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Comment on "Information management in DNA replication modeled by directional, stochastic chains with memory" [J. Chem. Phys. 145, 185103 (2016)]

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We previously introduced the independence limit theorem, within the context of directional, stochastic chains with memory.[1] For the early proof, we considered that partition functions for two different stochastic chains with memory do not strongly depend on the present. In the following, we prove this theorem for any configuration, i.e., for configurations that include any present and past events.

To herein discuss on a self-contained material, we bring in the necessary equations and include the theorem statement before its demonstration.

Let ν be a sequence of objects, $x_1, \ldots, x_n$, that stem from a multivariate random variable $\mathbf{X}$,

$$\nu = \{x_1, x_2, \ldots, x_i, \ldots, x_{n-1}, x_n\}. \tag{1}$$

Their alphabet or domain will be denoted by $\mathcal{X}$. The energy of state $\nu \in \mathcal{X}^n$ is

$$E_\nu \equiv E(x_1, \ldots, x_n) = \sum_{i=1}^{n} E(x_i; x_{i-1}, \ldots, x_1), \tag{2}$$

where the *partial energy* $E(x_i; x_{i-1}, \ldots, x_1)$ is the energy of object x_i, provided that the previous objects (which constitute a *partial sequence*) are $(x_1, \ldots, x_{i-1})$.

The equilibrium partition function reads as follows:

$$Z(\beta, n) \equiv \sum_{\nu=1}^{N} \exp(-\beta E_\nu) \tag{3}$$

$$= \sum_{x_1, \ldots, x_n} \exp(-\beta E(x_1, \ldots, x_n)) \tag{4}$$

$$= \sum_{x_1, \ldots, x_n} \exp\left(-\beta \sum_{i=1}^{n} E(x_i; x_{i-1}, \ldots, x_1)\right), \tag{5}$$

where $\beta = 1/\mathrm{kT}$, k is the Boltzmann constant, and T is the absolute temperature; $N = |\mathcal{X}|^n$ is the number of configurations, which is the result of combining n events and $|\mathcal{X}|$ possibilities for each event.

The two-sequence energy is

$$E_{\nu'\nu} \equiv \sum_{i=1}^{n} E(x_i'; x_{i-1}, \ldots, x_1), \tag{6}$$

and the sequence-dependent partition function is given by

$$Z_\nu(\beta, n) \equiv \sum_{\nu'=1}^{N} \exp(-\beta E_{\nu'\nu}) \tag{7}$$

$$= \sum_{x_1', \ldots, x_n'} \exp\left(-\beta \sum_{i=1}^{n} E(x_i'; x_{i-1}, \ldots, x_1)\right). \tag{8}$$

Theorem (Independence limit). *Let ν be a stochastic, linear chain with memory [Eq. (1)] sequentially constructed i: $1 \rightarrow n$. Let Z and Z_ν be the normal (equilibrium) and the sequence-dependent partition functions [Eqs. (3) and (5) and Eqs. (7) and (8), respectively],* *and let $E_i = E(x_i'; x_{i-1}', \ldots, x_1')$ and $E_i' = E(x_i'; x_{i-1}, \ldots, x_1)$ be the energies of object x_i' relative to two different partial sequences [Eq. (2)]. If the normalized energy difference $|E_i - E_i'|/kT \to 0$, $\forall i$, then $Z/Z_v \to 1$.*

We want to show that

$$\frac{Z}{Z_v} \approx 1 \tag{9}$$

for mild memory effects. We next provide two alternative demonstrations.

Proof 1. For mild memory effects, we can express the partial energies as follows:

$$E(x_i'; x_{i-1}', \ldots, x_1') = E(x_i'; x_{i-1}, \ldots, x_1) + \epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1),$$

where $\epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1)$ is the difference between energies associated with different, partial sequences $(x_{i-1}', \ldots, x_1')$ and $(x_{i-1}, \ldots, x_1)$.

For all i, $\epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1)$ fulfills

$$\epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1) = 0, \quad \text{if } (x_{i-1}, \ldots, x_1) = (x_{i-1}', \ldots, x_1'), \text{ and} \tag{10}$$

$$|\epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1)| \ll kT, \quad \text{otherwise.} \tag{11}$$

Then,

$$E_{v'} = \sum_{i=1}^{n} E(x_i'; x_{i-1}', \ldots, x_1') = \sum_{i=1}^{n} E(x_i'; x_{i-1}, \ldots, x_1) + \sum_{i=1}^{n} \epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1) = E_{v'v} + \epsilon_{v'v},$$

where $\epsilon_{v'v} \equiv \sum_{i=1}^{n} \epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1)$ is a small two-sequence energy. Consequently,

$$\frac{Z}{Z_v} = \frac{\sum_{v'=1}^{N} \exp(-\beta E_{v'})}{\sum_{v'=1}^{N} \exp(-\beta E_{v'v})} = \frac{\sum_{v'=1}^{N} \exp(-\beta E_{v'v}) \exp(-\beta \epsilon_{v'v})}{\sum_{v'=1}^{N} \exp(-\beta E_{v'v})} = \sum_{v'=1}^{N} p_{v'}(v) \exp(-\beta \epsilon_{v'v}), \tag{12}$$

where

$$p_{v'}(v) \equiv \frac{\exp(-\beta E_{v'v})}{\sum_{v'=1}^{N} \exp(-\beta E_{v'v})} \tag{13}$$

can be interpreted as a probability in v' with free parameter v. Certainly, $0 \le p_{v'}(v) \le 1$, $\forall v'$, $v = 1, \ldots, N$, and $\sum_{v'=1}^{N} p_{v'}(v) = 1$, $\forall v = 1, \ldots, N$. We now expand $\exp(-\beta\epsilon_{v'v})$ in the limit $\beta\epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1) \to 0$ [see Eqs. (10) and (11)],

$$\exp(-\beta\epsilon_{v'v}) = \exp\left(-\beta \sum_{i=1}^{n} \epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1)\right) \approx 1 - \beta \sum_{i=1}^{n} \epsilon(x_i'; x_{i-1}', x_{i-1}, \ldots, x_1', x_1) = 1 - \beta\epsilon_{v'v}. \tag{14}$$

Then,

$$\frac{Z}{Z_v} \approx \sum_{v'=1}^{N} p_{v'}(v)(1 - \beta\epsilon_{v'v}) = 1 - \sum_{v'=1}^{N} p_{v'}(v)\beta\epsilon_{v'v} = 1 + \varepsilon_v, \tag{15}$$

where we have introduced $\varepsilon_v \equiv -\sum_{v'=1}^{N} p_{v'}(v)\beta\epsilon_{v'v}$, a small number. Indeed, $|\varepsilon_v| \le \sum_{v'=1}^{N} \beta|\epsilon_{v'v}| \to 0$ for $\beta\epsilon_{v'v} \to 0$; we have used the following inequalities:

$$\left|\sum_{j=1}^{m} a_j b_j\right| \le \sum_{j=1}^{m} |a_j||b_j|, \qquad \left|\sum_{j=1}^{m} p_j a_j\right| \le \sum_{j=1}^{m} |a_j|,$$

with a_j, b_j, and p_j being real numbers and $0 \le p_j \le 1$, $\forall j = 1, \ldots, m$. Therefore, $\varepsilon_v \to 0$, which concludes the proof of Eq. (9) and the theorem.

Proof 2. For mild memory effects, we express $\forall x_i'$, $i = 1, \ldots, n$,

$$\beta|E(x_i'; x_{i-1}', \ldots, x_1') - E(x_i'; x_{i-1}, \ldots, x_1)| \le \varepsilon. \tag{16}$$

Then, $\beta|E_{v'} - E_{v'v}|$

$$= \beta\left|\sum_{i=1}^{n}[E(x_i'; x_{i-1}', \ldots, x_1') - E(x_i'; x_{i-1}, \ldots, x_1)]\right| \le \sum_{i=1}^{n} \beta|E(x_i'; x_{i-1}', \ldots, x_1') - E(x_i'; x_{i-1}, \ldots, x_1)| \le n\varepsilon. \tag{17}$$

The difference between partition functions is as follows:

$$|Z - Z_v| = \left|\sum_{v'}[\exp(-\beta E_{v'}) - \exp(-\beta E_{v'v})]\right| = \left|\sum_{v'} \exp(-\beta E_{v'v})[\exp(-\beta E_{v'} + \beta E_{v'v}) - 1]\right| \le \sum_{v'} \exp(-\beta E_{v'v})|\exp(-\beta(E_{v'} - E_{v'v})) - 1|. \tag{18}$$

To continue, we prove the following inequality:

$$|e^z - 1| \le e^{|z|}|z|, \tag{19}$$

which arises from the remainder in Taylor's theorem for $f(z) = e^z$. Indeed, since $f(z) = f(0) + f'(c)z$, for $|c| \le |z|$, it follows that $e^z = 1 + e^c z$, thus making $|e^z - 1| = |e^c z| = e^c|z| \le e^{|z|}|z|$.

We now use this inequality in Eq. (18) followed by Eq. (17). We obtain

$$|Z - Z_v| \le \sum_{v'} \exp(-\beta E_{v'v}) \exp(\beta|E_{v'} - E_{v'v}|)\beta|E_{v'} - E_{v'v}| \le \sum_{v'} \exp(-\beta E_{v'v}) \exp(n\varepsilon)n\varepsilon = Z_v n\varepsilon \exp(n\varepsilon).$$

Therefore,

$$\left|\frac{Z}{Z_v} - 1\right| \le n\varepsilon \exp(n\varepsilon) \Rightarrow \frac{Z}{Z_v} \xrightarrow[\varepsilon \to 0]{} 1,$$

which concludes the proof.

REFERENCE

[1] J. R. Arias-Gonzalez, J. Chem. Phys. **145**, 185103 (2016).