Test of error calculations for Ising model in 1D and 2D

May 23, 2014

This is short theoretical explanation of the test: **IsingTestError1D.h** and **IsingTestError2D.h**.

1 Standard deviation

In files IsingTestError1D.h and IsingTestError2D.h we test function *Ising::ERROR(string totalFname, ISING_ERROR_TYPE error_type)* which calculates standard daviation of choosen variable X using bootstrap algorithm.

Standard deviation of variable X can be expressed by:

$$\sigma(X) = \sqrt{\langle (X - \langle X \rangle)^2 \rangle} = \sqrt{\langle X^2 \rangle - \langle X \rangle^2}$$

and it tells as how far a set of numbers is spread out. Low standard deviation indicates that the data points tend to be near the mean value of the set, high - the opposite. Apart fom showing dispersion of a data set, standard deviation is usually used as a measure of confidence in statistical conclusions.

The standard deviation of some data set is a square root of its variance $V(X) = \langle X^2 \rangle - \langle X \rangle^2$. A useful property of the standard deviation is that, unlike the variance, it is expressed in the same units as the data.

2 Bootstrap method

If the sample size is insufficient to calculate the standard deviation from definition, we can use for this purpose bootstrap method. Bootstraping uses approximate distribution to estimate properties of an estimator (like standard deviation). To achieve it we can take set of observed data and (assuming independence of observation) construct a number of resamples. Such resamples have to be of equal size to the observed dataset and be obtained by random sampling with replacement from the original dataset. From a number of resamples we can create approximate distribution of variable and obtain estimator - in our case standard deviation.

The general bootstrap algorithm is as follows:

1. Let n be a number of elements in dataset. Pick at random n elements (with returns).
2. Calculate an observable X using n elements created in 1.
3. Repeat 1. and 2. m times. This gives a series X_1, X_2, ..., X_m of estimations of X.
4. Use this series to calculate the standard deviation $\sigma = \sqrt{\langle X^2 \rangle - \langle X \rangle^2}$.

We specifically want to use this algorithm for calculation of standard deviation of such physical quantities as specific heat C, magnetic susceptibility χ etc. However, as our Monte Carlo simulations are time- and memory-consuming, it's difficult to obtain suffiecient set of such quantities for calculating standard deviation. Instead we use data from one Monte Carlo simulation to construct set of resamples, from each we calculate the necessary quantity and find standard deviation of obtained distribution.

At this stage of project calculation of standard deviation of 3 quantities are implemented:

- specific heat C,
- magnetic susceptibility χ,
- magnetisation M.

You can choose proper quantity by choosing argument *error_type* in function *Ising::ERROR* as ERROR_CHI, ERROR_CC or ERROR_OP.

3 Tests

In the tests IsingTestError1D.h and IsingTestError2D.h we calculate error (standard deviation) of magnetic susceptibility in function of production time. We use bootstrap method implemented in function *Ising::ERROR*.

General result for error known in MC integration methods is inversely proportionate to square root of number of samples n:

$$error \propto 1/\sqrt{n}$$

Therefore, we expect our error would diminish with increase of production time like $1/\sqrt{prod\_t}$. Results agree with our predictions. On figures below you can see calculated error in function of production time as well as fits proportionate to $1/\sqrt{prod\_t}$.

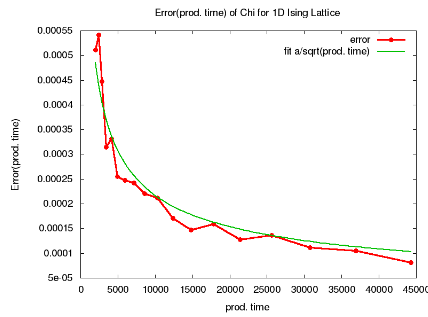

Figure 1: Error (standard deviation) of magnetic susceptibility in function of production time for 1D Ising lattice.

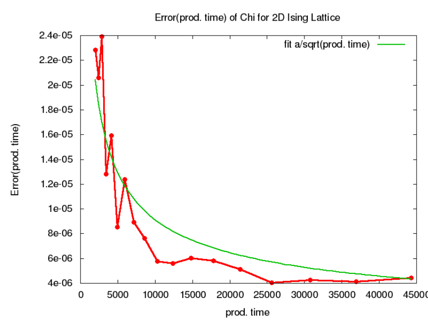

Figure 2: Error (standard deviation) of magnetic susceptibility in function of production time for 2D Ising lattice.

Additionally we calculate error of magnetic susceptibility in function of temperature and compare it with difference between analytical and numerical solution for χ. We do it only for 1D case because we do not now exact formula for χ in 2D. We can see both error and shown difference decrease with temperature and are of the same order of magnitude.

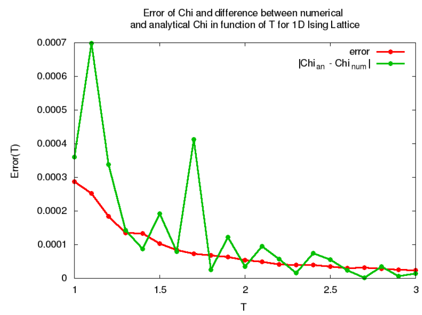

Figure 3: Comparison of error (standard deviation) and difference of analytical and numerical magnetic susceptibility in function of temperature.