Computational Physics Assignment 4: Ising Model

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Abstract

The following exercises showcase several uses of Monte Carlo methods, specifically highlighting their use in simulating the Ising model.

Contents

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1. Background

2. Program

The programs for this series of problems were written using Rust. A `nix flake` is used to manage the programming environment and necessary dependencies; the programming environment can be entered by running `nix develop` (assuming that `nix` is installed). From there, one can run `cargo run` in any directory containing a Rust project to compile and run the program.

Results can be plotted by running `python3 ./<plotting_script_name>` in the directory containing the corresponding python script.

3. Results

3.1. Task 1

3.1.1. Part A

The first part of task 1 asks us to calculate π numerically through a Monte Carlo simulation involving the random distribution of points (x, y) in the unit square.

The area of a circle is of course

$$a = \pi r^2 \tag{1}$$

and that of the unit square is 1. If we center a circle with radius 1 on the origin, then the fraction of the unit square covered by the circle f is given by

$$f = \frac{\pi r^2}{4} \cdot \frac{1}{1} = \pi \frac{r^2}{4} \tag{2a}$$

$$= \frac{\pi}{4} \tag{2b}$$

$$\implies \pi = 4f. \tag{2c}$$

Furthermore, we can easily determine if a point $(x, y,)$ is in a unit circle by checking if its radius r is less than 1.

$$x^2 + y^2 < r^2 \tag{3a}$$

$$\implies x^2 + y^2 < 1 \tag{3b}$$

Ergo, we can create a program for this task by generating q random points (x, y) with $x, y \in [0, 1)$, and calculate the number of points within the unit circle p , meaning that

$$\pi = \frac{4p}{q}. \tag{4}$$

To show convergence for this task with consistent results, a seed-based random number generator was used and the logarithm of percent error was plotted as a function of points used.

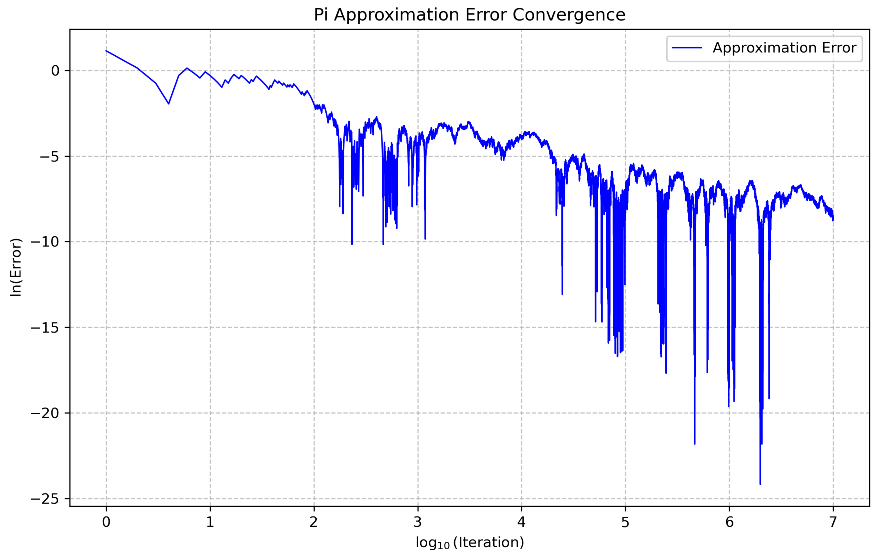

Figure 1: Plot of Pi Approximation as a function of Points used

As seen in 1, there is a steady decrease in the natural log of the error as a function of $\log_{10}$(iterations) , indicating the expected increase in precision following an increase in data points.

3.1.2. Part B

This task asks us to first create a random number generator following a Gaussian distribution with an average μ and a width σ . This function should then be used to calculate the following integral through MC Integration:

$$I = (2\pi)^{-2} \int_{-\infty}^{\infty} \mathrm{d}t \;\cos(t) \exp\left(-\frac{t^2}{2}\right). \tag{5}$$

We are given the analytical value $I = e^{-\frac{1}{2}} \approx 0.606531$ to check our answer.

We know that the standard normal distribution $f(x)$ is given by

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2}\sigma^2}. \tag{6}$$

In our case $\mu = 0$ and $\sigma = 1$, yielding

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}. \tag{7}$$

Knowing this, we can refactor our given integral as follows:

$$I = \frac{1}{(2\pi)^2} \int_{\infty}^{-\infty} \mathrm{d}t\ \cos(t) e^{-\frac{t^2}{2}} \tag{8a}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\infty}^{-\infty} \mathrm{d}t\ \cos(t) \left[\frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} \right] \tag{8b}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\infty}^{-\infty} \mathrm{d}t\ \cos(t) f(t). \tag{8c}$$

$f(x)$ is of course normalized, meaning that

$$\int_{\infty}^{-\infty} \mathrm{d}x\ f(x) = 1. \tag{9}$$

This in turn means that we replace $f(t)$ in the integral by selecting points according to this normal distribution:

$$I = \frac{1}{N} \sum_{i=0}^{N} \cos\left(x_i\right) \tag{10}$$

with N being the number of data points used and x being a normally distributed random value.

The required normal distribution was realized by using two uniformly generated numbers and a Box-Muller transform. The two random numbers $x, y \in (0, 1]$ were processed as follows:

$$R = \sqrt{-2 \cdot \ln x} \tag{11a}$$

$$\theta = 2\pi y, \tag{11b}$$

which can then be used to calculate the two normally distributed values Z_0, Z_1

$$Z_0 = R\cos(\theta) \tag{12a}$$

$$Z_1 = R\sin(\theta). \tag{12b}$$

We account for the modification of σ and μ by adding them as follows:

$$R = \sigma \cdot \sqrt{-2\ln x}, \tag{13a}$$

$$\theta = 2\pi y, \tag{13b}$$

$$Z_0 = R\cos(\theta) + \mu, \tag{14a}$$

$$Z_1 = R\sin(\theta) + \mu. \tag{14b}$$

3.2. Task 2

3.3. Task 3

3.4. Task 4