

CS537-002

Numerical Analysis

Lecture 4

Numerical Integration

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Definite Integral

A definite integral has an interval for integration. For a fixed integration interval, the result is a number

$$\int_0^{\frac{\pi}{2}} \sin x \, dx = 1$$

An indefinite integral does not have an integration interval. The result of an indefinite integral (antiderivative) is a class of functions

$$\int \sin x \, dx = -\cos x + C$$

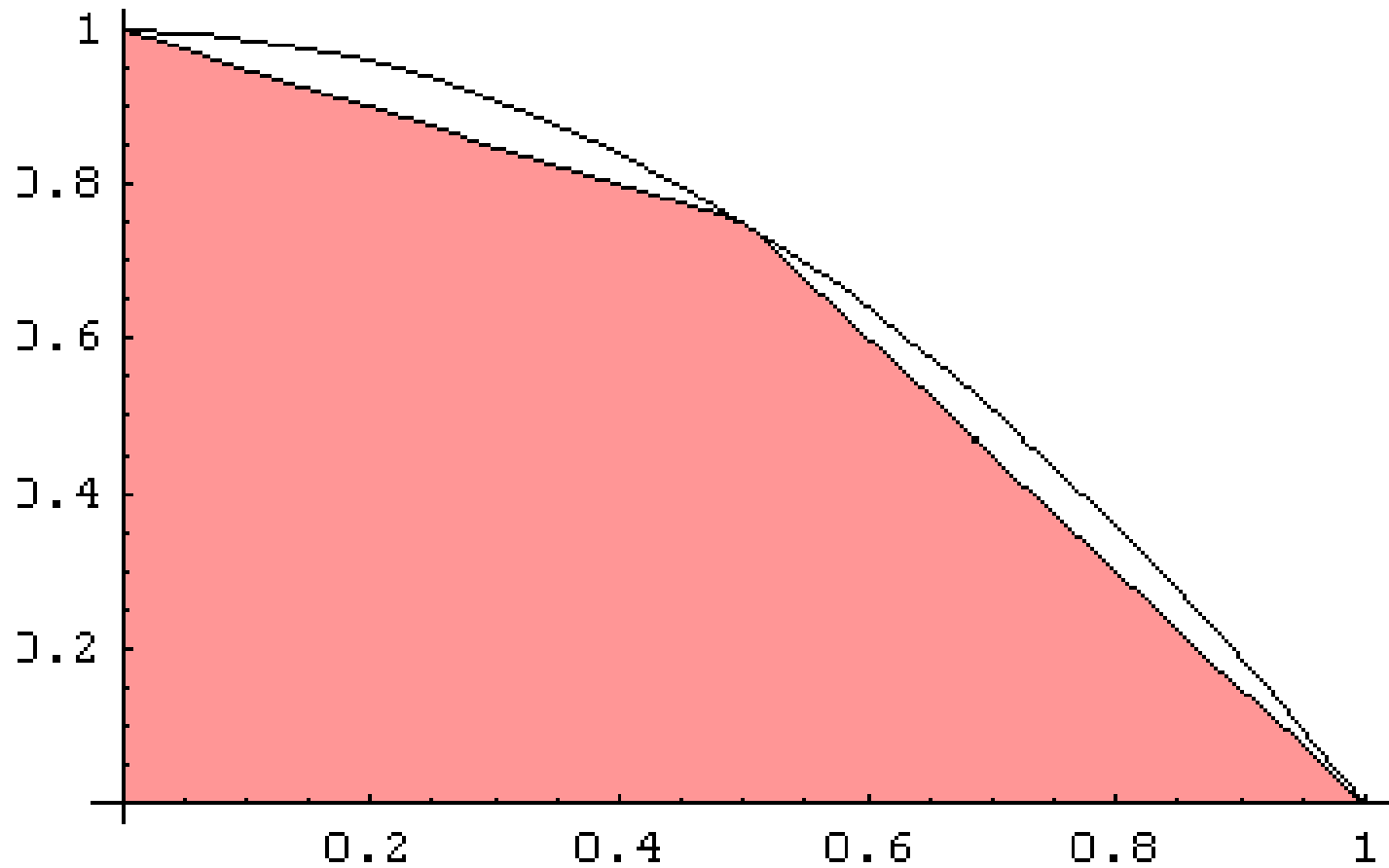
Numerical integration is for computing definite integrals

Fundamental Theorem of Calculus:

$$\int_a^b F'(x) \, dx = F(b) - F(a)$$

$$\int_a^x F'(t) \, dt = F(x) - F(a)$$

Numerical Integration



Partition

The definite integral of a function can be viewed as the area under a curve. This point of view lends us means to compute definite integral

Let P be a partition of the interval of $[a,b]$ as

$$P = \{a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b\}$$

We have n subintervals as $[x_i, x_{i+1}]$. Let m_i be the greatest lower bound of (a nonnegative function) $f(x)$ on $[x_i, x_{i+1}]$ as

$$m_i = \inf \{f(x) : x_i \leq x \leq x_{i+1}\}$$

And M_i as the least upper bound on the same subinterval

$$M_i = \sup \{f(x) : x_i \leq x \leq x_{i+1}\}$$

Partition



Lower and Upper Sums

The lower sums and upper sums of f corresponding to the given partition P is

$$L(f; P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$

$$U(f; P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$

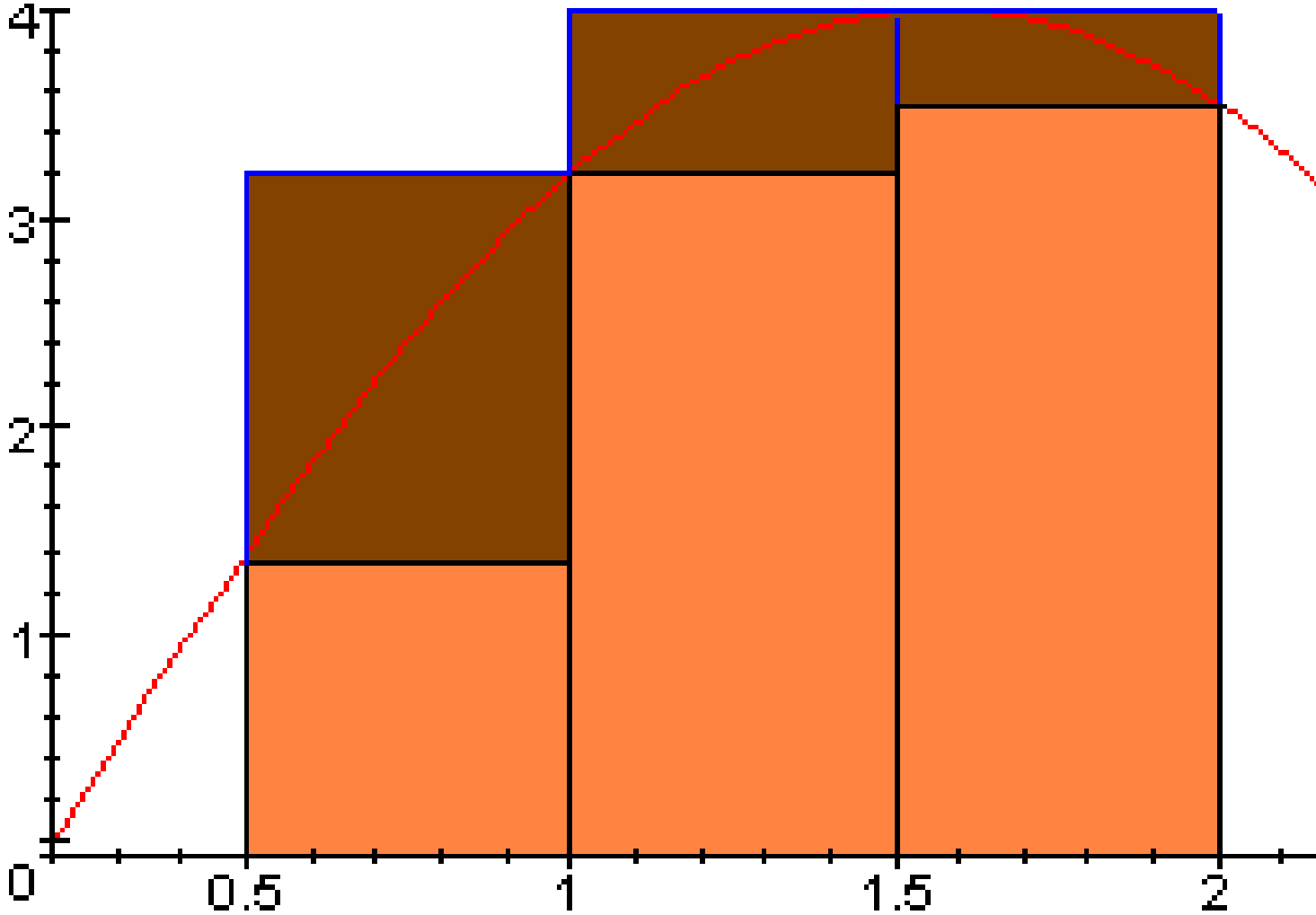
If we consider the definite integral of a nonnegative f as the area under the curve, we have

$$L(f; P) \leq \int_a^b f(x) dx \leq U(f; P)$$

for all partitions P

If f is continuous on $[a, b]$, then the above inequality defines the definite integral. The integral also exists if f is monotone (either increasing or decreasing) on $[a, b]$

Upper and Lower Bounds



Riemann-Integrable Functions

If the greatest lower bound equals the least upper bound for all partitions of $[a,b]$, i.e.,

$$\inf_P U(f; P) = \sup_P L(f, P)$$

Then f is said to be Riemann-integrable

Every continuous function defined on a closed and bounded interval of the real line is Riemann-integrable

We have

$$\lim_{n \rightarrow \infty} L(f; P_n) = \int_a^b f(x) dx = \lim_{n \rightarrow \infty} U(f; P_n)$$

where $P_0, P_1, \dots, P_n, \dots$ are a sequence of partitions such that the length of the largest subinterval in P_n converges to 0 as $n \rightarrow \infty$

We can construct nested (refined) partitions

Computation

- 1.) need a procedure to evaluate $f(x)$
- 2.) determine a partition (how many subintervals) of the interval $[a,b]$
- 3.) compute m_i and M_i on each subinterval
- 4.) compute the sums $L(f; P)$ and $U(f; P)$
- 5.) an approximate value is obtained

$$\int_a^b f(x) dx \approx \frac{1}{2}[U(f; P) + L(f; P)]$$

- 6.) the error of this approximation is bounded by

$$\frac{1}{2}[U(f; P) - L(f; P)]$$

Trapezoid Rule

A strategy that is better than estimating both the upper and the lower bounds of the area beneath the curve is to use trapezoids

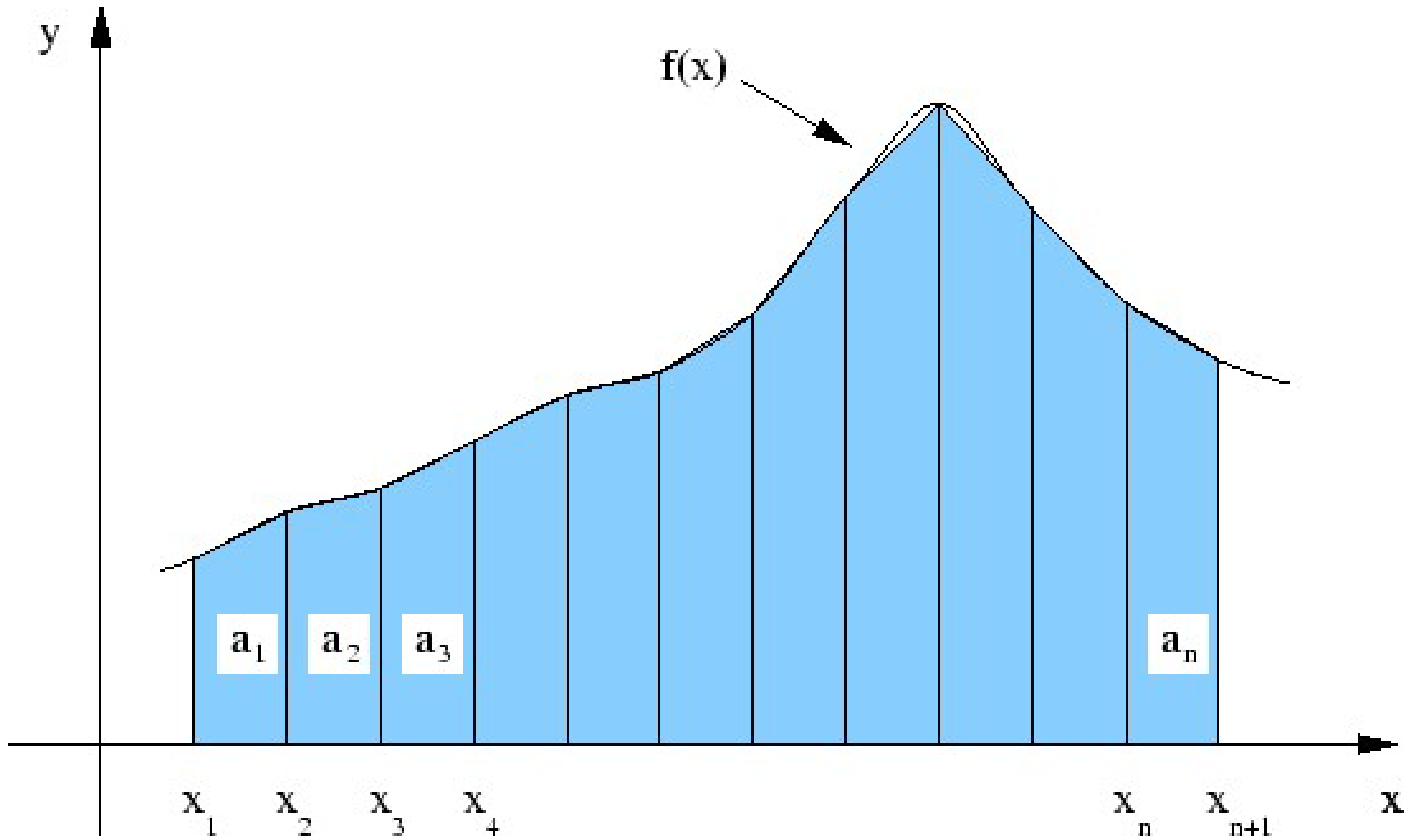
The interval $[a, b]$ is first divided into subintervals $[x_i, x_{i+1}]$, $0 \leq i \leq n - 1$. A typical trapezoid has the subinterval $[x_i, x_{i+1}]$ as its base, and the two vertical sides are $f(x_i)$ and $f(x_{i+1})$. The area is given by the base times the average height. The basic trapezoid rule for the subinterval $[x_i, x_{i+1}]$ is

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

The total area under the curve is

$$\begin{aligned} \int_a^b f(x) dx &\approx T(f; P) = \sum_{i=0}^{n-1} A_i \\ &= \frac{1}{2} \sum_{i=0}^{n-1} (x_{i+1} - x_i) [f(x_i) + f(x_{i+1})] \end{aligned}$$

Trapezoid Rule



Uniform Spacing

The lengths of the subintervals in a partition can be different. For fast computation, a uniform partition of the interval may be advantageous

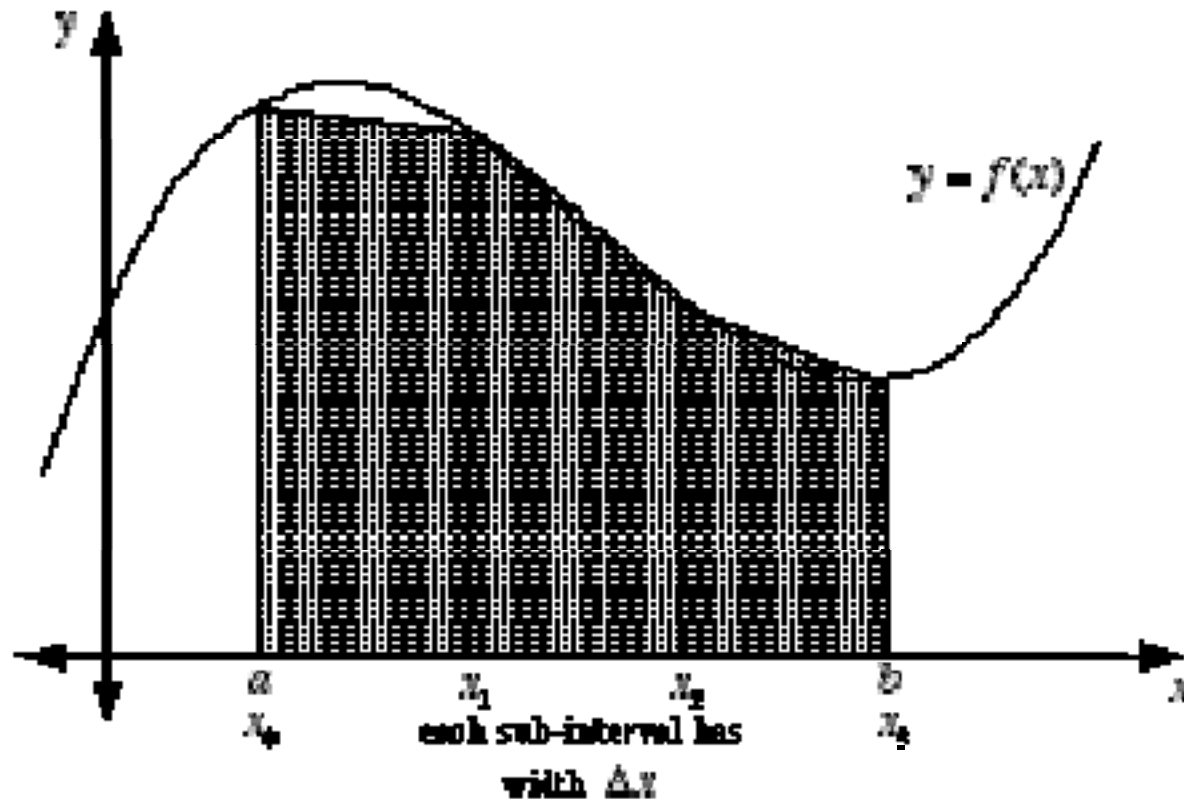
Let n be the number of subintervals, then $h = (b - a)/n$ is the uniform interval spacing. The nodal points are $x_i = a + i h, i = 0, 1, \dots, n$. Hence the composite trapezoid rule is

$$T(f; P) = \frac{h}{2} \sum_{i=0}^{n-1} [f(x_i) + f(x_{i+1})]$$

Note that the end point of an interval is the starting point of the next interval. This fact can save almost half of the computation,

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

Trapezoid Rule with Uniform Spacing



The area of the trapezoids (shaded) approximately equals the area bounded by $y = f(x)$.

$$\int_a^b f(x) dx \approx \frac{\Delta x}{2} [f(x_0) + 2f(x_1) + 2f(x_2) + f(x_3)].$$

Error Analysis (1)

If $f''(x)$ exists and is continuous on $[a,b]$, the error of the composite trapezoid rule T is

$$\int_a^b f(x) dx - T = -\frac{b-a}{12} h^2 f''(\xi) = O(h^2)$$

For some ξ in (a,b)

Proof. We first prove the result for $a=0$, $b=1$ and $h=1$. That is

$$\int_0^1 f(x) dx - \frac{1}{2} [f(0) + f(1)] = -\frac{1}{12} f''(\xi)$$

This simplified formula will be proved with the help of polynomial interpolation

Define a polynomial of degree that interpolates f at 0 and 1

$$p(x) = f(0) + [f(1) - f(0)]x$$

Error Analysis (2)

It follows that

$$\begin{aligned}\int_0^1 p(x) dx &= f(0) + \frac{1}{2}[f(1) - f(0)] \\ &= \frac{1}{2}[f(0) + f(1)]\end{aligned}$$

Using the error formula for the polynomial interpolation, we have

$$f(x) - p(x) = \frac{1}{12} f'''[\xi(x)]x(x-1)$$

Integrate it on both sides,

$$\int_0^1 f(x) dx - \int_0^1 p(x) dx = \frac{1}{2} \int_0^1 f'''[\xi(x)]x(x-1) dx$$

Error Analysis (3)

Using the Mean-Value Theorem for Integrals

$$\begin{aligned}\int_0^1 f''[\xi(x)]x(x-1) dx &= f''[\xi(s)]\int_0^1 x(x-1)dx \\ &= -\frac{1}{6}f''(\zeta)\end{aligned}$$

So we have

$$\int_0^1 f(x)dx - \frac{1}{2}[f(0) + f(1)] = -\frac{1}{12}f''(\zeta)$$

We then do a change of variable, and let

$$g(t) = f[a + t(b - a)], \quad x = a + (b - a)t$$

$$dx = (b - a)dt, \quad g'(t) = f'[a + t(b - a)](b - a)$$

$$g''(t) = f''[a + t(b - a)](b - a)^2$$

Error Analysis (4)

Then using the result for the special case,

$$\begin{aligned}\int_a^b f(x) dx &= (b-a) \int_0^1 f[a+t(b-a)] dt \\ &= (b-a) \int_0^1 g(t) dt \\ &= (b-a) \left\{ \frac{1}{2} [g(0) + g(1)] - \frac{1}{12} g''(\zeta) \right\} \\ &= \frac{b-a}{2} [f(a) + f(b)] - \frac{(b-a)^3}{12} f''(\xi)\end{aligned}$$

This is the error formula for the trapezoid rule with only one subinterval.

Let $[a, b]$ be divided into n equal subintervals by points

$$x_0, x_1, \dots, x_n, \text{ with subinterval } [x_i, x_{i+1}]$$

Error Analysis (5)

Let h be the interval length

$$\int_{x_i}^{x_{i+1}} f(x) dx = \frac{h}{2} [f(x_i) + f(x_{i+1})] - \frac{1}{12} h^3 f''(\xi)$$

Sum over all subintervals to get the composite trapezoid rule

$$\int_a^b f(x) dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x) dx = \frac{h}{2} \sum_{i=0}^{n-1} [f(x_i) + f(x_{i+1})] - \frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i)$$

Note that $h=(b-a)/n$, we use Intermediate-Value Theorem of Continuous Functions,

$$-\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\xi_i) = -\frac{b-a}{12} h^2 \left[\frac{1}{n} \sum_{i=0}^{n-1} f''(\xi_i) \right] = -\frac{b-a}{12} h^2 f''(\zeta)$$

Example 1

Show that

$$\int_a^{a+h} f(x) dx = \frac{h}{2} [f(a) + f(a+h)] - \frac{h^3}{12} f''(a) + \dots$$

Need to define

$$F(t) = \int_a^t f(x) dx$$

We can expand $F(a+h)$ using Taylor series

$$F(a+h) = F(a) + hF'(a) + \frac{h^2}{2} F''(a) + \frac{h^3}{3!} F'''(a) + \dots$$

Then by the Fundamental Theorem of Calculus, we have $F'(t) = f(t)$.

Note that $F(a) = 0$, $F''(t) = f'(t)$, $F'''(t) = f''(t)$, and so on.

Example 2

We have

$$(1) \quad \int_a^{a+h} f(x) dx = hf(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{3!} f''(a) + \dots$$

We can also apply the Taylor series directly on $f(t)$ as

$$(2) \quad f(a+h) = f(a) + hf'(a) + \frac{h^2}{2} f''(a) + \frac{h^3}{3!} f'''(a) + \dots$$

Adding $f(a)$ on both sides of (2) and multiplying by $h/2$, we obtain

$$(3) \quad \frac{h}{2}[f(a) + f(a+h)] = hf(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{4} f''(a) + \dots$$

Subtracting (3) from (1), we finally get

$$\int_a^{a+h} f(x) dx - \frac{h}{2}[f(a) + f(a+h)] = -\frac{1}{12} h^3 f''(a) + \dots$$

Estimate Grid Spacing

Example. If the composite trapezoid rule is used to compute

$$\int_0^1 e^{-x^2} dx$$

with an error of at most 0.5×10^{-4} , what is the uniform grid spacing h ?

From the graph of the second derivative (a decreasing function)

$$f''(x) = (4x^2 - 2)e^{-x^2}$$

We find that

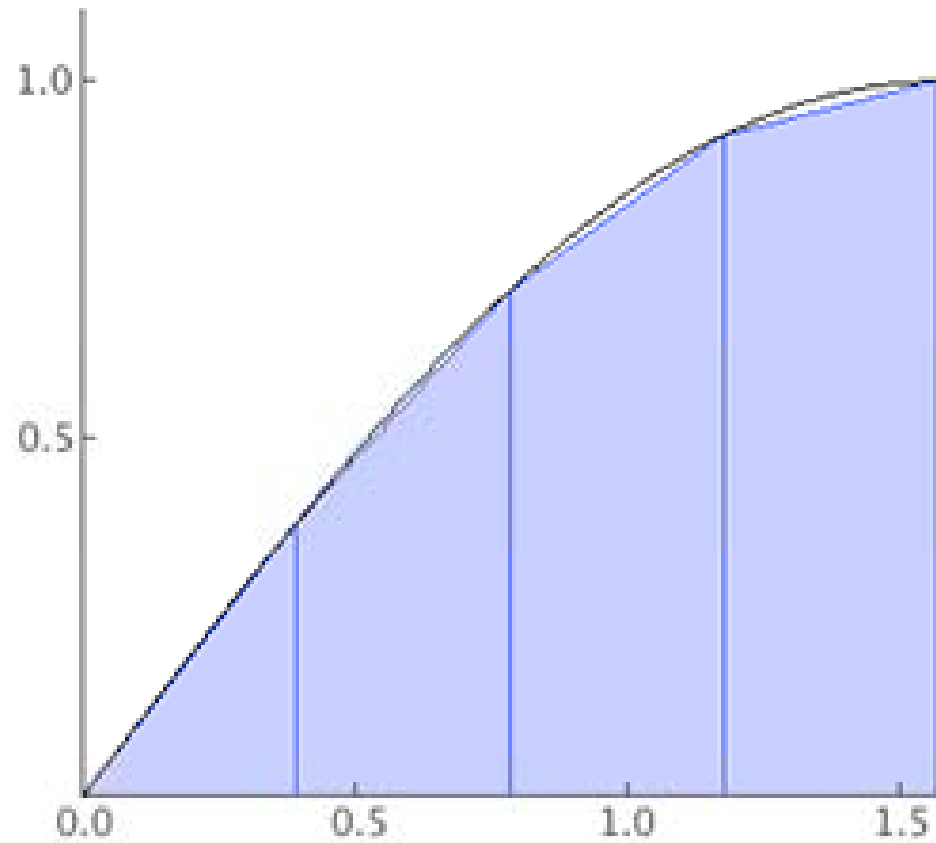
$$|f''(x)| \leq |f''(0)| = 2$$

We need

$$\left| -\frac{b-a}{12} h^2 f''(\xi) \right| \leq \frac{1}{6} h^2 < 0.5 \times 10^{-4}$$

It follows that $h \leq 0.01732$. The number of subintervals is $n \geq [1/h] = 58$

Recursive Trapezoid Idea



What we can do if the initial partition of interval is not fine enough?

Recursive Trapezoid Formula

Given a parameter n , dividing $[a,b]$ into 2^n equally spaced subintervals, we have

$$\begin{aligned} T(f; P) &= h \sum_{i=1}^{n-1} f(x_i) + \frac{h}{2} [f(x_0) + f(x_n)] \\ &= h \sum_{i=1}^{n-1} f(a + i h) + \frac{h}{2} [f(a) + f(b)] \end{aligned}$$

Note that $n = 2^n$ and $h = (b - a)/2^n$

$$R(n,0) = h \sum_{i=1}^{2^n-1} f(a + i h) + \frac{h}{2} [f(a) + f(b)]$$

Notice that $R(n,0)$ can be viewed as dividing each subinterval of $R(n-1,0)$ into two equal sub-subintervals. If we already computed $R(n-1,0)$, how can we compute $R(n,0)$ cheaply?

Recursive Formula

If $R(n-1,0)$ is available, $R(n,0)$ can be computed as

$$R(n,0) = \frac{1}{2}R(n-1,0) + h \sum_{k=1}^{2^n-1} f[a + (2k-1)h]$$

For $n \geq 1$ using $h = (b-a)/2^n$. Initial starting value is

$$R(0,0) = \frac{1}{2}(b-a)[f(a) - f(b)]$$

The trick is to only sum the function values at every other grid points

Proof. Note that

$$R(n,0) = h \sum_{i=1}^{2^n-1} f(a + i h) + C$$

With $C = h[f(a) + f(b)]/2$ and

$$R(n-1,0) = 2h \sum_{j=1}^{2^{n-1}-1} f(a + 2j h) + 2C$$

Recursive Formula

Hence, we have

$$\begin{aligned} R(n,0) - \frac{1}{2}R(n-1,0) &= h \sum_{i=1}^{2^n-1} f(a+ih) - h \sum_{j=1}^{2^{n-1}-1} f(a+2jh) \\ &= h \sum_{k=1}^{2^{n-1}} f[a+(2k-1)h] \end{aligned}$$

Each term in the first sum that corresponds to an even value of l is cancelled by a term in the second term. The final result has only the odd values of l

We can use the recursive trapezoid formula to compute a sequence of approximations to a definite integral using the trapezoid rule, without recomputing the values at points that have already been computed in the previous step

Two Dimensional Integration

For one dimensional numerical integration on $[0,1]$, using uniform space

$$h = 1/n \quad \int_0^1 f(x) dx \approx \frac{1}{2h} [f(0) + 2 \sum_{i=1}^{n-1} f\left(\frac{i}{n}\right) + f(1)]$$
$$= \sum_{i=0}^n A_i f\left(\frac{i}{n}\right)$$

For two dimensional integration on a unit square

$$\int_0^1 \int_0^1 f(x, y) dx dy \approx \int_0^1 \sum_{i=1}^n A_i f\left(\frac{i}{n}, y\right) dy$$
$$= \sum_{i=0}^n A_i \int_0^1 f\left(\frac{i}{n}, y\right) dy$$
$$\approx \sum_{i=0}^n A_i \sum_{j=0}^n A_j f\left(\frac{i}{n}, \frac{j}{n}\right)$$
$$= \sum_{i=0}^n \sum_{j=0}^n A_i A_j f\left(\frac{i}{n}, \frac{j}{n}\right)$$

Romberg Algorithm

Recursive composite trapezoid method

$$R(0,0) = \frac{1}{2}(b-a)[f(a) + f(b)]$$

For $h = 1/2^n$ and $n \geq 1$

$$R(n,0) = \frac{1}{2}R(n-1,0) + h \sum_{k=1}^{2^n-1} f[a + (2k-1)h]$$

Using Richardson extrapolation, we can have

$$R(i, j) = R(i, j-1) + \frac{1}{4^{j-1}}[R(i, j-1) - R(i-1, j-1)]$$

For $i \geq j$ and $j \geq 1$. This is the Romberg algorithm, which may yield better approximate values for larger j

$$\begin{array}{cccc} R(0, 0) & & & \\ R(1, 0) & R(1, 1) & & \\ R(2, 0) & R(2, 1) & R(2, 2) & \\ R(3, 0) & R(3, 1) & R(3, 2) & R(3, 3) \end{array}$$

Deriving Romberg Algorithm

Composite trapezoid rule on 2^{n-1} subintervals

$$\int_a^b f(x) dx = R(n-1,0) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots$$

With $h = (b-a)/2^{n-1}$ and the coefficients a_i depend on f but not on h

After one refinement and replacing $n-1$ with n and h with $h/2$, we have

$$\int_a^b f(x) dx = R(n,0) + \frac{1}{4} a_2 h^2 + \frac{1}{16} a_4 h^4 + \frac{1}{64} a_6 h^6 + \dots$$

Subtracting the 1st equation from 4 times the 2nd equation

$$\int_a^b f(x) dx = R(n,1) - \frac{1}{4} a_4 h^4 - \frac{5}{15} a_6 h^6 + \dots$$

where for $n \geq 1$

$$R(n,1) = R(n,0) + \frac{1}{3} [R(n,0) - R(n-1,0)]$$

More Romberg Algorithm

We could apply the extrapolation idea repeatedly to get

$$\int_a^b f(x) dx = R(n,2) + \frac{1}{4^3} a_6 h^6 + \frac{21}{4^5} a_8 h^8 + \dots$$

Where

$$R(n,2) = R(n,1) + \frac{1}{15} [R(n,1) - R(n-1,1)]$$

This time, the truncation error is of sixth order

A few steps of extrapolation may generate very accurate approximations

Too many extrapolations may make the computation tedious

General Extrapolation

Extrapolation processes can be applied in more general cases where the error term can be represented as

$$E = a h^\alpha + b h^\beta + c h^\gamma + \dots$$

With $0 < \alpha < \beta < \gamma$, we show how the first term of the error expansion is annihilated. Let

$$L = \phi(h) + a h^\alpha + b h^\beta + c h^\gamma + \dots \quad (1)$$

Replacing h by $h/2$ yields

$$L = \phi\left(\frac{h}{2}\right) + a \left(\frac{h}{2}\right)^\alpha + b \left(\frac{h}{2}\right)^\beta + c \left(\frac{h}{2}\right)^\gamma + \dots \quad (2)$$

Multiplying (2) by 2^α

$$2^\alpha L = 2^\alpha \phi\left(\frac{h}{2}\right) + a h^\alpha + 2^\alpha b \left(\frac{h}{2}\right)^\beta + 2^\alpha c \left(\frac{h}{2}\right)^\gamma + \dots \quad (3)$$

General Extrapolation – Cont.

Subtracting the previous two equations, we can remove the h^α term

$$(2^\alpha - 1)L = 2^\alpha \phi\left(\frac{h}{2}\right) - \phi(h) \\ + (2^{\alpha-\beta} - 1)b h^\beta + (2^{\alpha-\gamma} - 1)c h^\gamma + \dots$$

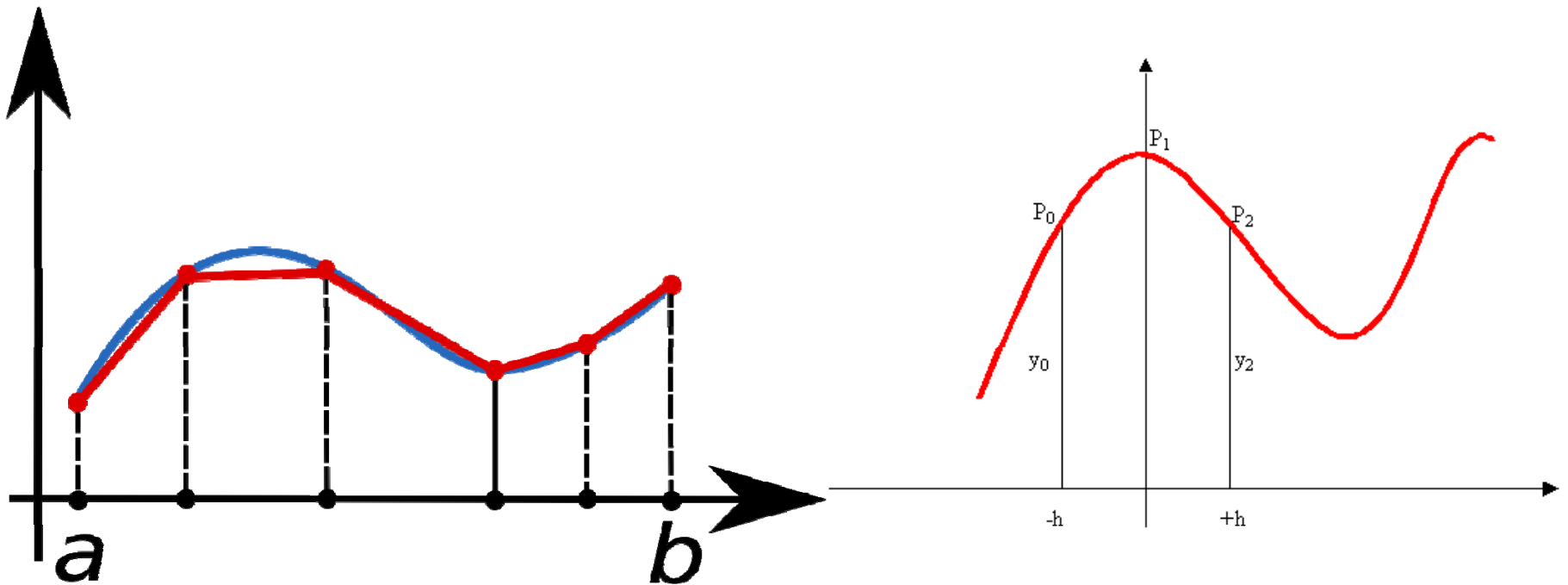
We can write the new approximation formula as

$$L = \frac{2^\alpha}{2^\alpha - 1} \phi\left(\frac{h}{2}\right) - \frac{1}{2^\alpha - 1} \phi(h) + b h^\beta + c h^\gamma + \dots$$

This approximation formula raises the order of truncation error from $O(h^\alpha)$ to $O(h^\beta)$ with $\alpha < \beta$

Please read the book on p. 217 for a concrete example to show how the approximation accuracy is improved using extrapolation

Basic Simpson's Rule



Simple trapezoid rule uses two points for approximations
Can we get more accurate approximation using more points?

Basic Simpson's Rule

A three point numerical integration rule using the middle point of the interval is known as the Simpson's rule with different weights for each point

$$\int_a^{a+2h} f(x) dx \approx \frac{h}{3} [f(a) + 4f(a+h) + f(a+2h)]$$

Using Taylor's expansion, we can find the error term of this approximation is

$$-\frac{h^5}{90} f^{(4)}(\xi)$$

For some point ξ in $(a, a+2h)$. This should be compared to the error term of the simple trapezoid rule $O(h^3)$

It is desirable to subdivide the interval adaptively so that refinement is only placed at the area of large fluctuation of function value

Basic Simpson's Rule

Using Taylor series for $f(x)$ at a , we have

$$f(a+h) = f(a) + hf'(a) + \frac{1}{2!}h^2 f''(a) + \frac{1}{3!}h^3 f'''(a) + \frac{1}{4!}h^4 f^{(4)}(a) + \dots$$

If we replace the interval size h by $2h$, we obtain

$$f(a+2h) = f(a) + 2hf'(a) + 2h^2 f''(a) + \frac{4}{3}h^3 f'''(a) + \frac{2^4}{4!}h^4 f^{(4)}(a) + \dots$$

By combining these two expansions, we get

$$f(a) + 4f(a+h) + f(a+2h) = 6f(a) + 6hf'(a) + 4h^2 f''(a) + 2h^3 f'''(a) + \frac{20}{4!}h^4 f^{(4)}(a) + \dots$$

Basic Simpson's Rule

On the other hand, define

$$F(x) = \int_a^x f(t) dt$$

We expand $F(a+2h)$ as

$$F(a+2h) = F(a) + 2hF'(a) + 2h^2F''(a) + \frac{4}{3}h^3F'''(a) + \frac{2}{3}h^4f^{(4)}(a) + \frac{2^5}{5!}h^5F^{(5)}(a) + \dots$$

Note that $F' = f$, $F(a) = 0$, $F'' = f'$, $F''' = f''$, we have

$$\int_a^{a+2h} f(x) dx = 2hf(a) + 2h^2f'(a) + \frac{4}{3}h^3f''(a) + \frac{2}{3}h^4f'''(a) + \frac{2^5}{5 \cdot 4!}h^5f^{(4)}(a) + \dots$$

From the previous page, we have

$$\begin{aligned} \frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] &= 2hf(a) + 2h^2f'(a) + \frac{4}{3}h^3f''(a) \\ &+ \frac{2}{3}h^4f'''(a) + \frac{20}{3 \cdot 4!}h^5f^{(4)}(a) + \dots \end{aligned}$$

Basic Simpson's Rule (1)

Subtracting the previous two terms, we have

$$\int_a^{a+2h} f(x)dx = \frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] - \frac{h^5}{90}f^{(4)} - \dots$$

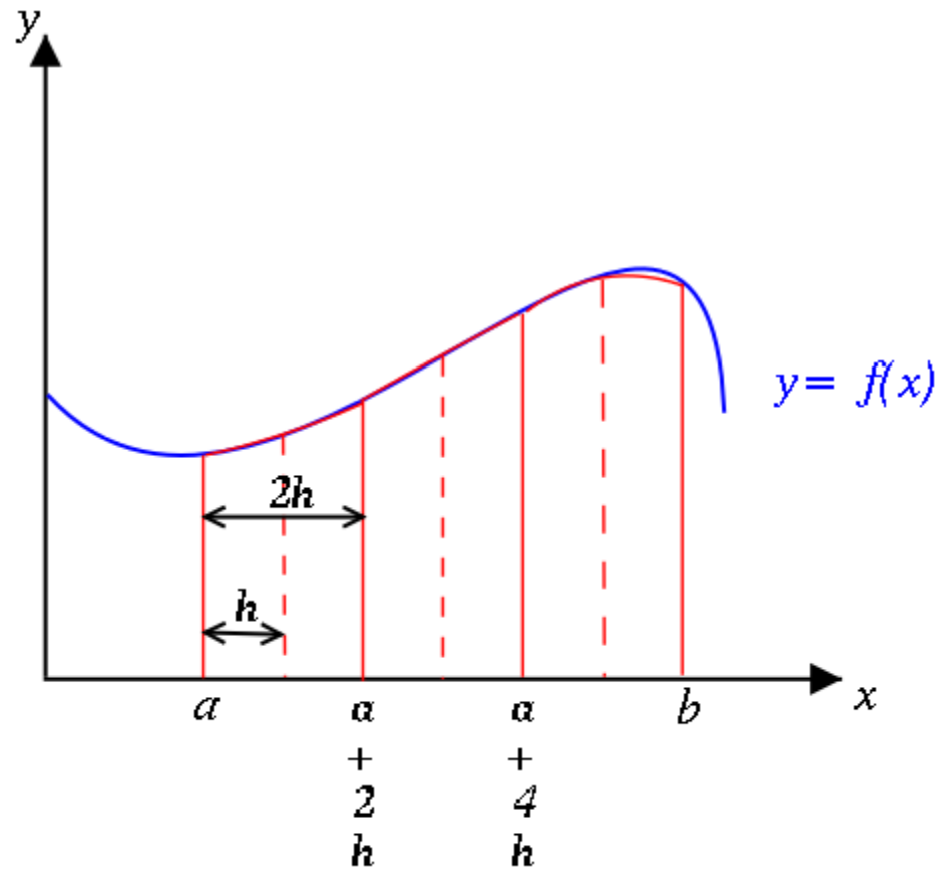
We have the Simpson's rule as

$$\int_a^{a+2h} f(x)dx \approx \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

The error term of the Simpson's rule is

$$-\frac{1}{90} \left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi)$$

Adaptive Simpson's Algorithm



Reduce the size of the intervals to get more accurate approximations

Adaptive Simpson's Algorithm

Given an interval $[a,b]$, we can use the basic Simpson's rule to compute an approximation to the integral as

$$I \equiv \int_a^b f(x) dx = S(a,b) + E(a,b)$$

Where the approximation part is

$$S(a,b) = \frac{(b-a)}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

And the error term is

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

For simplicity, we assume $f^{(4)}(x)$ remains constant on (a,b) . Let $h = b - a$, we have

$$I = S^{(1)} + E^{(1)}$$

For the first step approximation with

$$S^{(1)} = S(a,b)$$

Adaptive Simpson – (II)

And

$$E^{(1)} = -\frac{1}{90} \left(\frac{h}{2} \right)^5 f^{(4)}$$

We then subdivide the interval $[a,b]$ and apply the basic Simpson's rule on the subintervals $[a,c]$ and $[c,b]$ respectively. We have a new approximation on $[a,b]$ as the sum of two separate approximations

$$I = S^{(2)} + E^{(2)}$$

where $c = (a + b)/2$ with

$$S^{(2)} = S(a,c) + S(c,b)$$

And

$$E^{(2)} = -\frac{1}{90} \left(\frac{h/2}{2} \right)^5 f^{(4)} - \frac{1}{90} \left(\frac{h/2}{2} \right)^5 f^{(4)} = \frac{1}{16} E^{(1)}$$

This is certainly a better approximation since the subintervals are smaller than the original interval

Adaptive Simpson – (III)

Subtracting the two approximations yields

$$S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 15E^{(2)}$$

Hence the numerical integration can be

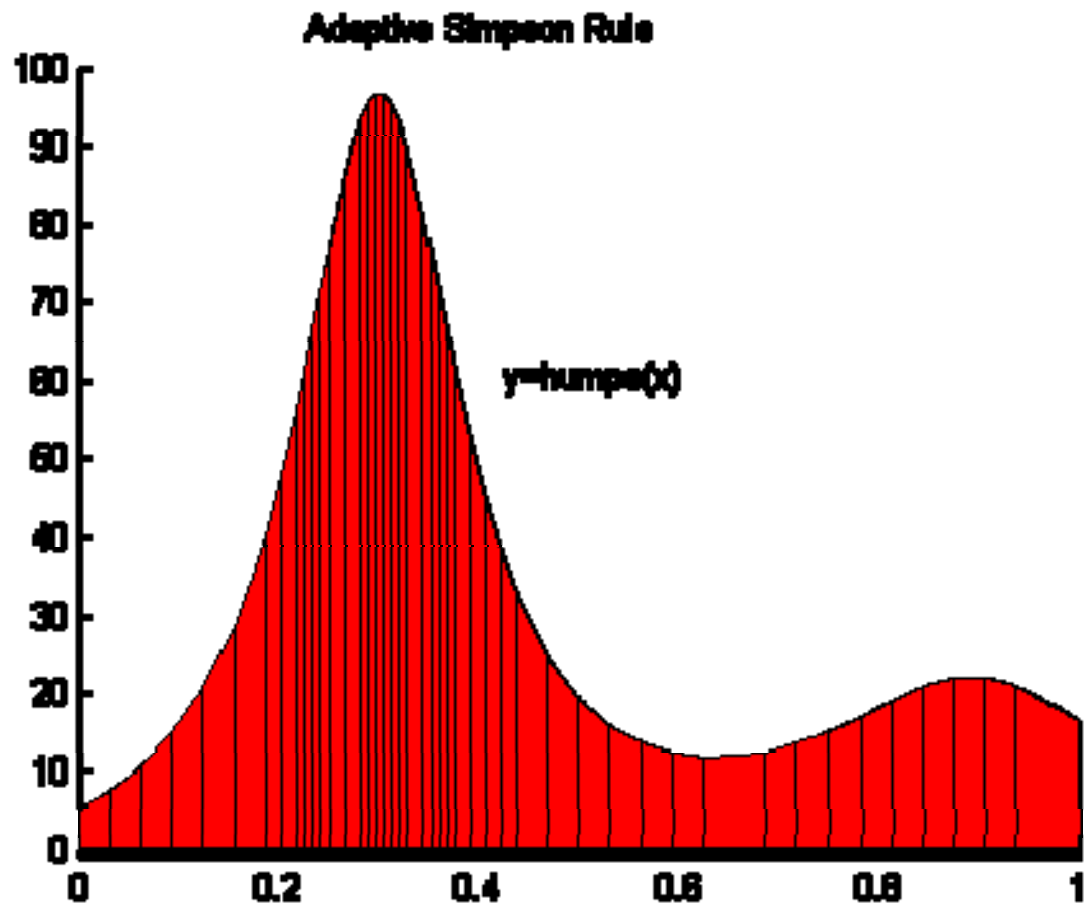
$$I = S^{(2)} + E^{(2)} = S^{(2)} + \frac{1}{15}(S^{(2)} - S^{(1)})$$

The error term is then computable and can be used for building the adaptive process

$$\frac{1}{15} |S^{(2)} - S^{(1)}| < \varepsilon$$

If this test shows that the error is larger than ε , the interval $[a,b]$ is split into two subintervals $[a,c]$ and $[c,b]$ with $c = (a + b)/2$. The previously described procedure is replaced by $\varepsilon/2$ to make sure that the error sum is smaller than ε

Adaptive Simpson's Algorithm



Refine the intervals at the places where the function changes quickly

Adaptive Simpson – (IV)

Numerical integration on subintervals

$$I = \int_a^b f(x) dx = \int_a^c f(x) dx + \int_b^c f(x) dx = I_L + I_R$$

Let S be the sum of $S_L^{(2)}$ on $[a,c]$ and $S_R^{(2)}$ on $[c,b]$, we have

$$\begin{aligned} |I - S| &= \left| I_L + I_R - S_L^{(2)} - S_R^{(2)} \right| \\ &\leq \left| I_L - S_L^{(2)} \right| + \left| I_R - S_R^{(2)} \right| \\ &= \frac{1}{15} \left| S_L^{(2)} - S_L^{(1)} \right| + \frac{1}{15} \left| S_R^{(2)} - S_R^{(1)} \right| \end{aligned}$$

If we want to have

$$|I - S| \leq \varepsilon$$

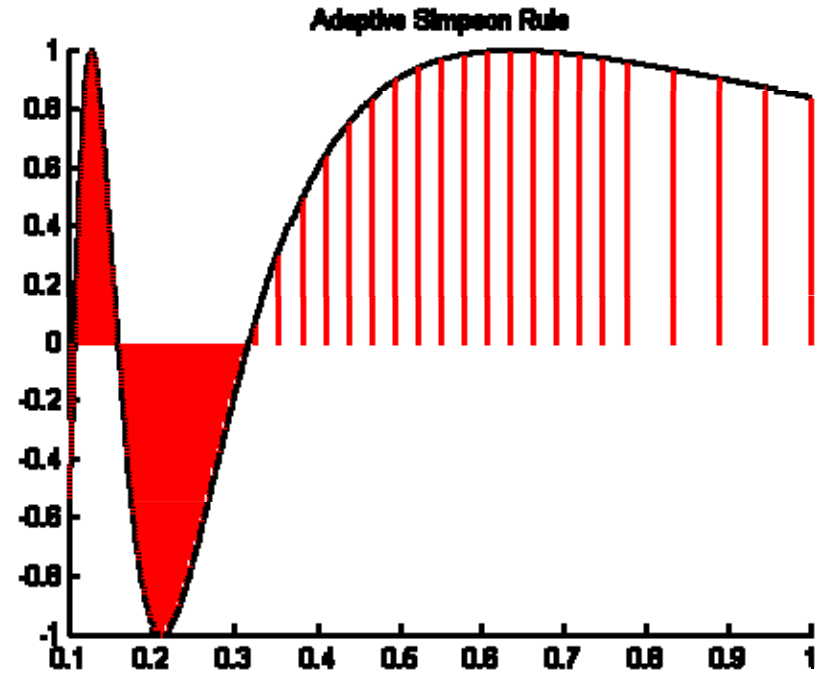
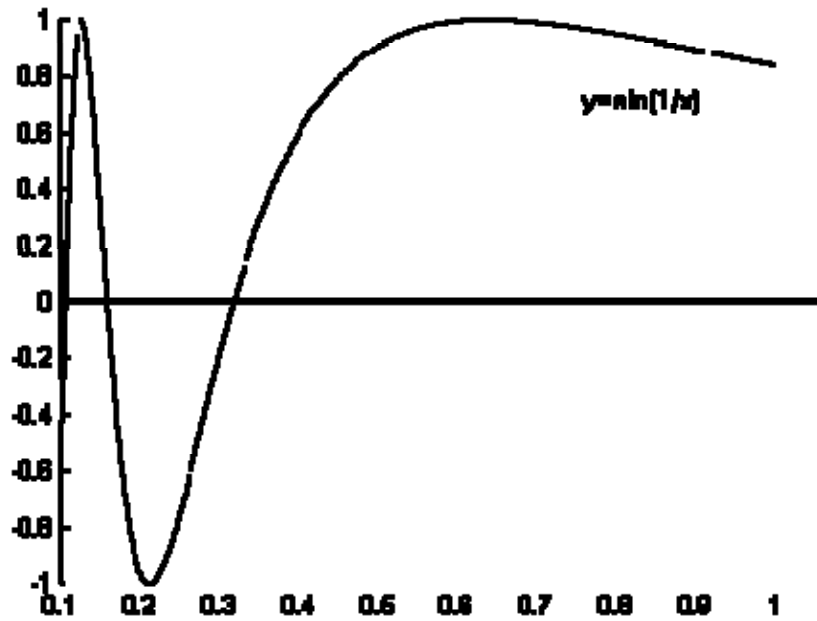
It is more than enough to have

$$\frac{1}{15} \left| S_L^{(2)} - S_L^{(1)} \right| \leq \frac{\varepsilon}{2}$$

and

$$\frac{1}{15} \left| S_R^{(2)} - S_R^{(1)} \right| \leq \frac{\varepsilon}{2}$$

Adaptive Simpson's Algorithm



One decision to make is to choose where to refine the interval

Computational Procedure

The interval $[a,b]$ is divided into four subintervals of equal length. Two Simpson approximations are computed using two double-width subintervals and four single-width subintervals

$$S_1 = \frac{h}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

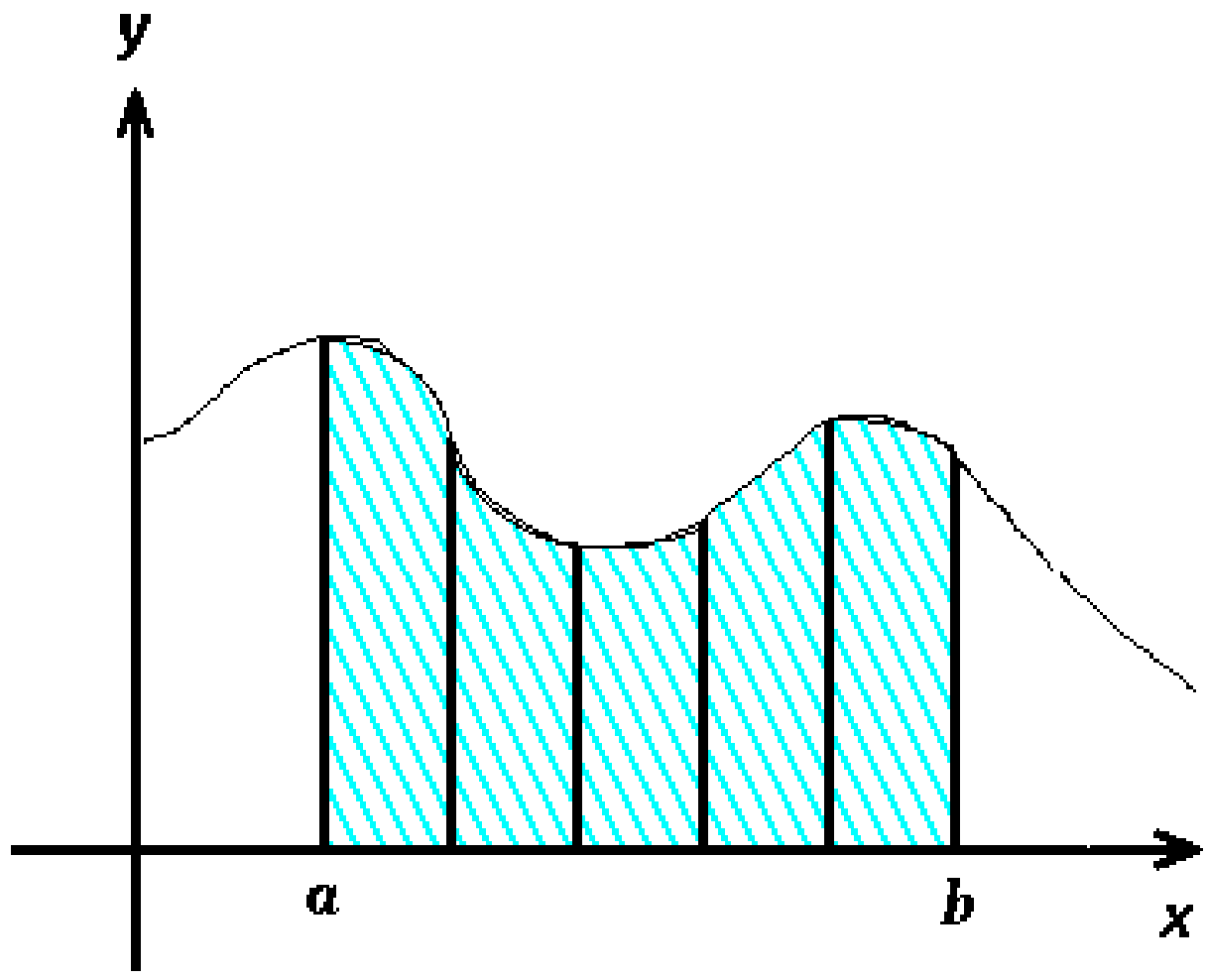
$$S_2 = \frac{h}{12} \left[f(a) + 4f\left(\frac{a+c}{2}\right) + 2f(c) + 4f\left(\frac{c+b}{2}\right) + f(b) \right]$$

If $|S_2 - S_1| \leq \varepsilon$, we have done, and set

$$S = \frac{1}{15} [16S_2 - S_1]$$

Otherwise the interval $[a,b]$ is divided in half and the recursive procedure is applied on the two subintervals $[a,c]$ and $[c,b]$, until either the error tolerance is satisfied or the maximum number of subdivisions is reached

Adaptive Simpson's Algorithm



Which sub-interval or both to divide for refinement

Gaussian Quadrature Formulas

A general numerical integration formula is

$$\int_a^b f(x) dx \approx A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n)$$

It suffices to know the nodes x_0, x_1, \dots, x_n and the weights A_0, A_1, \dots, A_n . For important special functions, they are listed in some reference books

Suppose a set of nodes is given, how to find the weights. This can be done using Lagrange interpolation polynomial as

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

With

$$l_i(x) = \prod_{j=0, j \neq i}^n \left(\frac{x - x_j}{x_i - x_j} \right)$$

If p is a good approximate to f , we anticipate $\int_a^b p(x) dx$ is a good approximate to $\int_a^b f(x) dx$

Gaussian Quadrature

We integrate over $p(x)$ as

$$\begin{aligned}\int_a^b f(x) dx &\approx \int_a^b p(x) dx \\ &= \sum_{i=0}^n f(x_i) \int_a^b l_i(x) dx = \sum_{i=1}^n A_i f(x_i)\end{aligned}$$

Where we can compute

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

Note that the polynomial interpolation is exact for a polynomial of degree at most n . It follows that the integration will be exact for such polynomials

If the nodes can be chosen carefully, it is possible to increase the order of polynomial with the exact integration remarkably. This was discussed by Karl Gauss

An Example

Determine a quadrature formula when the interval is $[-2,2]$ and the nodes are $-1, 0,$ and 1 .

We first need to compute the cardinal functions

$$l_0(x) = \prod_{j=1}^2 \left(\frac{x - x_j}{x_0 - x_j} \right) = \left(\frac{x - 0}{(-1) - 0} \right) \left(\frac{x - 1}{-1 - 1} \right) = \frac{1}{2} x(x - 1)$$

$$l_1(x) = \prod_{j=1}^2 \left(\frac{x - x_j}{x_1 - x_j} \right) = \left(\frac{x + 1}{0 - (-1)} \right) \left(\frac{x - 1}{0 - 1} \right) = 1 - x^2$$

$$l_2(x) = \prod_{j=1}^2 \left(\frac{x - x_j}{x_2 - x_j} \right) = \left(\frac{x - (-1)}{1 - (-1)} \right) \left(\frac{x - 0}{1 - 0} \right) = \frac{1}{2} x(x + 1)$$

The weights are computed by integrating these functions

$$A_0 = \int_{-2}^2 l_0(x) dx = \frac{1}{2} \int_{-2}^2 x(x - 1) dx = \frac{1}{2} \left[\frac{1}{3} x^3 - \frac{1}{2} x^2 \right]_{-2}^2 = \frac{8}{3}$$

An Example

Similarly, we have

$$A_1 = \int_{-2}^2 l_1(x) dx = \int_{-2}^2 (1 - x^2) dx = \left[x - \frac{1}{3} x^3 \right]_{-2}^2 = -\frac{4}{3}$$

$$A_2 = \int_{-2}^2 l_2(x) dx = \frac{1}{2} \int_{-2}^2 x(x+1) dx = \frac{1}{2} \left[\frac{1}{3} x^3 + \frac{1}{2} x^2 \right]_{-2}^2 = \frac{8}{3}$$

So the quadrature formula defined on the interval $[-2, 2]$ and using the node $-1, 0, 1$, is

$$\int_{-2}^2 f(x) dx \approx \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)$$

It can be verified that this formula gives exact values for the three functions

$$f(x) = 1, x, x^2$$

Gaussian Quadrature Theorem

Let q be a nontrivial polynomial of degree $n + 1$ such that

$$\int_a^b x^k q(x) dx = 0 \quad (0 \leq k \leq n)$$

Let x_0, x_1, \dots, x_n be zeroes of q . Then the formula

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

With these x_i 's as nodes, the approximation will be exact for all polynomials of degree at most $2n+1$. All these nodes lie in the open interval (a,b)

We can first figure out the quadrature for

$$\int_{-1}^1 f(t) dt \approx \sum_{i=0}^n A_i f(t_i)$$

Then use the transformation $t = [2x - (b - a)] / (b - a)$ for a Gaussian quadrature on the general interval $[a,b]$

Gaussian Theorem Proof

The transformed integral is

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

Proof of Gaussian Quadrature Theorem:

Let f be any polynomial of degree at most $(2n + 1)$. Dividing f by q with quotient p and a remainder r

$$f = p q + r$$

Both q and r are of degree at most n

By hypothesis, we have

$$\int_a^b q(x)p(x) dx = 0$$

Since x_i are roots of q , we have

$$f(x_i) = p(x_i)q(x_i) + r(x_i) = r(x_i)$$

Gaussian Theorem Proof (II)

Since the degree of r is at most n , the integration $\int_a^b r(x) dx$ is exact

$$\begin{aligned}\int_a^b f(x) dx &= \int_a^b p(x)q(x) dx + \int_a^b r(x) dx \\ &= \int_a^b r(x) dx = \sum_{i=0}^n A_i r(x_i) = \sum_{i=0}^n A_i f(x_i)\end{aligned}$$

Gaussian Quadrature Theorem guarantees high accuracy numerical integration with few nodes. However, finding these nodes is not an easy task. The roots of Legendre polynomials are the nodes for Gaussian quadrature on the interval $[-1,1]$. With $q_0(x) = 1$, $q_1(x) = x$, we have for $n \geq 2$

$$q_n(x) = \left(\frac{2n-1}{n}\right)xq_{n-1}(x) - \left(\frac{n-1}{n}\right)q_{n-2}(x)$$