3 Approximating a function using a polynomial

3.1 McLaurin series

Assume that $f(x)$ is a continuous function of x, then

$$f(x) = \sum_{i=0}^{\infty} a_i x^i = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} x^i$$

is known as the McLaurin Series, where a_i's are the coefficients in the polynomial expansion given by

$$a_i = \frac{f^{(i)}(x)}{i!}\Big|_{x=0}$$

and $f^{(i)}(x)$ is the i-th derivative of $f(x)$.

The McLaurin series is used to predict the value $f(x_1)$ (for any $x = x_1$) using the function's value $f(0)$ at the "reference point" ($x = 0$). The series is approximated by summing up to a suitably high value of i, which can lead to approximation or truncation errors.

Problem: When function $f(x)$ varies significantly over the interval from $x = 0$ to $x = x_1$, the approximation may not work well.

A better solution is to move the reference point closer to x_1, at which the function's polynomial expansion is needed. Then, $f(x_1)$ can be represented in terms of $f(x_r)$, $f^{(1)}(x_r)$, etc.

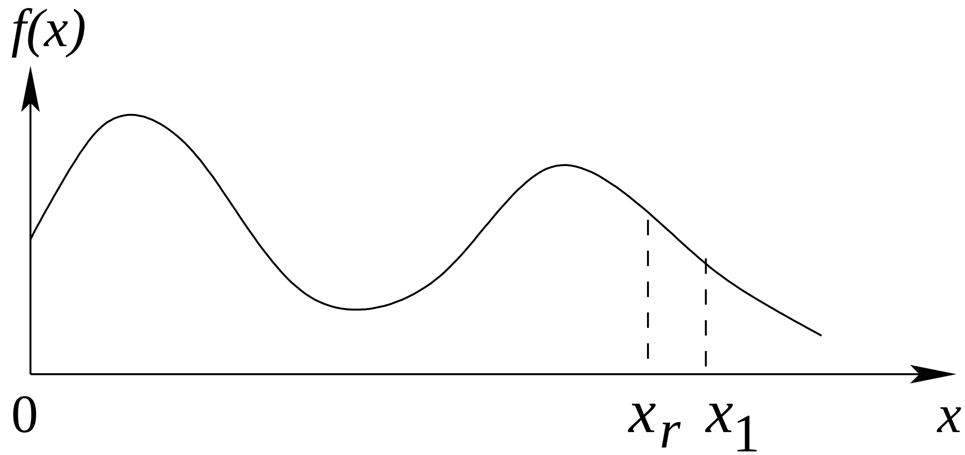


Figure 18: Taylor series

3.2 Taylor series

Assume that $f(x)$ is a continuous function of x, then

$$f(x) = \sum_{i=0}^{\infty} a_i (x - x_r)^i$$

where $a_i = \frac{f^{(i)}(x)}{i!}|_{x=x_r}$. Define $h = x - x_r$. Then,

$$f(x) = \sum_{i=0}^{\infty} a_i h^i = \sum_{i=0}^{\infty} \frac{f^{(i)}(x_r)}{i!} h^i$$

which is known as the Taylor Series.

If x_r is sufficiently close to x, we can approximate $f(x)$ with a small number of coefficients since $(x - x_r)^i \to 0$ as i increases.

Question: What is the error when approximating function $f(x)$ at x by $f(x) = \sum_{i=0}^{n} a_i h^i$, where n is a finite number (the order of the Taylor series)?

Taylor theorem:

A function $f(x)$ can be represented exactly as

$$f(x) = \sum_{i=0}^{n} \frac{f^{(i)}(x_r)}{i!} h^i + R_n$$

where R_n is the remainder (error) term, and can be calculated as

$$R_n = \frac{f^{(n+1)}(\alpha)}{(n+1)!} h^{n+1}$$

and α is an unknown value between x_r and x.

- Although α is unknown, Taylor's theorem tells us that the error R_n is proportional to h^{n+1}, which is denoted by
$$R_n = O(h^{n+1})$$
which reads "R_n is order h to the power of $n+1$".

- With n-th order Taylor series approximation, the error is proportional to step size h to the power $n+1$. Or equivalently, the truncation error goes to zero no slower than h^{n+1} does.

- With $h \ll 1$, an algorithm or numerical method with $O(h^2)$ is better than one with $O(h)$. If you half the step size h, the error is quartered in the former but is only halved in the latter.

Question: How to find R_n?

$$\begin{aligned} R_n &= \sum_{i=0}^{\infty} a_i h^i - \sum_{i=0}^{n} a_i h^i \\ &= \sum_{i=n+1}^{\infty} a_i h^i = \sum_{i=n+1}^{\infty} \frac{f^{(i)}(x_r)}{i!} h^i \end{aligned}$$

For small h ($h \ll 1$),

$$R_n \approx \frac{f^{(n+1)}(x_r)}{(n+1)!} h^{n+1}$$

The above expression can be used to evaluate the dominant error terms in the n-th order approximation.

For different values of n (the order of the Taylor series), a different trajectory is fitted (or approximated) to the function. For example:

- $n = 0$ (zero order approximation) $\rightarrow$ straight line with zero slope
- $n = 1$ (first order approximation) $\rightarrow$ straight line with some slope
- $n = 2$ (second order approximation) $\rightarrow$ quadratic function

Example 1: Expand $f(x) = e^x$ as a McLaurin series.

Solution:

$$\begin{aligned} a_0 &= f(0) = e^0 = 1, \\ a_1 &= \frac{f'(x)}{1!}\Big|_{x=0} = \frac{e^0}{1} = 1 \\ a_i &= \frac{f^{(i)}(x)}{i!}\Big|_{x=0} = \frac{e^0}{i!} = \frac{1}{i!} \end{aligned}$$

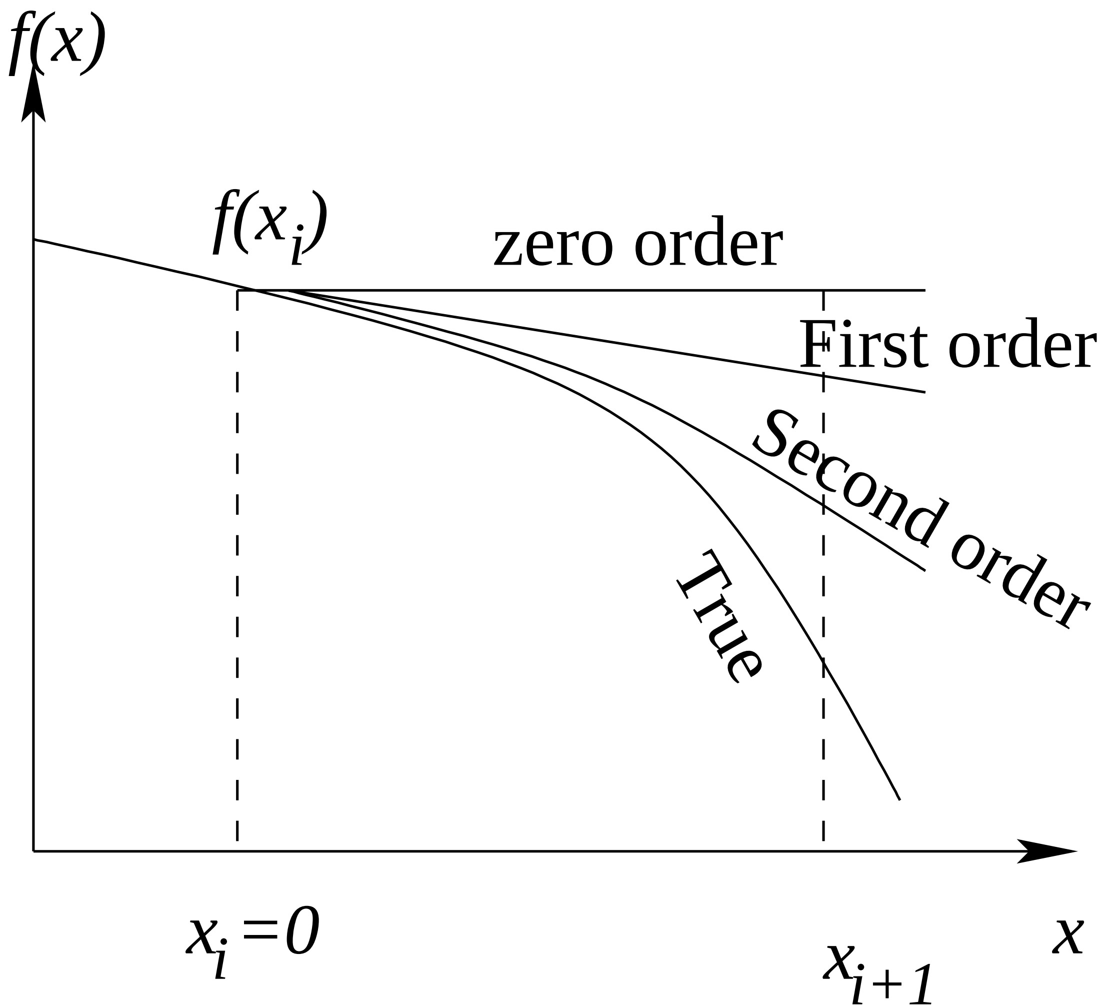


Figure 19: Taylor series

Then $f(x) = e^x = \sum_{i=0}^{\infty} \frac{x^i}{i!}$.

Example 2: Find the McLaurin series up to order 4, Taylor series (around $x = 1$) up to order 4 of function $f(x) = x^3 - 2x^2 + 0.25x + 0.75$.

Solution:

$$\begin{array}{lll} f(x) = x^3 - 2x^2 + 0.25x + 0.75 & f(0) = 0.75 & f(1) = 0 \\ f'(x) = 3x^2 - 4x + 0.25 & f'(0) = 0.25 & f'(1) = -0.75 \\ f''(x) = 6x - 4 & f''(0) = -4 & f''(1) = 2 \\ f^{(3)}(x) = 6 & f^{(3)}(0) = 6 & f^{(3)}(1) = 6 \\ f^{(4)}(x) = 0 & f^{(4)}(0) = 0 & f^{(4)}(1) = 0 \end{array}$$

The McLaurin series of $f(x) = x^3 - 2x^2 + 0.25x + 0.75$ can be written as

$$f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} x^i = \sum_{i=0}^{3} \frac{f^{(i)}(0)}{i!} x^i$$

Then the third order McLaurin series expansion is

$$\begin{aligned} f_{M3}(x) &= f(0) + f'(0)x + \frac{1}{2} f''(0)x^2 + \frac{1}{3!} f^{(3)}(0)x^3 \\ &= 0.75 + 0.25x - 2x^2 + x^3 \end{aligned}$$

which is the same as the original polynomial function.

The lower order McLaurin series expansion may be written as

$$\begin{aligned}
f_{M2}(x) &= f(0) + \frac{1}{2} f^{''}(0) x^2 \\
&= 0.75 + 0.25x - 2x^2 \\
f_{M1}(x) &= 0.75 + 0.25x \\
f_{M0}(x) &= 0.75
\end{aligned}$$

The Taylor series can be written as

$$f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(x_r)}{i!}(x - x_r)^i = \sum_{i=0}^{3} \frac{f^{(i)}(1)}{i!}(x-1)^i$$

Then the third order Taylor series of $f(x)$ is

$$\begin{aligned}
f_{T3}(x) &= f(1) + f^{'}(1)(x-1) + \frac{1}{2} f^{''}(1)(x-1)^2 + \frac{1}{3!} f^{(3)}(1)(x-1)^3 \\
&= 0.75 + 0.25x - 2x^2 + x^3
\end{aligned}$$

which is the same as the original function.

The lower order Taylor series expansion may be written as

$$\begin{aligned}
f_{T2}(x) &= f(1) + \frac{1}{2} f^{''}(1)(x-1)^2 \\
&= -0.75(x-1) + (x-1)^2 \\
&= 1.75 - 2.75x + x^2 \\
f_{T1}(x) &= f(1) + f^{'}(x-1) \\
&= -0.75(x-1) = 0.75 - 0.75x \\
f_{T0}(x) &= f(1) = 0
\end{aligned}$$

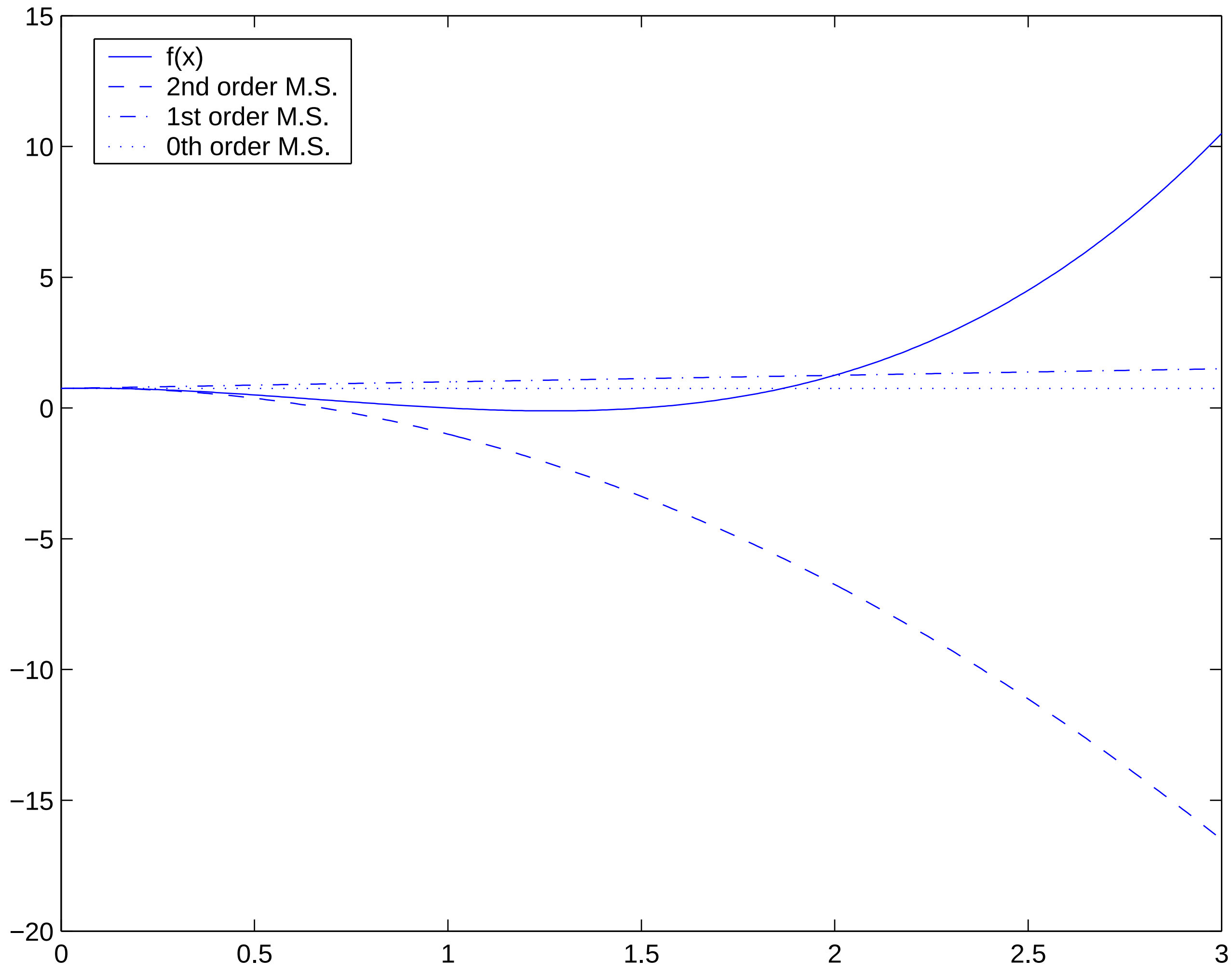


Figure 20: Example 1

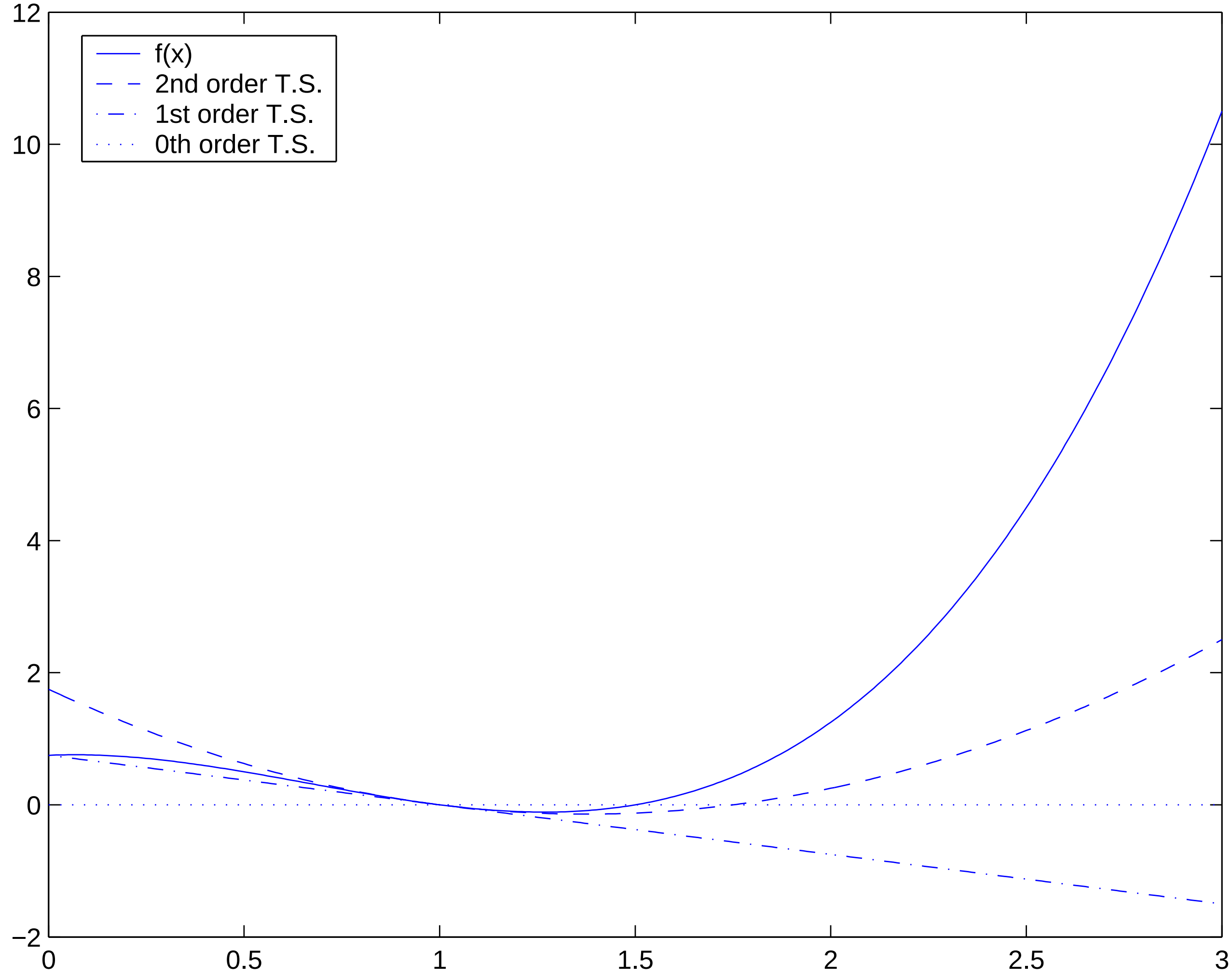


Figure 21: Example 2

Chapter 5: Numerical Integration and Differentiation

PART I: Numerical Integration

Newton-Cotes Integration Formulas

The idea of Newton-Cotes formulas is to replace a complicated function or tabulated data with an approximating function that is easy to integrate.

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

where $f_n(x) = a_0 + a_1x + a_2x^2 + \ldots + a_nx^n$.

1 The Trapezoidal Rule

Using the first order Taylor series to approximate $f(x)$,

$$I = \int_a^b f(x)dx \approx \int_a^b f_1(x)dx$$

where

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

Then

$$\begin{aligned} I &\approx \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx \\ &= (b - a)\frac{f(b) + f(a)}{2} \end{aligned}$$

The trapezoidal rule is equivalent to approximating the area of the trapezoidal

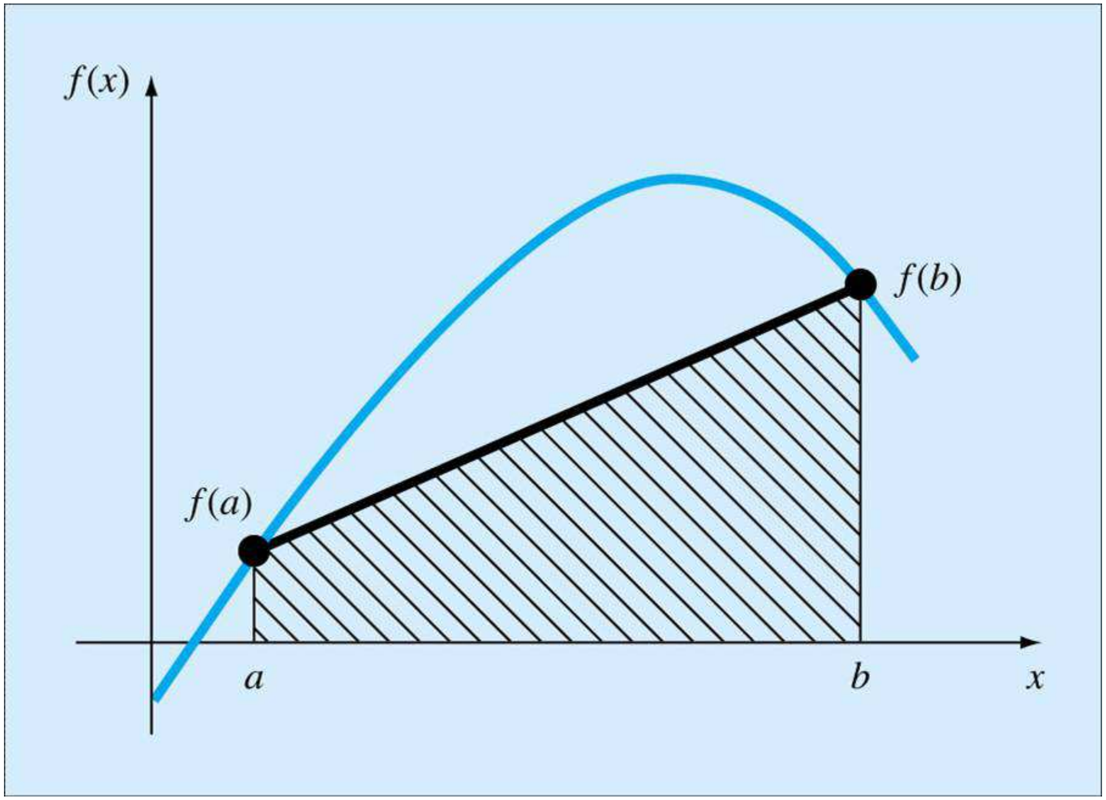


Figure 1: Graphical depiction of the trapezoidal rule

under the straight line connecting $f(a)$ and $f(b)$. An estimate for the local truncation error of a single application of the trapezoidal rule can be obtained using Taylor series as

$$E_t = -\frac{1}{12} f^{''}(\xi)(b-a)^3$$

where ξ is a value between a and b.

Example: Use the trapezoidal rule to numerically integrate

$$f(x) = 0.2 + 25x$$

from $a = 0$ to $b = 2$.

Solution: $f(a) = f(0) = 0.2$, and $f(b) = f(2) = 50.2$.

$$I = (b-a)\frac{f(b)+f(a)}{2} = (2-0) \times \frac{0.2+50.2}{2} = 50.4$$

The true solution is

$$\int_0^2 f(x)dx = (0.2x + 12.5x^2)|_0^2 = (0.2 \times 2 + 12.5 \times 2^2) - 0 = 50.4$$

Because $f(x)$ is a linear function, using the trapezoidal rule gets the exact solution.

Example: Use the trapezoidal rule to numerically integrate

$$f(x) = 0.2 + 25x + 3x^2$$

from $a = 0$ to $b = 2$.

Solution: $f(0) = 0.2$, and $f(2) = 62.2$.

$$I = (b-a)\frac{f(b)+f(a)}{2} = (2-0) \times \frac{0.2+62.2}{2} = 62.4$$

The true solution is

$$\int_0^2 f(x)dx = (0.2x + 12.5x^2 + x^3)|_0^2 = (0.2 \times 2 + 12.5 \times 2^2 + 2^3) - 0 = 58.4$$

The relative error is

$$|\epsilon_t| = \left|\frac{58.4 - 62.4}{58.4}\right| \times 100\% = 6.85\%$$

Multiple-application trapezoidal rule:

Using smaller integration interval can reduce the approximation error. We can divide the integration interval from a to b into a number of segments and apply the trapezoidal rule to each segment. Divide (a, b) into n segments of equal width. Then

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \ldots + \int_{x_{n-1}}^{x_n} f(x)dx$$

where $a = x_0 < x_1 < \ldots < x_n = b$, and $x_i - x_{i-1} = h = \frac{b-a}{n}$, for $i = 1, 2, \ldots, n$. Substituting the Trapezoidal rule for each integral yields

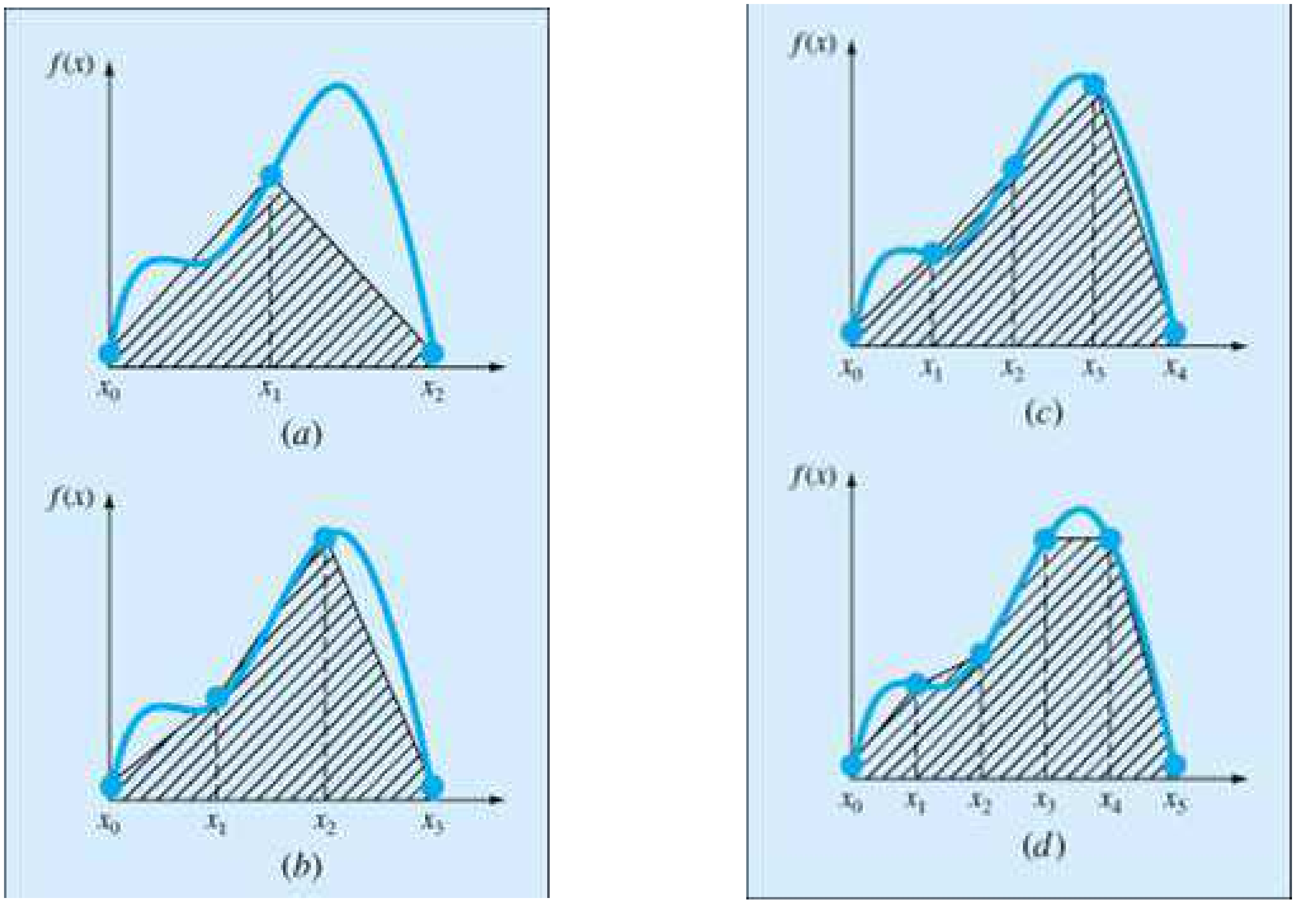
$$\begin{aligned} I &\approx h\frac{f(x_0) + f(x_1)}{2} + h\frac{f(x_1) + f(x_2)}{2} + \ldots + h\frac{f(x_{n-1}) + f(x_n)}{2} \\ &= \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right] \\ &= (b-a)\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n} \end{aligned}$$

The approximation error using the multiple trapezoidal rule is a sum of the individual errors, i.e.,

$$E_t = -\sum_{i=1}^{n} \frac{h^3}{12} f''(\xi_i) = -\sum_{i=1}^{n} \frac{(b-a)^3}{12n^3} f''(\xi_i)$$

Let $\overline{f''} = \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$. Then the approximate error is

$$E_t = -\frac{(b-a)^3}{12n^2}\overline{f''}$$



Example: Use the 2-segment trapezoidal rule to numerically integrate

$$f(x) = 0.2 + 25x + 3x^2$$

from $a = 0$ to $b = 2$.

Solution: $n = 2$, $h = (a - b)/n = (2 - 0)/2 = 1$.
$f(0) = 0.2$, $f(1) = 28.2$, and $f(2) = 62.2$.

$$I = (b - a)\frac{f(0) + 2f(1) + f(2)}{2n} = 2 \times \frac{0.2 + 2 \times 28.2 + 62.2}{4} = 59.4$$

The relative error is

$$|\epsilon_t| = \left|\frac{58.4 - 59.4}{58.4}\right| \times 100\% = 1.71\%$$

2 Simpson's Rules

Aside from using the trapezoidal rule with finer segmentation, another way to improve the estimation accuracy is to use higher order polynomials.

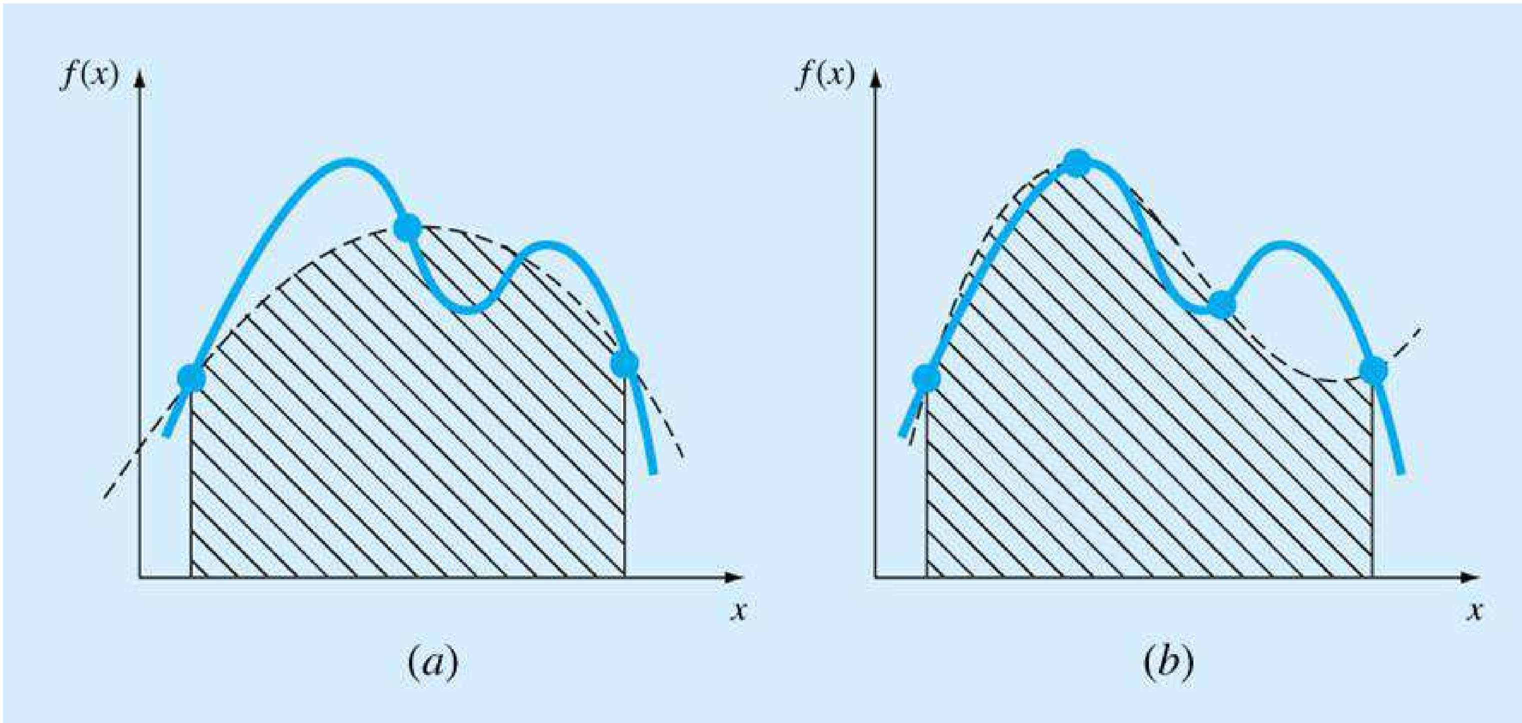


Figure 2: Illustration of (a) Simpson's 1/3 rule, and (b) Simpson's 3/8 rule

<u>Simpson's $1/3$ rule:</u>

Given function values at 3 points as $(x_0, f(x_0))$, $(x_1, f(x_1))$, and $(x_2, f(x_2))$, we can estimate $f(x)$ using Lagrange polynomial interpolation. Then

$$\begin{aligned} I &= \int_a^b f(x)dx \approx \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) \right. \\ &\left. + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx \end{aligned}$$

When $a = x_0$, $b = x_2$, $(a+b)/2 = x_1$, and $h = (b-a)/2$,

$$I \approx \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] = (b-a)\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$$

It can be proved that single segment application of Simpson's $1/3$ rule has a truncation error of

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi)$$

where ξ is between a and b.

Simpson's $1/3$ rule yields exact results for third order polynomials even though it is derived from parabola.

Example: Use Simpson's $1/3$ rule to integrate

$$f(x) = 0.2 + 25x + 3x^2 + 8x^3$$

from $a = 0$ to $b = 2$.

Solution: $f(0) = 0.2$, $f(1) = 36.2$, and $f(2) = 126.2$.

$$I = (b-a)\frac{f(0) + 4f(1) + f(2)}{6} = 2 \times \frac{0.2 + 4 \times 36.2 + 126.2}{6} = 90.4$$

The exact integral is

$$\int_0^2 f(x)dx = (0.2x{+}12.5x^2{+}x^3{+}2x^4)|_0^2 = (0.2{\times}2{+}12.5{\times}2^2{+}2^3{+}2{\times}2^4){-}0 = 90.4$$

Example: Use Simpson's $1/3$ rule to integrate

$$f(x) = 0.2 + 25x + 3x^2 + 2x^4$$

from $a = 0$ to $b = 2$.

Solution: $f(0) = 0.2$, $f(1) = 30.2$, and $f(2) = 94.2$.

$$I = (b-a)\frac{f(0) + 4f(1) + f(2)}{6} = 2 \times \frac{0.2 + 4 \times 30.2 + 94.2}{6} = 71.73$$

The exact integral is

$$\int_0^2 f(x)dx = (0.2x{+}12.5x^2{+}x^3{+}0.4x^5)|_0^2 = (0.2{\times}2{+}12.5{\times}2^2{+}2^3{+}0.4{\times}2^5){-}0 = 71.2$$

The relative error is

$$|\epsilon_t| = \left|\frac{71.2 - 71.73}{71.2}\right| = 0.7\%$$

Multiple-application Simpson's $1/3$ rule

Dividing the integration interval into n segments of equal width, we have

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots + \int_{x_{n-2}}^{x_n} f(x)dx$$

where $a = x_0 < x_1 < \ldots < x_n = b$, and $x_i - x_{i-1} = h = (b-a)/n$, for $i = 1, 2, \ldots, n$. Substituting the Simpson's $1/3$ rule for each integral yields

$$\begin{aligned} I &\approx 2h\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} \\ &\quad + \cdots + 2h\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6} \\ &= (b-a)\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n} \end{aligned}$$

Note that n has to be even.

Example: Use 4-segment Simpson's $1/3$ rule to integrate

$$f(x) = 0.2 + 25x + 3x^2 + 2x^4$$

from $a = 0$ to $b = 2$.

Solution: $n = 4$, $h = (b-a)/n = 0.5$.

$f(x_0) = f(0) = 0.2$, $f(x_1) = f(0.5) = 13.575$, $f(x_2) = f(1) = 30.2$, $f(x_3) =$

$f(1.5) = 54.575$, and $f(x_4) = f(2) = 94.2$.

$$\begin{aligned} I &= (b-a)\frac{f(0)+4f(0.5)+4f(1.5)+2f(1)+f(2)}{3\times 4} \\ &= 2\times\frac{0.2+4\times 13.575+4\times 54.575+2\times 30.2+94.2}{12} = 71.2333 \end{aligned}$$

The exact integral is

$$\int_0^2 f(x)dx = (0.2x+12.5x^2+x^3+0.4x^5)|_0^2 = (0.2\times 2+12.5\times 2^2+2^3+0.4\times 2^5)-0 = 71.2$$

The relative error is

$$|\epsilon_t| = \left|\frac{71.2-71.2333}{71.2}\right| = 0.047\%$$

Simpson's $3/8$ rule

This is to use a third-order Lagrange polynomial to fit to four points of $f(x)$ and yields

$$I \approx \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right]$$

where $h = (b-a)/3$. The approximation error using this rule is

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480}f^{(4)}(\xi)$$

where ξ is between a and b.

3 Integration of Equations

Newton-Cotes algorithms for equations

Compare the following two Pseudocodes for multiple applications of the trapezoidal rule.

Pseudocode 1: Algorithm for multiple applications of the trapezoidal rule

```
function Trapm(h,n,f)
  sum=f0
  for i=1:n-1
    sum=sum+2*fi
  end
  sum=sum+fn
  Trapm=h*sum/2
```

Pseudocode 2: Algorithm for multiple application of the trapezoidal rule when function $f(x)$ is available

```
 function TrapEq(n,a,b)
  h=(b-a)/n
  x=a
  sum=f(x)
  for i=1:n-1
```

```
    x=x+h
    sum=sum+2*f(x)
  end
  sum=sum+f(b)
  TraEq=(b-a)*sum/(2*n)
```

Pseudocode 1 can be used when only a limited number of points are given or the function is available. Pseudocode 2 is for the case where the analytical function is available. The difference between the two pseudocodes is that in Pseudocode 2 neigher the independent nor the dependent variable values are passed into the function via its argument as in Pseudocode 1. When the analytical function is available, the function values are computed using calls to the function being analyzed, $f(x)$.

4 Romberg Integration

Romberg integration is one technique that can improve the results of numerical integration using error-correction techniques.

Richardson's extrapolation uses two estimates of an integral to compute a third, more accurate approximation.

The estimate and error associated with a multiple-application trapezoidal rule can be represented as

$$I = I(h) + E(h)$$

where I is the exact value of the integral, $I(h)$ is the approximation from an n-segment application of the trapezoidal rule with step size $h = (b-a)/n$, and $E(h)$ is the truncation error. If we make two separate estimates using step sizes of h_1 and h_2 and have exact values for the error, then

$$I(h_1) + E(h_1) = I(h_2) + E(h_2) \tag{1}$$

The error of the multiple-application trapezoidal rule can be represented approximately as

$$E \approx -\frac{b-a}{12} h^2 \bar{f}''$$

where $h = (b-a)/n$. Assuming that $\bar{f}''$ is constant regardless of step size, we have

$$\frac{E(h_1)}{E(h_2)} \approx \frac{h_1^2}{h_2^2}$$

Then we have

$$E(h_1) \approx E(h_2) \left(\frac{h_1}{h_2}\right)^2$$

which can be substituted into (1):

$$I(h_1) + E(h_2) \left(\frac{h_1}{h_2}\right)^2 = I(h_2) + E(h_2)$$

Then $E(h_2)$ can be solved as

$$E(h_2) = \frac{I(h_2) - I(h_1)}{(h_1/h_2)^2 - 1}$$

This estimate can then be substituted into

$$I = I(h_2) + E(h_2)$$

to yield an improved estimate of the integral:

$$I \approx I(h_2) + \frac{I(h_2) - I(h_1)}{(h_1/h_2)^2 - 1}$$

It can be shown that the error of this estimate is $O(h^4)$. Thus, we have combined two trapezoidal rule estimates of $O(h^2)$ to yield a new estimate of $O(h^4)$. For the special case where the interval is $h_2 = h_1/2$, we have

$$I \approx I(h_2) + \frac{1}{2^2 - 1}[I(h_2) - I(h_1)] = \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1)$$

With two improved integrals of $O(h^4)$ on the basis of three trapezoidal rule estimates, we can combine them to yield an even better value with $O(h^6)$.

The Romberg integration algorithm has the general form as

$$I_{j,k} \approx \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

where $I_{j+1,k-1}$ and $I_{j,k-1}$ are the more and less accurate integrals, respectively, and $I_{j,k}$ is the improved integral. The index k signifies the level of the integration, where $k = 1$ corresponds to the original trapezoidal rule estimates, $k = 2$ corresponds to $O(h^4)$, $k = 3$ to $O(h^6)$, and so forth.

Example: $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$, find $\int_a^b f(x)dx$, $a = 0$, $b = 0.8$.

Solution:

True solution: $I = \int_0^{0.8} f(x)dx = \int_0^{0.8}(0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)dx = 1.640533$

$n_1 = 1$, $h_1 = 0.8$
$f(0) = 0.2$, $f(0.8) = 0.232$
$I_{1,1} = \int_0^{0.8} f_1(x)dx = 0.8 \times \frac{f(0)+f(0.8)}{2} = 0.1728$, $\epsilon_t = 89.5\%$

$n_2 = 2$, $h_2 = \frac{b-a}{2} = 0.4$, $(h_2 = h_1/2)$
$f(0) = 0.2$, $f(0.8) = 0.232$, $f(0.4) = 2.456$
$I_{2,1} = \int_0^{0.4} f_1(x)dx + \int_{0.4}^{0.8} f_1(x)dx = 0.4 \times \frac{f(0)+f(0.4)}{2} + 0.4 \times \frac{f(0.4)+f(0.8)}{2} = 1.0688$, $\epsilon_t = 34.9\%$

$n_3 = 4$, $h_3 = \frac{b-a}{4} = 0.2$, $(h_3 = h_2/2)$

$I_{3,1} = \frac{0.2}{2}[f(0) + 2f(0.2) + 2f(0.4) + 2f(0.6) + f(0.8)] = 1.4848$, $\epsilon_t = 9.5\%$

$I_{1,2} = \frac{4I_{2,1}-I_{1,1}}{4-1} = \frac{4}{3}I_{2,1} - \frac{1}{3}I_{1,1} = \frac{4}{3} \times 1.0688 - \frac{1}{3} \times 0.1728 = 1.367467$, $\epsilon_t = 16.6\%$

$I_{2,2} = \frac{4I_{3,1}-I_{2,1}}{4-1} = \frac{4}{3}I_{3,1} - \frac{1}{3}I_{2,1} = \frac{4}{3} \times 1.4848 - \frac{1}{3} \times 1.0688 = 1.623467$, $\epsilon_t = 1.0\%$

$I_{1,3} = \frac{4^2 I_{2,2}-I_{1,2}}{4^2-1} = \frac{16}{15}I_{2,2} - \frac{1}{15}I_{1,2} = \frac{16}{15} \times 1.623467 - \frac{1}{15} \times 1.367467 = 1.640533$,
$\epsilon_t = 0$

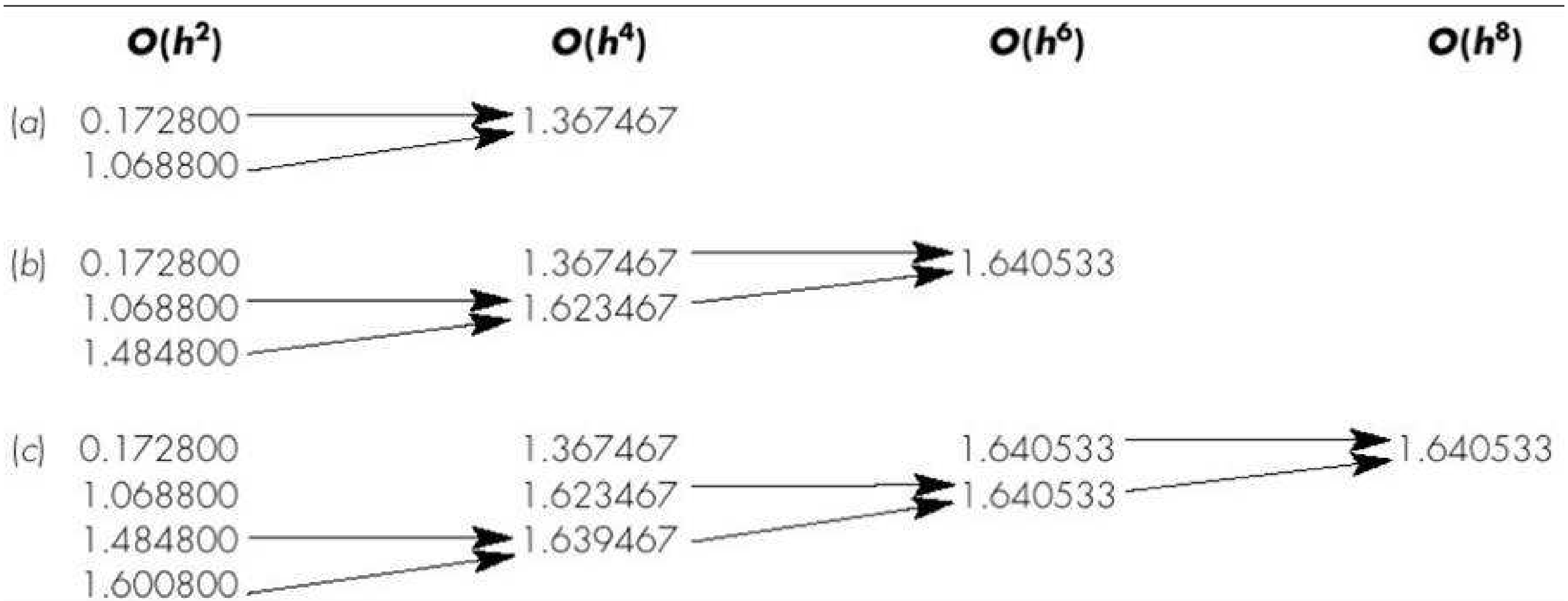


Figure 3: Example of Romberg integration

PART II: Numerical Differentiation

Finite Divided Difference

5 First Order Derivatives:

- The first forward finite divided difference

  Using Taylor series,

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + O(h^3)$$

  where $h = x_{i+1} - x_i$. Then $f'(x_i)$ can be found as

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

  The first forward finite divided difference is

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h}$$

- The first backward finite divided difference

  Using Taylor series,

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + O(h^3)$$

where $h = x_i - x_{i-1}$. Then $f^{'}(x_i)$ can be found as

$$f^{'}(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

and $f^{'}(x_i)$ can also be approximated as

$$f^{'}(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h}$$

which is called the first backward finite divided difference.

- The first centered finite divided difference

$$f(x_{i+1}) - f(x_{i-1}) = 2f^{'}(x_i)h + O(h^3)$$

and $f^{'}(x_i)$ can be found as

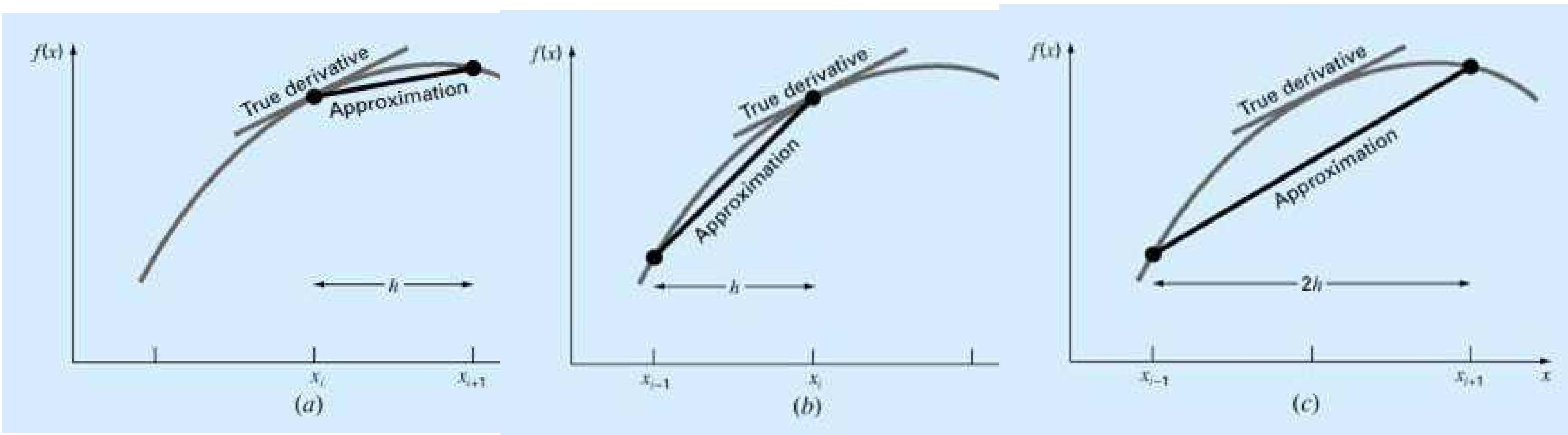
$$f^{'}(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - O(h^2)$$

and $f^{'}(x_i)$ can also be approximated as

$$f^{'}(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$$

which is called the first centered finite divided difference.

Notice that the truncation error is of the order of h^2 in contrast to the forward and backward approximations that are of the order of h. Therefore, the centered difference is a more accurate representation of the derivative.



Graphical depiction of (a) forward, (b) backward, and (c) centered finite-divided-difference approximations of the first derivative

Example: Estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$.

Solution:

The problem can be solved analytically

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$$

and $f'(0.5) = -0.9125$.

When $h = 0.5$, $x_{i-1} = x_i - h = 0$, and $f(x_{i-1}) = 1.2$; $x_i = 0.5$, $f(x_i) = 0.925$; $x_{i+1} = x_i + h = 1$, and $f(x_{i+1}) = 0.2$.

The forward divided difference:

$$f'(0.5) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{0.2 - 0.925}{0.5} = -1.45$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-1.45)}{-0.9125}\right| \times 100\% = 58.9\%$$

The backward divided difference:

$$f'(0.5) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{0.925 - 1.2}{0.5} = -0.55$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-0.55)}{-0.9125}\right| \times 100\% = 39.7\%$$

The centered divided difference:

$$f'(0.5) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{0.925 - 1.2}{2 \times 0.5} = -1.0$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-1.0)}{-0.9125}\right| \times 100\% = 9.6\%$$

When $h = 0.25$, $x_{i-1} = x_i - h = 0.25$, and $f(x_{i-1}) = 1.1035$; $x_i = 0.5$, $f(x_i) = 0.925$; $x_{i+1} = x_i + h = 0.75$, and $f(x_{i+1}) = 0.6363$.

The forward divided difference:

$$f^{'}(0.5) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{0.6363 - 0.925}{0.25} = -1.155$$

The percentage relative error:

$$|\epsilon_t| = \left| \frac{(-0.9125) - (-1.155)}{-0.9125} \right| \times 100\% = 26.5\%$$

The backward divided difference:

$$f^{'}(0.5) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{0.925 - 1.1035}{0.25} = -0.714$$

The percentage relative error:

$$|\epsilon_t| = \left| \frac{(-0.9125) - (-0.714)}{-0.9125} \right| \times 100\% = 21.7\%$$

The centered divided difference:

$$f^{'}(0.5) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{0.6363 - 1.1035}{2 \times 0.25} = -0.934$$

The percentage relative error:

$$|\epsilon_t| = \left| \frac{(-0.9125) - (-0.934)}{-0.9125} \right| \times 100\% = 2.4\%$$

Using centered finite divided difference and small step size achieves lower approximation error.

6 Higher Order Derivatives:

- The second forward finite divided difference

$$f(x_{i+2}) = f(x_i) + f^{'}(x_i)(2h) + \frac{f^{''}(x_i)}{2!}(2h)^2 + O(h^3) \tag{2}$$

$$f(x_{i+1}) = f(x_i) + f^{'}(x_i)h + \frac{f^{''}(x_i)}{2!}h^2 + O(h^3) \tag{3}$$

(2)-(3)$\times 2$:

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f^{''}(x_i)h^2 + O(h^3)$$

$f^{''}(x_i)$ can be found as

$$f^{''}(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

and $f^{''}(x_i)$ can be approximated as

$$f^{''}(x_i) \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$$

This is the second forward finite divided difference.

- The second backward finite divided difference

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + O(h)$$

and $f''(x_i)$ can be approximated as

$$f''(x_i) \approx \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$$

is the second backward finite divided difference.

- The second centered finite divided difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + O(h^4) \tag{4}$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f^{(3)}(x_i)}{3!}h^3 + O(h^4) \tag{5}$$

(4)+(5):

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)h^2 + O(h^4) \tag{6}$$

Then $f''(x_i)$ can be solved from (6) as

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2)$$

and

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$$

is the second centered finite divided difference.

7 High-Accuracy Numerical Differentiation

- The second forward finite divided difference

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \quad (7)$$

$$f''(x) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h) \quad (8)$$

Substitute (8) into (7),

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h} + O(h^2) \quad (9)$$

Then we have

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \quad (10)$$

- The second backward finite divided difference

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2) \quad (11)$$

- The second centered finite divided difference

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4) \quad (12)$$

Example: $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$, $x_i = 0.5$, $h = 0.25$.

$x_i = 0.5$, $x_{i-1} = x_i - h = 0.25$, $x_{i-2} = 0$, $x_{i+1} = x_i + h = 0.75$, $x_{i+2} = 1$.
$f(x_i) = 0.925$, $f(x_{i-1}) = 1.1035$, $f(x_{i-2}) = 1.2$, $f(x_{i+1}) = 0.6363$, and $f(x_{i+2}) = 0.2$.
Using the forward f.d.d., $f'(x_i) \doteq -1.155$, $\epsilon_t = -26.5\%$
Using the backward f.d.d., $f'(x_i) \doteq 0.714$, $\epsilon_t = 21.7\%$
Using the centered f.d.d., $f'(x_i) \doteq -0.934$, $\epsilon_t = -2.4\%$
Using the second forward f.d.d.,
$f'(x_i) = \frac{-f(x_{i+2})+4f(x_{i+1}-3f(x_i)}{2h} = \frac{-0.2+4\times0.6363-3\times0.925}{2\times0.25} = -0.8594$
$\epsilon_t = \left|\frac{-0.8594-(-0.9125)}{-0.9125}\right| \times 100\% = 5.82\%$

Using the second backward f.d.d., $f'(x_i) = \frac{3f(x_i)-4f(x_{i-1}+f(x_{i-2})}{2h} = -0.8781$, $\epsilon_t = 3.77\%$

Using the second centered f.d.d., $f^{'}(x_i) = \frac{-f(x_{i+2})+8f(x_{i+1}-8f(x_{i-1})+f(x_{i-2})}{12h} = -0.9125$, $\epsilon = 0\%$.

8 Richardson Extrapolation

This is to use two derivative estimates to compute a third, more accurate one.

$$D \approx \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1),\ h_2 = \frac{h_1}{2} \tag{13}$$

Example: $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$, $x_i = 0.5$, $h_1 = 0.5$, $h_2 = 0.25$.

Solution:

With h_1, $x_{i+1} = 1$, $x_{i-1} = 0$, $D(h_1) = \frac{f(x_{i+1})-f(x_{i-1})}{2h_1} = \frac{0.2-1.2}{1} = -1.0$, $\epsilon_t = -9.6\%$.

With h_2, $x_{i+1} = 0.75$, $x_{i-1} = 0.25$, $D(h_2) = \frac{f(x_{i+1})-f(x_{i-1})}{2h_2} = -0.934375$, $\epsilon_t = -2.4\%$.

$D = \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1) = \frac{4}{3} \times (-0.934575) - \frac{1}{3} \times (-1) = -0.9125$, $\epsilon_t = 0$.

For centered difference approximations with $O(h^2)$, using (13) yields a new estimate of $O(h^4)$.