Lecture 6

Last time we did Gaussian Quadrature

Let $\{Q_0, Q_1, Q_2, \ldots, Q_n, Q_{n+1}, \ldots\}$ be the Legendre polynomials

Let $\{x_0, x_1, \ldots, x_n\}$ be roots in $[-1, 1]$ of $Q_{n+1}(x)$

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

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

Then if $P(x)$ is a polynomial of degree $\leq 2n+1$

$$\text{then } \int_{-1}^{1} P(x)\, dx = \sum_{k=0}^{n} c_k f(x_k)$$

The roots of Legendre polynomial are known to a high degree of accuracy.
The c_i's are also known

Composite Trapezoidal Rules

We sub-divide the interval $[a, b]$ into N pairs

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

and then we apply Quadrature rule to each interval $[x_i, x_{i+1}]$

Composite Trapezoidal rule

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

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

Composite Simpsons Rule

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

Error for Composite Trapezoidal rule $= \dfrac{-f''(\xi)\,h^2(b-a)}{12}$

Error for composite Simpsons Rule $= \dfrac{-f^{(iv)}(\xi)\,(h/2)^4\,(b-a)}{180}$

Improper integrals

$$f(x) = \frac{g(x)}{(x-a)^p} \qquad 0 < p < 1$$

Then $\int_a^b f(x)\,dx$ exists

Question How to compute $\int_a^b f(x)\,dx$

Usual methods will involve $f(a) = \infty$

We assume that $g(x) \in C^4[a,b]$
(i.e g is 4 times differentiable in $[a,b]$
and $g^{(iv)}$ is continuous in $[a,b]$)

$P_4(x) = 4^{th}$ Taylor polynomial of g around a

$$P_4(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2}(x-a)^2 + \frac{g'''(a)}{6}(x-a)^3 + \frac{g^{(4)}(a)}{24}(x-a)^4$$

$$\int_a^b f(x)\,dx = \int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\,dx + \int_a^b \frac{P_4(x)}{(x-a)^p}\,dx$$

As $P_4(x)$ is a polynomial, we can determine the value of

$$\int_a^b \frac{P_4(x)}{(x-a)^p}\,dx = \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!}(x-a)^{k-p}\,dx$$

$$= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!\,(k+1-p)}(b-a)^{k+1-p}$$

This is generally the dominant part of the approximation, especially when the Taylor polynomial $P_4(x)$ agrees closely with $g(x)$ throughout the interval $[a,b]$

To approximate $\int_a^b f(x)\,dx$ we must add this value to the approximation of

$$\int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\, dx$$

Define $G(x) = \begin{cases} \dfrac{g(x) - P_4(x)}{(x-a)^p} & a < x < b \\ 0 & \text{if } x = a \end{cases}$

As $0 < p < 1$ and $P_4^{(k)}(a)$ agrees with $g^{(k)}(a)$ for $k = 0, 1, 2, 3, 4$, so $G(x) \in C^4[a, b]$

We can compute $\int_a^b G(x)\, dx$ by Composite Simpsons' Rule and get the final answer.

Example Approximate $\int_0^1 \frac{e^x}{\sqrt{x}}\,dx$

Ans

The fourth Taylor ~~formula~~ polynomial for e^x about $x=0$ is

$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24}$$

$$\int_0^1 \frac{P_4(x)}{\sqrt{x}}\,dx = \int_0^1 \left(\frac{1}{\sqrt{x}} + \sqrt{x} + \frac{x^{3/2}}{2} + \frac{x^{5/2}}{6} + \frac{x^{7/2}}{24} \right)$$

$$= 2x^{1/2} + \frac{2}{3}x^{3/2} + \frac{1}{5}x^{5/2} + \frac{1}{21}x^{7/2} + \frac{1}{108}x^{9/2}\Big|_0^1$$

$$= 2 + \frac{2}{3} + \frac{1}{5} + \frac{1}{21} + \frac{1}{108}$$

$$= 2.924$$

$$G(x) = \begin{cases} \frac{1}{\sqrt{x}}(e^x - P_4(x)) & 0 < x \le 1 \\ 0 & x = 0 \end{cases}$$

x	$g(x)$
0	0
0.25	0.0000170
0.5	0.0004013
0.75	0.0026026
1	0.009485

$$\int_0^1 g(x)\,dx \simeq 0.0018$$

$$I = 2.924 + 0.0018$$

$$= 2.9258$$

Example To find $\int_a^b f(x)\,dx$ where

$\lim_{x \to \infty} f(x) = \infty$

make substitution $z = -x$

$$\int_a^b f(x)\,dx = \int_{-a}^{-b} f(-z)(-dz)$$

$$= \int_{-b}^{-a} f(-z)\,dz$$

An improper integral with a singularity at c where $a < c < b$ is treated as the sum of improper integrals with end point singularities since

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx$$

Infinite lenghts of integration

$$\int_a^\infty f(x)\,dx \longrightarrow \text{put } t = \frac{1}{x}$$

$$dt = -\frac{1}{x^2}\,dx$$

$$= -t^2\,dx$$

$$\int_a^\infty f(x)\,dx = \int_{1/a}^0 -\frac{1}{t^2} f\left(\frac{1}{t}\right) dt \qquad dx = -\frac{1}{t^2}\,dt$$

$$= \int_0^{1/a} t^{-2} f\left(\frac{1}{t}\right) dt$$

Example $\quad I = \int_1^\infty x^{-3/2} \sin \frac{1}{x}\, dx$

$t = x^{-1}$

$dt = -x^{-2}\, dx \qquad dx = -t^{-2}\, dt$

$$I = \int_1^\infty x^{-3/2} \sin \frac{1}{x}\, dt$$

$$= \int_1^0 t^{3/2} (\sin t)\, -t^{-2}\, dt$$

$$= \int_0^1 \frac{\sin t}{\sqrt{t}}\, dt$$

$P_4(t) =$ fourth Taylor polynomial of $\sin t$

$$= t - \frac{t^3}{6}$$

$$\int_0^1 \frac{P_4(t)}{\sqrt{t}}\, dt = \int_0^1 \sqrt{t} - \frac{t^{5/2}}{6}$$

$$= \frac{2}{3} t^{3/2} - \frac{1}{21} t^{7/2} \Big|_0^1$$

$$= 6.190\ E{-1}$$

(10)

$$G(t) = \begin{cases} \dfrac{\sin t - t + \frac{1}{6}t^3}{\sqrt{t}} & * \quad 0 < t \leq 1 \end{cases}$$

x	$g(x)$
0	0
0.25	1.625 E-5
0.5	3.661 E-4
0.75	2.253 E-3
1	8.138 E-3

$$I_2 = \frac{0.5}{6}\left[0 + 4\times 1.625\,E{-}5 + 2\ 3.661\,E{-}4 + 4 \cdot 2.253\,E{-}3 + 8.138\,E{-}3\right\}$$

$$= 1.496\ E{-}3$$

$$I = 6.190\ E{-}1 + 1.496\ E{-}3$$

$$= 6.205\ E{-}1$$

Improper integrals using Lagrange interpolation

Suppose you have to estimate

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

here f is continuous on $[a,b]$ while $w(x)$ might be singular on $[a,b]$

Simple idea $f \overset{\text{replace}}{\rightsquigarrow} \sum_{i=0}^{n} l_i(x) f(x_i) = P_n(x)$

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

$$= \sum_{i=0}^{n} f(x_i)\, A_i$$

where $A_i = \int_a^b l_i(x)\, w(x)\, dx$

Note that A can be stored and used for many computations.

If $w(x) \geq 0$ on $[a,b]$ and $\int_a^b w(x)\,dx$ exists as an improper integral

Then we can define

$$\langle f, g \rangle = \int_a^b f(x)\, g(x)\, w(x)\, dx$$

"We will do the following later"

There exists monic polynomials $P_n(x)$ of degree n such that

$\langle P_n(x), q(x) \rangle = 0$ if $q(x)$ is a polynomial of degree $\leq n-1$

It can be shown that $P_n(x)$ has n simple zeros in (a,b)

Let $x_0, x_1, \ldots, x_n$ be roots of $P_{n+1}(x)$

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

Theorem :- If $Q(x)$ is a polynomial of degree $\leq 2n+1$ then

$$\int_a^b Q_n(x)\, w(x)\, dx = \sum_{i=0}^{n} Q(x_i)\, c_i$$

Proof :- **Case 1** $\deg Q(x) \leq n$

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

exactly (why?)

So we have

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

$$= \sum_{i=0}^{n} Q(x_i)\, c_i$$

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

$$Q(x) = P_{n+1}(x)\, h(x) + r(x)$$

$\deg h(x) \leq n$. $\deg r(x) \leq n$

$$\int_a^b Q(x)\,w(x)\,dx = \int_a^b P_{n+1}(x)\,h(x)\,w(x)\,dx + \int_a^b r(x)\,w(x)\,dx$$

$$= \int_a^b r(x)\,w(x)\,dx.$$

$$Q(x_i) = P_{n+1}(x_i)\,h(x_i) + r(x_i)$$

$$= r(x_i)$$

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

$$= \int_a^b r(x)\,w(x)\,dx \qquad \text{(by Gauss I)}$$

$$= \int_a^b Q(x)\,w(x)\,dx$$

Examples

1) $a = -1, \quad b = 1$ $\qquad w(x) = 1$ (i.e no singularity)

Then $P_n(x)$ = n^{th} Legendre polynomial

We get Gaussian Quadrature in this case.

2) $w(x) = \dfrac{1}{\sqrt{1-x^2}}$ $\qquad a = -1$, $b = 1$

We get Chebyshev Polynomials $T_n(x)$

$T_n(\cos\theta) = \cos n\theta$ is the defining relation of Chebyshev polynomials

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$T_0(x) = 1$

$T_1(x) = x$

$T_2(x) = 2x^2 - 1$

$T_3(x) = 4x^3 - 3x$

$T_4(x) = 8x^4 - 8x^2 + 1$

Roots of $T_{n+1}(x)$ are

$$\xi_{k,n+1} = \cos\left(\frac{2k+1}{2n+2}\pi\right)$$

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

$$c_i = \int_{-1}^{1} \frac{l_i(x)}{\sqrt{1-x^2}}\,dx = \frac{\pi}{n+1}$$

So $$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \approx \frac{\pi}{n+1} \sum_{i=0}^{n} f(\xi_{i,n+1})$$

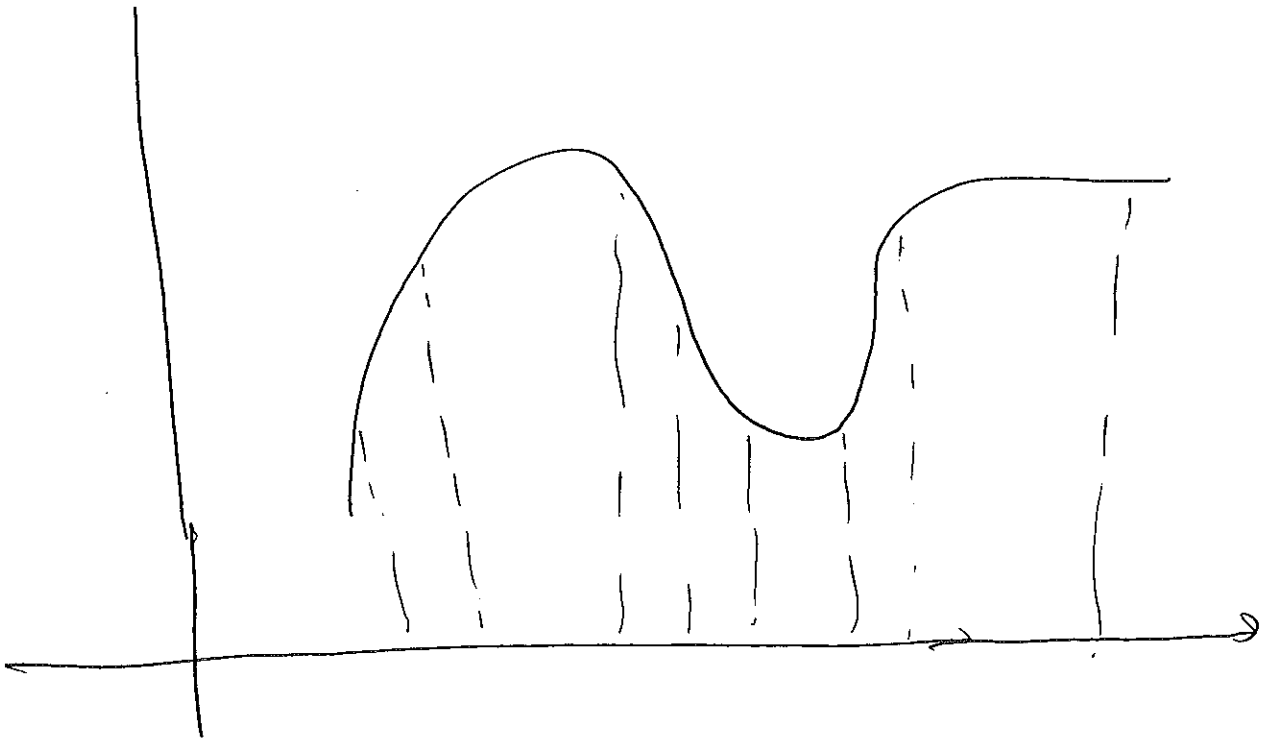
Adaptive Quadrature

Composite rules discussed so far are all based on N sub-intervals of equal size.

It is more economical to use subintervals whose length is determined by the local behaviour of the integrand

It is usually possible to evaluate $I(f) = \int_a^b f(x)\,dx$ to within a prescribed accuracy with fewer function evaluations if the subintervals are of properly chosen unequal size than if one insists on equal size sub-intervals

Basic Idea of Adaptive Quadrature



Use more subdivisions when function is varying a lot.

Use fewer subdivisions when function is not changing much.

Question :- How to determine such intervals ?

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

We describe on how to get an approximation P to I with

$$|P - I| \leq \varepsilon$$

ε ↑ prescribed error bound

We begin by dividing the interval ~~in~~ $[a, b]$ into N equally spaced subintervals

Let $[x_i, x_{i+1}]$ be one such subinterval

$$h = x_{i+1} - x_i$$

We now obtain two Simpson's rule approximations to the ~~integral~~ integral $\int_{x_i}^{x_{i+1}} f(x)\,dx$

$$S_i = \frac{h}{6}\left\{ f(x_i) + 4 f\left(x_i + \frac{h}{2}\right) + f(x_{i+1}) \right\}$$

$$\bar{S}_i = \frac{h}{12}\left\{ \begin{array}{l} f(x_i) + 4 f\left(x_i + \frac{h}{4}\right) + 2 f\left(x_i + \frac{h}{2}\right) \\ \quad + 4 f\left(x_i + \frac{3h}{4}\right) + f(x_{i+1}) \end{array} \right\}$$

From these two approximations we can estimate the error in the more accurate approximation $\bar{S}_i$ as follows

$$I_i - S_i = -\frac{f^{(iv)}(\eta)}{90}\left(\frac{h}{2}\right)^5 \qquad (1)$$

$$I_i - \bar{S}_i = -2\frac{f^{iv}(\xi)}{90}\left(\frac{h}{4}\right)^5 \qquad (2)$$

Assumption $f^{(iv)}$ is approximately constant in the sub-interval $[x_i, x_{i+1}]$

So $\eta \approx \xi$

① − ② yields

$$\bar{S}_i - S_i = \frac{f^{iv}(\xi)\, h^5}{2^5\, 90} \left(\frac{1 - 2^4}{2^4} \right)$$

$$\frac{f^{(iv)}(\xi)\, h^5}{2^5\, 90} = \frac{2^4}{1 - 2^4} (\bar{S}_i - S_i)$$

Substitute this in ②

$$\left| I_i - \bar{S}_i \right| = \frac{\bar{S}_i - S_i}{2^4 - 1} = \frac{1}{15} \left| \bar{S}_i - \bar{S}_i \right|$$

If the subinterval $[a, b]$ is covered by N subintervals and if each of these subintervals are arranged, that the error estimate satisfies

$$E_i = \frac{1}{15} |\bar{S}_i - S_i| \leq h/b-a \; \varepsilon \quad (*)$$

Then approximate to the integral obtained by summing $P = \sum_{i=1}^{N} \bar{S}_i$ will satisfy the error criterion

If (*) is Not satisfied by some subinterval then that sub-interval must be further sub-divided and the entire process repeated

Example Use adaptive Quadrature based on Simpson's rule to find an approximation of the integral

$$I = \int_0^1 \sqrt{x}\, dx$$

correct up to an error of $5E-4$

Ans Correct answer $= \frac{2}{3}$

However it is illustrative to do this problem by adaptive Simpsons rule

We first divide the interval $[0,1]$ into two part $[0, \frac{1}{2}]$ and $[\frac{1}{2}, 1]$

We now estimate $\int_{1/2}^{1} \sqrt{x}\, dx$

$$S\left[\tfrac{1}{2}, 1\right] = \frac{1}{12}\left\{\sqrt{1/2} + 4\sqrt{3/4} + \sqrt{1}\right\}$$

$$= 0.43093403$$

$$\bar{S}\left[\tfrac{1}{2}, 1\right] = \frac{1}{24}\left\{\sqrt{1/2} + 4\sqrt{5/8} + 2\sqrt{3/4} + 4\sqrt{7/8} + \sqrt{1}\right\}$$

$$= 0.43096219$$

$$E\left[\tfrac{1}{2}, 1\right] = \frac{1}{15}\left[\bar{S} - S\right] = 0.00000\ 18775$$

$$< \frac{1/2}{1}\,(0.00005)$$

$$= 0.00025$$

Thus our error criterion for $\int_{1/2}^{1} f(x)\, dx$

is satisfied

Sum $\leftarrow \bar{S}$

Now we estimate $\int_0^{1/2} \sqrt{x}\, dx$. (24)

$$S\left[0, \tfrac{1}{2}\right] = \frac{1}{12}\left\{0 + 4\sqrt{1/4} + \sqrt{1/2}\right\}$$

$$= 0.22559223$$

$$\bar{S}\left[0, \tfrac{1}{2}\right] = \frac{1}{24}\left\{0 + 4\sqrt{1/8} + 2\sqrt{1/4} + 4\sqrt{3/8} + \sqrt{1/2}\right\}$$

$$= 0.23211709$$

$$\bar{E}\left[0, \tfrac{1}{2}\right] = 0.0004399 \not< 0.00075$$

So the error test fails.
So we have to subdivide the interval into two part
So we have $\left[0, \frac{1}{4}\right]$ and $\left[1/4, \frac{1}{2}\right]$

applying simpsons rule

$$S\left[1/4, 1/2\right] = 0.15235819$$

$$\bar{S}\left[1/4, 1/2\right] = 0.15236814$$

$$E\left[1/4, 1/2\right] = 0.664\, 10^{-6} < \frac{1}{4}(0.0005)$$

$$0.000125$$

The error criterion is clearly satisfied

So we add $S[\frac{1}{4}, \frac{1}{2}]$ to the sum register to obtain the partial approximation

$$SOM[\tfrac{1}{4}, 1] = 0.43096219 + 0.15236819$$
$$= 0.58333033$$

Now we estimate $\int_0^{1/4} f(x)\,dx$

$$S[0, \tfrac{1}{4}] = 0.07975890$$

$$\overline{S}[0, \tfrac{1}{4}] = 0.08206578$$

$$E[0, \tfrac{1}{4}] = 0.00015379^{22}$$
$$+ 0.000125$$

Error criterion is not satisfied

So we must subdivide the interval $[0, 1/4]$ into two sub intervals $[0, 1/8]$ and $[1/8, 1/4]$

Proceeding as above with $h = 1/8$

$$S[1/8, 1/4] = 0.05386675$$

$$\bar{S}[1/8, 1/4] = 0.05387027$$

$$E[1/8, 1/4] = 0.00000000002346$$
$$< \frac{1}{8}(0.0005) = 0.0000625$$

We also get

$$S[0, 1/8] = 0.02819903$$

$$\bar{S}[0, 1/8] = 0.02901464$$

$$E[0, 1/8] = 0.00005437 < 0.0000625$$

So we can add $\bar{S}[0, 1/8] \cdot \ell\, \bar{S}[1/8, 1/4]$ to SUM and obtain

$$P = 0.66621524$$

$$|P - I| = 0.00045142 < 0.0005$$