Computational Physics

Exercises for Chapter 4

Exercise 4.1: Write a program to calculate and print the factorial of a number entered by the user. If you wish you can base your program on the user-defined function for factorial given in Section 2.6, but write your program so that it calculates the factorial using *integer* variables, not floating-point ones. Use your program to calculate the factorial of 200.

Now modify your program to use floating-point variables instead and again calculate the factorial of 200. What do you find? Explain.

Exercise 4.2: Quadratic equations

a) Write a program that takes as input three numbers, a, b, and c, and prints out the two solutions to the quadratic equation $ax^2 + bx + c = 0$ using the standard formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

Use your program to compute the solutions of $0.001x^2 + 1000x + 0.001 = 0$.

b) There is another way to write the solutions to a quadratic equation. Multiplying top and bottom of the solution above by $-b \mp \sqrt{b^2 - 4ac}$, show that the solutions can also be written as

$$x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}.$$

Add further lines to your program to print out these values in addition to the earlier ones and again use the program to solve $0.001x^2 + 1000x + 0.001 = 0$. What do you see? How do you explain it?

c) Using what you have learned, write a new program that calculates both roots of a quadratic equation accurately in all cases.

This is a good example of how computers don't always work the way you expect them to. If you simply apply the standard formula for the quadratic equation, the computer will sometimes get the wrong answer. In practice the method you have worked out here is the correct way to solve a quadratic equation on a computer, even though it's more complicated than the standard formula. If you were writing a program that involved solving many quadratic equations this method might be a good candidate for a user-defined function: you could put the details of the solution method inside a function to save yourself the trouble of going through it step by step every time you have a new equation to solve.

Exercise 4.3: Calculating derivatives

Suppose we have a function $f(x)$ and we want to calculate its derivative at a point x. We can do that with pencil and paper if we know the mathematical form of the function, or we can do it on the computer by making use of the definition of the derivative:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\delta\to 0} \frac{f(x+\delta) - f(x)}{\delta}.$$

On the computer we can't actually take the limit as δ goes to zero, but we can get a reasonable approximation just by making δ small.

a) Write a program that defines a function `f(x)` returning the value $x(x-1)$, then calculates the derivative of the function at the point $x = 1$ using the formula above with $\delta = 10^{-2}$. Calculate the true value of the same derivative analytically and compare with the answer your program gives. The two will not agree perfectly. Why not?

b) Repeat the calculation for $\delta = 10^{-4}$, 10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}, and 10^{-14}. You should see that the accuracy of the calculation initially gets better as δ gets smaller, but then gets worse again. Why is this?

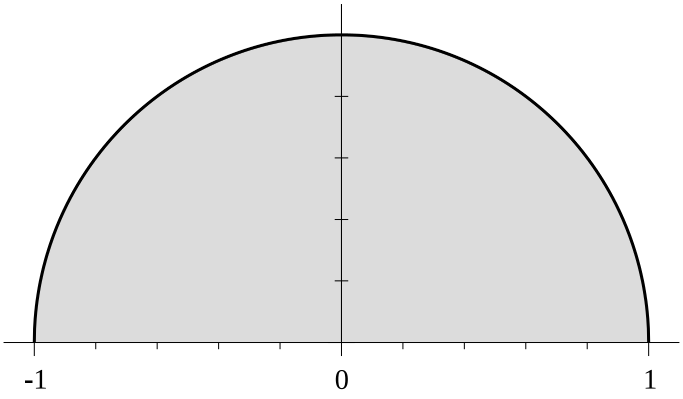
We will look at numerical derivatives in more detail in Section 5.10, where we will study techniques for dealing with these issues and maximizing the accuracy of our calculations.

Exercise 4.4: Calculating integrals

Suppose we want to calculate the value of the integral

$$I = \int_{-1}^{1} \sqrt{1-x^2}\,\mathrm{d}x.$$

The integrand looks like a semicircle of radius 1:



and hence the value of the integral—the area under the curve—must be $\frac{1}{2}\pi = 1.57079632679\ldots$

Alternatively, we can evaluate the integral on the computer by dividing the domain of integration into a large number N of slices of width $h = 2/N$ each and then using the Riemann definition of the integral:

$$I = \lim_{N\to\infty} \sum_{k=1}^{N} h y_k\,,$$

where

$$y_k = \sqrt{1 - x_k^2} \qquad \text{and} \qquad x_k = -1 + hk.$$

We cannot in practice take the limit $N \to \infty$, but we can make a reasonable approximation by just making N large.

a) Write a program to evaluate the integral above with $N = 100$ and compare the result with the exact value. The two will not agree very well, because $N = 100$ is not a sufficiently large number of slices.

b) Increase the value of N to get a more accurate value for the integral. If we require that the program runs in about one second or less, how accurate a value can you get?

Evaluating integrals is a common task in computational physics calculations. We will study techniques for doing integrals in detail in the next chapter. As we will see, there are substantially quicker and more accurate methods than the simple one we have used here.