PHY 4102: Numerical Simulation techniques in Physics

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Basic Error Analysis

(Also see: arXiv:1210.3781v2)

- We are interested in the expectation value of a quantity $\hat{A}$, given by

$$\langle A \rangle = \frac{1}{Z} \sum_x A_x e^{-\beta E_x}$$

The *variance* of $\langle A \rangle$ is, $\sigma^2 = \langle A^2 \rangle - \langle A \rangle^2$. σ is the *standard deviation*.

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- In Monte Carlo we estimate the quantity by the *estimator*,

$$\bar{A} = \frac{1}{M} \sum_{i=1}^{M} A_{x_i}$$

where the states x_i-s is selected from the proby distribution $p(x_i) = e^{-\beta E_{x_i}}/Z$.

- $\bar{A}$ is also called the *sample average* and the quantities A_{x_i}, which are the *samples*.

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First let us show that, $\langle \bar{A} \rangle = \langle A \rangle$:

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- What is the meaning of $\langle A_{x_i} \rangle$ in this context? Think of it as follows.
- We repeat the simulations very large number of times, that is, create a large number of Markov chains. From each chain, pick the states x_i realized at the i-th time step. Thus we have very large number of samples x_i picked from the same probability distribution $p(x_i)$. The average of these very large number of samples is $\langle A_{x_i} \rangle = \langle A \rangle$.

Next, let us calculate the quantity $\langle \bar{A}^2 \rangle$

$$
\begin{aligned}
\langle \bar{A}^2 \rangle = \left\langle \left(\frac{1}{M} \sum_{i=1}^{M} A_{x_i} \right)^2 \right\rangle &= \frac{1}{M^2} \sum_{i=1}^{M} \sum_{j=1}^{M} \langle A_{x_i} A_{x_j} \rangle \\
&= \frac{1}{M^2} \sum_{i=1}^{M} \langle A_{x_i}^2 \rangle + \frac{1}{M^2} \underbrace{\sum_{i=1}^{M} \sum_{j=1}^{M}}_{i \neq j} \langle A_{x_i} A_{x_j} \rangle
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Now *if* the samples are *independent*, $\langle A_{x_i} A_{x_j} \rangle = \langle A_{x_i} \rangle \langle A_{x_j} \rangle$ for $i \neq j$. Therefore,

$$\langle \bar{A}^2 \rangle = \frac{1}{M^2} \frac{1}{M} \sum_{i=1}^{M} \langle A^2 \rangle + \frac{M^2 - M}{M} \langle A \rangle^2$$

$$= \frac{1}{M} \langle A^2 \rangle + \frac{M-1}{M} \langle A \rangle^2$$

Standard deviation, σ_A

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\sigma_A^2 &= \left\langle \left(\bar{A} - \langle A \rangle\right)^2 \right\rangle = \langle \bar{A}^2 \rangle - \langle A \rangle^2 \\
&= \frac{1}{M} \langle A^2 \rangle + \frac{M-1}{M} \langle A \rangle^2 - \langle A \rangle^2 \quad \text{(using the prev. result)} \\
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s^2 = \frac{1}{M-1}\sum_{i=1}^{M}(A_{x_i} - \bar{A})^2
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- The best thing we can do is replace σ^2 by s^2. In fact it can be shown that $\langle s^2 \rangle = \sigma^2$.

- Finally, we can estimate *experimental error* of the Monte Carlo measurement as

$$\sigma_A = \left[\frac{1}{M(M-1)} \sum_{i=1}^{M} \left(A_{x_i} - \bar{A} \right)^2 \right]^{1/2}$$

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- Notice also that,

$$\sigma_A = \frac{s}{\sqrt{M}}$$

- Usually s does not vary much with M. Hence,

$$\sigma_A \propto \frac{1}{\sqrt{M}}$$

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- A simple stategy to obtain independent samples is to discard many states in between two measurements.
- But discard how many many exactly?
- A rigorous answer to the question would need calculation of a quantity called *autocorrelation time* τ_A. Time autocorrelation function,

$$\chi(t) = \int dt' \left[A(t')A(t'+t) - \bar{A}^2\right]$$
$$\chi(t) \sim e^{-t/\tau_A}$$