02635 Fall 2016 — Module 2

Homework

- Read chapters 3 and 4 in "Beginning C"
- Read chapters 1 and 2 in "Writing Scientific Software"

Exercises — Part I

- 1. Do exercises 3-1, and 4-1 in "Beginning C"
- 2. Do exercises 2, 3, and 4 (p. 39, chapter 5) in "Writing Scientific Software"
 - Remark: Exercise 4 should read "If b^2 is large compared to ac ..." (see errata)
- 3. Take this quiz to test your understanding of if statements
- 4. Take this quiz to test your understanding of loops

Exercises — Part II

Numerical integration

In this exercise, we will consider some basic methods for numerical integration. Specifically, given a function $f: \mathbb{R} \to \mathbb{R}$, we seek to compute or approximate definite integrals of the form

$$\int_{a}^{b} f(x) \, dx$$

where a, b (the limits of integration) are given. Many so-called *rules* exist for approximating such integrals. Here we will focus on two simple rules, namely the *rectangle rule* and the *trapezoidal rule*. For more information on numerical integration, take a quick look at the Wikipedia page about <u>Numerical Integration</u>.

Rectangle rule

The <u>rectangle rule</u> (also known as the midpoint rule) approximates the definite integral by the area of a rectangle that is b-a wide (i.e., the length of the interval [a,b]) and with height equal to the value of f at the midpoint (a+b)/2 of the interval [a,b], i.e.,

$$\int_{a}^{b} f(x) dx \approx (b - a) f\left(\frac{a + b}{2}\right).$$

Notice that only a single function evaluation is necessary to compute the approximation.

Trapezoidal rule

The trapezoidal rule approximates the definite integral by the area of a trapezoid, i.e.,

$$\int_a^b f(x) \, dx \approx (b-a) \frac{f(a) + f(b)}{2}.$$

Notice that the approximation requires two function evaluations.

Repeated/iterated rules

The approximation of the definite integral can be improved by dividing the interval into n subintervals. Specifically, if we define the width of each of these n subintervals as h = (b - a)/n, we can express the integral of interest as a sum of integrals over subintervals, i.e.,

$$\int_{a}^{b} f(x) dx = \sum_{i=1}^{n} \int_{a+(i-1)h}^{a+ih} f(x) dx.$$

Repeated rectangle rule

If we apply the rectangle rule to each of the subintervals in the above expression, we obtain the following approximation

$$\int_{a}^{b} f(x) dx \approx h \sum_{i=0}^{n-1} f(a + 0.5h + ih).$$

Note that this approximation requires n function evaluations.

Repeated trapezoidal rule

The repeated trapezoidal rule follows by applying the trapezoidal rule to each subinterval, i.e.,

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

which requires n+1 function evaluations (and not 2n since we can reuse function values for adjacent subintervals).

Exercises

1. Write a C program that computes an approximation of the following definite integral

$$\int_a^b e^{-x^2} dx.$$

The program should prompt the user to enter the integration limits a and b, the number of subintervals n, and the method of choice (rectangle rule or trapezoidal rule).

You may use the following main.c template:

```
#include <stdio.h>
#include <math.h>

int main(void) {

   /* Insert your code here */
   return 0;
}
```

Compiling your program

You can compile your program using the following command:

```
cc main.c -lm -o numint1
```

Notice the compiler option <code>-lm</code>. This tells the linker to link against the math library (<code>libm</code>). Implementations of what is defined in <code>stdlib.h</code> and <code>stdio.h</code> are included in a system C library (<code>libc</code>) which is automatically linked against, so it is not necessary to explicitly include any linking options when including <code>stdlib.h</code> and <code>stdio.h</code> in your program.

2. Write a new program that (i) prompts the user to enter the integration limits a, b and a positive integer N, and (ii), prints a table with the approximations obtained with the two numerical integration methods for n = 1, ..., N. For example, the output could look like this:

Parameters:

a = 0.0

b = 1.0

N = 50

Results:

n	Rectangle	Trapezoidal
1	7.78800783e-01	6.83939721e-01
2	7.54597944e-01	7.31370252e-01
3	7.50252350e-01	7.39986475e-01
:	:	:
49	7.46836901e-01	7.46798596e-01
50	7.46836396e-01	7.46799607e-01

Optional exercise

Monte Carlo integration is yet another method that can be used to approximate a definite integral of the form

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

Unlike the two methods described above, the Monte Carlo approach is based on randomization and is nondeterminstic.

To explain how Monte Carlo integration works, we'll need a random variable U with a uniform distribution on [a, b], i.e., the probability density function is given by

$$P_U(x) = \begin{cases} \frac{1}{b-a} & a \le x \le b \\ 0 & \text{otherwise.} \end{cases}$$

The expectation of f(U) is given by

$$\mathbb{E}[f(U)] = \int_{-\infty}^{\infty} f(x)P_U(x) dx = \frac{1}{b-a} \int_a^b f(x) dx$$

which is a constant multiple of the integral of interest. The expectation $\mathbb{E}[f(U)]$ may be estimated using a sample average approximation

$$\mathbb{E}[f(U)] \approx \frac{1}{N} \sum_{i=1}^{N} f(U_i)$$

where U_1,\ldots,U_N denote N independent and identically distributed random samples from the uniform

distribution on [a, b]. Thus, the definite integral of interest can be approximated as

$$\int_{a}^{b} f(x) dx \approx \frac{b-a}{N} \sum_{i=1}^{N} f(U_{i}).$$

Implement the Monte Carlo integration method for the function $f(x) = e^{-x^2}$ in C and compare it to your implementation of the two deterministic methods. Investigate numerically how the accuracy depends on the number of samples.

Hints:

- The approximation can be implemented recursively. To see this, let $s_1=f(U_1)$ and define

$$s_i = s_{i-1} + f(U_i), \quad i = 2, \dots, N,$$

i.e., $s_N = f(U_1) + \cdots + f(U_N)$. Dividing both sides by i yields the equation

$$\frac{s_i}{i} = \frac{s_{i-1}}{i} + \frac{f(U_i)}{i} \\ = \left(1 - \frac{1}{i}\right) \frac{s_{i-1}}{i-1} + \frac{1}{i} f(U_i),$$

and hence the approximation after i samples can be expressed recursively as

$$\int_{a}^{b} f(x) \approx (b - a)v_{i} = (b - a) \left[\left(1 - \frac{1}{i} \right) v_{i-1} + \frac{1}{i} f(U_{i}) \right]$$

where $v_i = \frac{s_i}{i}$, or equivalently,

$$v_i = \left(1 - \frac{1}{i}\right)v_{i-1} + \frac{1}{i}f(U_i)$$

for $i \geq 1$.

• The function <code>rand()</code>, which is defined in <code>stdlib.h</code>, can be used to generate pseudo-random integers between 0 and <code>RAND_MAX</code>, which is a constant that is defined in <code>stdlib.h</code>. The random number generator must be initialized with a so-called <code>seed</code> in order to produce a new pseudo-random series of numbers each time you run your program. The seed is set using the function <code>srand()</code> which takes an <code>unsigned int</code> as input. It is common to use the current time as a seed, i.e., to generate two pseudo-random numbers from a uniform distribution on <code>[a, b]</code>, we may use the following code:

It is only necessary to initialize the random number generator once before subsequent calls to rand(). The time() function is defined in the time.h header.