Babes-Bolyai University Cluj-Napoca

Faculty of Mathematics and Computer Science

Specialization: Mathematics and Computer Science

BACHELOR'S THESIS

Theme: Numerical integration methods

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Facultatea de Matematică şi Informatică

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LUCRARE DE LICENŢĂ

Temă: Metode de integrare numerică

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1 Differentiation

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

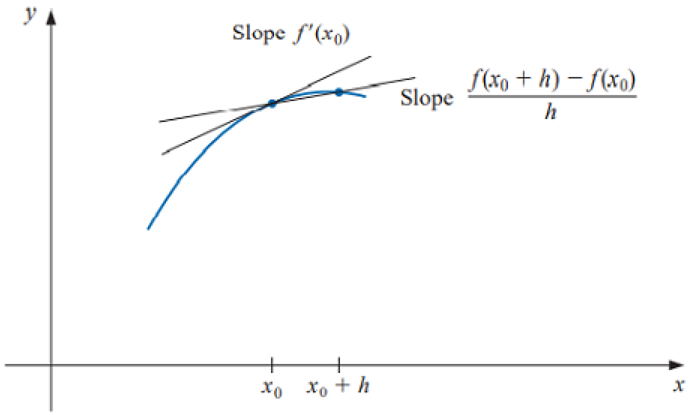
$$\frac{f(x_0+h)-f(x_0)}{h} \quad [8]$$

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)	$\frac{f(2.3+h)-f(2.3)}{h}$	$\frac{\lvert h\rvert}{2.3^3}$
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

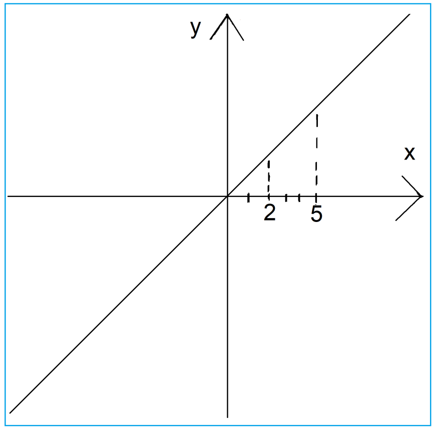
Definition 2.1 *Assume that* $f \in C[a,b]$ *, that the Riemann integral of g exists on [a, b], and that g(x) does not change sign on [a, b]. Then there exists a number c in (a, b) with*

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

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

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

Example: Apply Weighted Mean Value Theorem for Integrals to determine which x values the function f(x) $= 2 \cdot x$ have the average value over the interval [2,5]



There is a number c in [2,5] such that

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

$$f(c) = f_{avg} = \frac{1}{5-2}\int_2^5 (2\cdot x)dx$$

$$= \frac{1}{3}\left[\frac{2\cdot x^2}{2}\right]_2^5 = \frac{1}{3}\left[25-4\right]$$

$$= \frac{21}{3}$$

$$f(c) = f_{avg} = \frac{21}{3}$$

$$f(x) = 2\cdot x$$

$$f(c) = \frac{21}{3} = 2\cdot c$$

$$c = \frac{21}{6}$$

3 Trapezoidal vs Simpson

Trapezoidal Rule:

Let $x_0 = a, x_1 = b, h = b - a.$

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

Simpson's Rule:

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

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

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

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

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

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:

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

Example 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

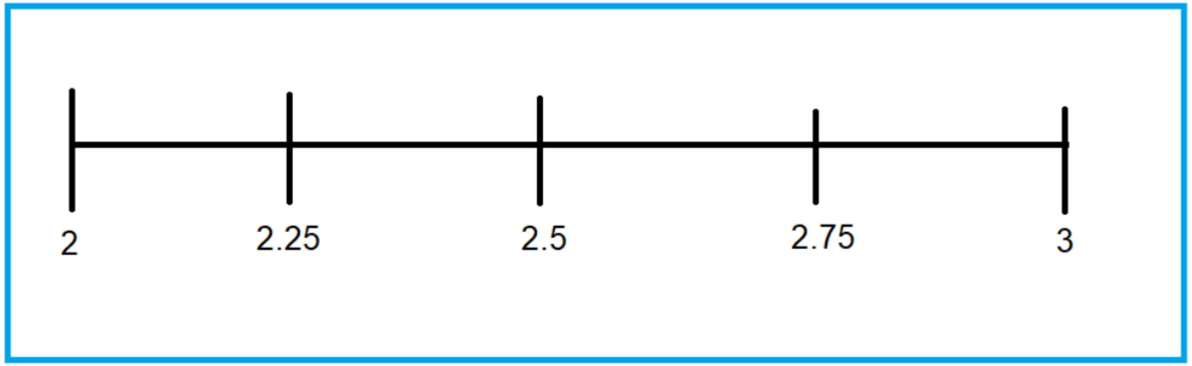
For the composite Simpson rule we have

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

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: $\int_2^3 x^2dx$ 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:

$$\begin{aligned}
\int_2^3 x^2 dx &\approx \frac{1/4}{3}\left[y_0 + y_4 + 4\left(y_1 + y_3\right) + 2y_2\right] = \\
&= \frac{0.25}{3}[f(2) + f(3) + 4\{f(2.75) + f(2.25)\} + 2f(2.5)] = \\
&= \frac{0.25}{3}[4 + 9 + 4(7.5625 + 5.0625) + 2 \cdot 6.25] = \\
&= \frac{0.25}{3} \cdot 76 = \\
&= 6.333
\end{aligned}$$

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

We set $x_{-1} = a$ and $x_{n+1} = b$.

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

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.

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

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

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

$S(a,(a+b)/2) + S((a+b)/2,b)$ 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

$$S\left(0,\frac{\pi}{4}\right) = \frac{\pi/8}{3}\left[\cos 0 + 4\cos\frac{\pi}{8} + \cos\frac{\pi}{4}\right] = \frac{\pi}{24}\cdot 5.4026249 = 0.70720194713$$

and

$$S\left(0,\frac{\pi}{8}\right) + S\left(\frac{\pi}{8},\frac{\pi}{4}\right) = \frac{\pi/16}{3}\left[\cos 0 + 4\cos\frac{\pi}{16} + 2\cos\frac{\pi}{8} + 4\cos\frac{3\pi}{16} + \cos\frac{\pi}{4}\right]$$
$$= 0.707112647.$$

So

$$\left|S\left(0,\frac{\pi}{4}\right) - S\left(0,\frac{\pi}{8}\right) - S\left(\frac{\pi}{8},\frac{\pi}{4}\right)\right| = |0.70720194713 - 0.707112647| = 0.00008930013$$

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

$$\frac{1}{15}\left|S\left(0,\frac{\pi}{4}\right) - S\left(0,\frac{\pi}{8}\right) - S\left(\frac{\pi}{8},\frac{\pi}{4}\right)\right| = 0.00000595334$$

which closely approximates the actual error

$$\left|\int_0^{\pi/4} \cos x dx - 0.707112\right| = 0.00000586581$$

8 Aplications

Most of the results of this section can be found in [6].

Computation of an ellipsoid surface

Consider an ellipsoid obtained by rotating the ellipse in Figure 2 around the x axis. The radius ρ is described as a function of axial coordinate by the equation

$$\rho^2(x) = \alpha^2\left(1 - \beta^2 x^2\right), \quad -\frac{1}{\beta} \leq x \leq \frac{1}{\beta}$$

where α and β are such that $\alpha^2\beta^2 < 1$

For test we chose the following values for the parameters: $\alpha = (\sqrt{2} - 1)/10, \beta = 10$

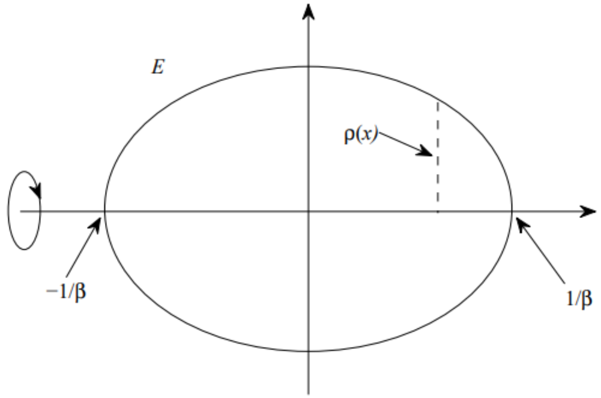
The surface is given by

$$I(f) = 4\pi\alpha \int_0^{1/\beta} \sqrt{1 - K^2 x^2}\, \mathrm{d}x$$

where $K^2 = \beta^2\sqrt{1 - \alpha^2\beta^2}$. An adaptive quadrature is gonna be applied.

We can compute the exact value and its floating point approximation using Symbolic Math Toolbox:

Figure 2:




```
clear
syms alpha beta K2 s2 x f vI
s2=sqrt(sym(2));
alpha=(s2-1)/10;
beta=sym(10);
K2=beta^2*sqrt(1-alpha^2*beta^2);
f=sqrt(1-K2*x^2);
vI=4*sym(pi)*alpha*int(f,0,1/beta)
vpa(vI,16)
```

The results are:

vI =

1/2 1/2 1/2 1/2 1/2

1/100 pi (-2 (-(-2 + 2 2) + 1) + 2 (-(-2 + 2 2)

1/2 1/2 1/2 3/4 1/2 1/4

+ 1) 2 + (-2 + 2 2) asin((-2 + 2 2)))

ans = 0.042347520940824 34

The next script approximates the surface with a tolerance of 1e-8 using the following functions: Romberg, adquad, and MATLAB quad and quadl.

```
err=1e-8;
beta=10;
alpha=(sqrt(2)-1)/10;
alpha2=alpha^2;
beta2=beta^2;
K2=beta2*sqrt(1-alpha2*beta2);
f=@(x) sqrt(1-K2*x.^2);
fpa=4*pi*alpha;
[vi(1), nfe (1) ] = Romberg (f,0,1/ beta, err, 100);
[vi(2),nfe(2)] = adquad (f,0,1/ beta, err );
[vi(3), nfe (3) ] = quad (f,0,1/beta, err)
```

$[\text{vi}(4), \text{nfe}(4)] = quadl(f, 0, 1/\text{ beta, err })$

vi=fpa*vi;

meth='Romberg','adquad','quad','quadl';

for i=1:4

fprintf('%8s %18.16f %3d\n',methi,vi(i),nfe(i))

end

Here is the output:

Romberg 0.0423475209214685 129

adquad 0.0423475209189811 65

quad 0.0423475203088494 37

quadl 0.0423475209279265 48

Romberg method is inferior to adaptive quadratures. Surprisingly, quad beats quadl.

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