Computer-Assisted Problem-Solving / Numerical Methods

Numerical Integration

version: October 16th, 2017

Legend: Method, Theory, Example, Advanced, Appendix

Theory

Numerical Integration

Calculate:

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

Can be interpreted as area under curve of $f(x)$

Divide interval $[a, b]$ in n parts: $h = \dfrac{b-a}{n}$

Mesh points: $x_i = a + ih \quad i = 0, 1, 2, ..., n$

(equidistant grid)

Approximate integral in each subinterval

$$Area_{\,i} \approx \int_{x_{i-1}}^{x_i} f(x)dx \quad (i = 1, 2, 3, ..., n).$$

Total integral (sum of sub-areas):

$$I \approx Area_{\,1} + Area_{\,2} + Area_{\,3} + ... + Area_{\,n}.$$

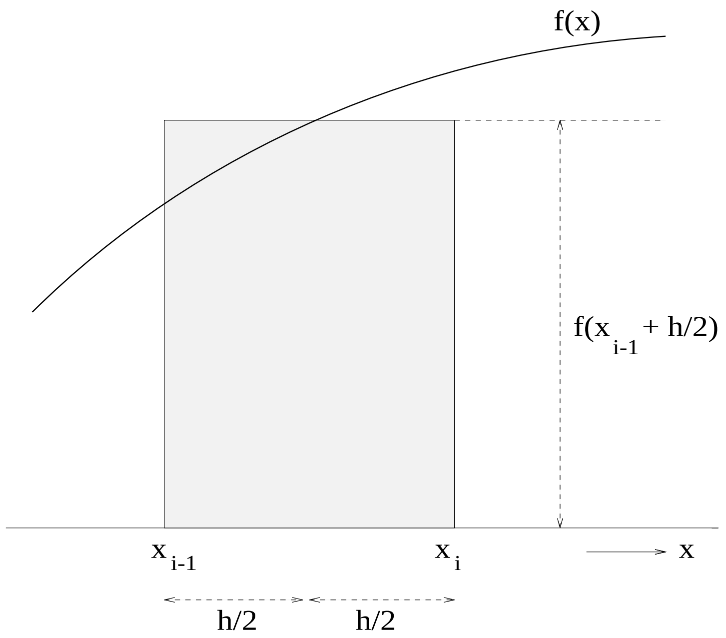
"Composite integral formula"

Special case of Quadrature formulas

(See Appendix)

Method

Midpoint Rule



The function $f(x)$ is approximated by the constant value $f(x_{i-1}+h/2)$ on the interval $[x_{i-1}, x_i]$ (value of f at midpoint $x_{i-1} + h/2$)

Partial integral:

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx hf(x_{i-1} + h/2) \quad i = 1, ..., n$$

Summing all partial integrals:

$$R(h) = h\{ \ f(a+\frac{1}{2}h) + f(a+\frac{3}{2}h) + ... + f(a+(n-\frac{1}{2})h) \ \}$$

What is the accuracy (truncation error) ?

Example

Example Midpoint Rule

Calculate the integral

$$I = \int_0^1 3x^2 dx$$

Exact answer: $I = 1$

Use $n = 1, 2, 4, 8, ...$ **subintervals**

n	$R(h)$	**error**
1	**0.75**	$2.50 * 10^{-1}$
2	**0.9375**	$6.25 * 10^{-2}$
4	**0.984375**	$1.56 * 10^{-2}$
8	**0.99609375**	$3.91 * 10^{-3}$
16	**0.9990234375**	$9.77 * 10^{-4}$
32	**0.999755859375**	$2.44 * 10^{-4}$
64	**0.9999389648438**	$6.10 * 10^{-5}$
128	**0.9999847412109**	$1.53 * 10^{-5}$

For $n = 128$ **(absolute) error** $\approx 1.53 * 10^{-5}$

For $n = \ 64$ **(absolute) error** $\approx 6.10 * 10^{-5}$

Quadratic convergence: $\epsilon_n \sim \mathcal{O}(h^2)$

Thus: $\epsilon_n / \epsilon_{2n} \approx 4$

Outlook

Always this order of accuracy (convergence)?

No! Depends on function $f(x)$.

Improving the Midpoint Rule:

- Approximate function $f(x)$ with straight line (linear interpolation) instead of constant value $\Longrightarrow$ Trapezoidal Rule

- Approximate function with parabola (2nd order interpolation) $\Longrightarrow$ Simpson's Rule

- "Extrapolation" of results after mesh refinement h, $h/2$, $h/4$, ... $\Longrightarrow$ methods of Richardson and Romberg

Theory

Local Error Midpoint Method

General definition local truncation error

$$\epsilon_i = \left| \int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x - Area_{\,i} \right|$$

Error of integral approximation on $[x_{i-1}, x_i]$

Local error for Midpoint Method

$$\epsilon_i(h) = \left| \int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x - \int_{x_{i-1}}^{x_i} f(x_m)\mathrm{d}x \right|,$$

with $x_m = x_{i-1} + \frac{h}{2}$ **the midpoint of** $[x_{i-1}, x_i]$

Use Taylor series for $f(x)$ **around** x_m

$$f(x) = f(x_m) + f'(x_m)(x - x_m) + \tfrac{1}{2} f''(x_m)(x - x_m)^2 + \cdots$$

Introduce: $f_m^{(k)}$ **is** $k\!-\!th$ **derivative of** $f(x)$ **in** x_m

This gives

$$\begin{aligned}
\epsilon_i(h) = &\int_{x_{i-1}}^{x_i} \{ f_m^{(1)}(x - x_m) + \frac{1}{2} f_m^{(2)}(x - x_m)^2 + \cdots \}\,\mathrm{d}x \\
= &\int_{x_{i-1}}^{x_i} f_m^{(1)}(x - x_m)\,\mathrm{d}x + \frac{1}{2}\int_{x_{i-1}}^{x_i} f_m^{(2)}(x - x_m)^2\,\mathrm{d}x \\
+ &\frac{1}{6}\int_{x_{i-1}}^{x_i} f_m^{(3)}(x - x_m)^3\,\mathrm{d}x + \frac{1}{24}\int_{x_{i-1}}^{x_i} f_m^{(4)}(x - x_m)^4\,\mathrm{d}x \\
+ &\cdots
\end{aligned}$$

Evaluate integrals

$$
\begin{aligned}
\epsilon_i(h) = \quad & \frac{1}{2} f_m^{(1)} (x - x_m)^2 \Big|_{x_{i-1}}^{x_i} + \quad \frac{1}{6} f_m^{(2)} (x - x_m)^3 \Big|_{x_{i-1}}^{x_i} \\
+ \; & \frac{1}{24} f_m^{(3)} (x - x_m)^4 \Big|_{x_{i-1}}^{x_i} + \; \frac{1}{120} f_m^{(4)} (x - x_m)^5 \Big|_{x_{i-1}}^{x_i} \\
+ \; & \qquad \cdots
\end{aligned}
$$

Local error

$$
\epsilon_i(h) = 0 \;\; + \;\; \frac{1}{24}\, f_m^{(2)} h^3 \;\; + \;\; 0 \;\; + \;\; \frac{1}{1920}\, f_m^{(4)} h^5 + \cdots
$$

Notice that even powers disappear

Theory

Global Error Midpoint Method

General definition global (total) error

$$\epsilon(h) = \sum \epsilon_i(h)$$

Error observed in tables

Global error for Midpoint Method

$$\epsilon(h) = \sum \frac{1}{24} f''(x_m)\, h^3 \; + \; \frac{1}{1920} f''''(x_m)\, h^5 \; + \; \cdots$$

If

$$\max_{x \in [a,b]} |f''(x)| \leq M$$

Then

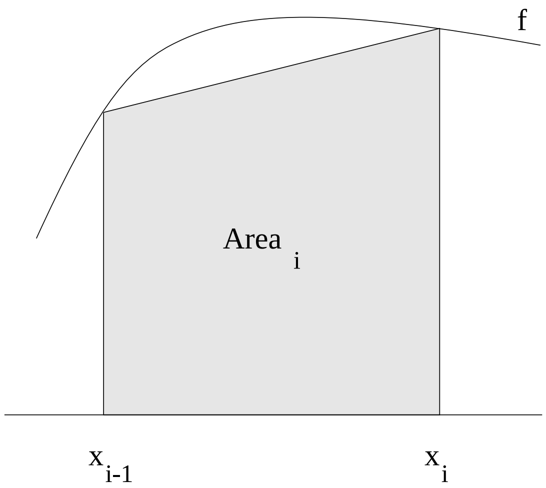
$$\epsilon \leq \frac{(b-a)}{24} h^2 M \quad \textbf{and hence} \quad \epsilon = \mathcal{O}(h^2)$$

Valid upon neglecting 4th-order terms and higher

So valid when h small enough

Method

Trapezoidal Rule



$f(x)$ is approximated by a straight line (linear interpolation) on the interval $[x_{i-1}, x_i]$

Partial integral:

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

Summing all partial integrals:

$$T(h) = h\{ \quad \frac{1}{2}f(a) + f(a+h) + f(a+2h) + \ldots. + f(a+(n-1)h) + \frac{1}{2}f(b) \quad \}$$

Quadratic convergence: $\epsilon_n \sim \mathcal{O}(h^2)$

Similar to Midpoint Rule!

Example

Example Trapezoidal rule

Calculate the integral

$$I = \int_0^1 e^x dx$$

Exact answer: $I = e - 1 \approx 1.718281828459$

Use $n = 1, 2, 4, 8$ **subintervals**

n	$T(h)$	$error$	$q(h)$
1	1.8591409	0.1408	
2	1.7539311	0.0356	3.94
4	1.7272219	0.0089	3.98
8	1.7205186	0.0022	

Quadratic convergence: $\epsilon_n \sim \mathcal{O}(h^2)$

Similar to Midpoint Rule!

Convergence ratio $q(h)$ **follows later**

Theory

Truncation Error Trapezoidal Rule

Theorem:

If integrand is not singular and $f \in C^\infty \Longrightarrow$

local truncation error Trapezoidal Rule

$$\epsilon_i(h) = \frac{h^3}{12} f''(x_{i-1}) + \mathcal{O}(h^4), \quad \textbf{or} \quad \epsilon_i = \mathcal{O}(h^3)$$

Remark: for Midpoint Rule

$$\epsilon_i(h) = \frac{h^3}{24} f''(x_{i-1}) + \mathcal{O}(h^4)$$

Proof

Local error Trapezoidal Method

$$\epsilon_i(h) = \left| \int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x - \int_{x_{i-1}}^{x_i} \frac{1}{2}\left(f(x_{i-1}) + f(x_i)\right) \mathrm{d}x \right|$$

Notation: $f_{i-1}^{(k)}$ **is** $k\!-\!th$ **derivative of** $f(x)$ **in** x_{i-1}

Taylor series for $f(x)$ **around** x_{i-1}

$$f(x) = f(x_{i-1}) + f_{i-1}^{(1)}(x - x_{i-1}) + \tfrac{1}{2} f_{i-1}^{(2)}(x - x_{i-1})^2 + \cdots$$

Integrate Taylor series: $\displaystyle\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x$

$$= f(x_{i-1})x|_{x_{i-1}}^{x_i} + f_{i-1}^{(1)} \frac{(x - x_{i-1})^2}{2}|_{x_{i-1}}^{x_i} + f_{i-1}^{(2)} \frac{(x - x_{i-1})^3}{6}|_{x_{i-1}}^{x_i} + \ldots$$

$$= f(x_{i-1})h + \frac{1}{2} f_{i-1}^{(1)} h^2 + \frac{1}{6} f_{i-1}^{(2)} h^3 + \cdots$$

Evaluate Local error Trapezoidal Method

$$\begin{aligned}\epsilon_i(h) &= \mid f(x_{i-1})h + \frac{1}{2}f^{(1)}_{i-1}h^2 + \frac{1}{6}f^{(2)}_{i-1}h^3 \; + \cdots \\ &\qquad - (f(x_{i-1}) + f(x_i))\frac{h}{2} \mid \\ &= \mid f(x_{i-1})\frac{h}{2} + \frac{1}{2}f^{(1)}_{i-1}h^2 + \frac{1}{6}f^{(2)}_{i-1}h^3 \; + \cdots - f(x_i)\frac{h}{2} \mid\end{aligned}$$

Eliminate last term with Taylor series

$$\begin{aligned}f(x_i) &= f(x_{i-1}) + f^{(1)}_{i-1}(x_i - x_{i-1}) + \tfrac{1}{2}f^{(2)}_{i-1}(x_i - x_{i-1})^2 + \cdots \\ &= f(x_{i-1}) + f^{(1)}_{i-1}\, h \; + \; \tfrac{1}{2}f^{(2)}_{i-1}\, h^2 \; + \; \cdots\end{aligned}$$

Final result:

$$\begin{aligned}\epsilon_i(h) &= \frac{1}{12}f^{(2)}_{i-1}h^3 + \frac{1}{24}f^{(3)}_{i-1}h^4 \\ &= \frac{1}{12}f''(x_{i-1})h^3 + \frac{1}{24}f'''(x_{i-1})h^4\end{aligned}$$

See Appendix B for a more formal proof

Theory

Global Error Trapezoidal Rule

Definition global (total) error

$$\epsilon(h) = \sum_{i=1}^{n} \epsilon_i(h)$$

Total error of approximation of integral in $[a, b]$

Error observed in tables

Theorem global truncation error (Trapezoidal Rule)

If

$$\max_{x\in[a,b]} |f''(x)| \leq M$$

Then

$$\epsilon \leq \frac{(b-a)}{12} h^2 M \quad \textbf{and hence} \quad \epsilon = \mathcal{O}(h^2)$$

(upon neglecting 4th-order terms and higher)

Proof:

$$\epsilon_i(h) = \frac{h^3}{12} f''(x_{i-1}) \leq \frac{h^3}{12} M \Longrightarrow$$

$$\epsilon = \sum_{i=1}^{n} \epsilon_i \leq n \frac{h^3}{12} M \quad \textbf{with } n = \frac{(b-a)}{h}$$

Theory

Convergence Ratio (q-factor)

For sufficiently small values of h:

$$T(h) \approx I \pm ch^2.$$

Trapezoidal integration with step size $h/2$ gives error which is (roughly) 4 times smaller:

$$T(h/2) \approx I \pm c(h/2)^2 = I \pm ch^2/4$$

Again halving gives

$$T(h/4) \approx I \pm ch^2/16$$

Thus the ratio

$$q(h/2) := \left| \frac{T(h) - T(h/2)}{T(h/2) - T(h/4)} \right|$$

is approximately equal to

$$q(h/2) \approx \left| \frac{I \pm ch^2 - (I \pm ch^2/4)}{I \pm ch^2/4 - (I \pm ch^2/16)} \right| = 4$$

Convergence ratio q is good measure for convergence order

If q not close to 4 then

- h not small enough $\Longrightarrow$ 3rd-order terms in ϵ not negligible w.r.t. 2nd-order term ch^2

or

- function f not smooth enough (e.g. cannot be differentiated enough times)

Example

Example Trapezoidal Rule (1)

Consider again the integral

$$I = \int_0^1 e^x dx = e - 1 \approx 1.718281828459.$$

Exact answer: $I = e - 1 \approx 1.718281828459$

Results of composite trapezoidal rule:

n	$T(h)$	$error$	$q(h)$
1	1.8591409	0.1408	
2	1.7539311	0.0356	3.94
4	1.7272219	0.0089	3.98
8	1.7205186	0.0022	

q **values** $\approx 4 \Longrightarrow$
quadratic convergence of $T(h)$

Estimate global error for $h = 1/8$**:**

$$|\epsilon| \leq (b-a)M\frac{h^2}{12} = (1-0)e^1\frac{(1/8)^2}{12} \approx 0.0035$$

Approximately equal to actual error 0.0022

Example

Example Trapezoidal Rule (2)

Consider

$$I = \int_0^1 \sqrt{x}dx = 2/3 \approx 0.66666666666$$

Approximations using Trapezoidal Rule:

n	$T(h)$	$error$	$q(h)$
1	0.5000000	0.1666	
2	0.6035535	0.0631	2.61
4	0.6432831	0.0234	2.68
8	0.6581303	0.0085	2.69
16	0.6635812	0.0031	2.89
32	0.6655590	0.0011	

q values much smaller than 4

$\Longrightarrow$ no quadratic convergence

Cause: integrand "singular" in $x = 0$

In this case: derivative of integrand not confined in integration interval $[0\ ,\ 1]$, indeed derivative of $\sqrt{x}$ is $1/(2\sqrt{x}) \to \infty$ if $x \to +0$

Second derivative even worse

Therefore the estimate $|\epsilon| \leq (b-a)Mh^2/12$ makes no sense in this case ($M = \infty$)

Improve weak convergence behaviour by changing integration variable

In this example use transformation $x = t^2$:

$$I = \int_0^1 \sqrt{x}dx = \int_0^1 2t^2 dt.$$

Now the integrand $2t^2$ is not singular

Trapezoidal Rule for transformed integral $\int_0^1 2t^2 dt$

n	$T(h)$	$error$	$q(h)$
1	1.000000	0.3333	
2	0.750000	0.0833	4.00
4	0.687500	0.0208	4.00
8	0.671875	0.0052	4.00
16	0.6679688	0.0013	4.00
32	0.6669922	0.0003	

Now convergence order (roughly) equal to 2
Error much faster $\to 0$ compared to original integration of $\sqrt{x}$

Error estimation for $h = 1/32$:

(absolute) max. of 2nd derivative of $2t^2$ on $[0, 1]$ is 4 $\Longrightarrow$

$$|\epsilon| \leq \frac{(1-0)}{12}(\frac{1}{32})^2 4 \approx 0.0003$$

This estimate exactly equals real error. Why?

Advanced

Singular Integrals

Problems in case of singular integrals:
i.e. when $f'(x)$ and/or $f''(x)$ not bounded
(or not existent)

Possible solutions:

1. **Partial integration**

$$\int_0^1 \frac{e^{-x}}{\sqrt{x}} dx = 2e^{-x}\sqrt{x}\Big|_0^1 + \int_0^1 2e^{-x}\sqrt{x}\, dx$$
$$= 2e^{-1} + \frac{4}{3}e^{-x}x^{3/2}\Big|_0^1 + \frac{4}{3}\int_0^1 e^{-x}x^{3/2}\, dx$$

2. **Transformation**

$$\int_0^1 \frac{e^{-x}}{\sqrt{x}}\, dx \overset{(x=t^2)}{=} 2\int_0^1 e^{-t^2}\, dt$$

3. **Split-off the unwanted behaviour**

$$\int_0^1 \frac{e^{-x}}{\sqrt{x}}\, dx = \int_0^1 \frac{e^{-x}-1+x-\frac{1}{2}x^2}{\sqrt{x}}\, dx + \int_0^1 \frac{1-x+\frac{1}{2}x^2}{\sqrt{x}}\, dx$$
$$= \frac{23}{15} + \int_0^1 \frac{e^{-x}-1+x-\frac{1}{2}x^2}{\sqrt{x}}\, dx$$

Reason: $e^{-x} = 1 - x + \frac{x^2}{2} - \frac{x^3}{3!} + \ldots$
Beware of number loss!

Advanced

Infinite Integration Interval

Problems in case of integration over $[a, \infty]$

Possible solutions:

1. **Transformation**

$$\int_1^{\infty} \frac{e^{-\frac{1}{t}}}{t^{3/2}} dt \overset{(t=1/x)}{=} \int_0^1 \frac{e^{-x}}{\sqrt{x}}\, dx, \quad \textbf{(see prev. page)}$$

2. **Cut off**

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx \approx \int_{-4}^{4} e^{-x^2}\, dx$$

3. **Split-off the unwanted behaviour**

$$\int_0^{\infty} (1+x^2)^{-\frac{4}{3}}\, dx =$$

$$\begin{aligned}
&= \int_0^R (1+x^2)^{-\frac{4}{3}}\, dx + \int_R^{\infty} x^{-\frac{8}{3}} (1+x^{-2})^{-\frac{4}{3}}\, dx \\
&= \int_0^R ..\, dx + \int_R^{\infty} \left(x^{-\frac{8}{3}} - \frac{4}{3} x^{-\frac{14}{3}} + \frac{14}{9} x^{-\frac{20}{3}} - \ldots \right) dx \\
&= \int_0^R ..\, dx + R^{-\frac{5}{3}} \left(\frac{3}{5} - \frac{4}{11} R^{-2} + \frac{14}{51} R^{-4} - \ldots \right)
\end{aligned}$$

For an accuracy of 5 digits: take $R = 8$ and evaluate the first integral numerically

Method

Simpson's Rule

Quadratic interpolation in $[x_{i-1}\ ,\ x_i]$

$$Area_{\,i} = \frac{h}{6}\{\ f(x_{i-1}) + 4f(\frac{x_{i-1}+x_i}{2}) + f(x_i)\ \}$$

Here we use $$x_m = \frac{x_{i-1}+x_i}{2}$$

Take notice: $h = x_i - x_{i-1}$ **!**

Use polynomial approximation (Lagrange)

$$f(x) \approx p_2(x) = \frac{(x-x_m)(x-x_i)}{(x_{i-1}-x_m)(x_{i-1}-x_i)} f(x_{i-1}) + \frac{(x-x_{i-1})(x-x_i)}{(x_m-x_{i-1})(x_m-x_i)} f(x_m) + \frac{(x-x_{i-1})(x-x_m)}{(x_i-x_{i-1})(x_i-x_m)} f(x_i)$$

If $f \in \mathcal{C}^4[a,b]$**, then local error** ϵ_i **in** $[x_{i-1}, x_i]$**:**

$$\epsilon_i = -\frac{\hat{h}^5}{90} f^{(4)}(\xi), \quad \xi \in [x_{i-1}, x_i]$$

with $\hat{h} = h/2$

Prove via interpolation error, mean-value theorem and partial integration

Global error Simpson in $[a, b]$:

If $\max_{x\in[a,b]} |f^{(4)}(x)| \leq M \Longrightarrow$

$$\textbf{global error} \quad \epsilon \leq \frac{\hat{h}^4}{180}(b-a)M$$

with again $\hat{h} = h/2$

Proof:

$$\epsilon_i = \frac{\hat{h}^5}{90} f^{(4)}(\xi) \leq \frac{\hat{h}^5}{90} M \Longrightarrow \epsilon = \sum_{i=1}^{n} |\epsilon_i| \leq n\frac{\hat{h}^5}{90} M$$

with

$$n = \frac{(b-a)}{h} = \frac{(b-a)/2}{h/2} = \frac{(b-a)/2}{\hat{h}}$$

Take notice:

$|f^{(4)}(x)| \leq M$ **for Simpson**

$|f^{(2)}(x)| \leq M$ **for Trapezoidal Rule**

Example

Example: Simpson vs. Trapezoidal

Numerical integration of $\int_0^1 x^3\sqrt{x}\,dx$

	Trapezoidal Rule		Simpson Rule	
n	Error	Ratio	Error	Ratio
2	–7.19720E–02		–3.37001E–03	
4	–1.81666E–02	3.961772	–2.31491E–04	14.557814
8	–4.55322E–03	3.989834	–1.54300E–05	15.002709
16	–1.13906E–03	3.997346	–1.00756E–06	15.314210
32	–2.84814E–04	3.999316	–6.48920E–08	15.526713
64	–7.12066E–05	3.999826	–4.14075E–09	15.671538
128	–1.78019E–05	3.999956	–2.62557E–10	15.770903
256	–4.45048E–06	3.999989	–1.65760E–11	15.839588
512	–1.11262E–06	3.999997	–1.04334E–12	15.887360

Numerical integration of $\int_0^5 \frac{1}{1+(x-\pi)^2}dx$

	Trapezoidal Rule		Simpson Rule	
n	Error	Ratio	Error	Ratio
2	1.73111E–01		–2.85329E–01	
4	7.10986E–02	2.434807	3.70944E–02	–7.691980
8	7.49582E–03	9.485108	–1.37051E–02	–2.706606
16	1.95340E–03	3.837313	1.05931E–04	–129.377902
32	4.89161E–04	3.993376	1.07999E–06	98.085254
64	1.22341E–04	3.998346	6.74324E–08	16.015873
128	3.05883E–05	3.999586	4.21692E–09	15.990914
256	7.64728E–06	3.999897	2.63594E–10	15.997765
512	1.91183E–06	3.999974	1.64752E–11	15.999443

Theory

Error Estimation by Halving h

Error of Trapezoidal Rule using step size h:

$$I = I_h + \epsilon_h$$

with exact answer I and approximation I_h

Halving step size:

$$I = I_{h/2} + \epsilon_{h/2}$$

Quadratic convergence: $\epsilon_h \approx 4\epsilon_{h/2} \Longrightarrow$

$$I_{h/2} + \epsilon_{h/2} = I_h + \epsilon_h \approx I_h + 4\epsilon_{h/2} \Longrightarrow$$

$$I_{h/2} - I_h \approx (4-1)\epsilon_{h/2} \Longrightarrow$$

$$\epsilon_{h/2} \approx \frac{1}{3}(I_{h/2} - I_h)$$

Thus: estimate error on basis of successive results of mesh refinement

Simpson has 4th-order convergence $\Longrightarrow$

$$\epsilon_{h/2} \approx \frac{1}{15}(I_{h/2} - I_h)$$

Proof: $I_{h/2} + \epsilon_{h/2} = I_h + \epsilon_h \approx I_h + 16\epsilon_{h/2} \Longrightarrow$

$$I_{h/2} - I_h \approx (16-1)\epsilon_{h/2} \Longrightarrow \epsilon_{h/2} \approx \tfrac{1}{15}(I_{h/2} - I_h)$$

Example

Example Error Estimation

$$I = \int_0^{\pi} e^x \cos x dx, \quad \text{'exact' solution } I = -12.0703463164\ldots$$

Trapezoidal Rule for $\int_0^{\pi} e^x \cos x dx$

n	I_n	$\lvert$error$\rvert$	ϵ_n/ϵ_{2n}	estimate $\lvert\epsilon_{h/2}\rvert$
2	-17.38925933	5.31891		
4	-13.33602285	1.26568	4.202427	1.351079
8	-12.38216243	3.11816E-01	4.059048	3.179535E-01
16	-12.14800410	7.76578E-02	4.015259	7.805278E-02
32	-12.08974212	1.93958E-02	4.003845	1.942066E-02
64	-12.07519410	4.84778E-03	4.000963	4.849340E-03
128	-12.07155819	1.21187E-03	4.000241	1.211970E-03
256	-12.07064928	3.02964E-04	4.000060	3.029700E-04
512	-12.07042206	7.57406E-05	4.000015	7.574000E-05

Simpson Rule for $\int_0^{\pi} e^x \cos x dx$

n	I_n	$\lvert$error$\rvert$	ϵ_n/ϵ_{2n}	estimate $\lvert\epsilon_{h/2}\rvert$
2	-11.59283955	4.77507E-01		
4	-11.98494402	8.54023E-02	5.591264	2.6140298E-02
8	-12.06420896	6.13736E-03	13.915154	5.2843293E-03
16	-12.06995132	3.94993E-04	15.537889	3.8282400E-04
32	-12.07032146	2.48603E-05	15.888486	2.4676000E-05
64	-12.07034476	1.55646E-06	15.972377	1.5533333E-06
128	-12.07034622	9.73205E-08	15.993110	9.7333333E-08
256	-12.07034631	6.08319E-09	15.998279	6.0000000E-09
512	-12.07034632	3.80210E-10	15.999566	6.6666672E-10

Method

Richardson Extrapolation

(Also known as: Simpson's procedure)

To estimate error of Trapezoidal Rule only "first part" of Taylor expansion considered

Theorem

If: integrand $f \in \mathcal{C}^{2m+1}$ in $[a,b]$

Then:

$$T(h) = I + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots + a_{2m} h^{2m} + \mathcal{O}(h^{2m+1}),$$

with coefficients $a_2, a_4, \ldots, a_{2m}$ depending on f, f', f'', ..., of a and b, but not(!) on h

Consequence:

for small h error of Trapezoidal Rule decreases with factor four when step size h halved

$$T(\frac{h}{2}) = I + a_2 \frac{h^2}{4} + a_4 \frac{h^4}{16} + \ldots + a_{2m} \frac{h^{2m}}{2^{2m}} + \mathcal{O}(h^{2m+1})$$

Remark:

to calculate $T(h/2)$ with given $T(h)$

only $n-1$ new evaluations of f needed,

namely in the "intermediate"-points

$a + h/2$, $a + 3h/2$, $a + 5h/2$, ...

Construction of new approximation with global error $\mathcal{O}(h^4)$ using $T(h)$ and $T(h/2)$:

Eliminate term a_2h^2 from $T(h)$ and $T(h/2)$ $\Longrightarrow$

$$T(h)-4T(h/2) = -3I+\frac{3}{4}a_4h^4+\frac{15}{16}a_6h^6+...+\mathcal{O}(h^{2m+1})$$

This gives

$$\frac{T(h)-4T(h/2)}{-3} = I-\frac{1}{4}a_4h^4-\frac{5}{16}a_6h^6-...-\mathcal{O}(h^{2m+1})$$

Result:

$$T_2(h/2) := T(h/2)+\frac{T(h/2)-T(h)}{3} \quad \sim \mathcal{O}(h^4)$$

Approximation of I with 4th order error $\frac{1}{4}a_4h^4$

Equivalent to Simpson's Rule

"Extrapolation" using known values

Order $\mathcal{O}(h^2)$ improvement

Compare approximations $T_2(h/2)$ and $T(h/2)$:

- $T_2(h/2)$ much more accurate for small h

- to calculate $T_2(h/2)$ little extra work

Repeat procedure:

starting with $T_2(h)$ and $T_2(h/2)$ extrapolation, another factor h^2 gain, etc. $\Longrightarrow$ Romberg

Example

Richardson Extrapolation

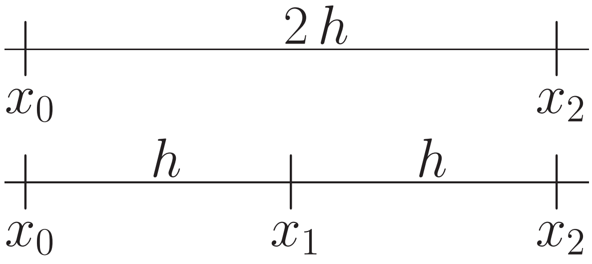
Consider $I = \int_0^1 e^x dx = 1.7182818284590449...$

n	$T_1(h)$	$T_2(h)$
2	**1.8591409142** ϵ_n =**1.409L−01**	
4	**1.7539310925** ϵ_n = **3.565L−02** f_n = **3.951**	**1.7188611519** ϵ_n = **5.793L−04** f_n = **not defined**
8	**1.7272219046** ϵ_n = **8.940L−03** f_n = **3.988**	**1.7183188419** ϵ_n = **3.701L−05** f_n = **15.65**
16	**1.7205185922** ϵ_n = **2.237L−03** f_n = **3.997**	**1.7182841547** ϵ_n = **2.326L−06** f_n = **15.91**
32	**1.7188411286** ϵ_n = **5.593L−04** f_n = **3.999**	**1.7182819741** ϵ_n = **1.456L−07** f_n = **15.98**
64	**1.7184216603** ϵ_n = **1.398L−04** f_n = **4.000**	**1.7182818376** ϵ_n = **9.103L−09** f_n = **15.99**

$$\epsilon_n = |\text{error}|, \; f_n = \frac{\epsilon_{n/2}}{\epsilon_n}$$

Theory

Trapezium+Richardson = Simpson



Trapezium approximations of $\int_{x_0}^{x_2} f(x)\mathrm{d}x$

Coarse grid: $T_{2h} = \frac{2h}{2}(f(x_0) + f(x_2))$

Fine grid: $T_h = \frac{h}{2}(f(x_0) + f(x_1)) + \frac{h}{2}(f(x_1) + f(x_2))$

$$= \frac{h}{2}(f(x_0) + 2f(x_1) + f(x_2))$$

Richardson: $\frac{4}{3}T_h - \frac{1}{3}T_{2h} = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$

Simpson approximation coarse grid:

$$\int_{x_0}^{x_2} f(x)\mathrm{d}x = \frac{2h}{6}\{\ f(x_0) + 4f(\frac{x_0 + x_2}{2}) + f(x_2)\ \}$$

Method

Romberg Integration

Start with $T_1(h) := T(h)$,

(approximation of I with Trapezoidal Rule)

and subsequently for $k = 1, 2, 3, \ldots$

$$T_{k+1}(h/2) := T_k(h/2) + \frac{T_k(h/2) - T_k(h)}{4^k - 1}.$$

Global truncation error in $T_k(h)$ has order h^{2k}:

$$T_k(h) = I + \mathcal{O}(h^{2k})$$

Romberg scheme:

$T(h)$				
$T(\frac{h}{2})$	$T_2(\frac{h}{2})$			
$T(\frac{h}{4})$	$T_2(\frac{h}{4})$	$T_3(\frac{h}{4})$		
$T(\frac{h}{8})$	$T_2(\frac{h}{8})$	$T_3(\frac{h}{8})$	$T_4(\frac{h}{8})$	
...	...	...	...	...

First calculate column T_1, then column T_2, etc.

For example: $T_1(h)$ **and** $T_1(h/2) \to T_2(h/2)$

$T_1(h/2)$ **and** $T_1(h/4) \to T_2(h/4)$

$T_2(h/2)$ **and** $T_2(h/4) \to T_3(h/4)$

Example

Example Romberg

Consider $I = \int_0^1 e^x dx = 1.7182818284590449...$

Romberg scheme:

n	$T_1(h)$	$T_2(h)$	$T_3(h)$	$T_4(h)$	$T_5(h)$
2	**1.8591409142**				
4	**1.7539310925**	**1.7188611519**			
8	**1.7272219046**	**1.7183188419**	**1.7182826879**		
16	**1.7205185922**	**1.7182841547**	**1.7182818422**	**1.7182818288**	
32	**1.7188411286**	**1.7182819741**	**1.7182818287**	**1.7182818285**	**1.7182818285**
64	**1.7184216603**	**1.7182818376**	**1.7182818285**	**1.7182818285**	**1.7182818285**

Romberg triangle of errors/factors:

2	**−1.409L−01**				
4	**−3.565L−02**	**−5.793L−04**			
	3.951L+00				
8	**−8.940L−03**	**−3.701L−05**	**−8.595L−07**		
	3.988L+00	**1.565L+01**			
16	**−2.237L−03**	**−2.326L−06**	**−1.376L−08**	**−3.355L−10**	
	3.997L+00	**1.591L+01**	**6.246L+01**		
32	**−5.593L−04**	**−1.456L−07**	**−2.163L−10**	**−1.344L−12**	**−3.308L−14**
	3.999L+00	**1.598L+01**	**6.361L+01**	**2.497L+02**	
64	**−1.398L−04**	**−9.103L−09**	**−3.386L−12**	**−5.995L−15**	**−8.882L−16**
	4.000L+00	**1.599L+01**	**6.389L+01**	**2.241L+02**	**3.725L+01**

Error decrease for $T_5 \neq (2^2)^5 = 1024$**:**
- loss of significant digits
- head term not sufficiently dominant

Theory

Rules Romberg Triangle

*) Every T_k in scheme approximates $I = \int_a^b f(x)dx$

*) Move one column to the right $\Longrightarrow$
convergence-order increased with 2

*) Move one row downwards $\Longrightarrow$
step size is halved

*) In k-th column of scheme: errors $\sim \mathcal{O}(h^{2k})$
of the form $\alpha_0 h^{2k} + \alpha_2 h^{2k+2} + \alpha_4 h^{2k+4} + \ldots$
with α_0, α_2, α_4, ... constants

*) If h small enough such that $\alpha_2 h^{2k+2}$, $\alpha_4 h^{2k+4}$,...
small compared to dominant term $\alpha_0 h^{2k}$ $\Longrightarrow$
error in k-th column decreases factor 4^k
when we move downwards one row

*) Performance Romberg worse in case of
singular integrals
Requirement integrand: $f \in \mathcal{C}^{2m+1}$ on $[a, b]$
(see Theorem Richardson Extrapolation)

Advanced

Error Estimates Romberg

Combination of

$$I \approx T_k(h) - \alpha_0 h^{2k}$$

and
$$T_k(h/2) \approx I + \alpha_0 \frac{h^{2k}}{4^k}$$

gives
$$T_k(h/2) \approx T_k(h) - \alpha_0 h^{2k} + \alpha_0 \frac{h^{2k}}{4^k}$$

Estimate for error in $T_k(h/2)$

$$\left|\frac{\alpha_0 h^{2k}}{4^k}\right| \approx \frac{T_k(h/2) - T_k(h)}{4^k - 1}$$

uses known values $T_k(h)$ **and** $T_k(h/2)$

Requirement for the error estimate:
h **small enough, such that higher-order terms in the error in** $T_k(h)$ **can be neglected**

Verification: check if the error decrease in k**-th column matches expected convergence order**

For this, we can use the convergence ratio

$$q_k(h/2) := \left|\frac{T_k(h) - T_k(h/2)}{T_k(h/2) - T_k(h/4)}\right|$$

If the higher order terms in the error in T_k **can be neglected, we have**

$$q_k(h/2) \approx \left|\frac{I + \alpha_0 h^{2k} - (I + \alpha_0 h^{2k}/4^k)}{I + \alpha_0 h^{2k}/4^k - (I + \alpha_0 h^{2k}/16^k)}\right| = 4^k$$

Advanced

Example Romberg Integration

Consider the integral

$$I = \int_0^1 \frac{dx}{1+x} = \ln 2 \approx 0.693147181...$$

Romberg-integration with $h = (1-0)/n$ **gives:**
(correct digits underlined)

n	T_1	T_2	T_3	T_4	T_5
1	$\underline{0}.750000000$				
2	$\underline{0}.708333333$	$\underline{0}.694444444$			
4	$\underline{0.69}7023810$	$\underline{0.693}253968$	$\underline{0.6931}74603$		
8	$\underline{0.69}4121850$	$\underline{0.6931}54531$	$\underline{0.69314}7901$	$\underline{0.69314}7478$	
16	$\underline{0.693}391202$	$\underline{0.693147}653$	$\underline{0.693147}194$	$\underline{0.69314718}3$	$\underline{0.69314718}2$

Remarks:

1. **For** T_5 **17 function evaluations are needed**
2. **Value convergence ratio:** $q_2(1/8) \approx 14.45 \approx 16$
   Hence, the error in the 2nd column is dominated by the 4-th order term $\alpha_2 h^4$

   Use error estimate (for $\alpha_0 h^{2k}/4^k$**) for errors** $\mathcal{O}(h^4)$ **in the 2nd column, e.g. for** $T_2(1/16)$**:**

$$|I - T_2(1/16)| \approx \left| \frac{T_2(1/16) - T_2(1/8)}{4^2 - 1} \right| \approx 4.585{*}10^{-7}$$

3. For the 3rd column: $q_3(1/8) \approx 37 \neq 64 \Longrightarrow$ **error estimation doubtful**

Similar for 4th and 5th column

This does not mean that results in 3rd, 4th, 5th column are worse than in 2nd column !

Accuracy increases when we move to the right in the scheme

Appendix

A: Quadrature formulas

Explicit formula to calculate

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

For example: replace f by approximation f_n
(with n number of mesh points,
interpolation order, ...)

Approximation $I_n(f) := I(f_n) = \int_a^b f_n(x)dx$

Error of approximation: $E_n(f) = I(f) - I_n(f)$

$$|E_n(f)| \leq \int_a^b |f(x) - f_n(x)|dx \leq (b-a)||f - f_n||_\infty$$

Normally $||f - f_n||_\infty \to 0$ **if** $n \to \infty$
(increasingly better approximation of f)

So: $|E_n(f)| \to 0$ **when** $n \to \infty$

General quadrature formula:

$$I_n(f) = \sum_{j=1}^{n} w_j f(x_j), \quad n \geq 1$$

with weighting factors w_j

Example:

$$I = \int_0^1 \frac{e^x - 1}{x} dx; \quad \textbf{so } f(x) = \frac{e^x - 1}{x}$$

Use Taylor expansion of e^x (order n; near $x_0 = 0$)

$$e^x = 1 + \sum_{j=1}^{n} x^j / j! + R_n|_{e_x}(x) \Longrightarrow$$

$$f(x) = \frac{e^x - 1}{x} = \sum_{j=1}^{n} \frac{x^{j-1}}{j!} + \frac{R_n|_{e_x}(x)}{x}$$

Approximation $f_n(x)$ of $f(x)$, use $R_n|_{e_x}(x) \approx 0$:

$$f_n(x) = \sum_{j=1}^{n} \frac{x^{j-1}}{j!} \Longrightarrow$$

$$I_n = \int_0^1 \sum_{j=1}^{n} \frac{x^{j-1}}{j!} dx = \sum_{j=1}^{n} \int_0^1 \frac{x^{j-1}}{j!} dx = \sum_{j=1}^{n} \frac{1}{j!\, j}$$

Series converges fast:

n	I_n
2	**1.25**
3	**1.30555556**
...	**...**
6	**1.31787037**
...	**...**
9	**1.31790212**
10	**1.31790215**
11	**1.31790215**

"Exact" value:

$I = 1.317902151...$

Error in integration with Taylor remainder:

$$R_n|_{e_x}(x) = \frac{x^{n+1}}{(n+1)!}\hat{f}|_{e_x}^{(n+1)}(\xi) = \frac{x^{n+1}}{(n+1)!}e^{\xi}, \quad \xi \in [0, x]$$

This gives:

$$f(x) - f_n(x) = \frac{R_n(x)}{x} = \frac{x^n}{(n+1)!}e^{\xi}, \quad \xi \in [0, x] \Longrightarrow$$

$$I - I_n = \int_0^1 \frac{x^n}{(n+1)!}e^{\xi}dx = \frac{x^{n+1}}{(n+1)!(n+1)}|_0^1 e^{\xi} = \frac{e^{\xi}}{(n+1)!(n+1)}$$

With $\xi \in [0, x]$ **en** $x \in [0, 1] \Longrightarrow$

$$\frac{1}{(n+1)!(n+1)} \leq I - I_n \leq \frac{e}{(n+1)!(n+1)}$$

Numerical values for $n = 6$**:**
Error estimate: $2.83\ \ 10^{-5} \leq I - I_6 \leq 7.70\ \ 10^{-5}$

$I_6 = 1.31787037$, **exact** $I = 1.317902151...$

Exact error $I - I_6$**:** $3.179\ \ 10^{-5}$

Appendix

B: Error Trapezoidal Method

Theorem:
If integrand is not singular and $f \in C^\infty \Longrightarrow$ **local truncation error Trapezoidal Rule**

$$\epsilon_i(h) = \frac{h^3}{12} f''(x_{i-1}) + \mathcal{O}(h^4), \quad \textbf{and hence} \quad \epsilon_i = \mathcal{O}(h^3)$$

Proof

Consider error ϵ_1 **on 1st subinterval** $[a, a+h]$
This (truncation) error equals, by definition,

$$\epsilon_1(h) := \frac{h}{2}\left(f(a) + f(a+h)\right) - \int_a^{a+h} f(x)dx. \qquad (1)$$

According to Taylor, $\epsilon_1(h)$ **can be written as**

$$\epsilon_1(h) = \epsilon_1(0) + h\epsilon_1'(0) + \frac{h^2}{2}\epsilon_1''(0) + \frac{h^3}{6}\epsilon_1'''(0) + \ldots \qquad (2)$$

Next we calculate $\epsilon_1(0), \epsilon_1'(0), \epsilon_1''(0)$ **and** $\epsilon_1'''(0)$

1. **Substitution of $h=0$ in (1) gives $\epsilon_1(0)=0$.**
2. **Take F the anti-derivative of f $(F'=f)$ $\Longrightarrow$ differentiate integral in r.h.s. of (1), w.r.t. h:**

   $$\frac{d}{dh}\int_a^{a+h} f(x)dx = \frac{d}{dh}\left(F(a+h)-F(a)\right) = F'(a+h)-0 = f(a+h)$$

   From (1) it then follows that $\epsilon_1'(h)$ is given by

   $$\epsilon_1'(h) = \frac{1}{2}\left(f(a)-f(a+h)\right) + \frac{h}{2}f'(a+h), \quad \textbf{so} \quad \epsilon_1'(0)=0.$$
3. **Differentiate again**

   $$\epsilon_1''(h) = -\frac{1}{2}f'(a+h) + \frac{1}{2}f'(a+h) + \frac{h}{2}f''(a+h) = \frac{h}{2}f''(a+h).$$

   So $\epsilon_1''(h)$ vanishes for $h=0$: $\epsilon_1''(0)=0$.
4. **Finally, the 3rd derivative of ϵ_1 is equal to**

   $$\epsilon_1'''(h) = \frac{1}{2}f''(a+h) + \frac{h}{2}f'''(a+h), \quad \textbf{so}: \quad \epsilon_1'''(0) = \frac{1}{2}f''(a).$$

Substitution of results 1–4 in Taylor-expansion (2) of ε_1 around $h=0$, gives

$$\epsilon_1(h) = \frac{h^3}{12}f''(a) + \frac{h^4}{4!}\epsilon_1''''(0) + \ldots \tag{3}$$

Normally step size h is small $\Longrightarrow$ 4-th and higher-order terms in (3) negligible:

$$\epsilon_1(h) \approx \frac{h^3}{12}f''(a).$$

Up to now we only considered ϵ_1
Other subintervals analogous $\Longrightarrow$

$$\epsilon_i(h) = \frac{h^3}{12}f''(x_{i-1}) + \frac{h^4}{4!}\epsilon_i''''(0) + \ldots$$

Appendix

C: Newton-Cotes Formulas

Formulas to approximate $I(f) = \int_a^b f(x)dx$

Trapezoidal and Simpson are examples

Equidistant grid:

$$h = (b-a)/n, \quad x_j = a + jh, \quad j = 0, 1, \cdots n$$

Approximation

$$I_n(f) = \int_a^b p_n(x)dx$$

with $p_n(x)$ **interpolation polynomial through** $x_0, x_1, \cdots, x_n$

Lagrange interpolation formula $\Longrightarrow$

$$I_n(f) = \int_a^b \sum_{j=0}^{n} l_j(x) f(x_j) dx = \sum_{j=0}^{n} w_j f(x_j)$$

with weighing factors

$$w_j = \int_a^b l_j(x)dx$$

Example: w_0 **when** $n = 3$**:**

$$w_0 = \int_a^b l_0(x)dx = \int_{x_0}^{x_3} \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} dx$$

Calculations can be simplified:

use $x = x_0 + \mu h$**, with** $0 \leq \mu \leq 3 \Longrightarrow$

$$\begin{aligned} w_0 &= -\frac{1}{6h^3}\int_{x_0}^{x_3}(x-x_1)(x-x_2)(x-x_3)dx \\ &= -\frac{1}{6h^3}\int_0^3(\mu-1)h(\mu-2)h(\mu-3)h\,h\,d\mu \\ &= -\frac{h}{6}\int_0^3(\mu-1)(\mu-2)(\mu-3)d\mu = \frac{3}{8}h \end{aligned}$$

Complete formula for $n = 3$**:**

$$I_3(f) = \frac{3}{8}h\{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\}$$

This is known as "Simpson's 3/8 rule"

Table: Newton-Cotes formulas for $I = \int_a^b f(x)dx$

$$\begin{array}{lll} n=0 & I_0 = & h\{f(\frac{a+b}{2})\} + \frac{h^3}{24}f''(\xi) \\ n=1 & I_1 = & \frac{h}{2}\{f(a)+f(b)\} - \frac{h^3}{12}f''(\xi) \\ n=2 & I_2 = & \frac{h}{3}\{f(a)+4f(\frac{a+b}{2})+f(b)\} - \frac{h^5}{90}f^{(4)}(\xi) \\ n=3 & I_3 = & \frac{3h}{8}\{f(a)+3f(a+h)+3f(b-h)+f(b)\} - \frac{3h^5}{80}f^{(4)}(\xi) \end{array}$$

Note: in these formulas $h = (b-a)/n$ **and not(!) some "in-between"-distance**

Appendix

D1: Error and Divided Differences

Integration methods (Midpoint, Trapezoidal, ...) use interpolation to approximate integrand $f(x)$

$\Longrightarrow$ (Truncation) Error in Integration can be derived from Interpolation Error and the Mean Value Theorem of Integration

Mean Value Theorem (normal):

If $f(x) \in \mathcal{C}[a,b]$ and differentiable on (a,b):

$$\exists \zeta \in (a,b) \text{ with } f(b) - f(a) = f'(\zeta)(b-a)$$

Mean Value Theorem (integration):

If $f(x) \in \mathcal{C}[a,b]$, $\quad w(x)$ constant sign on $[a,b]$ and $w(x)$ can be integrated on $[a,b]$:

$$\exists \zeta \in (a,b) \text{ with } \int_a^b w(x) f(x) dx = f(\zeta) \int_a^b w(x) dx$$

Theorem (interpolation error and differences):

$$\begin{aligned} f(x) - p_{n-1}(x) &= (x-x_0)\cdots(x-x_{n-1}) f[x_0, \cdots, x_{n-1}, x] \\ &= (x-x_0)\cdots(x-x_{n-1}) \frac{f^{(n)}(\xi)}{(n)!}, \end{aligned}$$

with $\xi \in I_x$, the smallest interval that contains $x_0, \cdots, x_{n-1}, x$

Appendix

D2: Truncation Error Trapezoidal

Trapezoidal interpolation on $[x_{i-1}\ ,\ x_i]$

$$I_1(f) = \frac{h}{2}(f(x_{i-1} + f(x_i))$$

This uses the polynomial approximation

$$f(x) \approx \frac{(x_i - x)f(x_{i-1}) + (x - x_{i-1})f(x_i)}{x_i - x_{i-1}} =: p_1(x)$$

Interpolation error (through some theorem):

$$E(x) = f(x) - p_1(x) = (x - x_{i-1})(x - x_i)f[x_{i-1}, x_i, x]$$

Local truncation error ϵ_i **on** $[x_{i-1}\ ,\ x_i]$**:**

$$\begin{aligned}\epsilon_i &= \int_{x_{i-1}}^{x_i} f(x)dx - I_1(f) \\ &= \int_{x_{i-1}}^{x_i} E(x)dx \\ &= \int_{x_{i-1}}^{x_i} (x - x_{i-1})(x - x_i)f[x_{i-1}, x_i, x]dx\end{aligned}$$

Mean Value Theorem $\{\,(x-x_{i-1})(x-x_i)\leq 0\,\} \Longrightarrow$

$$\epsilon_i = f[x_{i-1}, x_i, \zeta]\int_{x_{i-1}}^{x_i}(x-x_{i-1})(x-x_i)dx, \quad \zeta \in [x_{i-1}, x_i]$$

With shift $[x_0, x_1] \to [x_{i-1}, x_i]$

$$f[x_0, \ldots, x_{n-1}, x] = \frac{f^{(n)}(\xi)}{n!} \Longrightarrow f[x_{i-1}, x_i, \zeta] = \frac{f^{(2)}(\xi)}{2!}$$

and evaluation of the integral:

$$\begin{aligned} \epsilon_i &= \{\frac{1}{2} f''(\xi)\}\{-\frac{1}{6}(x_i - x_{i-1})^3\}, \quad \xi \in [x_{i-1}, x_i] \\ &= -\frac{(x_i - x_{i-1})^3}{12} f''(\xi) \end{aligned}$$

Comparable with previous result obtained by means of Taylor-series!