

$$= 1.934$$

By using Trapezoidal rule we get

$$\int_{-1}^{1} e^x \cos x \, dx \approx \frac{1}{2} \cdot 2 \left[f(-1) + f(1) \right]$$

$$= 0.1988 + 1.469$$

$$= 1.668$$

bad compared with Gaussian 2nd order &

By using Simpson's rule

$$\int_{-1}^{1} e^x \cos x \, dx \approx \frac{2}{6} \left[f(-1) + 4 f(0) + f(1) \right]$$

$$= \frac{1}{3} \left[0.1988 + 4 + 1.469 \right]$$

$$= 1.889$$

bad when compared with Gaussian of order 3.

Example 2

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

$$= 0.3103 \quad \text{(correct upto 4 sig digits)}$$

$I \approx 0.4208$ by Trapezoidal rule

$I \approx 0.3052$ by Simpson's rule

To apply Gaussian rules we need to change integral to -1 to 1

$$I = \int_0^1 \sin(x^2)\,dt$$

$t = 2x - 1 \qquad dt = 2\,dx$

$$= \int_{-1}^{1} \frac{1}{2} \sin\left(\frac{t+1}{2}\right)^2 dt$$

Gaussian 2pt rule

$$I \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = 0.3136$$

Gaussian 3 pt rule

$I \approx 0.3103$ exact upto 4 sig digits

Composite Rule

To compute $\int_a^b f(x)\,dx$ we developed some simple rules.

These rules do not give good estimates for I when [a, b] is reasonably large.

Example

$$I = \int_0^5 e^x dx = 1.474\ E2$$ correct upto 4 sig digits

By Trapezoidal rule

$$I \approx \frac{5}{2}\left[e^0 + e^5\right] = 3.735\ E+2$$

By Simpsons rule

$$I \approx \frac{5}{6}\left[e^0 + 4e^{2.5} + e^5\right]$$

$$= 1.347\ E2$$

Recall to approximate $\int_a^b f(x)\,dx$

We replaced $f(x)$ by an Interpolating polynomial $P_k(x)$ and then we

$$\int_a^b f(x)\,dx \approx \int_a^b P_k(x)\,dx.$$

If $b-a$ is large then there are two options

① • Increase # interpolation points.

This increases deg $P_k(x)$ and it creates lot of roundoff errors

② • Approximate f by piecewise polynomial function $P(x)\,dx$.

Option ② is good

In practise it divides $[a,b]$ into N smaller intervals and applies Quadrature rule to each of these subintervals

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

and apply Quadrature rule to each $[x_{i-1}, x_i]$.

We choose x_i's to be equally spaced

$$x_i = a + ih \qquad i = 0, 1, \ldots, N$$

$$h = \frac{b-a}{N}.$$

Composite Trapezoidal rule

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = \frac{h}{2}\left[f(x_{i-1}) + f(x_i)\right]$$

$$\int_a^b f(x)\,dx \cong \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x)\,dx$$

$$\approx \sum_{i=1}^{N} \frac{h}{2}\left(f(x_{i-1}) + f(x_i)\right)$$

$$T_N = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{N-1} f(x_i) + f(x_N)\right]$$

$I \approx T_N$ "Composite Trapezoidal rule"

$$\text{ERROR} = \sum_{i=1}^{N} \text{Error at } [x_{i-1}, x_i]$$

$$= \sum_{i=1}^{N} -\frac{f''(x_i)\, h^3}{12}$$

Recall $$\sum_{i=1}^{N} g(x_i)\, h(x_i) = g(\xi) \sum_{i=1}^{n} h(x_i)$$

if $h(x_i)$ is of one sign and g is cts.

So if f'' is continuous

$$\text{Error} = f''(\xi) \sum_{i=1}^{N} \frac{-h^3}{12} \qquad \xi \in (a,b)$$

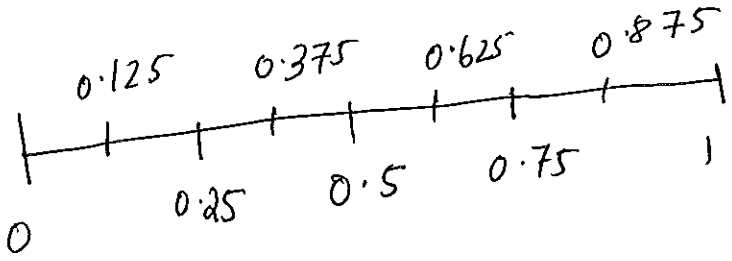
$$= -\frac{f''(\xi)\, h^3 N}{12} \qquad hN = b-a$$

$$= -\frac{f''(\xi)\, h^2 (b-a)}{12}.$$

Example

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

N	T_N
1	0.4208
2	0.3341
4	0.3159
8	0.3117



We compute Number of subdivisions required to get error $\leq 10^{-5}$

$$f(x) = \sin(x^2)$$

$$f^{(2)}(x) = -4x^2 \sin(x^2) + 2\cos(x^2)$$

$$|f^{(2)}(x)| \leq 6$$

$$\text{ERROR} = \frac{-f''(\xi)\, h^2 \cdot 1}{12}$$

$$|E| = \left| \frac{-f''(\xi)\, h^2}{12} \right| \leq \frac{6h^2}{12} < 10^{-5}$$

$$\frac{1}{2N^2} < 10^{-5}$$

$$N^2 > 5 \cdot 10^4$$

$$N > \sqrt{5}(10^2) \approx 224.$$

Composite Simpson's Rule

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = \frac{h}{6}\left[f(x_{i-1}) + 4f\left(x_{i-1}+\tfrac{h}{2}\right) + f(x_i)\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x_i)\,dx$$

$$\approx \sum_{i=1}^{N} \frac{h}{6}\left[f(x_{i-1}) + 4f\left(x_{i-1}+\tfrac{h}{2}\right) + f(x_i)\right]$$

Composite Simpson's Rule

$$\int_{x_{i-1}}^{x_i} f(x)\,dx \approx \frac{h}{6}\left[f(x_{i-1}) + 4f\left(x_{i-1}+\frac{h}{2}\right) + f(x_i)\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x)\,dx$$

$$\approx \sum_{i=1}^{N} \frac{h}{6}\left[f(x_{i-1}) + 4f\left(x_{i-1}+\frac{h}{2}\right) + f(x_i)\right]$$

$$S_N = \frac{h}{6}\left[f(x_0) + 2\sum_{i=1}^{N-1} f(x_i) + 4\sum_{i=1}^{N} f\left(x_{i-1}+\frac{h}{2}\right) + f(x_N)\right]$$

"Composite Simpson's Rule with N-nodes"

$$E_{RROR} = \sum_{i=1}^{N} \text{error at } [x_{i-1}, x_0]$$

$$= \sum_{i=1}^{N} -\frac{f^{(iv)}(\eta_i)}{90}\left(\frac{h}{2}\right)^5 \qquad \eta_i \in (x_{i-1}, x_i)$$

Assume $f^{(iv)}$ is continuous.

$$\text{ERROR} = -f^{(iv)}(\xi) \sum_{i=1}^{N} \frac{(h/2)^5}{90}$$

$\xi \in (a, b)$

$$= -f^{(iv)}(\xi) \frac{(h/2)^5}{90} \cdot N$$

$$= -f^{(iv)}(\xi) \frac{(h/2)^4}{180} \cdot (b-a)$$

Example

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

N	S_N
1	0.3052
2	0.3099
4	0.3103

→ correct upto 4 significant digits

We compute Number of subdivisons required to get error $< 10^{-5}$

$$f^{(iv)}(x) = \sin(x^2)\, 16x^4 - 48x^2 \cos x^2 - 12 \sin x^2$$

$$|f^{(iv)}(x)| \leq 76$$

$$|E_N^S| \leq \frac{|f^{iv}(\xi)| \left(\frac{h}{2}\right)^4 \cdot 1}{180}$$

$$\leq \frac{76}{180 \times 16 \times N^4} \leq 10^{-5}$$

$$N^4 \geq \frac{76 \times 10^5}{180 \times 16}$$

$$N \geq 7.1$$

Thus $N = 8$ will give answer correct upto 10^{-5}

Note $N \approx 224$ for composite Trapezoidal rule to give accuracy upto 10^{-6}.

Example

$$I = \int_0^4 e^x \, dx$$

Exact $= e^4 - e^0 = 53.59$ correct upto 4 sig digit

By Trapezoidal rule

N	T_N
1	111.2
2	70.37
4	57.99

By Simpson's Rule

N	S_N
1	56.76
2	53.86
4	53.61

Question (a) find N such that

$$|E_N^T| \leq 10^{-5}$$

(b) find N such that

$$|E_N^S| \leq 10^{-5}$$

(a) $E_N^T = -\dfrac{f''(\eta)\, h^2 (b-a)}{12}$

$f''(x) = e^x$

$|f^{(ii)}(x)| \le e^4 \quad \text{in } [0, 4]$

$|E_N^T| \le \dfrac{e^4}{12} \dfrac{4^2}{N^2} 4 < 10^{-5}$

(using $\dfrac{b-a}{N} = h$)

$N^2 > \dfrac{16}{3} e^4 \cdot 10^5$

$N > 4 e^2 10^2 \sqrt{\dfrac{10}{3}}$

$N > 5.396 \times 10^3$

$\boxed{N \ge 5397}$

(b) $E_N^S = -\dfrac{f^{(iv)}(\xi) \left(\frac{h}{2}\right)^4 (b-a)}{180}$

$f^{(iv)}(x) = e^x$

$|f^{(iv)}(x)| \le e^4 \quad \text{in } [0, 4)$

(30)

$$|E_N^S| \leq \frac{e^4}{180 \times 16} h^4 \cdot 4 \leq 10^{-5}$$

$$\therefore \frac{4}{N} = h$$

$$\frac{e^4 \; 4^4 \cdot 4}{16 \times 180 \times N^4} \leq 10^{-5}$$

$$N^4 \geq 10^5 \; \frac{e^4 \cdot 16 \times 4}{180}$$

$$N \geq \cdot e \times 10 \sqrt{\frac{16 \times 4}{18 \cdot}}$$

$$= 51.26$$

$N \geq 52$ will do the job