2 Examples for Lectures 7 – 8 (Numerical integration of functions)

Example 2.1 • For theory, see Lecture 7, pp. 9–15.

Compute the integral $I = \int\limits_0^{\frac{\pi}{4}} \sin x \, dx$ *using*

- *the trapezoidal rule*

  The trapezoidal rule is

$$\int\limits_a^b f(x)\,dx = \frac{b-a}{2}\left[f(a)+f(b)\right] + R(f)$$

  with

$$R(f) = -\frac{(b-a)^3}{12} f''(\xi), \ \ \xi \in (a,b).$$

  So,

$$I = \frac{\frac{\pi}{4}-0}{2}\left(\sin 0 + \sin\frac{\pi}{4}\right) = \frac{\pi}{8}\cdot\frac{\sqrt{2}}{2} = \frac{\pi\sqrt{2}}{16} \approx 0.277680183634898.$$

- *Simpson's rule*

  The Simpson's rule is

$$\int\limits_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right] + R(f)$$

  with

$$R(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi), \ \ \xi \in (a,b).$$

  So,

$$I = \frac{\frac{\pi}{4}-0}{6}\left(\sin 0 + 4\sin\frac{0+\frac{\pi}{4}}{2} + \sin\frac{\pi}{4}\right) = \frac{\pi}{24}\cdot\left(4\sin\frac{\pi}{8}+\frac{\sqrt{2}}{2}\right) \approx 0.292932637839748$$

The exact value is 0.2928932188134525.

Example 2.2 *Compute the integral* $\int_0^{\frac{\pi}{2}} \sin x \, dx$ *using the rectangle (midpoint) formula.*
The rectangle (midpoint) formula is

$$\int_a^b f(x)\,dx = (b-a) f\left(\frac{a+b}{2}\right) + R(f)$$

with

$$R(f) = \frac{(b-a)^3}{24} f''(\xi), \ \xi \in (a,b).$$

So,

$$\int_0^{\frac{\pi}{2}} \sin x\,dx = \left(\frac{\pi}{2}-0\right)\sin\left(\frac{0+\frac{\pi}{2}}{2}\right) = \frac{\pi}{2}\sin\frac{\pi}{4} = \frac{\pi\sqrt{2}}{4} \approx 1.11072073454$$

The actual value is $\cos 0 = 1$.

Example 2.3 *Does the trapezoidal rule reproduce for the integral* $\int\limits_0^2 3x\,dx$ *the exact value?*

Answer: Yes, because trapezoidal rule has the degree of precision 1, which means it gives the exact value for linear polynomials (=polynomials of degree 1).
Check:

$$\int\limits_0^2 3x\,dx = \frac{2-0}{2}(3\cdot 0 + 3\cdot 2) = 6 \text{ (with trapezoidal rule)}$$

$$\int_0^2 3x\,dx = 3\frac{x^2}{2}\Big|_0^2 = 3\frac{2^2}{2} - 3\frac{0^2}{2} = 6 \text{ (with usual computations).}$$

Remark 2.4 *The Simpson's rule has the degree of precision 3, which means that for polynomials of maximum degree 3, the formula returns the exact value.*

Example 2.5

$$\text{Simpson: } \int_1^2 (2x^3+3x)\,dx = \frac{2-1}{6}\left[\left(2\cdot 1^3+3\cdot 1\right)+4\cdot\left(2\cdot\left(\frac{3}{2}\right)^3+3\cdot\frac{3}{2}\right)+\left(2\cdot 2^3+3\cdot 2\right)\right] = \frac{1}{6}\cdot 72 = 12$$

$$\text{normal computation: } \int_1^2 (2x^3+3x)\,dx = \left(2\frac{x^4}{4}+3\frac{x^2}{2}\right)\Big|_1^2 = \left(2\frac{2^4}{4}+3\frac{2^2}{2}\right)-\left(2\frac{1^4}{4}+3\frac{1^2}{2}\right) = 8+6-\frac{1}{2}-\frac{3}{2} = 12.$$

Remark 2.6 *The remainder in each case also tells us about the degree of precision. Since in trapezoidal rule the remainder contains f'', it will be 0 for polynomials of maximum degree 1. The same happens in the rectangle rule. In the Simpson's rule, since we have $f^{(4)}$, the 4th derivative of polynomials of maximum degree 3 will be 0, so the degree of precision will be 3.*

Remark 2.7 *Other examples for trapezoidal, rectangle and Simpson formulas are found in Lecture 7, pp. 16–17.*

Example 2.8 *Compute $I = \int_1^2 \ln x\,dx$ using the composite (repeated) trapezoidal rule, for $n = 3$.*

The repeated trapezoidal rule is

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a)+2(f_1+\ldots+f_{n-1})+f(b)\right]+R_n(f)$$

with

$$R_n(f) = -\frac{h^2(b-a)}{12}f''(\xi),\quad \xi\in(a,b)$$

and

$$f_i = f(x_i),\quad x_i = a+ih,\quad h=\frac{b-a}{n},\quad i=\overline{0,n}.$$

We have: $i=\overline{0,3}$, $h=\frac{1}{3}$, $x_0=1$, $x_1=\frac{4}{3}$, $x_2=\frac{5}{3}$, $x_3=2$, $f(x)=\ln x$ and

$$I = \frac{1}{2\cdot 3}\left[\ln(1)+2\ln\left(\frac{4}{3}\right)+2\ln\left(\frac{5}{3}\right)+\ln(2)\right] = \frac{1}{6}\ln\left(\frac{16}{9}\cdot\frac{25}{9}\cdot 2\right) = \frac{1}{6}\ln\left(\frac{800}{81}\right)\approx 0.381693762165915.$$

The exact value is 0.3862943611198906.

Example 2.9 *Compute $I = \int_0^1 \frac{1}{1+x}\,dx$ using the composite (repeated) Simpson's rule and $n = 4$.*

The repeated Simpson's formula is

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a)+4\sum_{i=1}^{m} f_{2i-1}+2\sum_{i=1}^{m-1} f_{2i}+f(b)\right]+R_n(f)$$

with

$$R_n(f) = -\frac{h^4(b-a)}{180}f^{(4)}(\xi),\quad \xi\in(a,b)$$

and

$$f_i = f(x_i),\ x_i = a + ih,\ h = \frac{b-a}{n},\ i = \overline{0,n},\ \mathbf{n = 2m}.$$

We have: $m = 2$, $h = \frac{1-0}{4} = \frac{1}{4}$, $i = \overline{0,4}$, $x_0 = 0$, $x_1 = \frac{1}{4}$, $x_2 = \frac{1}{2}$, $x_3 = \frac{3}{4}$, $x_4 = 1$, $f(x) = \frac{1}{1+x}$ and

$$\begin{aligned}
I &= \frac{1}{4\cdot 3}\left[f(0) + 4\sum_{i=1}^{2} f_{2i-1} + 2\sum_{i=1}^{1} f_{2i} + f(1)\right] = \\
&= \frac{1}{12}\left[f(0) + 4\cdot(f_1 + f_3) + 2f_2 + f(1)\right] = \frac{1}{12}\left[1 + 4\left(\frac{1}{1+\frac{1}{4}} + \frac{1}{1+\frac{3}{4}}\right) + 2\cdot\frac{1}{1+\frac{1}{2}} + \frac{1}{2}\right] \\
&= \frac{1}{12}\left(\frac{3}{2} + \frac{16}{5} + \frac{16}{7} + \frac{4}{3}\right) = \frac{1}{12}\cdot\frac{1747}{210} \approx 0.693253968253968.
\end{aligned}$$

The exact value is $\ln 2 = 0.69314718056$.

Example 2.10 *Compute the integral $I = \int_1^2 \ln x\, dx$ using the composite (repeated) rectangle (midpoint) formula for $n = 3$.*

The repeated rectangle (midpoint) formula is

$$\int_a^b f(x)\, dx = h\sum_{i=0}^{n-1} f\left(a + \left(i + \frac{1}{2}\right)h\right) + R_n(f)$$

with

$$R_n(f) = \frac{h^2(b-a)}{24} f''(\xi),\ \xi \in (a,b)$$

and

$$h = \frac{b-a}{n}.$$

We have $h = \frac{1}{3}$ and

$$\begin{aligned}
I &= \frac{1}{3}\left[f\left(1 + \frac{1}{2}\cdot\frac{1}{3}\right) + f\left(1 + \frac{3}{2}\cdot\frac{1}{3}\right) + f\left(1 + \frac{5}{2}\cdot\frac{1}{3}\right)\right] = \\
&= \frac{1}{3}\left[f\left(\frac{7}{6}\right) f\left(\frac{9}{6}\right) + f\left(\frac{11}{6}\right)\right] = \frac{1}{3}\left(\ln\frac{7}{6} + \ln\frac{9}{6} + \ln\frac{11}{6}\right) = \frac{1}{3}\ln\left(\frac{693}{216}\right) \approx 0.38858386383.
\end{aligned}$$

The exact value is 0.3862943611198906.

Remark 2.11 *Other examples for repeated trapezium, repeated Simpson, repeated rectangle formulas are found in Lecture 7, pp. 17.*

The degree of exactness of a quadrature formula

$$\int_a^b f(x)\, dx = \sum_{k=0}^{m} A_k f(x_k) + R(f)$$

is n **if**:

- each $R(e_j) = 0$, for all $j = 0, 1, \ldots, n$ and $R(e_{n+1}) \neq 0$, where:
  - * $e_m(x) = x^m$;
  - * $R(e_j) = \int_a^b x^j\, dx - \sum_{k=0}^{m} A_k e_j(x_k)$

Practically, it reproduces exact the polynomials of maximum degree n.

Example 2.12 *Determine n such that the approximation error for the integral $\int_0^{\pi} \sin(x)\, dx$ is less than $2 \cdot 10^{-5}$ using*

a) *composite trapezoidal rule*

$a = 0,\ b = \pi,\ h = \frac{\pi}{n}$. The remainder should be less than $2 \cdot 10^{-5}$, so

$$|R(f)| < 2 \cdot 10^{-5}$$

For the remainder we need f''. $f'(x) = \cos(x)$ and $f''(x) = -\sin(x)$, so

$$|R(f)| = \left| -\frac{h^2(b-a)}{12} f''(\xi) \right| = \left| \frac{\pi^3}{12n^2}(-\sin(\xi)) \right| = \frac{\pi^3}{12n^2} |\sin(\xi)|$$

Since $\xi \in [0, \pi]$, to ensure that the inequality holds for every point of the interval, we can find n from

$$|R(f)| \leq \frac{\pi^3}{12n^2} \max_{x \in [0,\pi]} |\sin(x)| < 2 \cdot 10^{-5}$$

Now we work with the second inequality. $\max\limits_{x \in [0,\pi]} |\sin(x)| = 1$ which gives us

$$\frac{\pi^3}{12n^2} < \frac{2}{10^5} \implies \frac{12n^2}{\pi^3} > \frac{10^5}{2} \implies n^2 > \pi^3 \frac{10^5}{24} \approx 129192.8 \implies n = 360.$$

b) *composite Simpson's rule*

For the remainder in this case we need $f^{(4)}$. $f'(x) = \cos(x)$ and $f''(x) = -\sin(x)$, $f'''(x) = -\cos(x)$, $f^{(4)}(x) = \sin(x)$, so

$$|R(f)| = \left| -\frac{h^4(b-a)}{180} f^{(4)}(\xi) \right| = \frac{\pi^5}{180n^4} |\sin(\xi)|$$

Since $\xi \in [0, \pi]$, to ensure that the inequality holds for every point of the interval, we can find n from

$$|R(f)| \leq \frac{\pi^5}{180n^4} \max_{x \in [0,\pi]} |\sin(x)| < 2 \cdot 10^{-5}$$

Now we work with the second inequality. $\max\limits_{x \in [0,\pi]} |\sin(x)| = 1$ which gives us

$$\frac{\pi^5}{180n^4} < \frac{2}{10^5} \implies \frac{180n^4}{\pi^5} > \frac{10^5}{2} \implies n^4 > \pi^5 \frac{10^5}{360} \approx 85005.4 \implies n = 18.$$

Example 2.13 *Approximate $\ln 2$ with two correct decimals, using the repeated rectangle formula.*

Again we need to work with the remainder, and to obtain 2 correct decimals (see Lecture 1, pp. 12–13), we impose

$$|R(f)| < \frac{1}{2} \cdot 10^{-2}.$$

Furthermore, we need to determine the integral whose result is $\ln 2$, to obtain the function we will work with. For example, we can consider

$$\ln 2 = \int_1^2 \frac{1}{x}\, dx$$

so, $f(x) = \frac{1}{x},\ a = 1,\ b = 2,\ h = \frac{1}{n}$. This implies

$$\left| \frac{h^2(b-a)}{24} f''(\xi) \right| < \frac{1}{2} \cdot 10^{-2} \implies \frac{1}{24n^2} |f''(\xi)| < \frac{1}{2} \cdot 10^{-2}.$$

But for $\xi \in (1, 2)$:

$$\frac{1}{24n^2} |f''(\xi)| \leq \frac{1}{24n^2} \max_{x \in [1,2]} |f''(x)|$$

so we impose the condition

$$\frac{1}{24n^2}\max_{x\in[1,2]}|f''(x)| < \frac{1}{200}.$$

$f'(x) = -\frac{1}{x^2}$ and $f''(x) = \frac{2}{x^3} \implies \max\limits_{x\in[1,2]}|f''(x)| = 2$. We have:

$$\frac{2}{24n^2} < \frac{1}{200} \implies 12n^2 > 200 \implies n^2 > \frac{200}{12} = 16.(6) \implies n = 5.$$

$$\implies \ln 2 \approx \frac{1}{5}\left[f\left(\frac{11}{10}\right) + f\left(\frac{13}{10}\right) + f\left(\frac{15}{10}\right) + f\left(\frac{17}{10}\right) + f\left(\frac{19}{10}\right)\right] =$$
$$= \frac{1}{5}\left(\frac{10}{11} + \frac{10}{13} + \frac{10}{15} + \frac{10}{17} + \frac{10}{19}\right) = 0.69190788571.$$

$\ln 2 \approx 0.69314718056$.

Example 2.14 *Determine a quadrature formula of the form*

$$\int_{-1}^{1} f(x)\,dx = A_1 f(-1) + A_2 f(x_2) + A_3 f(1)$$

that has the degree of precision $d = 3$.

Since $d = 3$, the formula should be exact for polynomials of maximum degree 3. This means

$$R(e_0) = R(e_1) = R(e_2) = R(e_3) = 0,\ \ e_j = x^j. \tag{2.1}$$

$$\begin{cases} R(e_0) &= \int_{-1}^{1} e_0(x)\,dx - [A_1e_0(-1) + A_2e_0(x_2) + A_3e_0(1)] \\ R(e_1) &= \int_{-1}^{1} e_1(x)\,dx - [A_1e_1(-1) + A_2e_1(x_2) + A_3e_1(1)] \\ R(e_2) &= \int_{-1}^{1} e_2(x)\,dx - [A_1e_2(-1) + A_2e_2(x_2) + A_3e_2(1)] \\ R(e_3) &= \int_{-1}^{1} e_3(x)\,dx - [A_1e_3(-1) + A_2e_3(x_2) + A_3e_3(1)] \end{cases} \iff$$

$$\begin{cases} R(e_0) &= \int_{-1}^{1} 1\,dx - [A_1\cdot 1 + A_2\cdot 1 + A_3\cdot 1] \\ R(e_1) &= \int_{-1}^{1} x\,dx - [A_1\cdot(-1) + A_2x_2 + A_3\cdot 1] \\ R(e_2) &= \int_{-1}^{1} x^2\,dx - \left[A_1\cdot 1 + A_2x_2^2 + A_3\cdot 1\right] \\ R(e_3) &= \int_{-1}^{1} x^3\,dx - \left[A_1\cdot(-1) + A_2x_2^3 + A_3\cdot 1\right] \end{cases}$$

$$\xrightarrow{(2.1)} \begin{cases} A_1 + A_2 + A_3 = 2 \\ -A_1 + A_2x_2 + A_3 = 0 \\ A_1 + A_2x_2^2 + A_3 = \frac{2}{3} \\ -A_1 + A_2x_2^3 + A_3 = 0 \end{cases}$$

Remark 2.15 $e_0(1) = 1,\ e_0(x) = 1,$ *etc.* $e_1(x_1) = x_1,\ e_1(2) = 2,$ *etc.* $e_2(x_1) = x_1^2,\ e_2(2) = 2^2 = 4,$ *etc.*

From the 2nd and 4th eq. (substraction) we get

$$A_2x_2(1 - x_2^2) = 0.$$

$1 - x_2^2$ cannot be 0, because in this case x_2 would be 1 or -1 and the nodes should be distinct. So, we have either $A_2 = 0$ or $x_2 = 0$.

If we substract eq. (1) and (3), we have

$$A_2(1 - x_2^2) = \frac{4}{3}$$

so A_2 cannot be 0, which means that $x_2 = 0$. Then we get $A_2 = \frac{4}{3}$. From eq. (4) we have $A_1 = A_3$ (since $x_2 = 0$) and from eq. (1), $A_1 = A_3 = \frac{1}{3}$.

$$\implies \int_{-1}^{1} f(x)\,dx = \frac{1}{3}f(-1) + \frac{4}{3}f(0) + \frac{1}{3}f(1).$$

Example 2.16 *Evaluate $\int_1^3 \frac{1}{t}\,dt$ using Gauss-Legendre quadrature with $m = 3$.*

For the Legendre orthogonal polynomials, we have the weight function $w(x) = 1$ and the interval [-1,1].

We need first to transform the interval $[1,3]$ in $[-1,1]$.

We consider $x = t - 2 \implies t = x + 2,\ \ dt = dx$, so our integral becomes

$$I = \int_{-1}^{1} \frac{1}{x+2}\,dx.$$

The nodes of the quadrature are the zeros of the Legendre polynomial l_3 ($m = 3$) (see Lecture 8, pp. 14–15, Remark 3.10 and the table). We have

$$l_3(x) = \left[(x^2-1)^3\right]'''$$

$$\begin{aligned}
\left[(x^2-1)^3\right]' &= 3(x^2-1)^2 \cdot 2x = 6x(x^2-1)^2 \\
\left[(x^2-1)^3\right]'' &= \left[6x(x^2-1)^2\right]' = 6(x^2-1)^2 + 6x \cdot 2(x^2-1) \cdot 2x = 6(x^2-1)(5x^2-1) \\
\left[(x^2-1)^3\right]''' &= \left[6(x^2-1)(5x^2-1)\right]' = 6 \cdot 2x(5x^2-1) + 6(x^2-1) \cdot 10x = 24x(5x^2-3)
\end{aligned}$$

$$\implies l_3(x) = 24x(5x^2-3) = 0 \implies x_1 = -\sqrt{\frac{3}{5}},\ \ x_2 = 0,\ \ x_3 = \sqrt{\frac{3}{5}}.$$

For the coefficients A_1, A_2, A_3 we use the system (see Lecture 8, pp. 13, eq. (3.23)):

$$\begin{cases} A_1 + A_2 + A_3 = \mu_0 = \int_{-1}^{1} 1\,dx = 2 \\ A_1x_1 + A_2x_2 + A_3x_3 = \mu_1 = \int_{-1}^{1} x\,dx = 0 \\ A_1x_1^2 + A_2x_2^2 + A_3x_3^2 = \mu_2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3} \end{cases} \iff \begin{cases} A_1 + A_2 + A_3 = 2 \\ -\sqrt{\frac{3}{5}}A_1 + \sqrt{\frac{3}{5}}A_3 = 0 \\ \frac{3}{5}A_1 + \frac{3}{5}A_3 = \frac{2}{3} \end{cases}$$

From eq. (2) we have $A_1 = A_3$ and from eq. (3) we have $A_1 = A_3 = \frac{5}{9}$. Finally, from eq. (1) we have $A_2 = \frac{8}{9}$.

$$\implies I = \int_{-1}^{1} \frac{1}{x+2}\,dx \approx \frac{5}{9} \cdot f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} \cdot f(0) + \frac{5}{9} \cdot f\left(\sqrt{\frac{3}{5}}\right) \approx \frac{5}{9} \cdot \frac{1}{-\sqrt{\frac{3}{5}}+2} + \frac{8}{9} \cdot \frac{1}{0+2} + \frac{5}{9} \cdot \frac{1}{\sqrt{\frac{3}{5}}+2}$$

$$\implies I \approx 1.098039215686274.$$

The exact value is $\ln 3 = 1.098612288668110$.

- Other examples for Gauss quadratures are found in Lecture 8, pp. 11–12, 15.

Remark 2.17 *For examples of adaptive quadratures and Romberg's method, see Lecture 8, pp. 1–9 and what we have done at the lab.*