Numerically estimating the two-point correlation function in spin systems

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1 Motivation

Correlations are ubiquitous in physics, nature and life. In statistical mechanics the correlation is quantified by the correlation function. The most common definition of the latter is the canonical ensemble (thermal) average of the scalar product of two random variables, $\mathbf{s_1}$ and $\mathbf{s_2}$, at positions $R+r$ and times t and $t+\tau$:

$$C(r,\tau) = \langle \mathbf{s_1}(R,t) \cdot \mathbf{s_2}(R+r,t+\tau)\rangle \ - \langle \mathbf{s_1}(R,t)\rangle\langle \mathbf{s_2}(R+r,t+\tau)\rangle \, .$$

Here the brackets, $\langle\cdot\rangle$, indicate the above-mentioned thermal average. Here, we want to study the equal-time ($\tau = 0$) autocorrelation ($s_1 = s_2$) function where $s_1 = s_2 = \sigma$ are a scalar random variable with mean zero.

As the mean of σ is zero, the second part in Eq. (1) naturally is zero. Thus, from a purely analytical perspective it is clear that the term can be omitted. However, when the aim is to *estimate* $C(r,t)$ using a *finite* sample it is not clear whether and if, what to subtract from the first term.

The aim of this project is to study various possible estimators for the correlation function in Eq. (1) and to rank them by their suitability for practical applications.

2 Background

Throughout, we consider spin configurations $\{\sigma_i\}$ that consist of $N = L^d$ spins $\sigma_i \in \{-1,+1\}$, that lie on hyper-cubic lattice with linear length L and dimension $d = 1, 2$ or 3. At this point it is crucial to note, that there are 2^N possible spin configurations and that already for much smaller N than what we interested in we *cannot enumerate all of them.* Quite generally, the configuration $\{\sigma_i\}$ is a random variable that follows some probability mass function

$$P_\beta(\{\sigma_i\}), \tag{1}$$

where β is a control parameter which may be the inverse temperature but does not have to be[1].

The central quantity of interest is the two-point correlation function

$$C(i,j) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle, \tag{2}$$

where the angular brackets $\langle \cdot \rangle$ denote an average over all spin configurations weighted by Eq. (1), i.e.

$$\langle f\left(\{\sigma_i\}\right) \rangle = \sum_{\{\sigma_i\}} f(\{\sigma_i\}) P_\beta(\{\sigma_i\}) \tag{3}$$

and $f(\cdot)$ is a function that can be evaluated from a spin configuration. i and j in Eq. (2) refer to lattice sites and σ_i and σ_j are the respective spin values (-1 or $+1$) of a given spin configuration $\{\sigma_i\}$.

Further, we make the following assumptions on $P_\beta(\{\sigma_i\})$:

1. $P_\beta(\{\sigma_i\})$ is *translationally invariant*, that is for any $r \in \mathbb{Z}_L^d$:

$$P_\beta(\{\sigma_i\}) = P_\beta(\{\sigma_{i+r}\}). \tag{4}$$

   Note, that the addition $i + r$ is performed on the d-dimensional integer ring $\mathbb{Z}_L^d$ and that we automatically impose *periodic boundary conditions* on the system by requiring translational invariance.

2. $P_\beta(\{\sigma_i\})$ is *invariant under sign inversion*, that is

$$P_\beta(\{\sigma_i\}) = P_\beta(\{-\sigma_i\}). \tag{5}$$

As a consequence of the translational invariance (first assumption), the expectation value of a single spin $\langle \sigma_i \rangle$ is the same for all i and is equal to $m(\beta)$. If P is invariant under sign inversion it is easy to see that $m(\beta) = 0$. Coming back to Eq. (2), from the first assumption it follows that $C(i,j)$ only depends on $i - j$ and that the second term is equal to $[m(\beta)]^2$, which by imposing the second assumption is zero. This simplifies Eq. (2) to

$$C(r) = \langle \sigma_1 \sigma_{1+r} \rangle. \tag{6}$$

[1] In the context of equilibrium studies β corresponds to the inverse temperature $\beta \coloneqq 1/k_B T$ and we write down explicitly what we mean by Eq. (1). In nonequilibrium processes, e.g. the relaxation process triggered by a sudden change of the system's temperature, the control parameter is time t. Except for the simplest (nonequilibrium) cases, we cannot even write down an expression for Eq. (1) and usually describe in words what we mean by it.

3 Tasks

1. Familiarize yourself with the concept of *estimators*. Why do we need estimators? What is an unbiased estimator? How can there be two (different) estimators for the same quantity?

2. Using the example of the one-dimensional non-conserved Ising model with periodic conditions: Draw each $R^{\max}$ (uncorrelated) samples (= spin configurations) for the inverse temperatures $\beta \in \{0.5, 1, 2\}$ and using system sizes $L \in \{100, 1\,000, 10\,000\}$. Compare data for the energy and magnetization per spin to the known exact results.

3. Estimate $C(r)$ by using the following estimators (you may think of more and add more):

$$\hat{C}_1(r) = \frac{1}{R}\sum_{k=1}^{R}\frac{1}{L}\sum_{i=1}^{L}\sigma_i\sigma_{i+r} \tag{7a}$$

$$\hat{C}_2(r) = \frac{1}{R}\sum_{k=1}^{R}\frac{1}{L}\sum_{i=1}^{L}\sigma_i\sigma_{i+r} - \frac{1}{L}\sum_{i=1}^{L}\left(\frac{1}{R}\sum_{k=1}^{R}\sigma_i\right)\left(\frac{1}{R}\sum_{k=1}^{R}\sigma_{i+r}\right) \tag{7b}$$

$$\hat{C}_3(r) = \hat{C}_2(r)/\hat{C}_2(0) \tag{7c}$$

$$\hat{C}_4(r) = \frac{1}{R}\sum_{k=1}^{R}\frac{\frac{1}{L}\sum_{i=1}^{L}\sigma_i\sigma_{i+r} - \left(\frac{1}{L}\sum_{i=1}^{L}\sigma_i\right)^2}{1-\left(\frac{1}{L}\sum_{i=1}^{L}\sigma_i\right)^2} \tag{7d}$$

$$\hat{C}_5(r) = \frac{1}{R}\sum_{k=1}^{R}\frac{1}{L}\sum_{i=1}^{L}\sigma_i\sigma_{i+r} - \left(\frac{1}{R}\sum_{k=1}^{R}\frac{1}{L}\sum_{i=1}^{L}\sigma_i\right)^2 \tag{7e}$$

$$\hat{C}_6(r) = \hat{C}_5(r)/\hat{C}_5(0) \tag{7f}$$

   We know the *true* value for $C(r)$ (you may derive this yourself): $C(r) = (\tanh^r \beta J + \tanh^{L-r}\beta J)/(1+\tanh^L \beta J)$. By varying R, check whether the estimators $\hat{C}_k$ with $k \in \{1, 2, \ldots, 6\}$ are (asymptotically) unbiased. Check the variance of each estimator. Ultimately: Which estimator should be used in practice?

4. Possible further tasks:

   - For the $d = 1$ Ising model the bias and variance may be derived *exactly* for the estimators.
   - Repeat the analysis on the $d = 2$ Ising model. Also here some exact results can be used for comparison.
   - Repeat the analysis in a one- or two-dimensional Ising model when quenching the system from a high to a low temperature (= start at initial random configuration and simulate at a low temperature).