Computational Physics – Week 2

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1 Introduction

This week will discuss numerical integration. Mathematically, the integral is the area under the curve and we approximate this by breaking the interval into N bins of width $dx = (b-a)/N$ and replacing the integral with a sum. The *left-hand rule* corresponds to the following approximation

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N-1} f(a + i \times dx)dx \,. \tag{1}$$

This evaluates the function of the left edge of the interval and approximates the area under the curve in that inteval with the area of the rectangle determined by the left point. This approximation is of the order $\mathcal{O}(dx)$, since the error for each interval is $\mathcal{O}(dx^2)$ and there are $N \sim 1/dx$ bins.

A better approximation is provided by the midpoint rule, i.e.

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N-1} f(a + i \times dx + \frac{1}{2}dx)dx \,. \tag{2}$$

Here the function is evaluated at the middle of the interval and the approximation is of the order $\mathcal{O}(dx^2)$. During this week will investigate this two approximations for a simple mechanics problem.

2 Example problem

The problem we plan to solve is the following: take a point mass moving in one dimension under the influence of the potential $V(x) = \sin(x)$. Assume that the mass is equal to 1 and that the points starts at $x = 0$ with a velocity equal to 2. How long does it take to reach $x = \pi/2$? (Note that we choose this point to avoid accidental symmetries that will make the approximation used for integrations look better than expected.)

A straigtforward way to solve this problem is to integrate a second order differential equation. However, using conservation of energy we can reduce this problem to an integral

$$\tau = \int_0^\tau dt = \int_0^{\pi/2} \frac{dx}{v(x)} = \int_0^{\pi/2} \frac{dx}{\sqrt{\frac{2}{m}(E - V(x))}} = \int_0^{\pi/2} \frac{dx}{\sqrt{2(2-\sin x)}} \,. \tag{3}$$

3 Teaching objectives

- Numerical integration via left-hand and midpoint rule.
- Order of approximation and its importance.
- Determining the order empirically from log-log plot of error versus bin width.
- Separating code into functions.
- Learn how to bypass interactive prompt when using `scanf`.

- Use Mathematica to run and intercept the output of external programs.
- Use Mathematica to integrate using `Integrate` and `NIntegrate`.
- Define functions in Mathematica.
- Use `Table` to create lists in Mathematica.
- Use Mathematica to generate log-log plots using `ListLogLogPlot`.