MAT505E - Numerical Analysis I

Term Project - Euler-Maclaurin Summation Formula for Numerical Integration

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Content

Numerical Integration

- Numerical integration methods are used to approximate definite integrals.
- The main objective is to replace a definite integral with an approximate solution:

$$I = \int_a^b f(x)dx \approx \sum_{i=0}^{N} W_i f_i$$

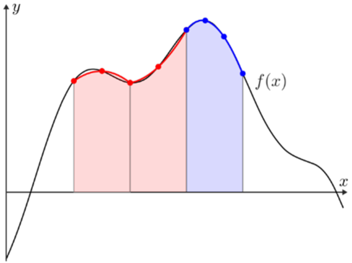


Figure: Numerical Integration (Source).

where x_i are the evaluation points, $f_i = f(x_i)$, and W_i is the weight given the i-th point.

Motivation and need

- The integrand $f(x)$ may be known only at certain points (sampling points).
- The integrated $f(x)$ may be known, but it may be difficult or impossible to find an antiderivative (e.g., $exp(-x^2)$).

Numerical Integration (cont'd.)

We want this approximation to be useful for a variety of integrals. Let us investigate the first two terms in a Taylor series expansion of any function,

$$\int_{x_0}^{x_1} 1dx = x_1 - x_0 \approx W_0 f_0 + W_1 f_1 = W_0 + W_1$$

$$\int_{x_0}^{x_1} xdx = \frac{x_1^2 - x_0^2}{2} \approx W_0 f_0 + W_1 f_1 = W_0 x_0 + W_1 x_1$$

The solution methods of linear algebra give,

$$W_0 = W_1 = \frac{x_1 - x_0}{2}$$

and finally, we can rewrite the integral using the solutions,

$$\int_{x_0}^{x_1} f(x)dx \approx W_0 f_0 + W_1 f_1 = \frac{x_1 - x_0}{2} f_0 + \frac{x_1 - x_0}{2} f_1 = \frac{x_1 - x_0}{2}(f_0 + f_1) = \frac{h}{2}(f_0 + f_1)$$

Numerical Integration (cont'd.): Trapezoid Rule

$$\int_{x_0}^{x_1} f(x)dx \approx W_0 f_0 + W_1 f_1 = \frac{x_1 - x_0}{2} f_0 + \frac{x_1 - x_0}{2} f_1 = \frac{x_1 - x_0}{2}(f_0 + f_1) = \frac{h}{2}(f_0 + f_1)$$

is called the **Trapezoid rule**. Of course, we are not limited to $N = 1$; for three points (quadratic), similarly, we can find the equations,

$$\int_{x_0}^{x_2} 1dx = x_2 - x_0 \approx W_0 f_0 + W_1 f_1 + W_2 f_2 = W_0 + W_1 + W_2$$
$$\int_{x_0}^{x_2} xdx = \frac{x_2^2 - x_0^2}{2} \approx W_0 f_0 + W_1 f_1 + W_2 f_2 = W_0 x_0 + W_1 x_1 + W_2 x_2$$
$$\int_{x_0}^{x_2} x^2 dx = \frac{x_2^3 - x_0^3}{3} \approx W_0 f_0 + W_1 f_1 + W_2 f_2 = W_0 x_0^2 + W_1 x_1^2 + W_2 x_2^2$$

Solving for the weights gives,

$$\int_{x_0}^{x_2} f(x)dx \approx W_0 f_0 + W_1 f_1 + W_2 f_2 = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

Numerical Integration (cont'd.): Simpson's Rule

$$\int_{x_0}^{x_2} f(x)dx \approx W_0 f_0 + W_1 f_1 + W_2 f_2 = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

is called the **Simpson's 1/3 rule**. Continuing in this fashion,

- 4 points: Simpson's 3/8 rule,
- 5 points: Boole's rule, ...

Method	**Degree**	**Step Size (h)**	**Formula**	**Error Term**
Trapezoid	1	$b-a$	$\frac{h}{2}(f_0 + f_1)$	$-\frac{1}{12}h^3 f^{(2)}(\xi)$
Simpson's 1/3	2	$\frac{b-a}{2}$	$\frac{h}{3}(f_0 + 4f_1 + f_2)$	$-\frac{1}{90}h^5 f^{(4)}(\xi)$
Simpson's 3/8	3	$\frac{b-a}{3}$	$\frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$	$-\frac{3}{80}h^5 f^{(4)}(\xi)$
Boole's	4	$\frac{b-a}{4}$	$\frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$	$-\frac{8}{945}h^7 f^{(6)}(\xi)$

Table: Summary table for numerical integration methods (Source).

Composite Formulas

As an alternative to higher-order approximations, we can also divide the total integration region into many segments. This allows us to use a low-order and relatively simple quadrature over each segment. Dividing the region from x_0 to x_N into N segments of width h for the Trapezoid rule,

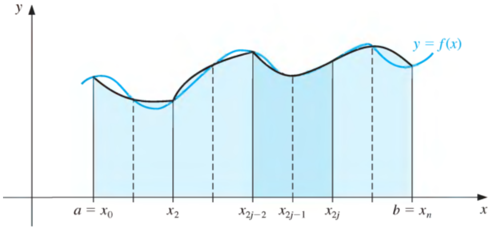


Figure: Composite integration [1].

$$\int_{x_0}^{x_N} f(x)dx \approx \frac{h}{2}(f_0+f_1)+\frac{h}{2}(f_1+f_2)+\cdots+\frac{h}{2}(f_{N-1}+f_N) = h(\frac{f_0}{2}+f_1+f_2+\cdots+f_{N-1}+\frac{f_N}{2})$$

is called the **composite Trapezoid rule**, a similar procedure for the Simpson's rule,

$$\int_{x_0}^{x_N} f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + 2f_2 + \cdots + 2f_{N-2} + 4f_{N-1} + f_N)$$

is called the **composite Simpson's rule**.

[1] Burden and Faires, *Numerical Analysis*

Errors … and Corrections:

Euler-Maclaurin Summation

Euler-Maclaurin Summation

So far, we derive the formulas by expanding the integrand in a Taylor series and integrating. Now, let us try to expand the function $f(x)$ in a Taylor series about $x = a$ [2],

$$\int_a^b f(x)dx \approx \int_a^b \left[f(a) + (x-a)f^{(1)}(a) + \frac{(x-a)^2}{2!} f^{(2)}(a) + \frac{(x-a)^3}{3!} f^{(3)}(a) + \cdots \right] dx$$

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

Similarly, the expansion about $x = b$,

$$\int_a^b f(x)dx \approx hf(b) - \frac{h^2}{2!} f^{(1)}(b) + \frac{h^3}{3!} f^{(2)}(b) - \frac{h^4}{4!} f^{(3)}(b) + \cdots$$

Adding these two equations yields,

$$\int_a^b f(x)dx \approx \frac{h}{2} [f(a) + f(b)] + \frac{h^2}{4} \left[f^{(1)}(a) - f^{(1)}(b) \right] + \frac{h^3}{12} \left[f^{(2)}(a) + f^{(2)}(b) \right] \cdots$$

[2] DeVries and Hasbun, *A First Course in Computational Physics*

Euler-Maclaurin Summation (cont'd.)

In the formula, we have the difference (even-order) and sum (odd-order) of derivatives. Let us see if we can eliminate the even-order ones by using the Taylor series expansion of $f'(x)$ about $x = a$,

$$f'(x) = f'(a) + (x-a)f^{(2)}(a) + \frac{(x-a)^2}{2}f^{(3)}(a) + + \frac{(x-a)^3}{6}f^{(4)}(a) + \cdots$$

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

Similarly, the expansion about $x = b$,

$$f'(b) = f'(b) + hf^{(2)}(b) + \frac{h^2}{2}f^{(3)}(b) + \frac{h^3}{6}f^{(4)}(b) + \cdots$$

Using these expressions, we can get the second-order derivative terms,

$$f^{(2)}(a) + f^{(2)}(b) = \frac{2}{h}\left[f'(b) - f'(a)\right] - \frac{h}{2}\left[f^{(3)}(a) - f^{(3)}(b)\right] - \frac{h^2}{6}\left[f^{(4)}(a) + f^{(4)}(b)\right] + \cdots$$

Euler-Maclaurin Summation (cont'd.)

We could also expand the $f^{(3)}(x)$ about $x = a$ and $x = b$ to find,

$$f^{(4)}(a) + f^{(4)}(b) = \frac{2}{h}\left[f^{(3)}(b) - f^{(3)}(a)\right] + \cdots$$

Using $f^{(2)}(a) + f^{(2)}(b)$ and $f^{(4)}(a) + f^{(4)}(b)$, the even-order terms can now be eliminated from the original equation,

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + f(b)] + \frac{h^2}{4}\left[f^{(1)}(a) - f^{(1)}(b)\right] + \frac{h^3}{12}\left[f^{(2)}(a) + f^{(2)}(b)\right]\cdots$$

$$\downarrow$$

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + f(b)] + \frac{h^2}{12}\left[f^{(1)}(a) - f^{(1)}(b)\right] - \frac{h^4}{720}\left[f^{(3)}(a) - f^{(3)}(b)\right] + \cdots$$

In general, we can write,

$$\int_{x_0}^{x_N} f(x)dx \approx h\left(\frac{f_0}{2} + f_1 + f_2 + \cdots + f_{N-1} + \frac{f_N}{2}\right) + \frac{h^2}{12}\left[f_0^{(1)} - f_N^{(1)}\right] - \frac{h^4}{720}\left[f_0^{(3)} - f_N^{(3)}\right] + \cdots$$

Applications:

Euler-Maclaurin Summation

Applications: Euler-Maclaurin Summation

- A research paper [3] is selected to compare the performance of the different numerical integration methods.
- The list of functions to be investigated from that paper:
  - $f(x) = sinx$ where $x \in [0, \pi/4]$
  - $f(x) = x^3$ where $x \in [0, 2.5]$
  - $f(x) = lnx$ where $x \in [1, 3]$
  - $f(x) = x^3 - x$ where $x \in [0, 2]$
- The list of the methods to be employed:
  - Trapezoid rule (from the paper),
  - Composite Simpson's 1/3 rule (with the code from scratch), and
  - Euler-Maclaurin summation (with the code from scratch)
- Three different numbers of panels (1,4,10) are investigated for each method.

[3] Winnicka, "Comparison of numerical integration methods"

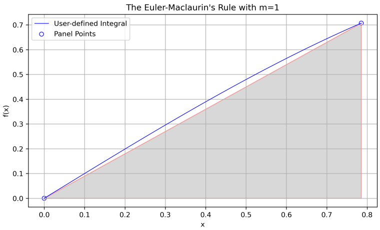
Applications: Euler-Maclaurin Summation (cont'd.)

f(x)	[a,b]	N	Exact Solution	Trapezoid [4]	Simpson's 1/3	Euler-Maclaurin
$sinx$	$[0, \pi/4]$	1		0.268012	0.185120	0.292891
		4	0.2928932188134525	0.281217	0.292896	0.292893
		10		0.281949	0.292893	0.292893
x^3	$[0, 2.5]$	1		19.53125	13.020833	9.765625
		4	9.765625	10.375976	9.765625	9.765625
		10		9.863281	9.765625	9.765625
lnx	$[1, 3]$	1		1.098612	0.732408	1.278036
		4	1.295836866004329	1.282105	1.295322	1.295826
		10		1.293619	1.295821	1.295837
$x^3 - x$	$[0, 2]$	1		6	4.000000	2.000000
		4	2	2.25	2.000000	2.000000
		10		2.04	2.000000	2.000000

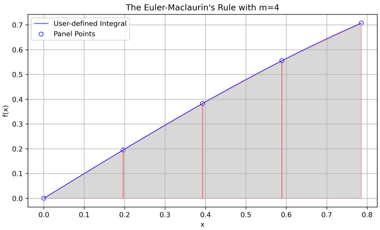
Table: Summary result table for the numerical integration methods.

[4] Winnicka, "Comparison of numerical integration methods"

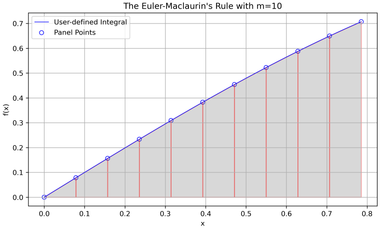
Example Plots for $sin(x)$: Euler-Maclaurin Summation



(a) EM with N=1

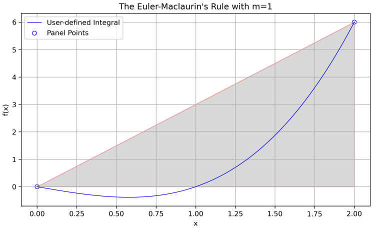


(b) EM with N=4

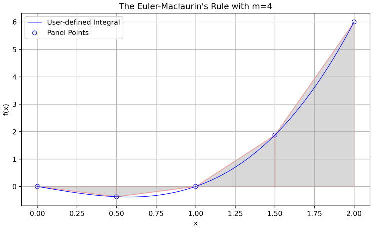


(c) EM with N=10

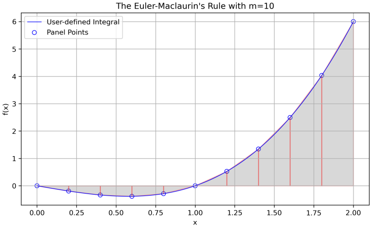
Example Plots for $x^3 - x$: Euler-Maclaurin Summation



(d) EM with N=1



(e) EM with N=4



(f) EM with N=10

References I

- Burden, Richard L. and J. Douglas Faires. *Numerical Analysis*. Fourth. The Prindle, Weber and Schmidt Series in Mathematics. Boston: PWS-Kent Publishing Company, 1989.
- DeVries, P.L. and J. Hasbun. *A First Course in Computational Physics*. Jones & Bartlett Learning, 2011. ISBN: 9780763773144. URL: https://books.google.com.tr/books?id=X3FEPiebLH0C.
- Winnicka, Alicja. "Comparison of numerical integration methods". In: *System (Linköping)*. 2019. URL: https://api.semanticscholar.org/CorpusID:261824322.

Questions?