Dynamical correlations from classical dynamics: Imposing causality through zero-padding

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1 Structure factor from dynamical correlations

Our interest is estimating dynamical expectation values for a classical system with a prescribed dynamics. For concreteness, consider a system of spins $\mathbf{S}$ in equilibrium, obeying the Boltzmann distribution, $P[\mathbf{S}] \sim \exp(-\beta H[\mathbf{S}])$. To estimate dynamical quantities, we must also introduce a model for the physical time-dynamics. This might be the energy-conserving Landau-Lifshitz (LL) equation, or a Langevin spin dynamics that includes damping and noise terms. The latter can be used to model the effective coupling of spins to a thermal bath.

Let $A(x,t)$ and $B(x,t)$ denote local observables at position x for the time-evolved spin configuration $\mathbf{S}(t)$, starting from some initial configuration, $\mathbf{S}(0) = \mathbf{S}_0$. A dynamical time correlation is then,

$$C(x,t) = \langle A(0,0)B(x,t)\rangle, \tag{1}$$

where the bracket denotes an average over initial conditions $\mathbf{S}_0$ sampled from thermal equilibrium. Time-evolution preserves the Boltzmann distribution (under either LL or Langevin dynamics), so the correlation function is invariant under an arbitrary time shift. The average over equilibrium configurations $\mathbf{S}_0$ also ensures translation invariance in space. This translation invariances justify averaging over many space-time shifts,

$$C(x,t) = \frac{1}{\Omega}\langle \int_\Omega A(x',t')B(x'+x,t'+t)dx'dt'\rangle, \tag{2}$$

where the volume Ω should be sufficiently large such that "surface effects" can be ignored.

This integral can be written compactly as a cross correlation,

$$C(x,t) = \frac{1}{\Omega}\langle (A \star B)(x,t)\rangle. \tag{3}$$

The convolution theorem allows simplification in Fourier space,

$$\hat{C}(q,\omega) = \frac{1}{\Omega}\langle \hat{A}^*(q,\omega)\hat{B}(q,\omega)\rangle. \tag{4}$$

For concreteness, we employ the Fourier transformation convention,

$$\hat{A}(q,\omega) = \mathcal{F}_{q,\omega}[A] \equiv \int e^{-i(qx+\omega t)} A(x,t). \tag{5}$$

Because the classical observable $A(x,t)$ is real, we can also write

$$\hat{C}(q,\omega) = \frac{1}{\Omega}\langle \hat{A}(-q,-\omega)\hat{B}(q,\omega)\rangle. \tag{6}$$

This makes contact with the usual notion of "structure factor".

2 Estimates of dynamical correlations

In practice, our data $A(x,t)$ and $B(x,t)$ will be periodic in x, but will be *nonperiodic* in t. If we naively take the FFT of this data to plug into Eq. (6), we are effectively assuming periodic boundaries in time, and this can lead to aliasing effects due to the discontinuity at the edges of the time interval.

An alternative approach, proposed by Sam, is to treat the real-space correlation function $C(x,t)$ of as the more fundamental object to be estimated, and only take its Fourier transform at the end of the calculation. This viewpoint is useful because it allows mitigation of artifacts that would otherwise arise when periodically extending time.

Since the data is properly periodic in x, it is convenient to work in a mixed space where the position variable x has been Fourier transformed, but time t has not,

$$C_q(t) \equiv \int dx e^{-iqx} C(x,t). \tag{7}$$

This evaluates to (I think),

$$C_q(t) = \frac{1}{V}\langle \frac{1}{T}\int A_q^*(t')B_q(t'+t)dt'\rangle, \tag{8}$$

where we have decomposed Ω into separate volumes for space V and time T.

Recall that the remaining integral over t' is optional. That is, we could get the same result (in principle) without any time averaging,

$$C_q(t) = \frac{1}{V}\langle A_q^*(t')B_q(t'+t)\rangle, \tag{9}$$

which is valid for arbitrary reference time t'. To improve the quality of the statistical estimate, however, it is best to make use of all possible data. Assuming there is trajectory data over the interval $0 \le t < T$,we can integrate over all reference times t' subject to the restriction that the indexing is within the allowed bounds,

$$C_q(t) = \frac{1}{V}\frac{\langle \int A_q^*(t')B_q(t'+t)P(t,t')dt'\rangle}{\int P(t,t')dt'}, \tag{10}$$

where

$$P(t,t') = \begin{cases} 1 & (0 \le t' < T \quad \text{and} \quad 0 \le t + t' < T) \\ 0 & \text{otherwise} \end{cases}. \tag{11}$$

An efficient way to implement the integral of Eq. (10) is to define a periodic extension of the data that includes zero-padding of length T, e.g.,

$$\tilde{A}_q(t) = \begin{cases} A_q(s) & (0 \le s < T) \\ 0 & (T \le s < 2T) \end{cases}, \tag{12}$$

where t can be any real number and

$$s = \mathrm{mod}(t, 2T). \tag{13}$$

This leads to,

$$C_q(t) = \frac{1}{V(T - |t|)} \langle \int_0^{2T} \tilde{A}_q^*(t') \tilde{B}_q(t' + t) dt' \rangle, \tag{14}$$

which is exactly consistent with Eq. (9).

The integral can be recognized as a discrete circular cross correlation,

$$C_q(t) = \frac{1}{V(T - |t|)} \langle (\tilde{A}_q \star \tilde{B}_q)_t \rangle, \tag{15}$$

which can be evaluated efficiently through the fast Fourier transform of the zero-padded data $\tilde{A}_q$ and $\tilde{B}_q$.

In a practical implementation, a final procedure might be:

1. Fourier transform the signals $A(x,t)$ and $B(x,t)$ in space to get $A_q(t)$ and $B_q(t)$.

2. Zero-pad in time to get $\tilde{A}_q(t)$ and $\tilde{B}_q(t)$, which effectively doubles the size of this dimension.

3. Use FFTs in time to naively perform a circular cross correlation in the t index, for each q independently.

4. Apply an overall scaling factor $V^{-1}(T - |t|)^{-1}$ to obtain $C_q(t)$.

5. The desired structure factor $\hat{C}(q,\omega)$ is related to $C_q(t)$ by a final Fourier transform in time.

3 Limiting artifacts due to finite trajectory length and equilibrium samples

The above procedure is formally correct, but suffers from two issues at finite trajectory length T:

1. The $C_q(t)$ data is available only over the finite range $-T < t < T$, whereas the true Fourier transformation requires data over *all* real time-shifts t.

2. The ensemble average $\langle \cdot \rangle$ will be estimated from a finite number of samples, and statistical estimates of $C_q(t)$ become especially noisy when $t \to \pm T$.

The first issue amounts to an unavoidable introduction of some windowing function which sets $C(t) = 0$ whenever $|t| > T$. Given the unavoidal presence of *some* window, it is advantageous to select a *smooth* window which moves continously to zero as $|t| \to T$. This empirically resolves the second issue, by damping statistical noise associated with low numbers of samples.

A reasonable choice for the smooth window function might be

$$f(t) = \cos^2(\pi t/2T). \tag{16}$$

Beyond $|t| > T$, we may zero-pad the estimated correlation function some arbitary amount,

$$C_q(t) \approx \begin{cases} \frac{f(t)}{V(T-|t|)} \langle (\tilde{A}_q \star \tilde{B}_q)_t \rangle & (-T \leq t < T) \\ 0 & (\text{some finite domain}) \end{cases}. \tag{17}$$

To obtain the structure factor estimate in Eq. (6), only the temporal Fourier transform remains to be evaluated,

$$\hat{C}(q, \omega) = \int e^{-i\omega t} C_q(t) dt. \tag{18}$$

In the special case that $t = 0$, the window function disappears, $f(0) = 1$, and

$$C_q(0) = \frac{1}{VT} \int_0^T A_q^*(t') B_q(t') dt'. \tag{19}$$

This ensures that the "classical sum rule" will be exactly respected.