Numerical Analysis

Numerical Differentiation and Integration

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Outline

Definition 1

1. $f'(x) \approx \dfrac{f(x+h)-f(x)}{h}$ is called the "forward difference approximation" provided that $h > 0$. The error of the approximation is bounded by $\dfrac{1}{2}hM$ where $|f''(x)| \leq M$ for $x \in (x, x+h)$.
2. $f'(x) \approx \dfrac{f(x+h)-f(x)}{h}$ is called the "backward difference approximation" provided that $h < 0$. The error of the approximation is bounded by $\dfrac{1}{2}hM$ where $|f''(x)| \leq M$ for $x \in (x+h, x)$.
3. $f'(x) \approx \dfrac{f(x+h)-f(x-h)}{2h}$ is called the "central difference approximation" provided $h > 0$. The error of the approximation is bounded by $\dfrac{1}{6}h^2M$ where $|f^{(3)}(x)| \leq M$ for $x \in (x-h, x+h)$.

Example 2

Values for $f(x) = xe^x$ are given by the following table

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957

Approximate $f'(2.0)$ using

1. forward difference approximation formula.
2. backward difference approximation formula.
3. central difference approximation formula.

1. $f'(2.0) \approx \frac{f(2.1)-f(2.0)}{2.1-2.0} = 23.70845$
2. $f'(2.0) \approx \frac{f(1.9)-f(2.0)}{1.9-2.0} = 20.74913$
3. $f'(2.0) \approx \frac{f(2.1)-f(1.9)}{2.1-1.9} = 22.22879$

Definition 3 ($(n+1)$ Points Formula)

Let $\{x_0, x_1, \dots, x_n\}$ be $n+1$ numbers in some interval I and $f \in C^{n+1}(I)$. Then, $f(x) = \sum_{i=0}^{n} f(x_i)L_{n,i}(x) + \frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!} f^{(n+1)}(\xi(x))$ and

$$f'(x) = \sum_{i=0}^{n} f(x_i)L'_{n,i}(x) + \frac{d}{dx}\left[\frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) + \frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!}\frac{d}{dx}\left[f^{(n+1)}(\xi(x))\right]$$

When x is one of the x_j where $j \in \{0, 1, \dots, n\}$,

$$f'(x_j) = \sum_{i=0}^{n} f(x_i)L'_{n,i}(x) + \frac{\prod_{\substack{i=0 \\ i\neq j}}^{n}(x_j-x_i)}{(n+1)!} f^{(n+1)}(\xi(x_j))$$

Let x_0, x_1, x_2 be three points with $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ for some $h \neq 0$. From the $(n+1)$ point formula, we get

1. $f'(x_0) = \dfrac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} + \dfrac{h^2}{3} f^{(3)}(\xi_0)$ where $\xi_0 \in (x_0, x_0 + 2h)$.
2. $f'(x_1) = \dfrac{-f(x_1 - h) + f(x_1 + h)}{2h} + \dfrac{h^2}{6} f^{(3)}(\xi_1)$ where $\xi_1 \in (x_1 - h, x_1 + h)$.
3. $f'(x_2) = \dfrac{f(x_2 - 2h) - 4f(x_2 - h) + 3f(x_2)}{2h} + \dfrac{h^2}{3} f^{(3)}(\xi_2)$ where $\xi_0 \in (x_2 - 2h, x_2)$.

Finally, note that the last of these equations can be obtained from the first by simply replacing h with $-h$, so there are actually only two formulas:

Three-Point Formula

1. Three-point endpoint formula

$$f'(x) = \frac{1}{2h}\left[-3f(x) + 4f(x+h) - f(x+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi(x))$$

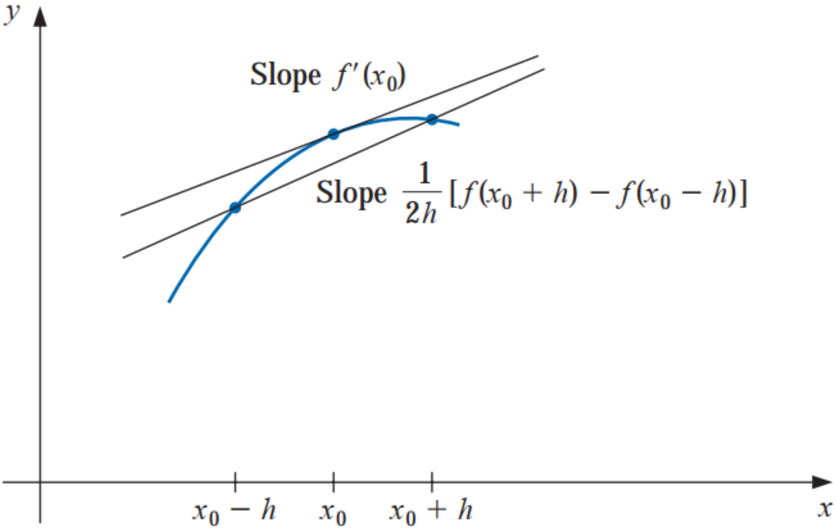
   where $\xi(x) \in (x, x+2h)$.

2. Three-point midpoint formula

$$f'(x) = \frac{1}{2h}\left[-f(x-h) + f(x+h)\right] + \frac{h^2}{6}f^{(3)}(\xi(x))$$

   where $\xi(x) \in (x-h, x+h)$.

Note that the last formula give the central difference approximation $f'(x) \approx \dfrac{1}{2h}\left[-f(x-h) + f(x+h)\right]$.



y
Slope $f'(x_0)$
Slope $\frac{1}{2h}[f(x_0+h) - f(x_0-h)]$
$x_0 - h$
x_0
$x_0 + h$
x

Five-Point Formula

1. Five-point endpoint formula

$$f'(x) = \frac{1}{12h}[-25f(x) + 48f(x+h) - 36f(x+2h) + 16f(x+3h) - 3f(x+4h)] + \frac{h^4}{5}f^{(5)}(\xi(x))$$

where $\xi(x) \in (x, x+4h)$.

2. Five-point midpoint formula

$$f'(x) = \frac{1}{12h}[f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)] + \frac{h^4}{30}f^{(5)}(\xi(x))$$

where $\xi(x) \in (x-2h, x+2h)$.

Example 4

Values for $f(x) = xe^x$ are given

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

1. Three-endpoint forward formula: $f'(2.0) \approx 22.032310$
2. Three-endpoint backward formula: $f'(2.0) \approx 22.054525$
3. Three-midpoint formula with $h = 0.1$: $f'(2.0) \approx 22.228790$
4. Three-midpoint formula with $h = 0.2$: $f'(2.0) \approx 22.414163$
5. Five-midpoint formula: $f'(2.0) \approx 22.166999$

1. Richardson extrapolation is a sequence acceleration method used to improve the rate of convergence of a sequence of estimates of some value $A^* = \lim_{h\to 0} A(h)$.
2. In essence, given the value of $A(h)$ for several values of h, we can estimate A^* by extrapolating the estimates to $h = 0$.
3. Let $A_0(h)$ be an approximation of A^* (exact value) that depends on a positive step size h with an error formula of the form

$$A^* = A_0(h) + a_0 h^{k_0} + a_1 h^{k_1} + a_2 h^{k_2} + \cdots$$

   where the a_i are unknown constants and the k_i are known constants such that $k_i < k_{i+1}$.
4. Furthermore, $O(h^{k_i})$ represents the trucation error of the $A_i(h)$ approximation such that $A^* = A_i(h) + O(h^{k_i})$.

5. Similarly, in $A^* = A_i(h) + O(h^{k_i})$, the approximation $A_i(h)$ is said to be an $O(h^{k_i})$ approximation.
6. Note that by simplifying with Big O notation, the following formulae are equivalent:

$$A^* = A_0(h) + a_0 h^{k_0} + a_1 h^{k_1} + a_2 h^{k_2} + \cdots$$
$$A^* = A_0(h) + a_0 h^{k_0} + O(h^{k_1})$$
$$A^* = A_0(h) + O(h^{k_0})$$

7. Richardson extrapolation is a process that finds a better approximation of A^* by changing the error formula from $A^* = A_0(h) + O(h^{k_0})$ to $A^* = A_1(h) + O(h^{k_1})$.
8. Therefore, by replacing $A_0(h)$ with $A_1(h)$ the truncation error has reduced from $O(h^{k_0})$ to $O(h^{k_1})$ for the same step size h.

9. Using the step sizes h and h/t for some constant t, the two formulas for A^* are:

$$A^* = A_0(h) + a_0 h^{k_0} + a_1 h^{k_1} + O(h^{k_2}) \tag{1}$$

$$A^* = A_0\left(\frac{h}{t}\right) + a_0\left(\frac{h}{t}\right)^{k_0} + a_1\left(\frac{h}{t}\right)^{k_1} + O(h^{k_2}) \tag{2}$$

10. Multiply the second equation (2) by t^{k_0} and subtract the first equation (1) to give us

$$(t^{k_0} - 1)A^* = \left[t^{k_0}A_0\left(\frac{h}{t}\right) - A_0(h)\right] + \left(t^{k_0}a_1\left(\frac{h}{t}\right)^{k_1} - a_1h^{k_1}\right) + O(h^{k_2})$$

$$\Rightarrow A^* = \frac{\left[t^{k_0}A_0\left(\frac{h}{t}\right) - A_0(h)\right]}{t^{k_0} - 1} + \frac{\left(t^{k_0}a_1\left(\frac{h}{t}\right)^{k_1} - a_1h^{k_1}\right)}{t^{k_0} - 1} + O(h^{k_2})$$

$$A^* = A_1(h) + a_1^{(1)}h^{k_1} + O(h^{k_2})$$

where $A_1(h) = \dfrac{t^{k_0}A_0\left(\frac{h}{t}\right) - A_0(h)}{t^{k_0} - 1}$.

11 A general recurrence relation can be defined for the approximations by

$$A_{i+1}(h) = \frac{t^{k_i} A_i\left(\frac{h}{t}\right) - A_i(h)}{t^{k_i} - 1} = A_i\left(\frac{h}{t}\right) + \frac{1}{t^{k_i} - 1}\left[A_i\left(\frac{h}{t}\right) - A_i(h)\right]$$

where k_{i+1} satisfies $A^* = A_{i+1}(h) + O(h^{k_{i+1}})$.

Example 5

Use the forward-difference method with $h = 0.1$ and $h/2 = 0.05$ to find approximations to $f'(1.8)$ for $f(x) = ln(x)$. Assume that this formula has truncation error $O(h)$ and use extrapolation on these values to see if this results in a better approximation.

1. $f'(1.8) \approx A_0(h) = \dfrac{f(1.8+0.1) - f(1.8-0.1)}{2(0.1)} = 0.5406722$
2. $f'(1.8) \approx A_0(h/2) = \dfrac{f(1.8+0.05) - f(1.8-0.05)}{2(0.05)} = 0.5479795$
3. $f'(1.8) \approx A_1(h) = A_0(h/2) + \dfrac{1}{2^1 - 1}[A(h/2) - A(h)] = 0.555287.$

It can be shown that

$$f'(x) = \frac{1}{2h}[f(x+h) - f(x-h)] - \frac{h^2}{6}f''(x) - \frac{h^4}{120}f^{(5)}(x) - \cdots$$

For $t = 2$, approximation of order $O(h^k)$ of $f'(x)$ by Richardson extrapolation can be summarized as

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$1 : A_0(h)$			
$2 : A_0(h/2)$	$3 : A_1(h)$		
$4 : A_0(h/4)$	$5 : A_1(h/2)$	$6 : A_2(h)$	
$7 : A_0(h/8)$	$8 : A_1(h/4)$	$9 : A_2(h/2)$	$10 : A_3(h)$

Example 6

Use the center-difference formula and the Richardson extrapolation iterations to find approximations of order $O(h^2), O(h^4), O(h^6)$, and $O(h^8)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

Definition 7 (Numerical Quadrature)

The basic method involved in approximating $\int_a^b f(x)dx$ is called numerical quadrature (numerical integration). It uses a sum $\sum_{k=0}^{n} a_k f(x_k)$ to approximate $\int_a^b f(x)dx$.

1. The basic idea is to select a set of $(n+1)$ distinct nodes $\{x_0, \dots, x_n\}$ from the interval $[a, b]$.
2. Then integrate the Lagrange interpolating polynomial

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

3. and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_{n,i}(x)\,dx + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n}(x - x_i)\,dx$$
$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x)) \prod_{i=0}^{n}(x - x_i)\,dx$$

where $a_i = \int_a^b L_{n,i}(x)\,dx$ for each $i = 0, 1, \ldots, n$.

4. The quadrature formula is, therefore, $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} a_i f(x_i)$

5. with error given by $E(f) = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x)) \prod_a^b (x - x_i)\,dx.$

Trapezoidal Rule (n=1)

Let $x_0 = a, x_1 = b$ and $h = b - a$. The numerical quadrature

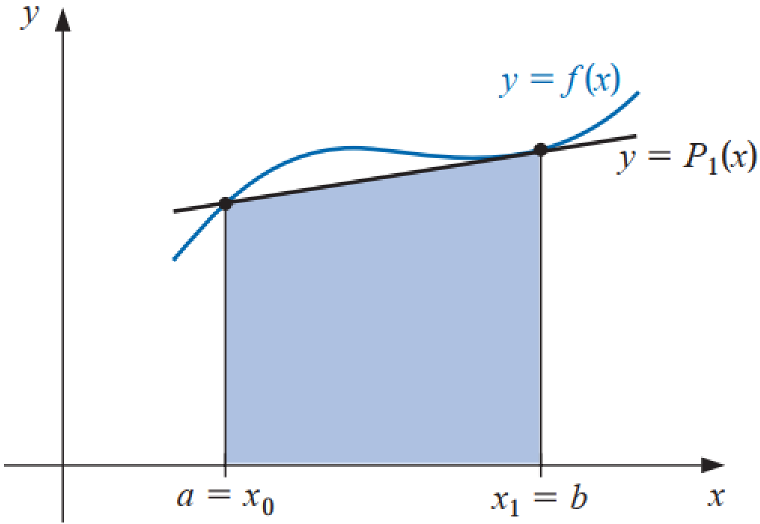
$$\int_a^b f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi)$$

where $\xi \in (x_0, x_1)$, is called trapezoidal rule.

1. Use the linear Lagrange polynomial $p_1(x) = \frac{(x-x_1)}{x_0-x_1}f(x_0) + \frac{(x-x_0)}{x_1-x_0}f(x_1)$,
2. we obtain $\int_a^b f(x)dx = \int_{x_0}^{x_1} p_1(x)dx + \frac{1}{2!}\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx$
3. By the Weighted Mean ValueTheorem for Integrals, there exist some $\xi \in (x_0, x_1)$,

$$E(f) = \frac{1}{2}f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)dx = -\frac{(x_1-x_0)^3}{12}f''(\xi) = -\frac{h^3}{12}f''(\xi)$$

3. Elements of Numerical Integration

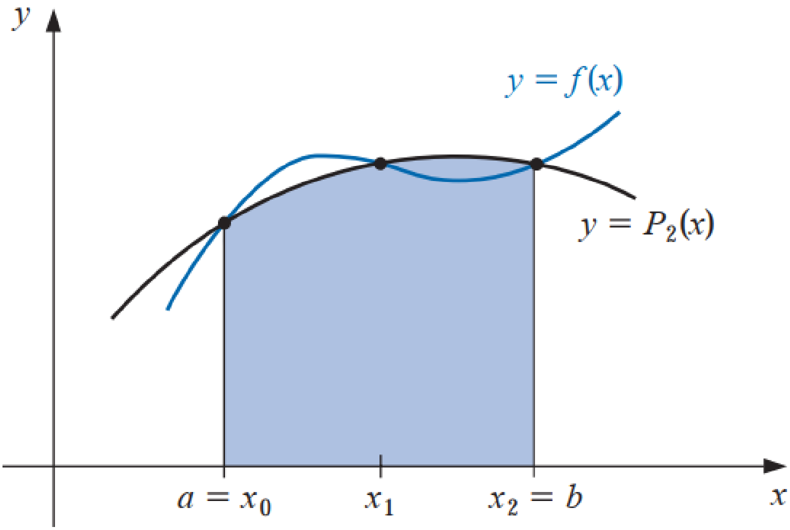


Simpson's Rule (n=2)

Let $x_0 = a, x_1 = a + h$ and $x_2 = b$ where $h = \dfrac{b-a}{2}$. The numerical quadrature

$$\int_a^b f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi)$$

where $\xi \in (x_0, x_2)$,is called Simpson's rule.



y
$y = f(x)$
$y = P_2(x)$
$a = x_0$
x_1
$x_2 = b$
x

Example 8

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^1 f_i(x)dx$ when $f_1(x) = x^2 + 1$, $f_2(x) = (x^2 + 1)^{-1}$, $f_3(x) = (x^2 + 1)^{1/2}$, $f_4(x) = \cos x$, and $f_5(x) = xe^x$.

Definition 9 (Measuring Precision)

The degree of accuracy, or precision, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.

The definition implies that the Trapezoidal and Simpson's (Three-Eighths) rules have degrees of precision one and three, respectively.

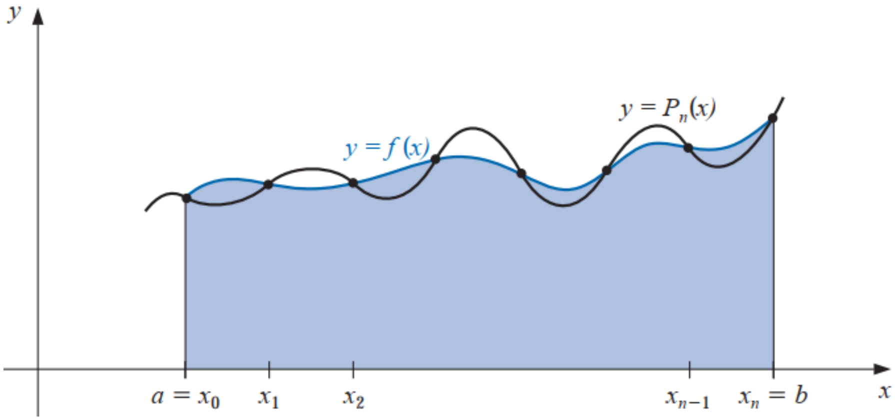
Definition 10 (Closed Newton-Cotes Formula)

The $(n+1)$-point closed Newton-Cotes formula uses nodes $x_i = x0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a, x_n = b$ and $h = (b-a)/n$. It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes. The formula assumes the form

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

where $a_i = \int_{x_0}^{x_n} L_{n,i}(x)dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x-x_j)}{(x_i-x_j)}dx.$

3. Elements of Numerical Integration



Theorem 11

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$*-point closed Newton-Cotes formula with* $x_0 = a, x_n = b$, *and* $h = (b-a)/n$. *There exists* $\xi \in (a, b)$ *for which*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3}}{(n+2)!} f^{(n+2)}(\xi) \int_0^n t^2(t-1)\cdots(t-n)\,dt,$$

if n *is even and* $f \in C^{n+2}[a, b]$, *and*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2}}{(n+1)!} f^{(n+1)}(\xi) \int_0^n t^2(t-1)\cdots(t-n)\,dt,$$

if n *is odd and* $f \in C^{n+1}[a, b]$.

Some of the common closed Newton-Cotes formulas with their error terms are listed. Note that in each case the unknown value ξ lies in (a, b).

1. $n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi)$$

2. $n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^4(\xi)$$

3. $n = 3$: Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80}f^4(\xi)$$

4. $n = 4$: Boole's rule

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945}f^6(\xi)$$

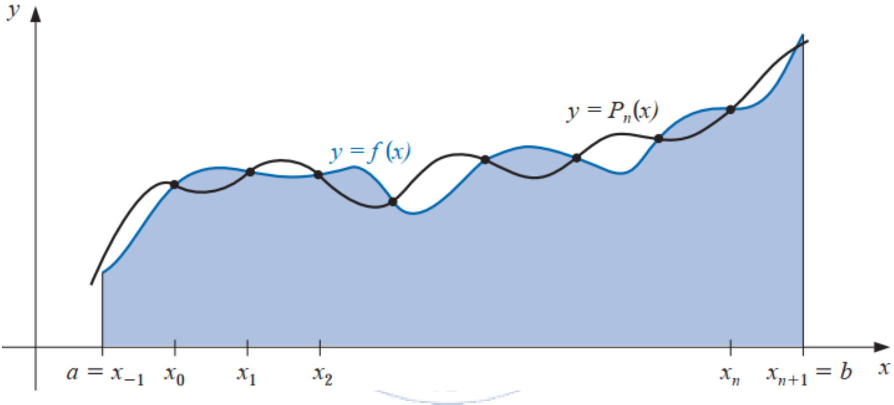
Definition 12 (Open Newton-Cotes Formula)

The open Newton-Cotes formulas do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$. Open formulas contain all the nodes used for the approximation within the open interval (a, b). The formulas become

$$\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where $a_i = \int_a^b L_{n,i}(x)dx$.

3. Elements of Numerical Integration



Theorem 13

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ *denotes the* $(n+1)$*-point open Newton-Cotes formula with* $x_{-1} = a, x_{n+1} = b$, *and* $h = (b-a)/(n+2)$. *There exists* $\xi \in (a,b)$ *for which*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3}}{(n+2)!} f^{(n+2)}(\xi) \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt,$$

if n *is even and* $f \in C^{n+2}[a,b]$, *and*

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2}}{(n+1)!} f^{(n+1)}(\xi) \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt,$$

if n *is odd and* $f \in C^{n+1}[a,b]$.

Some of the common open Newton-Cotes formulas with their error terms are as follows:

1. $n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi)$$

2. $n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(\xi)$$

3. $n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45}f^4(\xi)$$

4. $n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95h^5}{144}f^4(\xi)$$

Example 14

Compare the results of the closed and open Newton-Cotes formulas when approximating

$$\int_0^{\pi/4} \cos x \, dx \approx 0.70710678.$$

For the closed formulas we have

1. $n = 1: \; I \approx 0.67037927$
2. $n = 2: \; I \approx 0.70720195$
3. $n = 3: \; I \approx 0.70714899$
4. $n = 4: \; I \approx 0.70710669$

For the open formulas we have

1. $n = 0: \; I \approx 0.72561329$
2. $n = 1: \; I \approx 0.71940557$
3. $n = 2: \; I \approx 0.70702335$
4. $n = 3: \; I \approx 0.70704886$

Theorem 15 (Composite Simpson's Rule)

Let $f \in C^4[a,b]$, n be even, $h = \dfrac{b-a}{n}$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the Composite Simpson's rule for n subintervals can be written with its error term as

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu).$$

4. Composite Numerical Integration

With $h = (b-a)/n$ and $x_j = a + jh$, for each $j = 0, 1, \dots, n$, we have

$$\begin{aligned}
\int_a^b f(x)dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{2i} f(x)dx \\
&= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2i})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\} \\
&= \frac{h}{3} \left[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] + E(f)
\end{aligned}$$

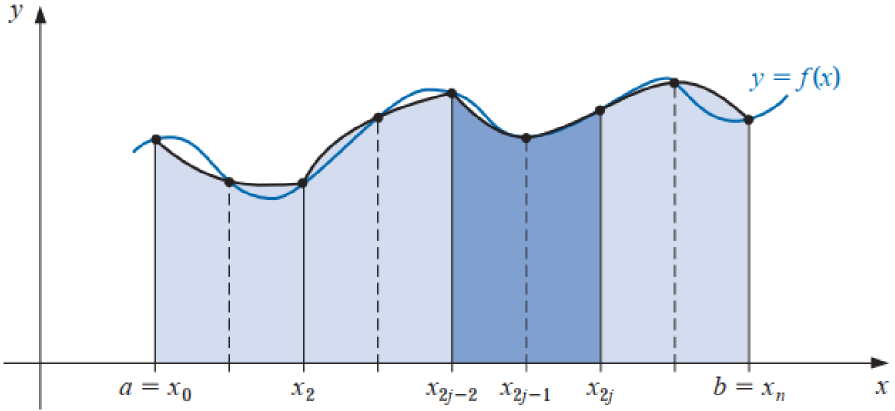
where $E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j)$. By the Extreme Value Theorem,

$$\begin{aligned}
\min_{x\in[a,b]} f^{(4)}(x) &\le f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x) \\
\Rightarrow \frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) &\le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x) \\
\Rightarrow \min_{x\in[a,b]} f^{(4)}(x) &\le \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x\in[a,b]} f^{(4)}(x)
\end{aligned}$$

By the Intermindiate Value Theorem, there exist $\mu \in (a, b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu) \Rightarrow E(f) = -\frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

4. Composite Numerical Integration



Algorithm: Composite Simpson's Rule

To approximate the integral $I^* = \displaystyle\int_a^b f(x)\,dx$:

INPUT endpoints a, b; even positive integer n.
OUTPUT approximation A to I^*.

1. Set $h = (b - a)/h$
2. Set $f0 = f(a) + f(b); f1 = 0; f2 = 0;$
3. For i from 1 to $n - 1$ do
   a. Set $x = a + ih$
   b. If i is even set $f2 = f2 + f(x)$
      else set $f1 = f1 + f(x)$
4. Set $A = h \cdot (f0 + 2 \cdot f2 + 4 \cdot f1)/3$
5. OUTPUT A;

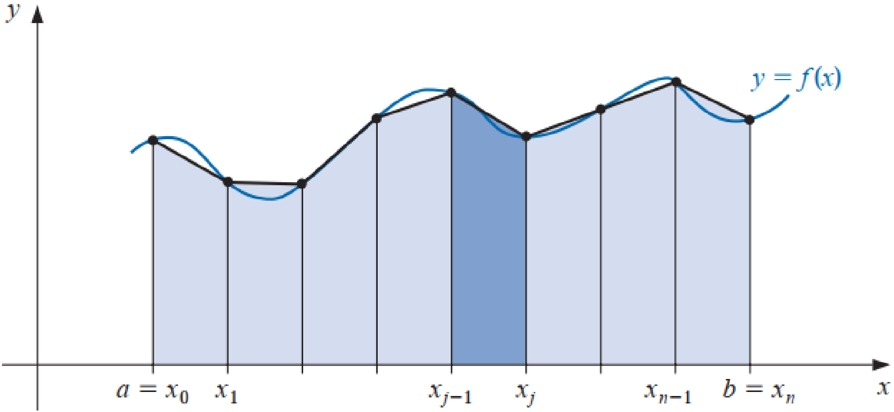
Theorem 16 (Composite Trapezoidal Rule)

Let $f \in C^2[a,b], h = \dfrac{b-a}{n}$, and $x_j = a + jh$, for each $j = 0, 1, \dots, n$. There exists a $\mu \in (a,b)$ for which the Composite Trapezoidal rule for n subintervals can be written with its error term as

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu).$$

The underlying reason follows exactly the same as Composite Simpson's Rule case.

4. Composite Numerical Integration

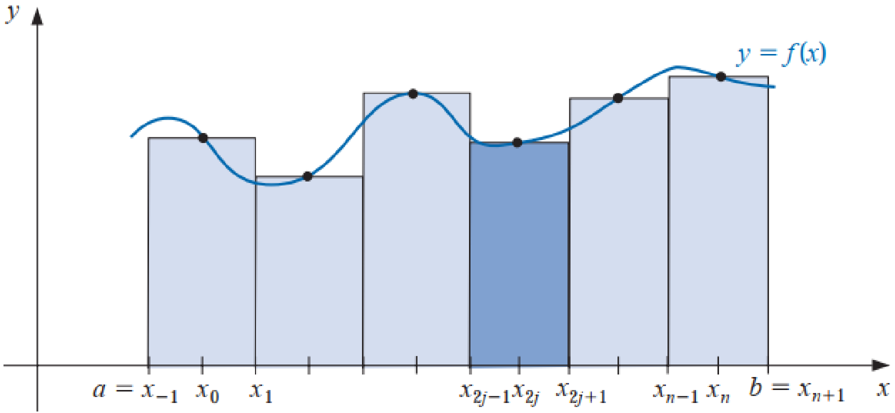


Theorem 17 (Composite Midpoint Rule)

Let $f \in C^2[a,b]$, n be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$ for each $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ for which the Composite Midpoint rule for $n+2$ subintervals can be written with its error term as

$$\int_a^b f(x)dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6} h^2 f''(\mu).$$

4. Composite Numerical Integration



Example 18

Approximate $I^* = \int_0^1 e^{-x^2}\, dx$ using the Composite Simpson's, Trapezoidal and Midpoint rules with the number of nodes $n = 2, 4, 6, 8, 10$.

To approximate the integral $\int_a^b f(x)dx$ we use the results of the Composite Trapezoidal rule with $n = 1, 2, 4, 8, \dots,$ (or $h, h/2, h/4, h/8, \dots$), and denote the resulting approximations, respectively, by $R_{0,0}, R_{1,0}, R_{2,0}$, etc. We then apply Richardson extrapolation, that is,

1. we obtain $O(h^4)$ approximations $R_{1,1}, R_{2,1}, R_{3,1}$, etc., by

$$R_{i,1} = R_{i,0} + \frac{1}{3}(R_{i,0} - R_{i-1,0}), \text{ for } i = 1, 2, 3, \dots$$

2. Then $O(h^6)$ approximations $R_{2,2}, R_{3,2}, R_{4,2}$, etc., by

$$R_{i,2} = R_{i,1} + \frac{1}{15}(R_{i,1} - R_{i-1,1}), \text{ for } i = 2, 3, 4, \dots$$

3. In general, after the appropriate $R_{i,j-1}$ approximations have been obtained, we determine the $O(h^{2j})$ approximations from

$$R_{i,j} = R_{i,j-1} + \frac{1}{4^j - 1}(R_{i,j-1} - R_{i-1,j-1}), \text{ for } i = j, j+1, \dots$$

Example 19

Use the Composite Trapezoidal rule to find approximations to $\int_0^{\pi} \sin x dx$ with $n = 1, 2, 4, 8,$ and $16.$ Then perform Romberg extrapolation on the results.

Next slide...

The Composite Trapezoidal rule for the various values of n gives the following approximations

$$R_{0,0} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0$$

$$R_{1,0} = \frac{\pi}{4}\left[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi\right] = 1.57079633$$

$$R_{2,0} = \frac{\pi}{8}\left[\sin 0 + 2\left(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + \sin\frac{3\pi}{4}\right) + \sin \pi\right] = 1.89611890$$

$$R_{3,0} = \frac{\pi}{16}\left[\sin 0 + 2\left(\sin\frac{\pi}{8} + \sin\frac{\pi}{4} + \cdots + \sin\frac{3\pi}{4} + \sin\frac{7\pi}{8}\right) + \sin \pi\right]$$
$$= 1.97423160$$

$$R_{4,0} = \frac{\pi}{32}\left[\sin 0 + 2\left(\sin\frac{\pi}{16} + \sin\frac{\pi}{8} + \cdots + \sin\frac{7\pi}{8} + \sin\frac{15\pi}{16}\right) + \sin \pi\right]$$
$$= 1.99357034$$

1. The $O(h^4)$ approximation are

$$R_{1,1} = R_{1,0} + \frac{1}{3}(R_{1,0} - R_{0,0}) = 2.09439511$$

$$R_{2,1} = R_{2,0} + \frac{1}{3}(R_{2,0} - R_{1,0}) = 2.00455976$$

$$R_{3,1} = R_{3,0} + \frac{1}{3}(R_{3,0} - R_{2,0}) = 2.00026917$$

$$R_{4,1} = R_{4,0} + \frac{1}{3}(R_{4,0} - R_{3,0}) = 2.00001659$$

2. The $O(h^6)$ approximation are

$$R_{2,2} = R_{2,1} + \frac{1}{15}(R_{2,1} - R_{1,1}) = 1.99857073$$

$$R_{3,2} = R_{3,1} + \frac{1}{15}(R_{3,1} - R_{2,1}) = 1.99998313$$

$$R_{4,2} = R_{4,1} + \frac{1}{15}(R_{4,1} - R_{3,1}) = 1.99999975$$

3. The $O(h^8)$ approximation are

$$R_{3,3} = R_{3,2} + \frac{1}{63}(R_{3,2} - R_{2,2}) = 2.00000555$$

$$R_{4,3} = R_{4,2} + \frac{1}{63}(R_{4,2} - R_{3,2}) = 2.00000001$$

4. and the $O(h^{16})$ approximation are

$$R_{4,4} = R_{4,3} + \frac{1}{255}(R_{4,3} - R_{3,3}) = 1.99999999$$

1. If the approximation error for an integral on a given interval is to be evenly distributed, a smaller step size is needed for the large-variation regions than for those with less variation.
2. An efficient technique for this type of problem should predict the amount of functional variation and adapt the step size as necessary.
3. These methods are called Adaptive quadrature methods.
4. The method we discuss is based on the Composite Simpson's rule, but the technique is easily modified to use other composite procedures.

5. Suppose that we want to approximate $\int_a^b f(x)dx$ to within a specified tolerance $\varepsilon > 0$. The first step is to apply Simpson's rule with step size $h = (b-a)/2$.

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi), \quad (1)$$

for some $\xi \in (a,b)$, where $S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)]$.

6. The next step is to determine an accuracy approximation that does not require $f^{(4)}(\varepsilon)$. To do this, we apply the Composite Simpson's rule with $n = 4$ and step size $(b-a)/4 = h/2$, giving

$$\int_a^b f(x)dx = S(a,a+h) + S(a+h,b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\xi}), \quad (2)$$

7. The error estimation is derived by assuming that $\xi \approx \tilde{\xi}$ or, more precisely, that $f^{(4)}(\xi) \approx f^{(4)}(\tilde{\xi})$. From (1) and (2),

$$S(a,a+h) + S(a+h,b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\xi}) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\xi)$$

$$\frac{15}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi) \approx S(a,b) - S(a,a+h) - S(a+h,b), \quad (3)$$

8. From (3) and (2), $|s_2 - s_1| \approx 15E = 15|I^* - s_2|, \quad (4)$
where $s_1 = S(a,b), s_2 = S(a,a+h) + S(a+h,b), E = \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi)$
and $I^* = \int_a^b f(x)dx.$

9. If $|s_2 - s_1| < 15\varepsilon$, we expect to have $|I^* - s_2| < \varepsilon$ and so s_2 is assumed to be a sufficiently accurate approximation to I^*.

Example 20

Approximate $I^* = \int_0^{\pi/2} \sin x dx$ with tolerance $\varepsilon = 0.00001$ using Simpson's Adaptive Quadrature.

On the interval $[0, \pi/2]$

1. $s_1 = S(0, \pi/2) = 1.00227988$
2. $s_2 = S(0, \pi/4) + S(\pi/4, \pi/2) = 1.00013458$
3. $|s_2 - s_1| = 0.00214529 > 15(0.00001)$
4. Does not meet the approximated tolerance $|s_2 - s_1| < 15\varepsilon$.

On the subinterval $[0, \pi/4]$

a. $s_1 = S(0, \pi/4) = 0.29293264$
b. $s_2 = S(0, \pi/8) + S(\pi/8, \pi/4) = 0.29289565$
c. $|s_2 - s_1| = 0.00003699 < 15(0.000005)$
d. Meet the approximated tolerance $|s_2 - s_1| < 15(\varepsilon/2)$.

On the subinterval $[\pi/4, \pi/2]$

a. $s_1 = S(\pi/4, \pi/2) = 0.70720195$
b. $s_2 = S(\pi/4, 3\pi/8) + S(3\pi/8, \pi/2) = 0.70711265$
c. $|s_2 - s_1| = 0.00008930 > 15(0.000005)$
d. Does not meet the approximated tolerance $|s_2 - s_1| < 15(\varepsilon/2)$.

On the subinterval $[\pi/4, 3\pi/8]$

i. $s_1 = S(\pi/4, 3\pi/8) = 0.32442604$
ii. $s_2 = S(\pi/4, 5\pi/16) + S(5\pi/16, \pi/2) = 0.32442352$
iii. $|s_2 - s_1| = 0.00000252 < 15(0.0000025)$
iv. Meet the approximated tolerance $|s_2 - s_1| < 15(\varepsilon/4)$.

On the subinterval $[3\pi/8, \pi/2]$

i. $s_1 = S(3\pi/8, \pi/2) = 0.38268661$
ii. $s_2 = S(3\pi/8, 7\pi/16) + S(7\pi/16, \pi/2) = 0.38268363$

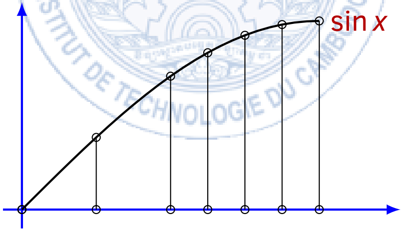
iii $|s_2 - s_1| = 0.00000298 < 15(0.0000025)$

iv Meet the approximated tolerance $|s_2 - s_1| < 15(\varepsilon/4)$.

Thus, $I^* \approx s_2([0, \pi/4]) + s_2([\pi/4, 3\pi/8]) + s_2([3\pi/8, \pi/2]) = 1.0000028$.

Note

The approximation on each subinterval is rounded to 8 decimal places and the factor of tolerance is 15. In practice, we choose 10 instead of 15 as the factor of tolerance.



1. Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced, way.
2. The nodes $x_1, x_2, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \ldots, c_n$, are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

3. To measure this accuracy, we assume that the best choice of these values produces the exact result for the largest class of polynomials, that is, the choice that gives the greatest degreeof precision.
4. The coefficients $c_1, c_2, \ldots, c_n$ in the approximation formula are arbitrary, and the nodes $x_1, x_2, \ldots, x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration. This gives us $2n$ parameters to choose.

5. If the coefficients of a polynomial are considered parameters, the class of polynomials of degree at most $2n - 1$ also contains $2n$ parameters.
6. To illustrate the procedure for choosing the appropriate parameters, we will show how to select the coefficients and nodes when $n = 2$ and the interval of integration is $[-1, 1]$.
7. Suppose we want to determine $c_1, c_2, x_1,$ and x_2 so that the integration formula

$$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

8. gives the exact result whenever $f(x)$ is a polynomial of degree $2(2) - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3,$$

for some collection of constants, $a_0, a_1, a_2,$ and a_3.

9. Because

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

this is equivalent to showing that the formula gives exact results when $f(x)$ is $1, x, x^2$, and x^3.

10. Hence, we need c_1, c_2, x_1, and x_2, so that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1dx = 2,$$

$$c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} xdx = 0,$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2dx = \frac{2}{3},$$

$$c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3dx = 0.$$

11. Solve the system of above equations gives

$$c_1 = 1, c_2 = 1, x_1 = -\frac{\sqrt{3}}{3}, x_2 = \frac{\sqrt{3}}{3}$$

12. which gives the approximation formula

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

13. This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less.

Definition 21 (Legendre Polynomials)

The Legendre polynomials constitute a set $p_0, p_1, \ldots, p_n, \ldots$ of polynomials satisfying the following conditions:

1. Each polynomial $p_n(x)$ is monic of degree n, that is, the coefficient multiplying x^n is 1.
2. The polynomial p_n is orthogonal to $p_0, p_1, \ldots, p_{n-1}$ with respect to the inner product defined by $\langle p, q\rangle = \displaystyle\int_{-1}^{1} p(x)q(x)dx$, that is,

$$\int_{-1}^{1} p_k(x)p_n(x)dx = 0, \text{ for } k = 0, 1, \ldots, n-1.$$

To obtain the Legendre polynomials we apply to Gram-Schmidt orthonormalization process on the set $\{1, x, x^2, \ldots, x^n, \ldots\}$ with respect to the mentioned inner product.

The first few Legendre polynomials are as follows:

$$
\begin{aligned}
p_0(x) &= 1,\\
p_1(x) &= x,\\
p_2(x) &= -\frac{1}{3} + x^2,\\
p_3(x) &= -\frac{3}{5}x + x^3,\\
p_4(x) &= \frac{3}{35} - \frac{6}{7}x^2 + x^4,\\
p_5(x) &= \frac{5}{21}x - \frac{10}{9}x^3 + x^5\\
p_6(x) &= -\frac{5}{231} + \frac{5}{11}x^2 - \frac{15}{11}x^4 + x^6,\\
p_7(x) &= -\frac{35}{429}x + \frac{105}{143}x^3 - \frac{21}{13}x^5 + x^7
\end{aligned}
$$

Theorem 22

Suppose that $x_1, x_2, \dots, x_n$ are the roots of the n-th Legendre polynomial $p_n(x)$ and that for each $i = 1, 2, \dots, n$, the numbers c_i are defined by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx.$$

If $p(x)$ is any polynomial of degree less than or equal to $2n-1$, then

$$\int_{-1}^{1} p(x)dx = \sum_{i=1}^{n} c_i p(x_i).$$

1. The coefficients $c_i = \int_{-1}^{1} L_{n,i}(x)dx$'s can be generated by Adaptive Simpson's Quadrature.
2. The roots of Legendre's polynomials can be generated by Müller's method with the help of Horn's algorithm.
3. Here are some coefficients c_i's and roots x_i's with 10^{-10} accuracy for $n = 2, 3, 4, 5$.

Table: Coefficients and Roots for Gaussian Quadrature

i	1	2	3	4	5
$c[2]$	1.0000000000	1.0000000000			
$x[2]$	0.5773502692	-0.5773502692			
$c[3]$	0.8888888889	0.5555555556	0.5555555556		
$x[3]$	-0.0000000000	-0.7745966692	0.7745966692		
$c[4]$	0.6521451549	0.6521451549	0.3478548451	0.3478548451	
$x[4]$	0.3399810436	-0.3399810436	-0.8611363116	0.8611363116	
$c[5]$	0.5688888889	0.4786286705	0.4786286705	0.2369268851	0.2369268851
$x[5]$	-0.0000000000	0.5384693101	-0.5384693101	-0.9061798459	0.9061798459

4. An integral $\int_a^b f(x)dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables

$$u = \frac{2x - a - b}{b - a} \Leftrightarrow x = \frac{1}{2}[(b - a)u + a + b]$$

5. This permits Gaussian quadrature to be applied to any interval $[a, b]$, because

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{1}{2}[(b - a)u + a + b]\right) \frac{b - a}{2} du$$
$$= 0.5(b - a) \int_{-1}^{1} f\left(0.5[(b + a) + (b - a)x]\right) dx$$

Example 23

Approximate $\displaystyle\int_0^1 e^{-x^2}dx$ using Gaussian quadrature with $n = 2$.

First, note that the exact integral is 0.7468241328.

$$
\begin{aligned}
\int_0^1 e^{-x^2}dx &= \int_{-1}^1 \exp\left(-\left[\frac{(1+0)+(1-0)x}{2}\right]^2\right)\frac{(1-0)}{2}dx \\
&= \int_{-1}^1 \exp\left(-\left(\tfrac{x+1}{2}\right)^2\right)\tfrac{1}{2}dx \\
&\approx 1.0000000000\cdot\tfrac{1}{2}\exp\left(-\left(\tfrac{0.5773502692+1}{2}\right)^2\right) \\
&\qquad + 1.0000000000\cdot\tfrac{1}{2}\exp\left(-\left(\tfrac{-0.5773502692+1}{2}\right)^2\right) \\
&= 0.7465946883
\end{aligned}
$$