Lecture 9

Last time we introduced 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

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

Trapezoidal rule

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

Simpson's 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

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

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

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

If f is a cubic polynomial then

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

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

So Simpson's rule is exact if

$f(x)$ is polynomial of degree ≤ 3

Basic idea for deriving the formula.

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

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

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

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

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

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

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

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

Thus $\int_a^b P_n(x)\,dx = f(x_0)c_0 + f(x_1)c_1 + \cdots + f(x_n)c_n$

Thus $I = \int_a^b f(x)\,dx \approx f(x_0)c_0 + f(x_1)c_1 + \cdots + f(x_n)c_n$

Does $\exists$ choice of $x_0, x_1, \ldots, x_n$ such that 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 formula

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

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 $$\int_{-1}^{1} f(x)\,dx = a_0 \int_{-1}^{1} 1\,dx + a_1 \int_{-1}^{1} x\,dx + a_2 \int_{-1}^{1} x^2\,dx + a_3 \int_{-1}^{1} x^3\,dx$$

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) $c_0 x_0^2 + c_1 x_1^2 = \int_{-1}^{1} x^2 dx = 2/3$

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

$c_0 = 1 \qquad c_1 = 1$

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

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

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

:

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

Note that
$$\int_a^b f(x)\,dx = \int_{-1}^{1} f(t)\,dt$$ by a change of variables.

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

This solution is called Gaussian Quadrature

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

Introduction to Legendre polynomials

$\{Q_0, Q_1, \ldots Q_n, Q_{n+1}, \ldots\}$ is the set of Legendre polynomials. It has the following properties

- $Q_0(x) = 1$
- $Q_n(x)$ is monic has degree n for $n = 1, 2, \ldots$.

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

$Q_1(x) = x$

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

$Q_3(x) = x^3 - \frac{3}{5}x$ $\quad$ $Q_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$

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

<u>Notation</u>

$x_0, x_1, \dots x_n$ zero's of $Q_{n+1}(x)$

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

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

<u>Theorem</u> If $P(x)$ is any 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 $\qquad \deg P(x) \le n$

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

exactly why?

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

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 $\qquad n+1 \le \deg P(x) \le 2n+1$

We divide $P(x)$ by $\phi_{n+1}(x)$

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

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

$\deg r(x) \leq n$ or $r(x) = 0$

Note $p(x_i) = h(x_i) Q_{n+1}(x_i) + r(x_i)$

$= 0 + r(x_i)$

$= r(x_i)$

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

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

(by property of Legendré polynomials)

$$\sum_{i=0}^{n} p(x_i) c_i = \sum_{i=0}^{n} r(x_i) c_i$$

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

by case 1

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

Legendres polynomials are known
roots are also known
c_i are computed to a high degree of precision

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

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

$c_0 = 1 \qquad c_1 = 1$

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

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

$x_1 = 0$

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

$c_0 = 0.5556$

$c_1 = 0.8889$

$c_2 = 0.5556$

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 $= 1.933$ (upto 4 sig digits)

Gaussian of order 3

$$\int_{-1}^{1} e^{x}\cos x \, dx \simeq f(-0.7746) \times 0.5556$$

$$+ f(0) \times 0.8889$$

$$+ f(0.7746) \times 0.5556$$

$$= 0.3294 \times 0.5556$$
$$+ 1 \times 0.8889$$
$$+ 1.551 \times 0.5556$$
$$= 1.934$$

(*) by using Trapezoidal rule we get

$$\int_{-1}^{1} e^x \cos x \, dx \approx \frac{1}{2} \cdot 2 \left[f(-1) + f(1) \right]$$
$$= 1 \cdot (0.1988 + 1.469)$$
$$= 1.668$$

bad compared with Guassian 2^{nd} order

* Using Simpson's rule

$$\int_{-1}^{1} e^x \cos x \, dx \approx \frac{2}{6} \left[f(-1) + 4f(0) + f(1) \right]$$
$$= \frac{1}{3} \cdot \left[0.1988 + 4 + 1.469 \right]$$
$$= 1.889$$

bad when compared with Gaussian of order 3.

Example 2

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

$I = 0.3103$ (correct upto 4 sig digit

$I \approx 0.4208$ (by Trapezoidal rule)

$I' \approx 0.3052$ by simpson's rule)

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

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

put $t = 2x - 1$ $\quad dt = 2\,dx$

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

Guassian 2 pt rule

$$I \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = \begin{array}{l} 2.232\ E{-2} \\ + 2.913\ E{-1} \end{array}$$

$= 0.3136$

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

by Gaussian 3 pt rule

$$I \approx \begin{aligned} & f(-0.7746) \times 0.5556 \\ & f(0) \times 0.8889 \\ & + f(0.7746) \times 0.5556 \end{aligned}$$

$$\begin{aligned} = \; & 6.350\,E{-3} \times 0.5556 \\ & + 1.237\,E{-1} \times 0.8889 \\ & + 3.542\,E{-1} \times 0.5556 \end{aligned}$$

$$= 0.3103$$

(exact upto 4 sig digits)