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1993 J. Phys. A: Math. Gen. 26 2269

(http://iopscience.iop.org/0305-4470/26/9/022)

J. Phys. A: Math. Gen. 26 (1993) 2269–2273. Printed in the UK

COMMENT

Explicit mean energies for the thermodynamics of systems of finite sequences

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Received 21 June 1992, in final form 26 October 1992

Abstract. Wiślicki has suggested that the Hamming distance between binary sequences (or strings, or bit-strings) might serve as an interaction energy. The partition function and related thermodynamic quantities could then be calculated and used to investigate ensembles of binary string systems evolving, for example, according to cellular automata rules. In this note we construct the *explicit* mean energies for ensembles whose elements consist of N bit-strings, each of length M. The N bit-strings have $n_1, n_2, \ldots, n_N$ 1s and $M - n_1, M - n_2, \ldots, M - n_N$ 0s, respectively, where $0 \leqslant n_i \leqslant M, i = 1, 2, \ldots, N$. The energy of N interacting bit-strings is taken to be the pairwise sum of the Hamming distances between individual pairs of bit-strings.

Recently Wiślicki (1990) investigated the possibility of characterizing the output of finite sequences of symbols from a dynamical system by constructing thermodynamic-like characteristics of the output ensemble. Specifically, he considered a system consisting of N binary strings (or bit-strings) of length M, i.e. N sequences whose individual elements are M 0s and 1s. The strings in this set interact with each other through some specified relation structure, and Wiślicki concentrated on the important case where each string in the system interacts with every other string in the system, giving rise to $N(N-1)/2$ interactions.

Interacting strings S_i and S_j were characterized by an energy of interaction E_{ij}, the Hamming distance $d(S_i, S_j)$, so that

$$E_{ij} = d(S_i, S_j) \,. \tag{1}$$

The Hamming distance $d(S_i, S_j)$ is the number of places where the strings S_i and S_j differ, or equivalently, the number of 1s in the string $S_i \oplus S_j$, where $\oplus$ stands for bitwise addition of strings modulo 2. Equation (1) implies that the production of either string from the other costs at least $d(S_i, S_j)$ 'energy units', where the latter measures the cost of changing a bit.

Wiślicki's intention was to introduce a method for characterizing ensembles of binary strings representing the output of a formal system; for example, an ensemble of N bit-strings evolving according to cellular automata rules. Cellular automata have been used to model pattern formation in dendritic structures, reaction-diffusion processes, molecular dynamics, soliton behaviour and a number of other physical systems (see Wolfram 1986, for example). Though the author is unaware of any physical systems which can be directly modelled by the formal system considered by Wiślicki, it is quite possible that his ideas could find application in some models of physical systems.

For a system of N interacting binary strings $(S_1, S_2, \ldots, S_N)$, each of length M, suppose that the location of 0s and 1s in the strings is random except for the constraint that the

N strings $S_1, S_2, \ldots, S_N$ have $n_1, n_2, \ldots, n_N$ 1s and $M - n_1, M - n_2, \ldots, M - n_N$ 0s respectively. The ensemble of all possible such N strings has $\binom{M}{n_1}\binom{M}{n_2}\cdots\binom{M}{n_N}$ elements. We assume the N strings interact pairwise (all known interactions in physics occur this way) so that from (1) the combined energy of interaction of these N strings is

$$E_{12\ldots N} = \sum_{i<j\leqslant N} E_{ij} = \sum_{i<j\leqslant N} d(S_i, S_j)\,. \tag{2}$$

There are $\binom{N}{2}$ terms in the sum in (2).

In order to calculate thermodynamic analogues for systems of binary strings, Wiślicki used statistical mechanics (e.g. Huang 1963) to define the thermodynamic energy U and the thermodynamic entropy S as

$$U = -\frac{\partial}{\partial\beta}(\log Z_N) \qquad S = -\beta^2\frac{\partial}{\partial\beta}\left(\frac{1}{\beta\log Z_N}\right) \tag{3}$$

where Z_N, the partition function of the fixed N system, is defined by

$$Z_N = \sum_k \exp(-\beta E_k)\,. \tag{4}$$

The quantity E_k in the sum in (4) is the energy of the kth state. The formal parameter β is called the inverse temperature. If the energy spectrum is known, Z_N can be calculated from (4) and the energy U and the entropy S can be determined from (3). Alternatively, one can determine the probability p_k of finding the system in the energy state E_k and thus calculate the mean energy $\langle E\rangle$, where

$$\langle E\rangle = \sum_k p_k E_k\,. \tag{5}$$

Equating the thermodynamic energy U in (3) and the mean energy $\langle E\rangle$ in (5) yields

$$U(\beta) = \langle E\rangle \tag{6}$$

and the solution of (6) for β yields the equilibrium temperature. One can see from (6) that explicit knowledge of $\langle E\rangle$ would be useful in determining the equilibrium inverse temperature β, a parameter which could be used to describe the ensemble.

Wiślicki (1990) considered the simplest non-trivial case ($N = 2$) of two interacting strings of length M with n_1 and n_2 1s and $M - n_1$ and $M - n_2$ 0s respectively. In the special case for which $n_1 = n_2 = n$ and $M \geqslant 2n$ he determined the partition function Z_2 and, using (3) and (6), gave asymptotic formulas (as $n \to \infty$) for U, β, and S in terms of $\langle E\rangle$. Using an expression for p_k obtained from combinatorial arguments together with (5), he gave an explicit expression for $\langle E\rangle$, $\langle E\rangle = n$, in the special case when $n_1 = n_2 = n$ and $M = 2n$. Wiślicki remarked that the determination of $\langle E\rangle$ in general from (5) was difficult because of the presence of factorials in the sum and that, in practice, numerical methods were usually necessary.

The purpose of this note is to *explicitly* calculate $\langle E\rangle$ for arbitrary N, M, and $n_1, n_2, \ldots, n_N$. This result is given in (19). It should be useful in future investigations of the thermodynamics of systems of finite sequences.

Suppose the positive integers N and M and the N-tuple $(n_1, n_2, \ldots, n_N)$ are given, with $0 \leqslant n_i \leqslant M$ for $i = 1, 2, \ldots, N$. The sample space Ω_N has $\binom{M}{n_1}\binom{M}{n_2}\cdots\binom{M}{n_n}$ elements, each consisting of an N-tuple of binary-strings of length M, $(S_1, S_2, \ldots, S_N)$. Each S_i has n_i 1s and $M - n_i$ 0s, $i = 1, 2, \ldots, N$. Note that $n_1, n_2, \ldots, n_N$ are the same for all elements in the sample space Ω_N.

Pick i and j so that $1 \leqslant i < j \leqslant N$ and define the energy of interaction of the pair of strings (S_i, S_j) to be $E_{ij} = d(S_i, S_j)$ as in (1). This defines a random variable E_{ij} on the sample space Ω_N. Its mean value will allow us to determine the mean energy of an element in Ω_N.

To determine the possible energies E_{ij} for an element in Ω_N and the distribution of these values over the sample space Ω_N we proceed in the following way. For an element in Ω_N there are $\binom{M}{n_i}$ ways to place the n_i 1s in S_i—leaving the remaining $M - n_i$ bits in S_i as 0s. After selecting the positions of the n_i 1s in S_i in some manner, construct the S_j of that element by putting k 0s and $n_i - k$ 1s in the spaces in S_j which coincide with the locations of the n_i 1s in S_i. The integer k is constrained by the inequalities

$$0 \leqslant k \leqslant n_i \qquad n_i - k \leqslant n_j \tag{7}$$

since S_i and S_j have n_i and n_j 1s respectively. This method of placing k 0s and $n_i - k$ 1s in S_j contributes an amount k to $d(S_i, S_j)$. In the remaining $M - n_i$ spaces in S_j we must place $n_j - (n_i - k)$ 1s and

$$M - n_i - [n_j - (n_i - k)] = M - n_j - k$$

0s, where k satisfies the inequality

$$k \leqslant M - n_j \tag{8}$$

since S_j has $M - n_j$ 0s. The inequalities in (7) and (8) together imply that

$$k_{\min} \leqslant k \leqslant k_{\max} \tag{9}$$

where

$$k_{\min} = \max\{0, n_i - n_j\} \qquad k_{\max} = \min\{n_i, M - n_j\}\,. \tag{10}$$

Since the remaining $M - n_i$ spaces in S_j coincide with 0s in S_i and we are placing $n_j - (n_i - k)$ 1s into them, we get an additional contribution of $k + n_j - n_i$ to $d(S_i, S_j)$. Therefore $\mathrm{d}(S_i, S_j) = 2k + n_j - n_i$, and we define the energy E_k^{ij} of this state to be

$$E_k^{ij} = 2k + n_j - n_i \tag{11}$$

where the index k satisfies (9) and (10).

For a given k, how many elements of the sample space Ω_N have energy E_k^{ij} given by (11)? By the process used to determine the energy state E_k^{ij}, it is clear that there are

$$\binom{M}{n_i}\binom{n_i}{k}\binom{M - n_i}{k + n_j - n_i}\binom{M}{n_r}\binom{M}{n_s}\cdots\binom{M}{n_t}$$

elements in Ω_N for which the random variable E_{ij} defined by (1) has the value E_k^{ij}. The integer k satisfies (9), and and the subscript indices $i, j, r, s, \ldots, t$ are related by

$$\{r, s, \ldots t\} = \{1, 2, \ldots, N\}/\{i, j\}\,.$$

Consequently the probability p_k^{ij} that the random variable E_{ij} takes the value E_k^{ij} in (11) on Ω_N is given by

$$p_k^{ij} = \frac{\binom{n_i}{k}\binom{M-n_i}{k+n_j-n_i}}{\binom{M}{n_j}} . \tag{12}$$

Now when m and n are integers and l is a non-negative integer,

$$\sum_k \binom{l}{m+k}\binom{s}{n+k} = \binom{l+s}{l-m+n} \tag{13}$$

where the sum in (13) extends over all integers k and the binomial coeffients $\binom{r}{k}$ are defined by

$$\binom{r}{k} = \begin{cases} \dfrac{r(r-1)\cdots(r-k+1)}{k(k-1)\cdots 1} & k \text{ integer} \quad k > 0 \\ 1 & k \text{ integer} \quad k = 0 \\ 0 & k \text{ integer} \quad k < 0 \end{cases} \tag{14}$$

(see, for example, Graham *et al* 1989 p 169). In (13) and (14) s and r are real numbers; the definition in (14) is notationally useful because the limits on the sum in (13) need not be explicitly given.

Combining (12) and (13) then gives

$$\sum_k p_k^{ij} = \frac{\binom{M}{n_j}}{\binom{M}{n_j}} = 1 . \tag{15}$$

Observe, in accordance with the previous remark, that because of the definitions of p_k^{ij} and $\binom{r}{k}$ in (12) and (14), the only non-zero terms in the sum in (15) are those for which k satisfies (9).

To compute $\langle E_{ij} \rangle$, the expected value of the random variable E_{ij} on Ω_N, we use (11) and (15) to write

$$\langle E_{ij} \rangle = \sum_k p_k^{ij} E_k^{ij} = \sum_k p_k^{ij} (n_j - n_i + 2k) = n_j - n_i + \sum_k 2kp_k^{ij} . \tag{16}$$

(Note that in the $N = 2$ case (where $i = 1$ and $j = 2$) Wiślicki inexplicably fails to include the $n_2 - n_1$ term of (16) in his equation (11).) Now

$$k\binom{n_i}{k} = \begin{cases} n_i \binom{n_i - 1}{k-1} & k \text{ integer} \quad k \geqslant 1 \\ 0 & k \text{ integer} \quad k \leqslant 0 \end{cases} \tag{17}$$

and so by combining (12), (13), (16) and (17) we obtain

$$\begin{aligned} \langle E_{ij} \rangle &= n_j - n_i + \frac{2n_i}{\binom{M}{n_j}} \sum_k \binom{n_i - 1}{k-1}\binom{M - n_i}{k + n_j - n_i} = n_j - n_i + 2n_i \frac{\binom{M-1}{n_j}}{\binom{M}{n_j}} \\ &= n_j - n_i + 2n_i \frac{(M - n_j)}{M} = n_i\left(1 - \frac{n_j}{M}\right) + n_j\left(1 - \frac{n_i}{M}\right) . \end{aligned} \tag{18}$$

For a given $i < j \leqslant N$, (18) explicitly gives the mean value of the interaction energy E_{ij}, or equivalently, the mean value of the Hamming distance $d(S_i, S_j)$, on Ω_N. The mean interaction energy $\langle E_{ij}\rangle$ is symmetric in n_i and n_j and tends to $n_i + n_j$ as n_i/M and n_j/M both tend to zero.

To compute $\langle E_{12\ldots N}\rangle$, the expected value of the random variable $E_{12\ldots N}$ defined on Ω_N by equation (2), note that $E_{12\ldots N}$ is the sum of the $N(N-1)/2$ individual random variables $E_{ij} = d(S_i, S_j)$, $i < j \leqslant N$, each of which is defined on the sample space Ω_N. The possible values of $E_{12\ldots N}$ and their corresponding probabilities could be found from the the joint distribution of the $d(S_i, S_j)$ and so $\langle E_{12\ldots N}\rangle$ could be calculated. This is a rather daunting task and a much simpler way to proceed is to observe that the mean or expected value of a finite sum of random variables is the sum of their mean or expected values (see, for example, Feller 1968). Equations (2) and (18) then imply

$$\langle E_{12\ldots N}\rangle = \sum_{i<j\leqslant N} \langle E_{ij}\rangle = \sum_{i<j\leqslant N} \left[n_i\left(1 - \frac{n_j}{M}\right) + n_j\left(1 - \frac{n_i}{M}\right)\right] \tag{19}$$

giving an explicit formula for the mean energy of an element in Ω_N. Note that when $N = 2, n_1 = n_2 = n$, and $M = 2n$, equation (19) reduces to

$$\langle E_{12}\rangle = n$$

the special case considered by Wiślicki following his equation (17).

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