Numerical Analysis : [MA214]
Lecture 5

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Recall

Last time we learnt cubic Spline Interpolation and some method to compute $\int_a^b f(x)dx$ numerically.

Rectangle rule

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

Midpoint rule

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

Trapezoidal rule

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

Simpsen'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

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

Example:-

$$I=\int_0^1 sinxdx=-cos|_0^1=4.597E{-1}$$

1. **Rectangle rule**
   $Ans = f(a)(b-a) = 0$
2. **Midpoint rule**
   $Ans = sin(0.5) = 4.794E{-1}$

3. **Trapezoidal rule**
   $Ans = 4.207E{-1}$
4. **Simpsen's rule**
   $Ans = 4.599E{-1}$
5. **Corrected Trapezoidal rule**
   $Ans = 4.590E{-1}$

It is important to keep track of the errors involved

$$\text{Always } \int_a^b f(x)dx = Approximation + error$$

$$
\begin{aligned}
E^R &= f'(\eta)\frac{(b-a)^2}{2}, \text{ for some } \eta \in [a,b] \\
E^M &= \frac{f''(\eta)}{2}\frac{(b-a)^3}{24}, \text{ for some } \eta \in [a,b] \\
E^T &= -\frac{f''(\eta)(b-a)^3}{12}, \text{ for some } \eta \in [a,b] \\
E^S &= -\frac{1}{90}f^{(4)}(\eta)\left(\frac{b-a}{2}\right)^5, \text{ for some } \eta \in [a,b] \\
E^{CT} &= \frac{f^{(4)}(\eta)(b-a)^5}{720}, \text{ for some } \eta \in [a,b]
\end{aligned}
$$

Thus if f is a linear polynomial then $f''(x) = 0$. So

$$E^M = \frac{f''(\eta)}{2}\frac{(b-a)^3}{24} = 0$$

Thus midpoint rule is exact.

Similarly

$$E^T = -\frac{f''(\eta)(b-a)^3}{12} = 0$$

If f is cubic polynomial then $f^{(4)}(x) = 0$. So

$$E^S = -\frac{1}{90} f^{(4)}(\eta) \left(\frac{b-a}{2}\right)^5 = 0$$

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

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

$$\text{Exact} \int_a^b f(x)dx$$

$$\text{approximate} \int_a^b P_n(x)dx$$

$$f(x) = P_n(x) + f[x_0, x_1, \cdots, x_n, x]\Psi_n(x)$$

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

$$\text{E}_{\text{RROR}} = \int_a^b f[x_0, x_1, \cdots, x_n, x]\Psi_n(x)dx$$

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

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

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

$$\int_a^b P_n(x)dx = f(x_i) \int_a^b l_i(x)dx$$

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 there exists choice of $x_0, x_1, \cdots, x_n$ 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 $\{f(x_0), c_0, f(x_1), c_1, \cdots, f(x_n), c_n\}$

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

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

Since

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

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

So we get the following equations

1. $c_0.1 + c_1.1 = \int_{-1}^{1} 1dx = 2$
2. $c_0x_0 + c_1x_1 = \int_{-1}^{1} \int_{-1}^{1} xdx = 0$
3. $c_0x_0^2 + c_1x_1^2 = \int_{-1}^{1} x^2dx = \frac{2}{3}$
4. $c_0x_0^3 + c_1x_1^3 = \int_{-1}^{1} x^3dx = 0$

If we solve this system we get $c_0 = 1, c_1 = 1, x_0 = \frac{-\sqrt{3}}{3}, x_1 = \frac{\sqrt{3}}{3}$

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

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

Example:- $I = \int_0^1 sinxdx$

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

$$\begin{aligned} I &= \int_{-1}^{1} \frac{1}{2} sin\left(\frac{t+1}{2}\right) dt \\ &\approx \frac{1}{2} sin\left(\frac{\frac{-\sqrt{3}}{3}+1}{2}\right) + \frac{1}{2} sin\left(\frac{\frac{\sqrt{3}}{3}+1}{2}\right) \\ &\approx 4.596E{-1} \\ \text{Correct answer} &= 4.597E{-1} \end{aligned}$$

Note that 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 this interval $[-1, 1]$ there exists a choice of nodes $x_0, x_1, \cdots, x_n$ 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 Quadratures.

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

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

is the set of Legendre's polynomials.

$$Q_0(x) = 1$$

$Q_n(x)$ is monic and degree n

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

$$\begin{aligned} Q_1(x) &= x \\ Q_2(x) &= x^2 - \frac{1}{3} \\ Q_3(x) &= x^3 - \frac{3}{5}x \\ Q_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{25} \end{aligned}$$

Important properties of Legendre's polynomials

$Q_n(x)$ has n distinct roots in $(-1, 1)$.
Furthermore the roots are symmetric $w.r.t.$ the origin

Notation:-

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

$$c_i = \int_{-1}^{1} \left(\prod_{k=0, k\neq i}^{n} \frac{x - x_k}{x_i - x_k} \right) dx \ , \ i = 0, 1, 2, \cdots, n$$

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:- degree of $P(x) \leq n$

$$\begin{aligned} P(x) &= f(x_0)l_0(x) + f(x_1)l_1(x) + \cdots + f(x_n)l_n(x) \text{ (exactly) [Why} \\ \int_{-1}^{1} P(x)dx &= f(x_0)\int_{-1}^{1} l_0(x)dx + f(x_1)\int_{-1}^{1} l_1(x)dx + \cdots + f(x_n)\int_{-1}^{1} l_n(x \end{aligned}$$

$$\text{Note that } c_i = \int_{-1}^{1} l_i(x)dx \text{ , } i = 0, 1, 2, \cdots, n$$

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

Case 2:- $n + 1 \leq degP(x) \leq 2n + 1$. We divide $P(x)$ by $Q_{n+1}(x)$

$$P(x) = h(x)Q_{n+1}(x) + r(x) \text{ , Note that } deg\ h(x) \leq n$$

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

$$P(x) = h(x)Q_{n+1}(x) + r(x)$$
$$P(x_i) = 0 + r(x_i) = r(x_i)$$

$$\begin{aligned}
\int_{-1}^{1} P(x)dx &= \int_{-1}^{1} h(x)Q_{n+1}(x)dx + \int_{-1}^{1} r(x)dx \\
&= \int_{-1}^{1} r(x)dx \text{ by property of Legendre polynomials} \\
\sum_{i=0}^{n} P(x_i)c_i &= \sum_{i=0}^{n} r(x_i)c_i \\
&= \int_{-1}^{1} r(x)dx \text{ by case 1} \\
&= \int_{-1}^{1} P(x)dx
\end{aligned}$$

Legendre polynomials are known. Roots are also known. c_i are computed to a high degree of precision.

$$
\begin{aligned}
Q_1(x) &= x \text{ and } x_0 = 0 \\
Q_2(x) &= x^2 - \frac{1}{3} \\
& \quad x_0 = \frac{-1}{\sqrt{3}}, x_1 = \frac{1}{\sqrt{3}}, c_0 = 1, c_1 = 1 \\
Q_3(x) &= x^3 - \frac{3}{5}x \\
& \quad x_0 = -\sqrt{\frac{3}{5}} = -0.7746, x_1 = 0, x_2 = \sqrt{\frac{3}{5}} = 0.7746 \\
& \quad c_0 = 0.5556, c_1 = 0.8889, c_2 = 0.5556
\end{aligned}
$$

Example 1:- Approximate $\int_{-1}^{1} e^x cosx\ dx$ using Gaussian Quadrature of order 2 and 3.

Ans:- Order 2

$$
\begin{aligned}
\int_{-1}^{1} e^x cosxdx &\approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \\
&= 0.4704 + 10493 = 1.963 \\
\text{Exact Answer} &= 1.933(\text{ correct upto 4 sig digits })
\end{aligned}
$$

Gaussian of order 3:-

$$
\begin{aligned}
\int_{-1}^{1} e^x cosxdx &\approx f(-0.7746) \times 0.5556 + f(0) \times 0.8889 + f(0.7746) \times 0.55 \\
&= 1.934
\end{aligned}
$$

By using trapezoidal rule we get

$$\begin{aligned}\int_{-1}^{1} e^x cosxdx &\approx \frac{1}{2}2[f(-1)+f(1)]\\ &= 0.1988 + 1.469 = 1.668\end{aligned}$$

bad compared with Gaussian 2^{nd} order.

By using Simpson's rule we get

$$\begin{aligned}\int_{-1}^{1} e^x cosxdx &\approx \frac{2}{6}[f(-1)+4f(0)+f(1)]\\ &= \frac{1}{3}[0.1988+4+1.469] = 1.889\end{aligned}$$

Bad when compared with Gaussian of order 3.

Example 2:-

$$I = \int_0^1 sin(x^2)dx = 0.3103 \text{ , (correct upto 4 sig digits)}$$

$$I \approx 0.4208 \text{ , by Trapezoidal rule}$$

$$I \approx 0.0.3052 \text{ , by Simpson's rule}$$

To apply Gaussian rule we need to change integral from -1 to 1.

$$\begin{aligned} I &= \int_0^1 sin(x^2)dx \\ & \quad t = 2x - 1 \text{ then } dt = 2dx \\ I &= \int_{-1}^1 \frac{1}{2} sin\left(\frac{t+1}{2}\right)^2 dt \end{aligned}$$

Gaussian 2pt rule

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

Gaussian 3pt rule

$$I \approx 0.3103 \text{ , exact upto 4 sig digits}$$

Composite Rule

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

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

Example

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

By Trapezoidal rule

$$I \approx \frac{5}{2}[e^0 + e^5] = 3.735E2$$

By Simpson's rule

$$I \approx \frac{5}{6}[e^0 + e^{2.5} + e^5] = 3.735E2 = 1.347E2$$

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 number of interpolation points. This increases degree of $P_k(x)$ and it creates lot of round off error.
2. Approximate f by piecewise polynomial function $P(x)dx$

Option 2 is good

In practice it divides $[a, b]$ into N smaller intervals and applies Quadrature rule to each 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

$$x_i = a + ih, \ h = \frac{b-a}{N}, \ i = 0, 1, 2, \cdots, N$$

Composite Trapezoidal Rule

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

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

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

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

$$I \approx T_N \text{ , "Composite Trapezoidal rule"}$$

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

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 continuous.

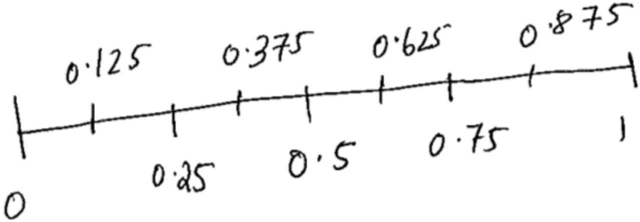
So if f'' is continuous

$$\begin{aligned} E_{RROR} &= f''(\xi)\sum_{i=1}^{N} -\frac{h^3}{12} \text{ where } \xi \in [a, b] \\ &= -\frac{f''(\xi)h^3 N}{12} \text{ where } hN = b - a \\ &= -\frac{f''(\xi)h^2(b-a)}{12} \end{aligned}$$

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 $\leq 10^{-5}$

$$\begin{aligned} f(x) &= sin(x^2) \\ f^{(2)}(x) &= -4x^2 sin(x^2) + 2cos(x^2) \\ |f^{(2)}(x)| &\leq 6 \end{aligned}$$

$$\begin{aligned} E_{RROR} &= -\frac{f''(\xi)h^2.1}{12} \\ |E| &= \left|-\frac{f''(\xi)h^2}{12}\right| \\ &= \frac{6h^2}{12} < 10^{-5} \end{aligned}$$

$$\begin{aligned} \frac{1}{2N^2} &< 10^{-5} \\ N^2 &\geq 5 \times 10^4 \\ N &\geq \sqrt{5}(10^2) \approx 224 \end{aligned}$$

Composite Simpson's Rule

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

$$\begin{aligned}\int_a^b f(x)dx &\approx \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x)dx \\ &\approx \sum_{i=1}^{N} \frac{h}{6}\left[f(x_{i-1}) + 4f\left(x_{i-1} + \frac{h}{2}\right) + f(x_i)\right]\end{aligned}$$

$$\begin{aligned}S_N &= \frac{h}{6}\left[f(x_0) + 2\sum_{i=1}^{N-1} f(x_i) + 4\sum_{i=1}^{N-1} f\left(x_{i-1} + \frac{h}{2}\right) + f(x_N)\right] \\ I &\approx S_N \text{ , "Composite Simpson's rule with } N\text{-nodes"}\end{aligned}$$

$$
\begin{aligned}
E_{RROR} &= \sum_{i=1}^{N} \text{Error at } [x_{i-1}, x_i] \\
&= \sum_{i=1}^{N} -\frac{f^{(4)}(\eta_i)}{90}\left(\frac{b-a}{2}\right)^5 \ , \ \eta_i \in [x_{i-1}, x_i]
\end{aligned}
$$

Assume $f^{(4)}$ is continuous.

$$
\begin{aligned}
E_{RROR} &= -f^{(4)}(\xi)\sum_{i=1}^{N} \frac{(h/2)^5}{90} \ , \text{ where } \xi \in [a, b] \\
&= -\frac{f^{(4)}(\xi)(h/2)^5 N}{90} \ , \text{ where } hN = b - a \\
&= -\frac{f^{(4)}(\xi)(h/2)^4(b-a)}{180}
\end{aligned}
$$

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 subdivisions required to get error $< 10^{-5}$

$$\begin{aligned} f(x) &= sin(x^2) \\ f^{(4)}(x) &= 16x^4 sin(x^2) - 48x^2 cos(x^2) - 12 sin(x^2) \\ |f^{(4)}(x)| &\leq 76 \end{aligned}$$

$$
\begin{aligned}
|E_N^S| &= \left| \frac{f^{(4)}(\xi)(h/2)^4.1}{180} \right| \\
&\leq \frac{|f^{(4)}(\xi)|(h/2)^4}{180} \\
&\leq \frac{76}{180 \times 16 \times N^4} \leq 10^{-5}
\end{aligned}
$$

$$
\begin{aligned}
N^4 &\geq \frac{76 \times 10^5}{180 \times 16} \\
N &\geq 7.1
\end{aligned}
$$

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

Note $N \approx 224$ for composite Trapezoidal rule to give accuracy upto 10^{-5}.

Example

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

$$\text{Exact } = e^4 - e^0 = 53.59 \text{ correct upto 4 sig digits}$$

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

Questions:-

1. Find N such that $E_N^T \leq 10^{-5}$
2. Find N such that $E_N^S \leq 10^{-5}$

Answer (1) :-

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

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

$$|f''(x)| \leq e^4 \text{ in } [0,4]$$

$$|E_N^T| \leq \frac{e^4 4^2 .4}{12N^2} < 10^{-5}$$

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

$$N^2 > \frac{16e^4.10^5}{3}$$

$$N > 4e^2 100\sqrt{\frac{10}{3}}$$

$$N > 5.396 \times 10^3$$

$$N \geq 5397$$

Answer (2) :-

$$\begin{aligned}
E_N^S &= -\frac{f^{(4)}(\xi)(h/2)^4(b-a)}{180} \\
f^{(4)}(x) &= e^x \\
|f^{(4)}(x)| &\leq e^4 \text{ in } [0,4]
\end{aligned}$$

$$|E_N^S| \leq \frac{e^{(4)}h^4.4}{180 \times 16} \leq 10^{-5}$$

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

$$\begin{aligned}
\frac{e^{(4)}4^4.4}{180 \times 16 \times N^4} &\leq 10^{-5} \\
N^4 &\geq \frac{e^{(4)}64 \times 10^5}{180 \times 16} \\
N &\geq e \times 10\sqrt{\frac{64}{18}} = 51.26
\end{aligned}$$

Thus $N \geq 52$ will do the job