2 Examples for Lectures 6 – 9 (Numerical integration of functions)

Example 2.1 *Compute the integral* $I = \int_0^{\frac{\pi}{4}} \sin x \, dx$ *using*

- *the trapezium's formula*

  The trapezium's formula is

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\left[f(a)+f(b)\right] + R_1 f(x)$$

with

$$R_1 f(x) = -\frac{(b-a)^3}{12} f''(\xi), \ \ \xi \in (a,b).$$

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

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right] + R_2 f(x)$$

with

$$R_2 f(x) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi), \ \ \xi \in (a,b).$$

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 *Does trapezium's formula reproduce for the integral* $\int_0^2 3x\,dx$ *the exact value?*

Answer: Yes, because trapezium's formula has the degree of exactness 1, which means it gives the exact value for linear polynomials (=polynomials of degree 1).
Check:

$$\int_0^2 3x\,dx = \frac{2-0}{2}(3\cdot 0 + 3\cdot 2) = 6 \text{ (with trapezium's formula)}$$

$$\int_0^2 3x\,dx = 3\frac{x^2}{2}\bigg|_0^2 = 3\frac{2^2}{2} - 3\frac{0^2}{2} = 6.$$

Remark 2.3 *The Simpson's rule has the degree of exactness 3, which means that for polynomials of maximum degree 3, the formula returns the exact value.*

Example 2.4

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

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

Remark 2.5 *Other examples for trapezium and Simpson formulas are found in Course 7, slides 4–6.*

Example 2.6 *Compute* $I = \int_1^2 \ln x \, dx$ *with a precision of* $\epsilon = 10^{-2}$ *using the repetead trapezium's formula.*

The repetead trapezium's formula is

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

with

$$R_n(f) = -\frac{(b-a)^3}{12n^2} f''(\xi), \;\; \xi \in (a,b)$$

and

$$x_k = a + kh, \;\; h = \frac{b-a}{n}, \;\; k = \overline{0,n}.$$

For our problem, since the precision should be attained, we first have to find n. We find it from

$$|R_n(f)| \le \frac{(b-a)^3}{12n^2} M_2 f, \quad \text{with } M_2 f = \max_{x\in[a,b]} |f''(x)|.$$

We should have that $|R_n(f)| < \epsilon$. For $f(x) = \ln x$, $f'(x) = \frac{1}{x}$ and $f''(x) = -\frac{1}{x^2}$ which means that $M_2 f = \max_{x\in[1,2]} |-\frac{1}{x^2}| = 1$, so since $\epsilon = 10^{-2}$ we have that

$$|R_n(f)| \le \frac{(2-1)^3}{12n^2} \cdot 1 < 10^{-2} \iff 12n^2 > \frac{1}{10^{-2}} \iff n^2 > \frac{100}{12} \approx 8.33... \implies n = 3$$

So, we have $k = \overline{0,3}$, $h = \frac{1}{3}$, $x_0 = 1$, $x_1 = \frac{4}{3}$, $x_2 = \frac{5}{3}$, $x_3 = 2$ and

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

The exact value is 0.3862943611198906.

Example 2.7 *Compute* $I = \int_0^1 \frac{1}{1+x}\, dx$ *with a precision of* $\epsilon = 10^{-3}$ *using the repeated Simpson's rule.*

The repetead Simpson's formula is

$$\int_a^b f(x)\,dx = \frac{b-a}{6n}\left[f(a) + f(b) + 4\sum_{k=1}^{n} f\left(\frac{x_{k-1}+x_k}{2}\right) + 2\sum_{k=1}^{n-1} f(x_k)\right] + R_n(f)$$

with

$$R_n(f) = -\frac{(b-a)^5}{2880n^4} f^{(4)}(\xi), \;\; \xi \in (a,b)$$

and

$$x_k = a + kh, \;\; h = \frac{b-a}{n}, \;\; k = \overline{0,n}.$$

For our problem, since the precision should be attained, we first have to find n. We find it from

$$|R_n(f)| \le \frac{(b-a)^5}{2880n^4} M_4 f, \quad \text{with } M_4 f = \max_{x\in[a,b]} |f^{(4)}(x)|.$$

We should have that $|R_n(f)| < \epsilon$. In our case

$$f'(x) = -(1+x)^{-2}, \;\; f''(x) = 2(1+x)^{-3}, \;\; f^{(3)}(x) = -6(1+x)^{-4}, \;\; f^{(4)}(x) = 24(1+x)^{-5}.$$

The function $|f^{(4)}(x)|$ attains its maximum in $[0,1]$ at $x = 0$ and it is $M_4 f = 24$, so, since $\epsilon = 10^{-3}$ we get

$$|R_n(f)| \le \frac{(1-0)^5}{2880n^4}\cdot 24 < 10^{-3} \iff \frac{1}{120n^4} < 10^{-3} \iff 120n^4 > \frac{1}{10^{-3}} = 1000 \implies n^4 > \frac{1000}{120} \approx 8.33.. \implies n = 2.$$

So we have $h = \frac{1-0}{2} = \frac{1}{2}$, $k = 0, 1, 2$ and $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_2 = 1$, that gives us

$$\begin{aligned}
I &= \frac{1-0}{6 \cdot 2}\left[f(0) + f(1) + 4f\left(\frac{0+\frac{1}{2}}{2}\right) + 4f\left(\frac{\frac{1}{2}+1}{2}\right) + 2f\left(\frac{1}{2}\right)\right] = \\
&= \frac{1}{12}\left(1 + \frac{1}{2} + 4 \cdot \frac{1}{1+\frac{1}{4}} + 4\frac{1}{1+\frac{3}{4}} + 2\frac{1}{1+\frac{1}{2}}\right) = \\
&= \frac{1}{12}\left(\frac{3}{2} + \frac{16}{5} + \frac{16}{7} + \frac{4}{3}\right) = \frac{1}{12} \cdot \frac{1747}{210} \approx 0.693253968253968.
\end{aligned}$$

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

Remark 2.8 *Other examples for repeated trapezium and repeated Simpson formulas are found in Course 7, slides 12–14.*

Example 2.9 *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 2.10 *Compute the integral $I = \int_1^2 \ln x \, dx$ with a precision of $\epsilon = 10^{-2}$ using the repetead rectangle (midpoint) formula.*
The repetead rectangle (midpoint) formula is

$$\int_a^b f(x)\,dx = \frac{b-a}{n}\sum_{k=1}^{n} f(x_k) + R_n(f)$$

with

$$R_n(f) = \frac{(b-a)^3}{24n^2} f''(\xi),\ \ \xi \in (a,b)$$

and

$$x_1 = a + \frac{b-a}{2n},\ \ x_k = x_1 + (k-1)\frac{b-a}{n},\ \ k = \overline{2,n}.$$

For our problem, since the precision should be attained, <u>we first have to find n</u>. <u>We find it from</u>

$$|R_n(f)| \leq \frac{(b-a)^3}{24n^2} M_2 f, \quad \text{with } M_2 f = \max_{x\in[a,b]} |f''(x)|.$$

We should have that $|R_n(f)| < \epsilon$. For $f(x) = \ln x$, $f'(x) = \frac{1}{x}$ and $f''(x) = -\frac{1}{x^2}$ which means that $M_2 f = \max_{x\in[1,2]} |-\frac{1}{x^2}| = 1$, so since $\epsilon = 10^{-2}$ we have that

$$|R_n(f)| \leq \frac{(2-1)^3}{24n^2} \cdot 1 < 10^{-2} \iff 24n^2 > \frac{1}{10^{-2}} \iff n^2 > \frac{100}{24} \approx 4.16... \implies n = 3$$

So, we have $k = 2, 3$, $x_1 = 1 + \frac{2-1}{2\cdot 3} = \frac{7}{6}$ and $x_2 = \frac{7}{6} + (2-1)\cdot\frac{1}{3} = \frac{9}{6}$, $x_3 = \frac{7}{6} + (3-1)\cdot\frac{1}{3} = \frac{11}{6}$ and

$$I = \frac{2-1}{3}\left(f\left(\frac{7}{6}\right) + f\left(\frac{9}{6}\right) + f\left(\frac{11}{6}\right)\right) = \frac{1}{2}\left(\ln\frac{7}{6} + \ln\frac{9}{6} + \ln\frac{11}{6}\right) = \frac{1}{3}\ln\left(\frac{693}{216}\right) \approx 0.38858386383.$$

The exact value is 0.3862943611198906.

Remark 2.11 *Other examples for repetead rectangle formula are found in Course 8, slides 17–18.*

Example 2.12 *For Gauss quadrature formulas, see examples on slides 13-14 and 18-19 in Course 8.*

Example 2.13 *Determine a general quadrature formula of the form*

$$I = \int_a^b f(x)\,dx = Af'(a) + Bf(b) + R(f)$$

and determine the degree of exactness. (See Course 9, slide 1.)
This is a general quadrature formula. Since we have information about $f'(a)$ and $f(b)$ ($f(a)$ is missing), we have to work with **the Birkhoff interpolation**.

$$x_0 = a,\ x_1 = b\ \ I_0 = \{1\},\ I_1 = \{0\} \implies m = |I_0| + |I_1| - 1 = 1 + 1 - 1 = 1.$$

So our polynomial will have the degree 1 and we find the coefficients A and B by integrating the fundamental Birkhoff interpolation polynomials.

$$B_1(f) = \sum_{k=0}^{1} \sum_{j \in I_k} b_{kj}(x) f^{(j)}(x_k) = b_{01}(x) f'(x_0) + b_{10}(x) f(x_1)$$

Since the polynomial should have the degree 1, we write the fundamental pol. b_{01}, b_{10} as general linear polynomials (ex. $tx + v$, with the derivative t) and determine the coefficients t and v. (see the examples from Birkhoff to additional information about how to construct these polynomials.)

$$\begin{cases} b'_{01}(a) = 1 \\ b_{01}(b) = 0 \end{cases} \iff \begin{cases} \quad t = 1 \\ tb + v = 0 \implies v = -b. \end{cases}$$

$$b_{01}(x) = x - b.$$

$$\begin{cases} b'_{10}(a) = 0 \\ b_{10}(b) = 1 \end{cases} \iff \begin{cases} \quad t = 0 \\ tb + v = 1 \implies v = 1. \end{cases}$$

$$b_{10}(x) = 1.$$

And now, our integral will be written as

$$I = f'(a) \int_a^b b_{01}(x)\,dx + f(b) \int_a^b b_{10}(x)\,dx + R(f)$$

so,

$$A = \int_a^b b_{01}(x)\,dx = \int_a^b (x - b)\,dx = \frac{(x-b)^2}{2}\Big|_a^b = \frac{(b-b)^2}{2} - \frac{(a-b)^2}{2} = -\frac{(a-b)^2}{2}.$$

$$B = \int_a^b b_{10}(x)\,dx = \int_a^b 1\,dx = x\,\Big|_a^b = b - a.$$

We shall now find the degree of exactness of this formula. **The degree of exactness of a quadrature formula is n if:**

- each $R(e_k) = 0$, for all $k = 0, 1, ..., n$ and $R(e_{n+1}) \neq 0$, where:
  - $e_m(x) = x^m$;
  - $R(e_k) = \int_a^b x^k dx - \sum_{j=0}^{m} A_j e_k(x_j)$

In our case, we compute $R(e_0)$, $R(e_1)$ and so on until we find one that is not 0. Practically, *f is substituted with e_k*. So, if you have $f(2)$ somewhere, it will be substituted by $e_2(2)$ which is 2^2.

$$R(e_0) = \int_a^b x^0 dx - A \cdot e_0'(a) - B \cdot e_0(b) =$$

$$= \int_a^b 1dx + \frac{(a-b)^2}{2} \cdot 0 - (b-a) \cdot 1 = (b-a) - (b-a) = 0$$

$$R(e_1) = \int_a^b x^1 dx - A \cdot e_1'(a) - B \cdot e_1(b) =$$

$$= \frac{x^2}{2}\bigg|_a^b + \frac{(a-b)^2}{2} \cdot 1 - (b-a) \cdot b = \frac{b^2 - a^2 + a^2 - 2ab + b^2 - 2b^2 + 2ab}{2} = 0.$$

$$R(e_2) = \int_a^b x^2 dx - A \cdot e_2'(a) - B \cdot e_2(b) =$$

$$= \frac{x^3}{3}\bigg|_a^b + \frac{(a-b)^2}{2} \cdot 2a - (b-a) \cdot b^2 = \frac{2b^3 - 2a^3 + 6a^2 - 12ab + 6b^2 - 6b^3 + 6ab^2}{6} \neq 0.$$

So, the degree of exactness is 1. (= it reproduces exactly polynomials of degree 1.)

Remark 2.14 *For $e_2'(a)$, we first compute the derivate of $e_2(x)$ which is $2x$, since $e_2(x) = x^2$ and then we substitute x with a. This procedure was done in all the cases.*

Remark 2.15 *The same idea is used when we have to compute Hermite quadrature formulas. For example, if we have to construct a general quadrature of the form*

$$I = \int_0^1 f(x)\,dx = Af(0) + Bf(1) + Cf'(1) + R(f),$$

we determine the fundamental Hermite polynomials h_{00}, h_{10}, h_{11} and integrate them on $[0,1]$ to obtain the coefficients A, B, C. (See another example in Course 9, slide 2.)

Example 2.16 *Find a quadrature formula of the form*

$$I = \int_0^1 f(x)\,dx = af(0) + bf\left(\frac{1}{2}\right) + cf(1) + R(f)$$

that is exact for all polynomials of maximum degree 2.

Since the formula should have the degree of exactness 2, we need to have $R(e_0) = R(e_1) = R(e_2) = 0$, where

$$R(e_0) = \int_0^1 x^0\,dx - \left[ae_0(0) + be_0\left(\frac{1}{2}\right) + ce_0(1)\right]$$
$$R(e_1) = \int_0^1 x^1\,dx - \left[ae_1(0) + be_1\left(\frac{1}{2}\right) + ce_1(1)\right]$$
$$R(e_2) = \int_0^1 x^2\,dx - \left[ae_2(0) + be_2\left(\frac{1}{2}\right) + ce_2(1)\right]$$

$e_0(x) = x^0 = 1,\ e_1(x) = x,\ e_2(x) = x^2$. So, we have

$$\begin{cases} \int_0^1 x^0\,dx - \left[ae_0(0) + be_0\left(\frac{1}{2}\right) + ce_0(1)\right] = 0 \\ \int_0^1 x^1\,dx - \left[ae_1(0) + be_1\left(\frac{1}{2}\right) + ce_1(1)\right] = 0 \\ \int_0^1 x^2\,dx - \left[ae_2(0) + be_2\left(\frac{1}{2}\right) + ce_2(1)\right] = 0 \end{cases} \Longleftrightarrow \begin{cases} x\,|_0^1 = a \cdot 1 + b \cdot 1 + c \cdot 1 \\ \frac{x^2}{2}\,|_0^1 = a \cdot 0 + b \cdot \frac{1}{2} + c \cdot 1 \\ \frac{x^3}{3}\,|_0^1 = a \cdot 0^2 + b \cdot \left(\frac{1}{2}\right)^2 + c \cdot 1^2 \end{cases}$$

which gives us the system

$$\begin{cases} a+b+c=1 \\ \dfrac{b}{2}+c=\dfrac{1}{2} \\ \dfrac{b}{4}+c=\dfrac{1}{3} \end{cases} \text{ with the solution } \begin{cases} a=\dfrac{1}{6} \\ b=\dfrac{2}{3} \\ c=\dfrac{1}{6} \end{cases}.$$

Remark 2.17 One can see that

$$I=\frac{1}{6}\left[f(0)+4f\left(\frac{1}{2}\right)+f(1)\right]+R(f)$$

is the Simpson's quadrature formula on $[0,1]$. Also, if one computes $R(e_3)$, it can be seen that this is also equal to 0, but $R(e_4)\neq 0$, which means that this formula's degree of exactness is 3, and it is correct, since one knows that Simpson's quadrature formula reproduces polynomial of maximum degree 3, i.e., it has the degree of exactness 3.

Example 2.18 For the Romberg's algorithms (iterative and with Aitken) and Adaptive quadratures, see the formulas in Course 8 and also what we have done at the lab.