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1990 J. Phys. A: Math. Gen. 23 L121

(http://iopscience.iop.org/0305-4470/23/3/008)

J. Phys. A: Math. Gen. 23 (1990) L121-L125. Printed in the UK

LETTER TO THE EDITOR

Thermodynamics of systems of finite sequences

Wojciech Wiślicki
Institute for Nuclear Studies, Warsaw, Poland

Received 1 August 1989, in final form 1 November 1989

Abstract. It is proposed that the Hamming distance between bit-strings plays the role of interaction energy. The statistical sum and thermodynamic functions are calculated for the canonical ensemble of bit-sequences. The method is illustrated with an ensemble of two-sequence systems which evolve according to cellular automata rules.

Recently much attention has been devoted to developing new tools to study high-dimensional dynamical systems, e.g. many-body and fluid mechanics, neural networks and lasers. The complexity of the objects under consideration requires effectively computable methods to characterise their behaviour. There exists a wealth of nonlinear models too complex for analytical treatment. Algorithmic methods, however, often render difficult any synthetic approach to the process and results of computations are often treated as experimental data. Let us imagine the situation when the system we are studying consists of a number of outputs of computations represented as finite sequences of symbols. The state of our system depends on inputs and by changing inputs randomly one can form the ensemble of outputs. A single sequence of symbols is considered here as the basic constituent, analogously to a molecule in physical systems such as gases or crystals. For simplicity we take into account only a two-symbol alphabet, i.e. strings composed of zeros and ones. Extensions to larger numbers of symbols are straightforward. We show the possibility of constructing thermodynamic characteristics of the output ensemble and thus describe the formal system it represents. We illustrate this method by studying in more detail the simple example of the two-string system evolving according to the rules of legal class-3 automata.

Let us consider a system consisting of N bit-strings of length M, i.e. sequences built from M 0s and 1s. We allow the set of strings to have a relation structure specified by the set of links between elements. Of interest to us are connected sets, i.e. those where a path exists for any pair of elements. In the extreme case there may exist a link between each pair of strings and we call this the maximum connection scheme. The state of our system is completely described by specifying the connection scheme and values of bits (0 or 1) in each string.

If two strings are connected by a link we call them interacting elements and we propose an analogue of the energy for this interaction. For given two strings S_1 and S_2 we identify the energy E_{12} with the Hamming distance between them, i.e. the number of bits which differ by

$$E_{12} = d(S_1, S_2) \tag{1}$$

where $d(S_1, S_2)$ is the number of 1s in the string $S_1 \oplus S_2$. Symbol $\oplus$ stands for exclusive-or operator. To make this definition more intuitive we recall the interpretation

0305-4470/90/030121+05$03.50

of the Hamming distance as the minimal number of bit-flips necessary to make two strings identical. In other words, production of $S_{1(2)}$ from $S_{2(1)}$ costs at least $d(S_1, S_2)$ elementary energy units.

Generally, we call the sum of E_{ij} over all links (i, j) the energy of the given state

$$E_A = \sum_{(i,j)} E_{ij}. \tag{2}$$

In order to find thermodynamic characteristics we use standard statistical mechanics methods (Huang 1963) and define the partition function Z_N of the fixed-N system as

$$Z_N = \sum_k \exp(-\beta E_k) \tag{3}$$

where E_k stands for energy of the kth state and we shall call the formal parameter β the inverse temperature.

In many cases the energy spectrum is known; Z_N can be calculated explicitly and then the energy U and the entropy S can be found by using the formulae

$$U = -\frac{\partial}{\partial \beta}(\log Z_N) \tag{4}$$

$$S = -\beta^2 \frac{\partial}{\partial \beta}\left(\frac{1}{\beta \log Z_N}\right). \tag{5}$$

It should be mentioned here that the term 'entropy' is often used in the literature in the other sense. For example, the Kolmogorov entropy and 'thermodynamic' entropy defined here are not the same thing.

On the other hand it is often possible to estimate the probability of finding a state of energy E_k and calculate the mean energy $\langle E \rangle$ of the system from combinatorics. Comparing $\langle E \rangle$ found in this way and U from (4) one gets the equation

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

Equation (6) should be solved in order to get the equilibrium temperature.

As the simplest non-trivial case let us consider two interacting random strings of length M with n_1 and n_2 1s. Without loss of generality we may assume $n_2 \leqslant n_1$. The equilibrium probability for the state of energy $E_k = 2k + n_2 - n_1$ in the canonical ensemble is given by (cf, e.g., Huang 1963)

$$p_k = \exp[-\beta(2k + n_2 - n_1)]/Z_2 \tag{7}$$

where

$$Z_2 = \sum_{k=0}^{k_{max}} \exp[-\beta(2k + n_2 - n_1)] \tag{8}$$

and

$$k_{max} = \begin{cases} n_1 & \text{for } n_1 + n_2 \leqslant M \\ M - n_2 & \text{for } n_1 + n_2 > M. \end{cases} \tag{9}$$

For random strings the probability p_k can be found from combinatorics and is equal to

$$p_k = \binom{n_1}{k}\binom{M - n_1}{k + n_2 - n_1}\binom{M}{n_2}^{-1}. \tag{10}$$

For the ensemble of random strings the mean energy is

$$\langle E \rangle = \sum_{k=0}^{k_{max}} 2k p_k. \tag{11}$$

Let us take the special case of $n_1 = n_2 = n$ and $M \geqslant 2n$, corresponding to two strings produced by the same source with probabilities n/M and $1-n/M$ for producing 1 and 0, respectively. We require the strings to be distinguishable, i.e. that the minimal energy be greater than zero. The partition function in this case is equal to

$$Z_2 = \sum_{k=1}^{n} e^{-2\beta k} = (1-e^{-2\beta n})/(e^{2\beta}-1). \tag{12}$$

For sufficiently long strings the statistical sum (12) in its asymptotic form reads

$$Z = \lim_{n\to\infty} Z_2 = 1/(e^{2\beta}-1). \tag{13}$$

The energy U calculated from (4) is equal to

$$U = 2/(1-e^{-2\beta}) \tag{14}$$

and from (6) follows the formula for equilibrium temperature

$$T = 1/\beta = -\tfrac{1}{2}\log^{-1}(1-2/\langle E\rangle). \tag{15}$$

The equilibrium entropy (5) is given by

$$\begin{aligned} S &= \log(\tfrac{1}{2}\langle E\rangle - 1) - \tfrac{1}{2}\langle E\rangle \log(1-2/\langle E\rangle) \\ &= 2/T(e^{2/T}-1) - \log(1-e^{-2/T}). \end{aligned} \tag{16}$$

The entropy (16) is an increasing function of both the mean energy $\langle E\rangle$ and the temperature T. From (16) it also follows that for low temperature the entropy tends to zero.

The statements above are valid generally for all long distinguishable strings with the same non-zero probabilities of finding 1, not necessarily random. In the random case the mean energy $\langle E\rangle$ can be calculated explicitly by using formulae (10) and (11). However, for long sequences the calculation of factorials in (10) may be difficult and in practice one has to determine $\langle E\rangle$ by Monte Carlo methods. The only simple case is $n = M/2$ where the formula (cf, e.g., Gradshteyn and Ryzhik 1971)

$$\sum_{k=1}^{n} k\binom{n}{k}^2 = (2n-1)!/[(n-1)!]^2 \tag{17}$$

is to be applied and $\langle E\rangle = n$.

As an illustration of our method we consider time evolution of the entropy for simple cellular automata (Wolfram 1983). We will investigate six computational rules, so called legal class-3 automata. The rules are labelled with numbers 18, 22, 90, 122, 126 and 150.

Our starting point is the ensemble of a thousand pairs of random strings with equal probabilities of 1s and 0s. To fulfil the requirements for applying asymptotic thermodynamic formulae we take strings of length 20 000. For each pair of the ensemble the evolution is followed up to one hundred steps, the energy (Hamming distance) calculated at each step and averaged over the ensemble. Then the entropy is calculated by using the formula (16).

It is known that for some rules densities of 1s do not remain constant during evolution. We have found the probabilities of 1s after one hundred steps to be equal to 0.26, 0.35, 0.55, 0.50, 0.51 and 0.50 for rules 18, 22, 90, 122, 126 and 150, respectively. For comparison, the numbers observed by the other authors (Kaspar and Schuster 1987) are 0.25, 0.35, 0.5, 0.5, 0.5 and 0.5. In order to show that the observed behaviour

of the entropy is not produced by the variable density of 1s itself we have studied the ratio S/S_{rand}, where S is the entropy for strings evolving according to a given rule and S_{rand} is the entropy for random strings with actual numbers of 1s.

The results obtained are displayed in figures 1-6 where the reduced entropy is presented for rules 18, 22, 90, 122, 126 and 150, respectively. Inspection of the figures reveals that for rules 122 and 150 there is no significant deviation of S/S_{rand} from 1. For rules 18 and 22 the reduced entropy decreases. The effect is stronger for rule 18. Rule 90 exhibits slow relaxation to the constant value of 1 after an initial slight decrease. For rule 126, after an initial rapid fall, the S/S_{rand} remains approximately constant slightly below 1.

Class-3 automata have been studied with a few other methods for complexity and pattern selection (Grassberger 1984, Kaspar and Schuster 1987, Wolfram 1984) and it

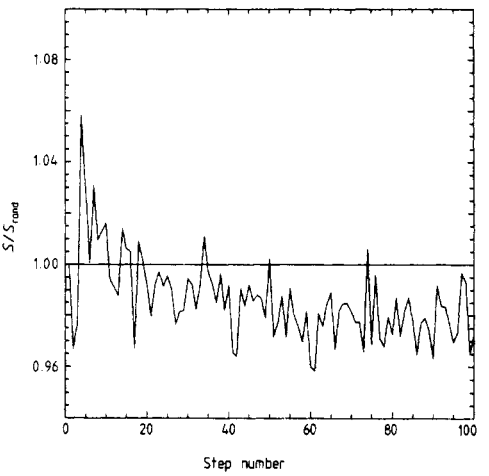

Figure 1. Evolution of the reduced entropy of the two-string system for the automaton rule 18.

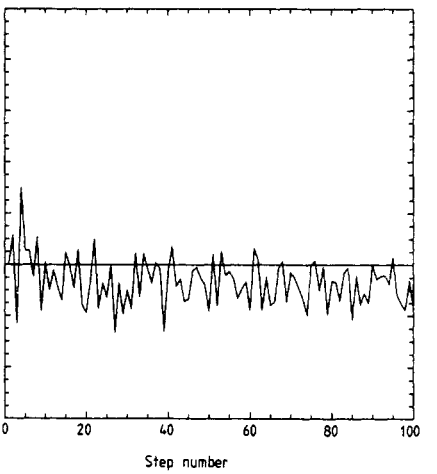

Figure 2. Evolution of the reduced entropy of the two-string system for the automaton rule 22.

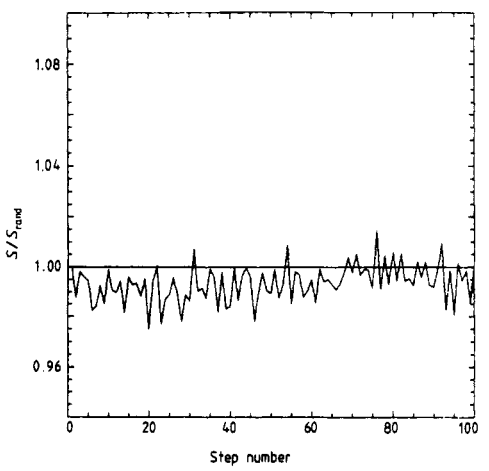

Figure 3. Evolution of the reduced entropy of the two-string system for the automaton rule 90.

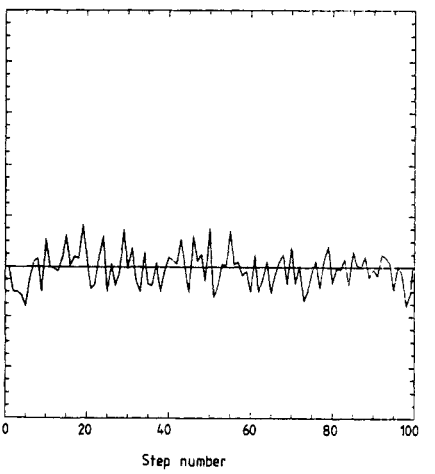

Figure 4. Evolution of the reduced entropy of the two-string system for the automaton rule 122.

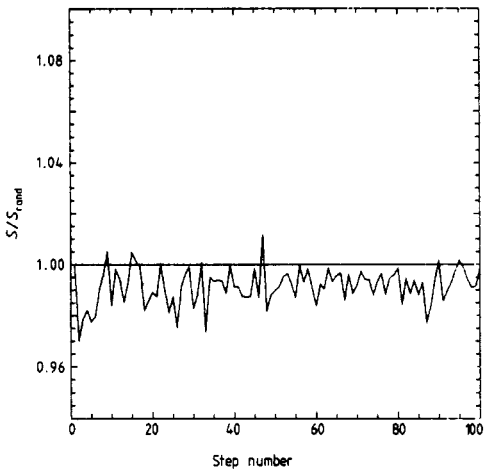

Figure 5. Evolution of the reduced entropy of the two-string system for the automaton rule 126.

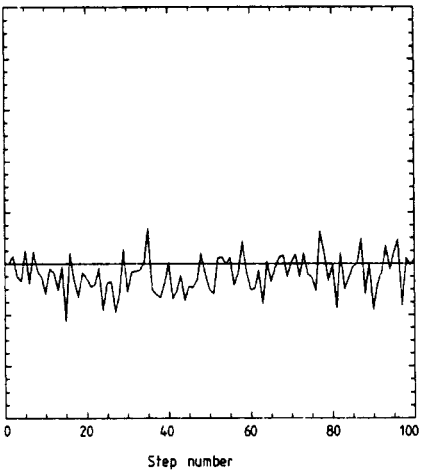

Figure 6. Evolution of the reduced entropy of the two-string system for the automaton rule 150.

has been found that no patterns appear for rules 90 and 150 and a reduction of the complexity was found for rules 18, 22, 122 and 126. Those investigations have been done for single strings. It is worth noting that the method presented here sheds light on the other feature of the automata, namely the ability to correlate chaotic sequences. Rules 18, 22 and 126 exhibit both complexity reduction and reduction of the entropy introduced in the present work.

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