MTMM.00.005 Numerical Methods
Practical lesson 13–15: Numerical integration

May 7-21, 2019

To get a positive result, student has to solve all of the exercises given in practical lessons, explain the programming code and answer the questions.

The deadline for the 13th and last set of exercises is May 28th.

NB! In order to use the nonstandard packages as *numpy* and *matplotlib* one could use Command Prompt and type

```
H:\nm> "C:\Program Files\Anaconda3\python" <filename>.py
```

Here `H:\nm` is the folder for `<filename>.py`.

Newton-Cotes formulae

Assume that one has to calculate the definite integral

$$\int_a^b f(x)dx.$$

Let $x_i = a + ih$, $i = 0, \ldots, n$, $h = \dfrac{b-a}{n}$, and approximate $f(x)$ by the Lagrange polynomial $P_n(x) = \sum\limits_{i=0}^{n} f(x_i) l_{ni}(x)$ interpolating the values at x_i, i.e., $P_n(x_i) = f(x_i)$, $i = 0, \ldots, n$. Newton-Cotes formulae have the form

$$\int_a^b f(x)dx = \int_a^b \big(P_n(x) + r_n(f,x)\big)dx = \sum_{i=0}^{n} A_i f(x_i) + R_n(f),$$

where $A_i = \displaystyle\int_a^b l_{ni}(x)dx$. Denote $B_i = \dfrac{A_i}{b-a}$, then the coefficients B_i have the next properties:

1) $\sum\limits_{i=0}^{n} B_i = 1$; 2) $B_i = B_{n-i}$, $i = 0, \ldots, n$.

Trapezoidal rule

Let $n = 1$, $x_0 = a$, $x_1 = b$. The coefficients satisfy

$$B_0 + B_1 = 1,$$
$$B_0 = B_1,$$

thus $B_0 = B_1 = \dfrac{1}{2}$. The trapezoidal rule is

$$\boxed{\int_a^b f(x)dx = \frac{b-a}{2}\big(f(a) + f(b)\big) + R_1(f),}$$

where $R_1(f) = -\frac{(b-a)^3}{12}f''(\xi)$, $\xi \in [a,b]$. Divide interval $[a,b]$ into N equal parts with the length $h = \frac{b-a}{N}$, the subintervals have endpoints $x_i = a + ih$, $i = 0, \dots, N$. Apply on each interval the trapezoidal rule yielding the composite trapezoidal rule

$$\boxed{\int_a^b f(x)dx = \sum_{i=1}^{N} \int_{x_{i-1}}^{x_i} f(x)dx = \frac{b-a}{2N}(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{N-1} + f_N) + R_1(f,N),}$$

where $f_i = f(x_i)$, $i = 0, \dots, N$, and $R_1(f,N) = -\frac{(b-a)^3}{12N^2}f''(\xi)$, $\xi \in [a,b]$.

Simpson's rule

For $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$ we have $B_0 = B_1 = \frac{1}{6}$, $B_2 = \frac{4}{6}$. The Simpson's rule is

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

where $R_2(f) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{IV}(\xi)$, $\xi \in [a,b]$. Divide interval $[a,b]$ into N equal parts, where now let N be an even number, but still $h = \frac{b-a}{N}$. Write the integral as a sum of integrals over the intervals $[a, a+2h]$, $[a+2h, a+4h]$, $\ldots$, $[b-2h, b]$, and apply on each interval the Simpson's rule yielding the composite Simpson's rule

$$\boxed{\int_a^b f(x)dx = \frac{b-a}{3N}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 4f_{N-1} + f_N) + R_2(f,N),}$$

where $f_i = f(x_i)$, $i = 0, \dots, N$, and $R_2(f,N) = -\frac{(b-a)^5}{180N^4}f^{IV}(\xi)$, $\xi \in [a,b]$.

Newton's $\frac{3}{8}$ rule

Let $n = 3$, then $B_0 = B_3 = \frac{1}{8}$, $B_1 = B_2 = \frac{3}{8}$ and $x_0 = a$, $x_1 = a + h$, $x_2 = a + 2h$, $x_3 = b$, $h = \frac{b-a}{3}$. The Newton's $\frac{3}{8}$ rule is

$$\boxed{\int_a^b f(x)dx = \frac{b-a}{8}\left(f(a) + 3f(a+h) + 3f(a+2h) + f(b)\right) + R_3(f),}$$

where $R_3(f) = -\frac{3}{80}\left(\frac{b-a}{3}\right)^5 f^{IV}(\xi)$. Corresponding composite formula is

$$\boxed{\int_a^b f(x)dx = \frac{3(b-a)}{8N}(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + \ldots + 3f_{N-1} + f_N) + R_3(f,N),}$$

where $N = 3m$, $m \in \mathbb{N}$, $f_i = f(x_i)$, $i = 0, \dots, N$, and $R_3(f,N) = -\frac{(b-a)^5}{80N^4}f^{IV}(\xi)$, $\xi \in [a,b]$.

Some other Newton-Cotes formulae

n	$B_0 = B_n$	$B_1 = B_{n-1}$	$B_2 = B_{n-2}$	B_3
4	$\frac{7}{90}$	$\frac{32}{90}$	$\frac{12}{90}$	
5	$\frac{19}{288}$	$\frac{75}{288}$	$\frac{50}{288}$	
6	$\frac{41}{840}$	$\frac{216}{840}$	$\frac{27}{840}$	$\frac{272}{840}$

$$\int\limits_a^b f(x)dx \approx (b-a)\sum_{i=0}^{n} B_i f(x_i)$$

$$x_i = a + ih,\, h = \frac{b-a}{n}$$

Rectangular rule

In case of rectangular rule function f is approximated by a (piecewise) constant function which interpolates the value(s) at midpoint(s) of interval(s). Rectangular rule has the form

$$\boxed{\int_a^b f(x)dx = (b-a)f\left(\frac{a+b}{2}\right) + R_0(f),}$$

where $R_0(f) = \dfrac{(b-a)^3}{24} f''(\xi),\, \xi \in [a,b]$. The composite rectangular rule has the form

$$\boxed{\int_a^b f(x)dx = \frac{b-a}{N}\left(f\left(a+\frac{h}{2}\right) + f\left(a+\frac{3h}{2}\right) + \ldots + f\left(b-\frac{h}{2}\right)\right) + R_0(f,N),}$$

where $h = \dfrac{b-a}{N}$, $R_0(f,N) = \dfrac{(b-a)^3}{24N^2} f''(\xi),\, \xi \in [a,b]$.

Runge's method

Let us use the symbol I for the integral, and let the quadrature sum be I_h at step h. If the remainder R_h is in form $R_h = I - I_h = \kappa h^q + O(h^{q+1})$, where κh^q is the main part of remainder term, then it holds

$$I - I_h = \frac{I_h - I_{2h}}{2^q - 1} + O(h^{q+1}).$$

For trapezoidal and rectangular rule $q = 2$, for Simpson's and Newton's $\frac{3}{8}$ rule $q = 4$. This method allows us to estimate the actual remainder term $R_h \approx \dfrac{I_h - I_{2h}}{2^q - 1}$.

Exercise 1. Use Newton-Cotes formulae to calculate a definite integral

$$\int_a^b f(x)dx \approx (b-a)\sum_{i=0}^{n} B_i f(x_i), \quad x_i = a + ih,\ h = \frac{b-a}{n},$$

for $n = 1, \ldots, 6$.

n	$B_0 = B_n$	$B_1 = B_{n-1}$
1	$\frac{1}{2}$	
2	$\frac{1}{6}$	$\frac{4}{6}$
3	$\frac{1}{8}$	$\frac{3}{8}$

n	$B_0 = B_n$	$B_1 = B_{n-1}$	$B_2 = B_{n-2}$	B_3
4	$\frac{7}{90}$	$\frac{32}{90}$	$\frac{12}{90}$	
5	$\frac{19}{288}$	$\frac{75}{288}$	$\frac{50}{288}$	
6	$\frac{41}{840}$	$\frac{216}{840}$	$\frac{27}{840}$	$\frac{272}{840}$

Choose the integral according to your α-value:

1) if $\alpha \vdots 4$, then $\int\limits_{0.1}^{5} \frac{\sin x}{x} dx$;

2) if $(\alpha - 1) \vdots 4$, then $\int\limits_{0}^{2} x^x dx$;

3) if $(\alpha - 2) \vdots 4$, then $\int\limits_{0.2}^{2} \frac{e^x}{x} dx$;

4) if $(\alpha - 3) \vdots 4$, then $\int\limits_{0}^{2} e^{-x^2} dx$.

Exercise 2. Use Newton-Leibniz formula to calculate

$$\int_1^2 x e^{(1+0.1\alpha)x} dx.$$

To find the antiderivative, you may use, for example, `www.WolframAlpha.com`.
Use composite trpezoidal rule to calculate the integral for $N = 2, 4, 8, 16, \ldots$. Terminate the process if the error, estimated by Runge's method, is less or equal to 10^{-6}, i.e.,

$$|R_h| = \left| \frac{I_h - I_{2h}}{2^q - 1} \right| \le 10^{-6}.$$

Print out the quadrature sums I_h, errors R_h estimated by Runge's method and actual errors for each $N = 2, 4, 8, 16, \ldots$.
Repeat the exercise by using the composite Simpson's rule and the composite rectangular rule.