Babes-Bolyai University Cluj-Napoca

Faculty of Mathematics and Computer Science

Specialization: Mathematics and Computer Science

BACHELOR'S THESIS

Theme: Numerical integration methods

Kohan Alexandru

Assoc. Prof. Cătinaş Teodora

2022

Universitatea Babeş-Bolyai

Facultatea de Matematică şi Informatică

Specializare: Matematică şi Informatică

LUCRARE DE LICENŢĂ

Temă: Metode de integrare numerică

Kohan Alexandru

Assoc. Prof. Cătinaş Teodora

2022

1 Differentiation

This formula demonstrates how to generate a good estimate of $f'(x_0)$

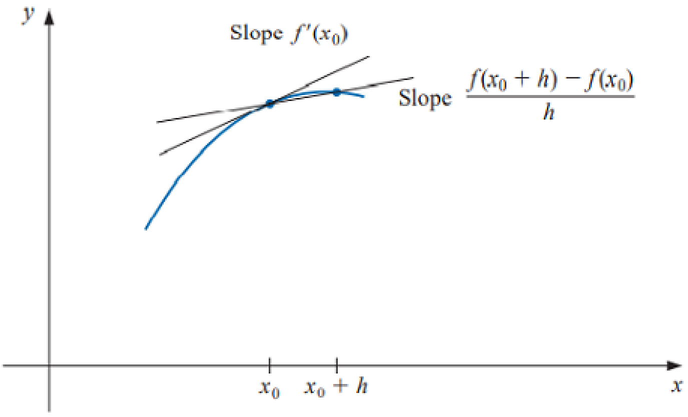
$$\frac{f(x_0+h)-f(x_0)}{h} \quad [8]$$

Example: Using h = 0.2, h = 0.1, and h = 0.02, approximate the derivative of $f(x) = 1/x$ at $x_0 = 2.3$ using the forward-difference formula, and calculate bounds for the approximation errors.

Solution

$$\frac{f(2.3+h)-f(2.3)}{h}$$

Figure 1:



with h = 0.2 gives

$$\frac{1/2.5-1/2.3}{0.2} = \frac{0.4-0.434}{0.2} = -0.17$$

Because $f''(x) = 2/x^3$ and $2.3 < \xi < 2.5$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h*2|}{2\xi^3} < \frac{0.2}{2.3^3} = 0.01643$$

with h = 0.1 gives

$$\frac{1/2.4 - 1/2.3}{0.1} = \frac{0.416 - 0.434}{0.1} = -0.18$$

$$\frac{|hf''(\xi)|}{2} = \frac{|h * 2|}{2\xi^3} < \frac{0.1}{2.3^3} = 0.00821$$

with h = 0.02 gives

$$\frac{1/2.32 - 1/2.3}{0.02} = \frac{0.431 - 0.434}{0.02} = -0.15$$

$$\frac{|hf''(\xi)|}{2} = \frac{|h * 2|}{2\xi^3} < \frac{0.02}{2.3^3} = 0.00164$$

Table 1:

h	f(2.3+h)	$\frac{f(2.3+h)-f(2.3)}{h}$	$\frac{\|h\|}{2.3^3}$
0.2	0.4	-0.17	0.01643
0.1	0.416	-0.18	0.00821
0.02	0.431	-0.15	0.00164

2 Weighted-mean-value

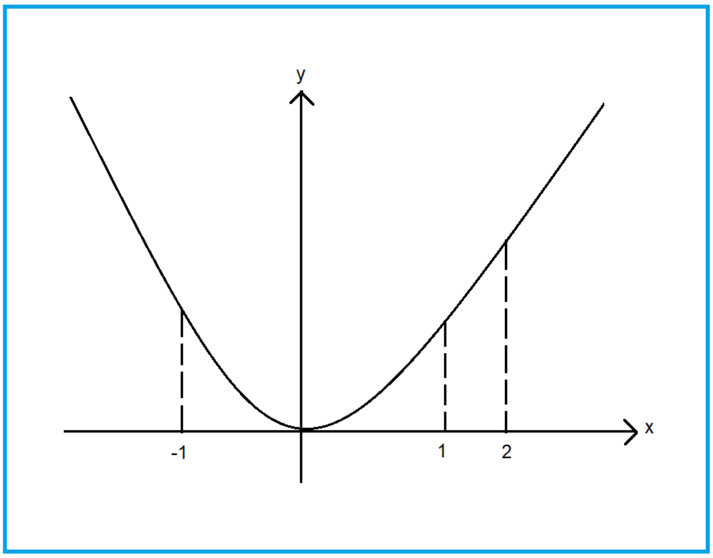
Definition 2.1 *Assume that $f \in C[a,b]$, that the Riemann integral of g exists on [a, b], and that g(x) does not change sign on [a, b]. Then there exists a number c in (a, b) with*

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx \quad [8]$$

When $g(x) \equiv 1$, Theorem 2.1 is the usual Mean Value Theorem for Integrals. It calculates the average value of the function f over the interval [a, b] as (See Figure 2.)

$$f(c) = \frac{1}{b-a}\int_a^b f(x)dx \quad [8]$$

Example: Apply Weighted Mean Value Theorem for Integrals to determine which x values the function f(x) $= 1 + x^2$ have the average value over the interval [-1,2]



There is a number c in [-1,2] such that

$$f(c) = \frac{1}{b-a}\int_a^b f(x)dx$$

$$h_{avg} = \frac{Area}{Width}$$

$$f(c) = f_{avg} = \frac{1}{2-(-1)}\int_{-1}^{2}(1+x^2)dx$$

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

$$= \frac{1}{3}\left[3 + \frac{9}{3}\right] = \frac{1}{3}\left[3+3\right] = \frac{6}{3} = 2$$

$$f(c) = f_{avg} = 2$$

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

$$f(c) = 2 = 1 + c^2$$

$$c^2 = 1$$

$$c = \pm\sqrt{1} = \pm 1$$

3 Trapezoidal vs Simpson

Trapezoidal Rule:

$$\int_a^b f(x)dx = \frac{h}{2}\left[f\left(x_0\right)+f\left(x_1\right)\right]-\frac{h^3}{12}f''(\xi) \quad [8]$$

Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f\left(x_0\right)+4f\left(x_1\right)+f\left(x_2\right)\right]-\frac{h^5}{90}f^{(4)}(\xi) \quad [8]$$

Example: Compare the Trapezoidal rule and Simpson's rule approximations to $\int_1^3 f(x)dx$ when f(x) is x^3

Solution on [1, 3] the Trapezoidal and Simpson's rule have the forms

$$Trapezoid: \int_1^3 f(x)dx \approx f(1)+f(3)$$

and

$$Simpson's: \int_1^3 f(x)dx \approx \frac{1}{3}[f(1)+4f(2)+f(3)].$$

When $f(x)=x^3$ they give

Let $\xi = 2$ in (1, 3)

$$\text{Trapezoid: } \int_1^3 f(x)dx \approx 1^3+3^3=28 \text{ and}$$

$$\text{Simpson's: } \int_1^3 f(x)dx \approx \frac{1}{3}\left[\left(1^3\right)+4\cdot 2^3+3^3\right]=20.$$

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^3$

Table 2 summarizes the findings for the function in three locations. It's worth noting that Simpson's Rule is far superior.

Table 2:

$f(x)$	x^3
Exact value	20
Trapezoidal	28
Simpson's	20

4 Composite-Rules

Both rules are obtained by applying the simplest kind of interpolation on subintervals of the decomposition

$$a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b, \quad x_k = a + kh, \quad h = \frac{b-a}{n}$$

of the interval $[a, b]$. [6]

The composite trapezoidal rule:

$$\int_a^b f(x)dx = h\left(\frac{1}{2}f_0 + f_1 + \cdots + f_{n-1} + \frac{1}{2}f_n\right) - \frac{1}{12}h^3 \sum_{k=0}^{n-1} f''\left(\xi_k\right) \quad [6]$$

<u>**Example**</u> The following integral is given:

$$\int_{1.3}^{4.3} 5xe^{-2x}dx$$

a) Estimate the value of this integral using the composite trapezoidal rule. Three segments should be used.

b) Find the true error E_t for part (a).

$$a) \int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a) + 2\sum_{i=1}^{n-1} f(a+ih) + f(b)\right]$$

$$h = \frac{b-a}{n} = \frac{4.3-1.3}{3} = 1$$

$$\int_{1.3}^{4.3} f(x)dx \simeq \frac{1}{2}\left[f(1.3) + 2\sum_{i=1}^{3-1} f(1.3+i\cdot 1) + f(4.3)\right]$$

$$= \frac{1}{2}\left[f(1.3) + 2\sum_{i=1}^{2} f(1.3+i\cdot 1) + f(4.3)\right]$$

$$= \frac{1}{2}\left[f(1.3) + 2f(1.3+(1)\cdot 1) + 2f(1.3+(2)\cdot 1) + f(4.3)\right]$$

$$= 0.5[f(1.3) + 2f(2.3) + 2f(3.3) + f(4.3)]$$

$$= 0.5\left[5(1.3)e^{-2(1.3)} + 2(5)(2.3)e^{-2(2.3)} + 2(5)(3.3)e^{-2(3.3)} + 5(4.3)e^{-2(4.3)}\right] =$$

$$= 0.5\left[0.4827 + 0.2311 + 0.0448 + 0.0039\right]$$

$$= 0.3812$$

$$b) \int_{1.3}^{4.3} 5xe^{-2x}dx = 0.3320$$

$$E_t = 0.3320 - 0.3812 = -0.0492$$

Composite Simpson Rule

For the composite Simpson rule we have

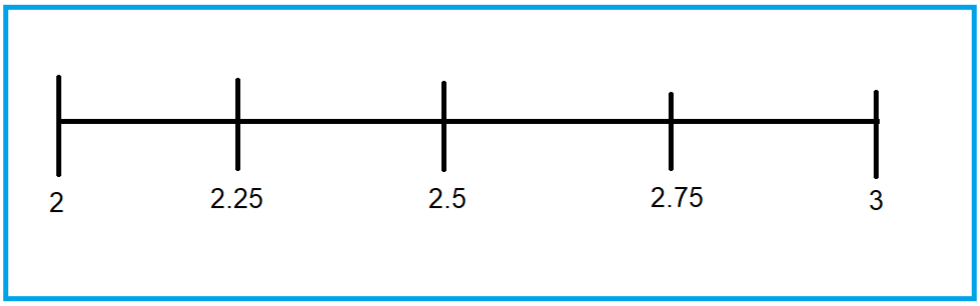
$$\int_a^b f(x)dx = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f_n\right) + R_{2,n}(f) \quad [6]$$

with

$$R_{2,n}(f) = -\frac{1}{180}(b-a)h^4 f^{(4)}(\xi) = -\frac{(b-a)^5}{2880n^4} f^{(4)}(\xi), \quad \xi \in (a,b) \quad [6]$$

Example The integral is as follows: $\int_2^3 x^2 dx$ and n=4. Using composite

Simpson's Rule, find the value of the integral.



When n=4 then $h = \frac{3-2}{4}$. The approximation is:

$$\int_2^3 x^2 dx \approx \frac{1/4}{3}\left[y_0 + y_4 + 4\left(y_1 + y_3\right) + 2y_2\right] =$$

$$= \frac{0.25}{3}[f(2) + f(3) + 4\{f(2.75) + f(2.25)\} + 2f(2.5)] =$$

$$= \frac{0.25}{3}[4 + 9 + 4(7.5625 + 5.0625) + 2 \cdot 6.25] =$$

$$= \frac{0.25}{3} \cdot 76 =$$

$$= 6.333$$

5 Closed-Newton-Cotes

n=1: Trapezoidal Rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}\left[f\left(x_0\right) + f\left(x_1\right)\right] - \frac{h^3}{12}f''(\xi) \quad [8]$$

Example: Aproximate the integral $\int_0^{\pi/4} \cos x dx$ using Closed Newton Cotes with n=1.

$$\int_0^{\pi/4} \cos x dx \approx 0.70710$$

$$\int_0^{\pi/4} \cos x dx = \frac{h}{2}\left[f\left(x_0\right) + f\left(x_1\right)\right]$$

$$= \frac{\pi/4}{2}[\cos(0) + \cos(\pi/4)]$$

$$\approx 0.67037$$

6 Open-Newton-Cotes

n=0: Midpoint Rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf\left(x_0\right) + \frac{h^3}{3}f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1 \quad [8]$$

Example: Aproximate the integral $\int_0^{\pi/3} \cos x dx$ using Open Newton Cotes with n=0.

$$\int_0^{\pi/3} \cos x dx \approx 0.866025$$

$$I = 2hf\left(x_0\right)$$

$$h = \frac{b-a}{n+2} = \frac{\pi/3 - 0}{2} = \pi/6$$

$$x_0 = a + h = 0 + \pi/6$$

$$x_0 = \pi/6$$

$$I = 2(\pi/6)\cos(\pi/6) \approx 0.90689$$

7 Adaptive Quadrature

Assume that we need to approximate $\int_a^b f(x)dx$ to within a certain tolerance $\epsilon > 0$. The first step is to use Simpson's rule with step size h = (b - a)/2.

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90}f^{(4)}(\xi), \quad \text{for some } \xi \text{ in } (a,b) \quad [8]$$

where the Simpson's rule approximation on [a, b] is denoted by

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)] \quad [8]$$

This implies that $S(a,(a+b)/2) + S((a+b)/2, b)$ approximates $\int_a^b f(x)dx$ about 15 times better than it agrees with the computed value S(a, b). Thus, if

$$\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\varepsilon \quad [8]$$

we expect to have

$$\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < \varepsilon \quad [8]$$

and

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) \quad [8]$$

is expected to be a sufficiently accurate approximation to $\int_a^b f(x)dx$.

Example: Examine the error estimate's accuracy when applied to the integral:

$$\int_0^{\pi/4} \cos x dx = \frac{\sqrt{2}}{2}$$

by comparing

$$\frac{1}{15}\left|S\left(0,\frac{\pi}{4}\right)-S\left(0,\frac{\pi}{8}\right)-S\left(\frac{\pi}{8},\frac{\pi}{4}\right)\right| \quad \text{to} \quad \left|\int_0^{\pi/4}\cos x dx - S\left(0,\frac{\pi}{8}\right)-S\left(\frac{\pi}{8},\frac{\pi}{4}\right)\right|.$$

We have

$$S\left(0,\frac{\pi}{4}\right)=\frac{\pi/8}{3}\left[\cos 0+4\cos\frac{\pi}{8}+\cos\frac{\pi}{4}\right]=\frac{\pi}{24}\cdot 5.4026249=0.707201$$

and

$$S\left(0,\frac{\pi}{8}\right)+S\left(\frac{\pi}{8},\frac{\pi}{4}\right)=\frac{\pi/16}{3}\left[\cos 0+4\cos\frac{\pi}{16}+2\cos\frac{\pi}{8}+4\cos\frac{3\pi}{16}+\cos\frac{\pi}{4}\right]$$
$$=0.707112.$$

So

$$\left|S\left(0,\frac{\pi}{4}\right)-S\left(0,\frac{\pi}{8}\right)-S\left(\frac{\pi}{8},\frac{\pi}{4}\right)\right|=|0.707201-0.707112|=0.002145293$$

The estimate for the error obtained when using S(a,(a+b))+S((a+b), b) to approximate $\int_a^b f(x)$ is consequently

$$\frac{1}{15}\left|S\left(0,\frac{\pi}{2}\right)-S\left(0,\frac{\pi}{4}\right)-S\left(\frac{\pi}{4},\frac{\pi}{2}\right)\right|=0.000089$$

which closely approximates the actual error

$$\left|\int_0^{\pi/4}\cos x dx-0.707112\right|=0.00000521$$

References

[1] C.H. Edwards - The Historical Development of the Calculus (p. 99)- Springer-Verlag

[2] Daffodil International University: Application of numerical integration and differentiation in real life, https://www.slideshare.net/ashaf15-7473/application-of-numerical-integration-and-differentiation-in-real-life

[3] Felix Klein - Elementary Mathematics from an Advanced Standpoint. Arithmetic, Algebra, Analysis (p. 209) - Dover Publications

[4] Gheorghe Coman, Ioana Chiorean, Teodora Cătinaş: Numerical Analysis. An Advanced Course.

[5] Petronas Twin Towers, https://www.petronastwintowers.com.my/design-and-structures/

[6] Radu T. Trîmbiţaş: Numerical Analysis in MATLAB, Cluj-Napoca, July 2008

[7] Radu T. Trîmbiţaş: Romberg.m electronic file

[8] Richard L. Burden, J. Douglas Faires: Numerical Analysis, 2010

[9] The Volume of a wine barrel, http://www.matematicasvisuales.com/english/html/history/kepler/keplerbarrel.html

[10] https://www.youtube.com/watch?v=Dx7fDb6boRA&ab_channel=numericalmethodsguy

[11] https://www.chegg.com/homework-help/use-composite-simpson-s-rule-approximate-integrals-exercise-chapter-4.4-problem-3e-solution-9781305253667-exc

[12] https://www.youtube.com/watch?v=ts-zBjsqiX0&ab_channel=DrSajjadKhanMathAcademy