

Worksheet 5: Monte-Carlo

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1 Simple Sampling- Intrgration

First we were asked to program a function `runge(x)` that computes the runge function $f(x) = \frac{1}{1+x^2}$ and to plot it on the interval $[-5, 5]$.

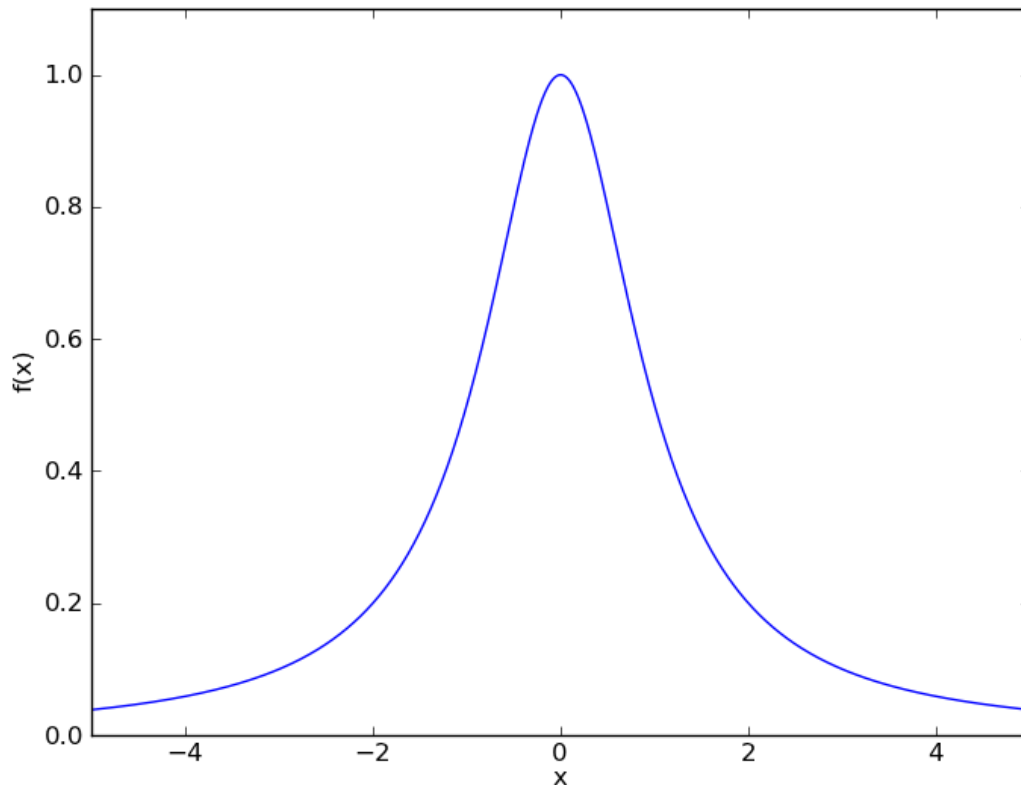


Figure 1: Runge function $f(x)$ on the interval $[-5, 5]$

Then we had to write a function that computes the exact integral of the runge function. The exact result is:

$$\int_{-5}^5 \frac{1}{1+x^2} = \arctan(5) - \arctan(-5) \approx 2.7468$$

After that we were asked to program a function `simple_sampling(f,a,b,N)` that performs N steps of a simple sampling Monte-Carlo integration and to use this function to compute the Integral for $N = 2^i$ with $2 \leq i \leq 20$. Furthermore we were asked to determine the actual and statistical error and to plot them against the number of integration steps N . In the following are two plots of the error from two different runs.

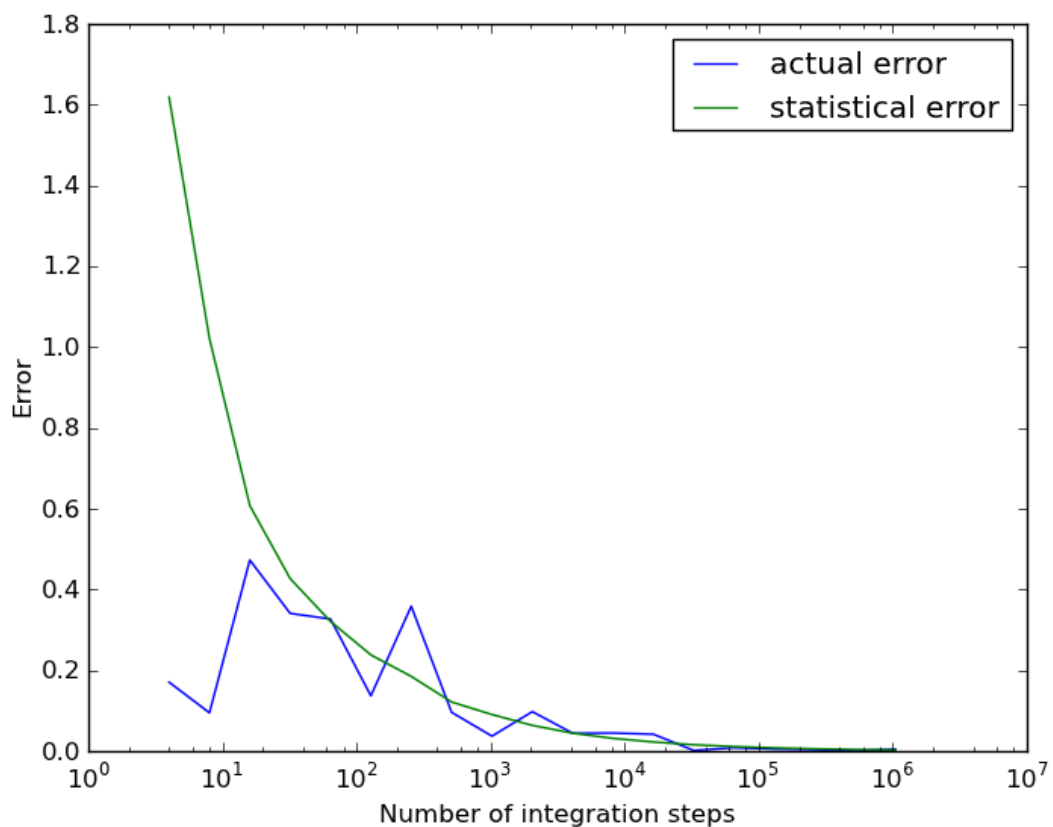
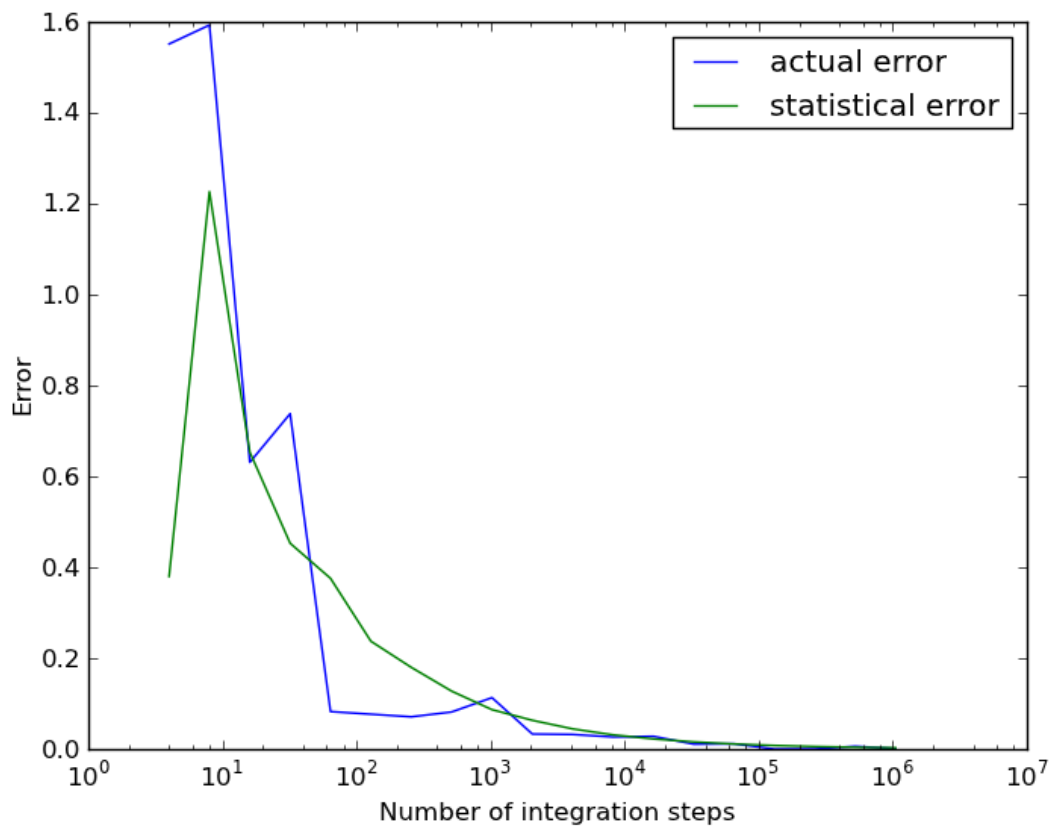


Figure 2: Statistical and actual error of the Integration with the simple sampling method

As it can be seen due to the randomness of the points in which f is evaluated the actual error behaves quite different from run to run. Furthermore it also varies for small numbers of integration steps quite a lot from the statistical error. In contrast to this the statistical error has a much more comparable behavior in different runs.

2 Importance Sampling- Metropolis-Hastings-Algorithm

In this task we were asked to implement the Metropolis-Hastings-algorithm and to use that function to generate a given number of samples for several Δx being used in the trial move. The resulting histograms can be found in the following plots

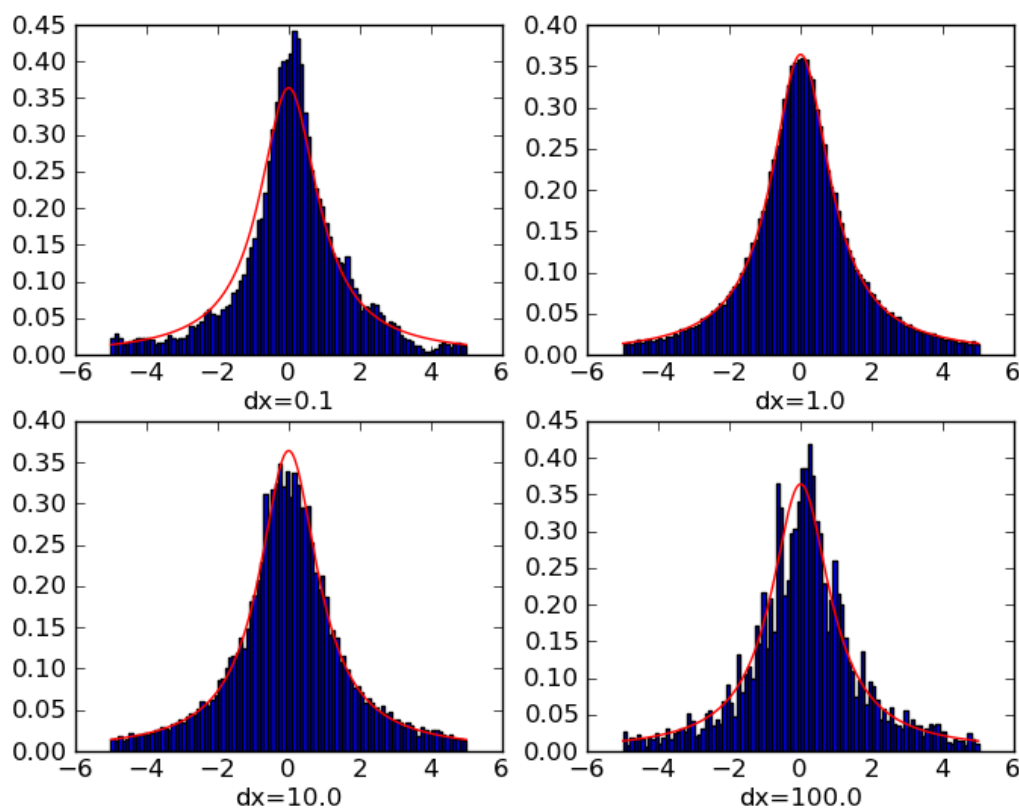


Figure 3: Distribution histograms of the Metropolis samples with 100 bins compared to the normalized runge function (red)

By eye it is hard to say whether $dx = 1.0$ or $dx = 10.0$ is the better choice. Having a look at the acceptance rates - $\approx 84.8\%$ for $dx = 1.0$, $\approx 32.5\%$ for $dx = 10.0$ - and taking into account that it was stated on the worksheet that an acceptance rate of about 30% is optimal, it can be said that $dx = 10.0$ is a better choice than $dx = 1.0$.

3 Simulating the Ising Model

The exact solution of the Ising Model was obtained by using the canonical partition function. The metropolis Monte-Carlo algorithm was implemented according to worksheet 5.

To determine the statistical errors Binning errors was used. Here you can see the calculated error of the mean energy as a function of the block size k .

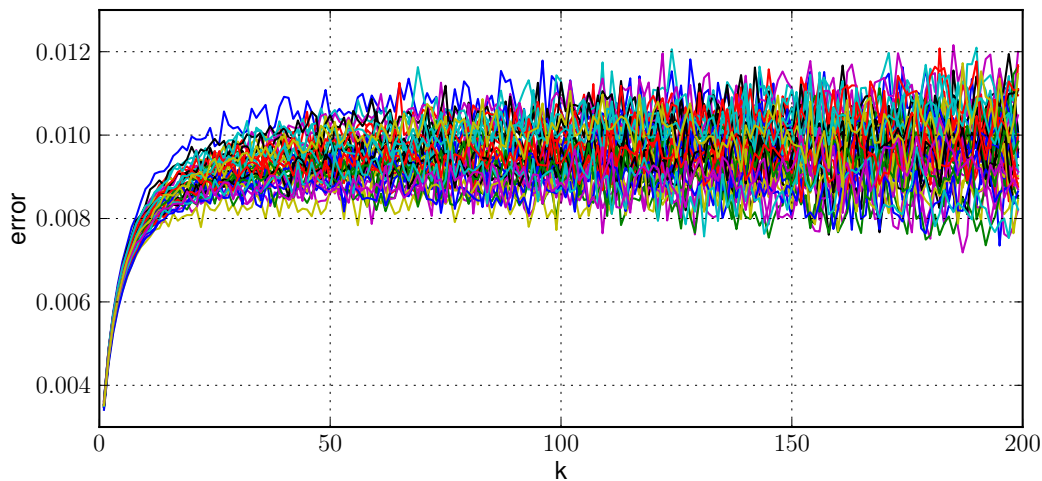


Figure 4: Binning error as a function of the block size k . Fifty seems to be a good value for k .

However there's much noise. Maybe it's because the energy of a fixed configuration of the finite Ising Model can only have discrete values.

3.0.1 Mean energy

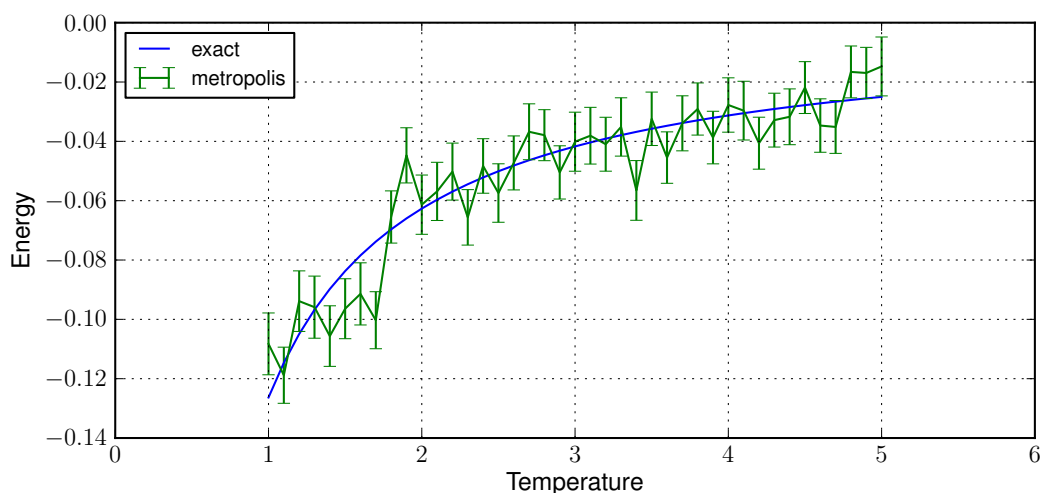


Figure 5: The energy becomes higher, when the temperature raises. The metropolis Monte-Carlo curve is in acceptable conformity to the exact one.

3.0.2 Mean magnetization

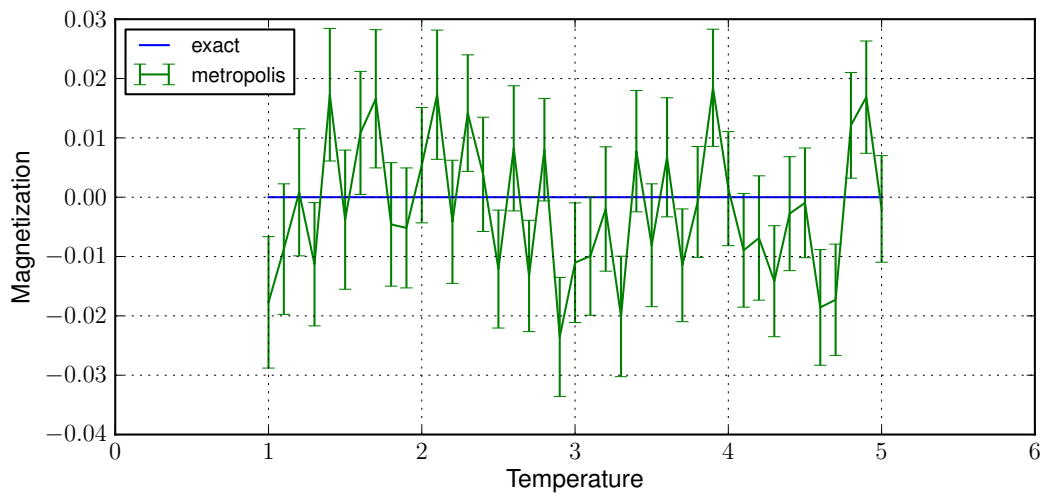


Figure 6: The mean magnetization is around zero. This full fills our expectations because for every magnetization below zeros there's a equiprobable magnetization above zero.

3.0.3 Mean absolute magnetization

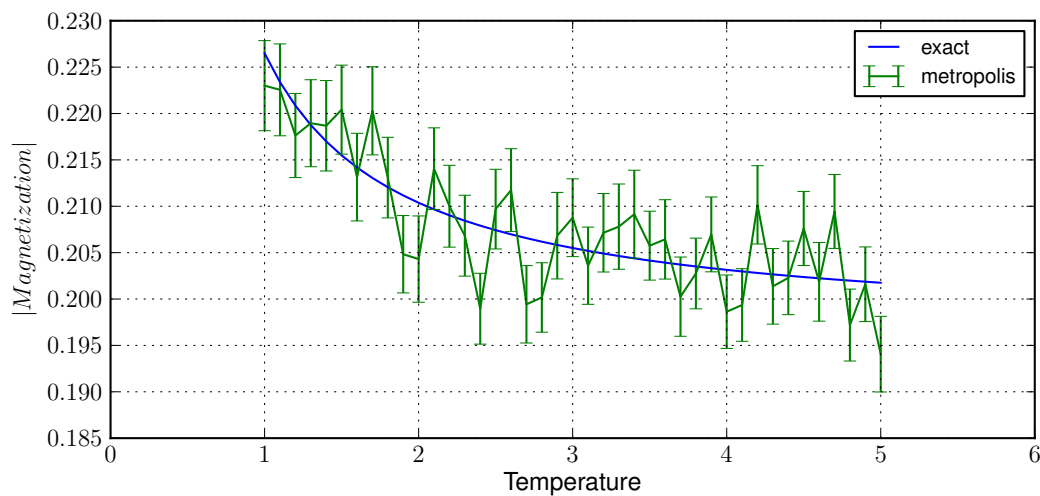


Figure 7: The curve of the absolute magnetization is interesting. It clearly shows that a high temperature destroys regimes of equal orientated spins.