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We define the entropy function $S(\rho)=\mathrm{Lim}_{n\to\infty}2n^{-2}\ln N(n,\rho)$, where $N(n,\rho)$ is the number of distinct partial order relations which may be defined on a set of n elements such that a fraction ρ of the possible $n(n-1)/2$ pairs are comparable. We derive upper bounds to $S(\rho)$ to show that $S(\rho)<(1/2)\ln 2$ if $\rho\geq .699$.

I. Introduction. In an earlier paper [1, hereafter referred to as I] we have studied the asymptotic enumeration of partial order relations defined over a set of n distinct objects, subject to a constraint that a given fraction ρ of the $n(n-1)/2$ pairs are comparable. Let this number be denoted by $N(n,\rho)$. We showed that $N(n,\rho)$ increases as an exponential of n^2 for large n (except in the trivial cases when ρ is either zero or one), and defined a function $S(\rho)$ by the equation

$$S(\rho) = \lim_{n\to\infty} 2n^{-2}\ln N(n,\rho)\ . \tag{1}$$

This function $S(\rho)$ may be called the entropy function as it is related to the thermodynamic entropy of a lattice-gas with a long-range three-body interaction. For details of this equivalence, the reader is referred to I.

Using upper and lower bounds on $S(\rho)$, we showed that $S(\rho)$ is a continuous function of ρ for the allowed range of ρ, $0\leqq\rho\leqq 1$. It is, however, not an analytic function of ρ. It was proved that

$$S(\rho) = \frac{1}{2}\ln 2 \quad \text{if} \quad \frac{1}{4}\leqq\rho\leqq\frac{3}{8} \tag{2}$$

and

$$S(\rho) < \frac{1}{2}\ln 2\ , \quad \text{if} \quad \rho\leqq .083 \quad \text{or if} \quad \rho\geqq 48/49\ . \tag{3}$$

The equality in (2) could be proved, because in this range of ρ, we derived a lower bound to $S(\rho)$ which coincides with an earlier known ρ-independent upper bound due to Kleitmen and Rothschild [2]. We conjectured that the lower bound (derived in I) gives the exact value of $S(\rho)$ for all ρ. This, however, could not be proved because the corresponding upper bounds to $S(\rho)$ were too weak. We have subsequently improved the upper bounds. Using these improved bounds we can show that

$$(4) \qquad S(\rho) < \frac{1}{2}\ln 2\,, \quad \text{if} \quad \rho \leqq .154 \quad \text{or} \quad \rho \geqq .699\,.$$

While these bounds fall short of the conjectured result

$$(5) \qquad S(\rho) < \frac{1}{2}\ln 2\,, \quad \text{if} \quad \rho < \frac{1}{4} \quad \text{or if} \quad \rho > \frac{3}{8}\,,$$

they are considerably better than the earlier bounds. These can be improved somewhat by a more extensive numerical calculation. A substantial improvement will perhaps require a different technique. In this paper, we report these bounds.

More recently Kleitman and Rothschild [3] have been able to determine $S(\rho)$ exactly in the range $0 \leqq \rho \leqq 1/4$. Their results, in particular, imply the first part of the inequality (5). Their result is obviously better than our bound for $\rho < .154$. However, their method does not seem to be generalizable to higher ρ values.

II. Preliminaries and notation. Consider a set $\mathscr{S}$, consisting of n distinct elements. Let R be a partial order relation defined on this set. We shall use the notation $a \geqq b (a, b \in \mathscr{S})$ iff a is related to b under R. We write $a > b$ iff $a \geqq b$ and $a \neq b$. A pair (a, b) is said to be comparable iff $a \geqq b$ or $b \geqq a$. It is nontrivial if $a \neq b$.

An ordered sequence $a_1, a_2, a_3, \cdots, a_l$ of elements of $\mathscr{S}$ constitutes a chain of length l iff $a_1 > a_2 > a_3 \cdots > a_l$. The rank of an element a, denoted by $r(a)$, is defined as the length of the longest chain in $\mathscr{S}$ which starts with a. By $r(T)$ we shall denote the specification of rank of each of the elements of $T \subseteqq \mathscr{S}$.

The relation R induces a decomposition into maximal disjoint chains $C_1, C_2, \cdots, C_p$. (This decomposition need not be unique.) The chains C_i are constructed as follows: C_1 is a longest chain in $\mathscr{S}$. C_2 is a longest chain in $\mathscr{S} - C_1$. C_3 is longest chain in $\mathscr{S} - C_1 - C_2$, and so on. The process is continued till all the elements of $\mathscr{S}$ are exhausted. The length of a chain C_i will be denoted by l_i. Clearly, we have $l_1 \geqq l_2 \geqq l_3, \cdots$. Also, any element of a chain C_i is incomparable to at least one element in each of the preceding chains C_j, $j < i$.

Let $N_n(m)$ be the number of different partial order relations R definable over $\mathscr{S}$, having exactly m nontrivial, comparable pairs. Let $\Omega_n(z)$ be the generating function for $N_n(m)$, i.e.,

$$(6) \qquad \Omega_n(z) = \sum_{m=0}^{n(n-1)/2} N_n(m) z^m\,.$$

Let A and B be disjoint, ordered subsets of $\mathscr{S}$. By an ordered subset here we mean a subset whose first, second elements

are identified. Let $|A| = i$ and $|B| = j$. Also let $\tilde{r}$ be a mapping from the set $A \cup B$ to the set of integers. Let $\tilde{R}$ be a partial order relation on $A \cup B$. We say that $\tilde{R}$ is consistent with the maximal chain structure $\{A, B\}$ and the rank function $\tilde{r}$ iff there exists a partial order relation R defined over $\mathscr{S}$ such that

(i) $\tilde{R}$ is the restriction of R to the domain $A \cup B$.

(ii) A and B are chains under some maximal chain decomposition of $\mathscr{S}$ under R.

(iii) For all $x \in A \cup B$, $\tilde{r}(x)$ is the rank of x under R. We now define

$P_k(\tilde{r}; A, B) =$ The number of distinct partial order relations $\tilde{R}$, which are consistent with the maximal chain structure $\{A, B\}$, and the rank function $\tilde{r}$, and have exactly k comparable pairs of the form (a, b) where $a \in A$, $b \in B$.

Clearly, $P_k(\tilde{r}; A, B)$ depends on the chains A and B only through their lengths. Hence, we may write

$$P_k(\tilde{r}; A, B) = P_{ij,k}(\tilde{r}) \,. \tag{7}$$

We further define the generating functions $P_{ij}(z)$ by

$$P_{ij}(z) = P_{ji}(z) = \sum_{k=0}^{ij} z^k P_{ij,k} \,, \tag{8}$$

where

$$P_{ij,k} = \max_{\tilde{r}} [P_{ij,k}(\tilde{r})] \,. \tag{9}$$

In eq. (9), the maximum is taken over all possible rank assignments. We shall assume that n is sufficiently large so that $P_{ij,k}$ is independent of n.

These polynomials $P_{ij}(z)$ are easily determined for small values of i and j, by exhaustive enumeration. Some low order polynomials are listed in the appendix, where an outline of the method used for their determination is also given. We used a computer program to determine all the polynomials for $i, j \leqq 6$. For higher values of i and j, the computation time increases very sharply.

We define polynomial $\bar{P}_{ij}(z)$ similarly. These are generating functions $\bar{P}_{ij,k} \overset{\text{def}}{=} \text{Max}_{\tilde{r}}\, \bar{P}_{ij,k}(\tilde{r})$, where $\bar{P}_{ij,k}(\tilde{r})$ is defined similar to $P_{ij,k}(\tilde{r})$, except that we do not require the chains A and B to be maximal. These too were determined by exhaustive search.

The general properties of these polynomials $P_{ij}(z)$ and $\bar{P}_{ij}(z)$ are not very obvious. For large i, with i/j held fixed, $P_{ij}(z)z^{-ij}$ is ex-

pected to behave like $[g(z)]^i$, where $g(z)$ is some (as yet unknown) function of z. The study of these polynomials is interesting on its own, but not really necessary for our discussion here.

III. **The upper bound.** We may now state the main result of this paper.

THEOREM. *Let z, ρ, f_i by any nonnegative real numbers satisfying the following conditions*:

(i) $\sum_i i f_i = 1$.

(ii) $0 \leqq \rho \leqq 1$.

Then $S(\rho) \leqq \mathrm{Max}_{\{f_i\}} [\sum_{i,j} f_i f_j \ln P_{ij}(z) - \rho \ln z]$.

Proof. Consider a particular decomposition of $\mathscr{S}$ in maximal disjoint chains $C_1, C_2 \cdots C_p$. Let the lengths of these chains be $l_1, l_2 \cdots l_p$ respectively, where $l_1 \geqq l_2 \geqq \cdots \geqq l_p$. Consider, also, a rank function $r(\mathscr{S})$.

Let R' be a binary relation defined over $\mathscr{S}$ satisfying the following property for all i and j, the restriction of R' to the set $C_i \cup C_j$ is a partial order relation consistent with the maximal chain structure $\{C_1, C_2 \cdots C_p\}$, and the rank function $r(\mathscr{S})$. Clearly, not all such relations R', define a partial order relation over the full set $\mathscr{S}$. The enumeration of all relations satisfying the above property, gives an upper bound on the enumeration of all partial order relations R satisfying the above property. The relations R' are easily enumerated in terms of the polynomials $P_{ij}(z)$ defined earlier, and we get quite easily

$$\Omega_n(z) \leqq \sum_{\{C_i\}} \sum_{r(\mathscr{S})} [z^{\sum_i l_i(l_i-1)/2} \prod_{(i,j)}{}' P_{l_i l_j}(z)] \,. \tag{10}$$

In this inequality, the summations over $\{C_i\}$ and over $r(\mathscr{S})$ are over all possible chain decompositions of $\mathscr{S}$ and all possible rank functions $r(\mathscr{S})$. The term $z^{l_i(l_i-1)/2}$ comes from the $l_i(l_i-1)/2$ comparable pairs in the chain C_i, and $P_{l_i l_j}(z)$ is the contribution of the mutual pairs between the chains C_i and C_j. The prime over the product sign indicates the fact that $i = j$ term is excluded from the product. This inequality (10), clearly holds term by term for each power of z.

Now, the rank of an element in $\mathscr{S}$ can take values 1 to n. Hence total number of possible rank assignments is certainly less than n^n. Also, the total number of ways, the set $\mathscr{S}$ may be broken into disjoint subsets is at most ${}^{2n}P_n$. Hence we get from the inequality (10)

$$\Omega_n(z) \leqq {}^{2n}P_n n^n \operatorname*{Max}_{\{l_i\}} \left[z^{\sum_i l_i(l_i-1)/2} \prod_{(i,j)}' P_{l_i l_j}(z) \right] , \tag{11}$$

where the maximal is taken over all possible partitions $\{l_i\}$ of n ($\sum_i l_i = n$).

$\Omega_n(z)$ is a polynomial in z with positive coefficients. Hence for all real positive values of z

$$N_n(m) \leqq \Omega_n(z) z^{-m} . \tag{12}$$

Taking logarithms of both sides we get

$$\begin{aligned} \ln N_n(m) &\leqq \ln ({}^{n^n}\ {}^{2n}P_n) \\ &+ \operatorname*{Max}_{\{l_i\}} \left[\sum_i \frac{l_i(l_i-1)}{2} \ln z - m \ln z + \sum_{(i,j)}' \ln P_{l_i l_j}(z) \right] . \end{aligned} \tag{13}$$

In the chain decomposition $\{C_i\}$, let the chains of length i be F_i in number. Since the total number of elements is n, we have

$$\sum_i i F_i = n . \tag{14}$$

The double summation on the right hand side of the inequality (13) may be rewritten as

$$\sum_{(i,j)}' \ln P_{l_i l_j}(z) = \sum_i \frac{F_i(F_i-1)}{2} \ln P_{ii}(z) + \sum_{i \neq j} \frac{F_i F_j}{2} \ln P_{ij}(z) . \tag{15}$$

Substituting in (13) and taking the limit of large n, with $f_i = F_i/n$, we get

$$S(\rho) \leqq \operatorname*{Max}_{\{f_i\}} \left[\sum_{i,j} f_i f_j \ln P_{ij}(z) - \rho \ln z \right] , \tag{16}$$

which proves the theorem.

This theorem is not very useful for numerical calculation of upper bounds on $S(\rho)$, as knowledge of all the polynomials $P_{ij}(z)$ is required. For explicit calculation we use the following modified version of the theorem.

THEOREM. *Let p be any positive integer, and let z, f_i ($i = 1$ to p), be any nonnegative real numbers satisfying the following conditions*:

$$\text{(i)} \quad \sum_{i=1}^{p} i f_i = 1 , \tag{17}$$

$$\text{(ii)} \quad 0 \leqq \rho \leqq 1 ,$$

then

$$S(\rho) \leqq \underset{\{f_k\}}{\text{Max}} \left[\sum_{i,j=1}^{p} f_i f_j \ln Q_{ij}(z) - \rho \ln z \right], \tag{18}$$

where

$$Q_{ij}(z) = P_{ij}(z), \quad \textit{iff } (i \neq p \quad \textit{and} \quad j \neq p), \tag{19}$$

$$Q_{ij}(z) = \bar{P}_{ij}(z), \quad \textit{iff } (i = p \quad \textit{or} \quad j = p). \tag{20}$$

Proof. Express $\mathscr{S}$ as a union of disjoint chains of length less than or equal to p. Then the chains of length p need not be maximal. Rest of the proof is as before.

We use variational calculus to maximize the right hand side of inequality (18), and then minimize the result with respect to z, to get the best upper bound. The constraint (17) is taken care of by a Lagrange multiplier. This gives the equations

$$\rho = z \frac{\partial}{\partial z} \sum_{i,j=1}^{p} f_i f_j \ln Q_{ij}(z), \tag{21}$$

and

$$\sum_{j=1}^{p} [\ln Q_{ij}(z)] f_j = \lambda i, \quad \text{if} \quad f_i > 0. \tag{22}$$

Here λ is the Lagrange multiplier. Corresponding to any value of z, we first determine f_i by solving the linear equations (17) and (22); and substitute in (21) and (18) to get the corresponding value ρ and $S(\rho)$. By varying z, bounds for different values of ρ are obtained. If for any value of z, the solution of equation (17) and (22) gives negative values of f_i for some i, we choose that f_i to be exactly zero and variationally optimize over the remaining variables. For $p = 6$, the numerical results show that

$$S(\rho) < \frac{1}{2} \ln 2, \quad \text{if} \quad \rho \leqq .154 \quad \text{or if} \quad \rho > .699, \tag{23}$$

which is the promised result.

APPENDIX

Let $A = \{a_1, a_2, \cdots, a_i\}$ and $B = \{b_1, b_2, \cdots, b_j\}$. The rank function $\tilde{r}$ on AUB may be specified by a list of the form $a_1 a_3 b_1 a_3 b_2 \cdots$, where the elements are arranged in order of decreasing rank. Consistency with the rank r implies that no element can be greater than any element preceding it in the rank list. The exact values of ranks assigned are not relevant. The total number of rank functions to be tested is thus ${}^{i+j}C_j$.

The relation R may be represented by two lists, of the same

form as the rank list. For $x, y \in AUB$, $x \geqq y$ if x appears before y in both of these lists. The computer program generates all possible relations R, and rejects those inconsistent with the rank list.

To save computation time, the maximality constraint was replaced by the following weaker constraint: If $i \geqq j$, then $a_p \not> b_{j-i+p}$ and $a_p \not< b_p$ for all p. If this condition fails, clearly the A chain is not maximal, as we can form a chain of length $(i+1)$ from AUB. Clearly, this relaxation of constraints does not affect the validity of the bounds derived. We list below some lower order polynomials $P_{ij}(z)$ and $\bar{P}_{ij}(z)$.

$$P_{11}(z) = 1$$
$$P_{12}(z) = 1 + 2z$$
$$P_{22}(z) = 1 + 2z + z^2$$
$$P_{13}(z) = 1 + 2z + 2z^2$$
$$P_{23}(z) = 1 + 2z + 5z^2 + 6z^3 + 4z^4$$
$$P_{33}(z) = 1 + 2z + 5z^2 + 6z^3 + 6z^4 + 4z^5 + z^6$$
$$\bar{P}_{11}(z) = 1 + z$$
$$\bar{P}_{12}(z) = 1 + 2z + z^2$$
$$\bar{P}_{16}(z) = 1 + 2z + 3z^2 + 4z^3 + 3z^4 + 2z^5 + z^6$$
$$\bar{P}_{26}(z) = 1 + 2z + 5z^2 + 8z^3 + 14z^4 + 18z^5 + 22z^6 + 22z^7 + 21z^8 + 16z^9 + 10z^{10} + 4z^{11} + z^{12}$$

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