Numerical Analysis : [MA214]
Lecture 6

Instructor: Prof. Tony J. Puthenpurakal

Department of Mathematics
Indian Institute of Technology Bombay

tputhen@math.iitb.ac.in

Recall

Last time we did Gaussian Quadrature. Let

$$\{Q_0, Q_1, Q_2, \cdots, Q_n, Q_{n+1}, \cdots\}$$

be the set of Legendre's polynomials.

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

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

$$c_i = \int_{-1}^{1} l_i(x)dx$$

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

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

The roots of Legebdre polynomial are known to be a high degree of

Composite Rules

We subdivide the interval $[a, b]$ into N smaller intervals.

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

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

Composite Trapezoidal Rules

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

Composite Simpson's Rules

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

$$E_{RROR} \text{ For Composite Trapezoidal rules } = -\frac{f''(\xi)h^2(b-a)}{12}$$

$$E_{RROR} \text{ For Composite Simpson's rules } = -\frac{f^{(4)}(\xi)(h/2)^4(b-a)}{}$$

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

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 $g^{(4)}$ is continuous in $[a,b]$).

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

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

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

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

$$\begin{aligned}
\int_a^b \frac{P_4(x)}{(x-a)^p}dx &= \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(x)}{k!}(x-a)^{k-p}dx \\
&= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k+1-p)}(b-a)^{k+1-p}
\end{aligned}$$

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

$$G(x) = \left\{ \begin{array}{ll} \frac{g(x)-P_4(x)}{(x-a)^p} & \text{if } a < x < b \\ 0 & \text{if } x = a \end{array} \right\}$$

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 Simpson's Rule and get the final answer.

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

Answer:- The fourth Taylor polynomial for e^x about $x = 0$ is

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

$$\begin{aligned}
\int_0^1 \frac{P_4(x)}{\sqrt{x}}dx &= \int_0^1 \left(\frac{1}{\sqrt{x}} + \sqrt{x} + \frac{x^{3/2}}{2} + \frac{x^{5/2}}{6} + \frac{x^{7/2}}{24} \right) \\
&= \left[2\sqrt{x} + \frac{2x^{3/2}}{3} + \frac{x^{5/2}}{5} + \frac{x^{7/2}}{21} + \frac{x^{9/2}}{108} \right]_0^1 \\
&= 2 + \frac{2}{3} + \frac{1}{5} + \frac{1}{21} + \frac{1}{108} \\
&= 2.924
\end{aligned}$$

$$G(x) = \left\{ \begin{array}{ll} \frac{1}{\sqrt{x}}(e^x - P_4(x)) & \text{if } 0 < x < 1 \\ 0 & \text{if } x = 0 \end{array} \right\}$$

x	$G(x)$
0	0
0.25	0.0000170
0.5	0.0004013
0.75	0.0026026
1.0	0.009485

$$\int_0^1 G(x)dx \approx 0.0018$$

$$I = 2.924 + 0.0018 = 2.9258$$

Example:- To find $\int_a^b f(x)dx$ where $\lim_{x \to b} f(x) = \infty$

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 integral with end point singularity since

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

Infinite length of integration

$$\int_a^\infty f(x)dx \to \text{ put } t = \frac{1}{x}, \text{ so } dt = -\frac{1}{x^2}dx = -t^2dx$$

$$\int_a^\infty f(x)dx = \int_{\frac{1}{a}}^0 \frac{-1}{t^2} f(\frac{1}{t})dt = \int_0^{\frac{1}{a}} t^{-2} f(\frac{1}{t})dt$$

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

$$\text{put } t = \frac{1}{x}, \text{ so } dt = -\frac{1}{x^2}dx = -t^2 dx$$

$$\begin{aligned} I &= \int_1^\infty x^{-3/2} sin(\frac{1}{x})dx \\ &= \int_1^0 t^{3/2} sin(t)(-t^{-2}dt) \\ &= \int_0^1 \frac{sin(t)}{\sqrt{t}}dt \end{aligned}$$

The fourth Taylor polynomial for $sin(t)$ about $t = 0$ is

$$P_4(t) = t - \frac{t^3}{6}$$

$$\begin{aligned}\int_0^1 \frac{P_4(t)}{\sqrt{t}}dt &= \int_0^1 \sqrt{t} - \frac{t^{5/2}}{6}dt \\ &= \left[\frac{2t^{3/2}}{3} - \frac{t^{7/2}}{21}\right]_0^1 \\ &= 6.190E{-1}\end{aligned}$$

$$G(t) = \left\{ \begin{array}{ll} \frac{sin t - t + \frac{t^3}{6}}{\sqrt{t}} & \text{if } 0 < t < 1 \\ 0 & \text{if } t = 0 \end{array} \right\}$$

t	$G(t)$
0	0
0.25	$1.625E{-5}$
0.5	$3.661E{-4}$
0.75	$2.253E{-3}$
1.0	$8.138E{-3}$

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

$$I_2 = 1.496E{-}3$$

$$I = 6.190E{-}1 + 1.496E{-}3 = 6.205E{-}1$$

Improper integral 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 $[a, b]$.

Basic Idea

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

$$\begin{aligned}\int_a^b f(x)w(x)dx &= \int_a^b \sum_{i=0}^{n} l_i(x)f(x_i)w(x)dx \\ &= \sum_{i=0}^{n} f(x_i)A_i\end{aligned}$$

$$\text{where} \quad A_i = \int_a^b l_i(x)w(x)dx$$

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

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 polynomial $P_n(x)$ of degree n such that

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

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

Let $x_0, x_1, \cdots, x_n$ 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

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

Proof.

Case 1 : degree $Q(x) \leq n$. Then

$$Q(x) = \sum_{i=0}^{n} l_i(x) Q(x_i) \text{ , (exactly why?)}$$

So we have

$$\begin{aligned} \int_a^b Q(x)w(x)dx &= \sum_{i=0}^{n} Q(x_i) \int_a^b l_i(x)w(x)dx \\ &= \sum_{i=0}^{n} Q(x_i)c_i \end{aligned}$$

$\square$

Case 2 : $n+1 \leq \text{degree } Q(x) \leq 2n+1$

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

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

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

$$\begin{aligned}
\sum_{i=0}^{n} Q(x_i)c_i &= \sum_{i=0}^{n} r x_i c_i \\
&= \int_a^b r(x)w(x)dx \text{ (by case 1)} \\
&= \int_a^b Q(x)w(x)dx
\end{aligned}$$

1. $a = -1,\ b = 1,\ w(x) = 1$ (*i.e.* no singularity)
Then $P_n(x) = n^{th}$ Legendre polynomial. We get Gaussian Quadrature in this case.

2. $a = -1,\ b = 1$

$$w(x) = \frac{1}{\sqrt{1-x^2}}$$

We get Chebyshev Polynomial $T_n(x)$

$$T_n(cos\theta) = cosn\theta$$

is the defining relation of Chebyshev polynomial

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \\ T_2(x) &= 2x^2 - 1 \\ T_3(x) &= 4x^3 - 3x \\ T_4(x) &= 8x^4 - 8x^2 + 1 \end{aligned}$$

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

$$\xi_{k,n+1} = cos\left(\frac{2k+1}{2n+2}\pi\right) \ , \ k = 0, 1, 2, \cdots, n$$

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

So

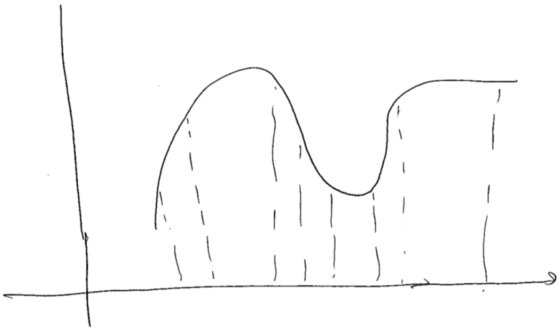
$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n+1} \sum_{i=0}^{n} f(\xi_{i,n+1})$$

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 behavior 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 evaluation if the subintervals are of properly chosen unequal size then if one insists on equal size subintervals.

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

$$|P - I| \leq \epsilon \text{ (prescribed error bound)}$$

We begin by dividing the interval $[a, b]$ 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 approximation to the integral $\int_{x_i}^{x_{i+1}} f(x)dx$

$$\begin{aligned} S_i &= \frac{h}{6}\{f(x_i) + 4f\left(x_i + \frac{h}{2}\right) + f(x_{i+1})\} \\ \overline{S_i} &= \frac{h}{12}\left\{f(x_i) + 4f\left(x_i + \frac{h}{2}\right) + 2f\left(x_i + \frac{h}{2}\right) + 4f\left(x_i + \frac{3h}{4}\right) + f(x_{i+1})\right. \end{aligned}$$

From these two approximations we can estimate the error in the more accurate approximate $\overline{S_i}$ as follows

$$
\begin{aligned}
I_i - S_i &= -\frac{f^{(4)}(\eta)}{90}\left(\frac{h}{2}\right)^5 &(1)\\
I_i - \overline{S_i} &= -\frac{2f^{(4)}(\xi)}{90}\left(\frac{h}{4}\right)^5 &(2)
\end{aligned}
$$

Assumption:- $f^{(4)}$ is approximately constant in the subinterval $[x_i, x_{i+1}]$. So $\eta \approx \xi$

equation(1) − *equation*(2) yields

$$
\begin{aligned}
\overline{S_i} - S_i &= \frac{f^{(4)}(\xi)h^5}{2^5.90}\left(\frac{1-2^4}{2^4}\right)\\
\frac{f^{(4)}(\xi)h^5}{2^5.90} &= \frac{2^4}{1-2^4}(\overline{S_i} - S_i)
\end{aligned}
$$

Substitute this in equation 2

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

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

$$E_i = \frac{1}{15}|\overline{S_i} - S_i| \leq \frac{h}{b-a}\epsilon \tag{3}$$

Then approximate to the integral obtained by summing $P = \sum_{i=1}^{N} \overline{S_i}$ will satisfies the error criterion.

If equation 3 is not satisfied by some subinterval then that subinterval must be further subdivided and the entire process repeated.

Examples

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 Simpson's rule.

We first devide the interval $[0, 1]$ into two parts $[0, 1/2]$ and $[1/2, 1]$.

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

$$
\begin{aligned}
S[1/2, 1] &= \frac{1}{12}[\sqrt{1/2} + 4\sqrt{3/4} + \sqrt{1}] \\
&= 0.43093403 \\
\overline{S}[1/2, 1] &= \frac{1}{24}[\sqrt{1/2} + 4\sqrt{5/8} + 2\sqrt{3/4} + 4\sqrt{7/8} + \sqrt{1}] \\
&= 0.43096219 \\
E[1/2, 1] &= \frac{1}{15}[\overline{S} - S] = 0.0000018775 < \frac{1}{2}(0.00005) = 0.00025
\end{aligned}
$$

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

$$Sum \longleftarrow \overline{S}$$

We now estimate $\int_0^{1/2} \sqrt{x}dx$

$$\begin{aligned} S[0,1/2] &= \frac{1}{12}[0 + 4\sqrt{1/4} + \sqrt{1/2}] \\ &= 0.22559223 \\ \overline{S}[0,1/2] &= \frac{1}{24}[0 + 4\sqrt{1/8} + 2\sqrt{1/4} + 4\sqrt{3/8} + \sqrt{1/2}] \\ &= 0.23211709 \\ E[0,1/2] &= 0.0004399 \nless 0.00025 \end{aligned}$$

So the error test fails.

So we have to subdivide the interval into two part. So we have $[0, 1/4]$ and $[1/4, 1/2]$.

Applying Simpson's rule

$$\begin{aligned}
S[1/4, 1/2] &= 0.15235819 \\
\overline{S}[1/4, 1/2] &= 0.15236814 \\
E[1/4, 1/2] &= 0.664 \times 10^{-6} < \frac{1}{4}(0.0005) = 0.000125
\end{aligned}$$

The error criterion is clearly satisfied. So add $S[1/4, 1/2]$ to the sum register to obtain the partial approximation

$$SUM[1/4, 1] = 0.43096219 + 0.15236814 = 0.58333033$$

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

$$\begin{aligned}
S[0, 1/4] &= 0.07975890 \\
\overline{S}[0, 1/4] &= 0.08206578 \\
E[0, 1/4] &= 0.0001537922 \not< 0.000125
\end{aligned}$$

Error criterion is not satisfied

So we must subdivide the interval $[0, 1/4]$ into subintervals $[0, 1/8]$ and $[1/8, 1/4]$.

Proceeding as above with $h = \frac{1}{8}$

$$
\begin{aligned}
S[1/8, 1/4] &= 0.05386675 \\
\overline{S}[1/8, 1/4] &= 0.05387027 \\
E[1/8, 1/4] &= 0.000000002346 < \frac{1}{8}(0.0005) = 0.0000625
\end{aligned}
$$

We also get

$$
\begin{aligned}
S[0, 1/8] &= 0.02819903 \\
\overline{S}[0, 1/8] &= 0.02901464 \\
E[0, 1/8] &= 0.00005437 < 0.0000625
\end{aligned}
$$

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

$$P = 0.66621524$$

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