Bounds on the Size of Ultrametric Structures

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We present theorems on the possible sizes of ultrametric and almost-ultrametric structures and discuss implications for the entropy of spin-glasses, the traveling salesman problem, and neural network memories.

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It has proved fruitful to the understanding of spin-glasses to study the free-energy landscape. A decade of research has indicated[1-5] that the glassy phase is characterized by a large number of deep free-energy valleys. In the thermodynamic limit, that is, the limit as the number of spins N is taken to infinity, there are believed to be infinitely many valleys, called equilibrium states, separated by infinite free-energy barriers. Remarkably, it has recently been shown[3,4] that these equilibrium states are organized in a hierarchy characterized by an ultrametric structure. More precisely, if a natural definition of distance between equilibrium states is introduced, then any triangle formed by three equilibrium states is either equilateral or isosceles with the third edge shortest.

Ultrametricity is a very strong constraint. If k points, say in R^N, are to be chosen to be ultrametric, then the $\binom{k}{3}$ possible triangles must have this special form. We have studied the consequences of this constraint. We find, for example, that no ultrametric set of spin-glass configurations on N sites contains more than $N+1$ configurations. Since the theorems of Refs. 3 and 4 in fact only show that in the $N \to \infty$ limit almost every triangle satisfies the constraint, we have also investigated this case. Given a reasonable assumption on the number of triangles violating ultrametricity, we have proved a polynomial bound on the size of any almost-ultrametric set.

A polynomial bound on the number of equilibrium states would be extremely interesting since it would immediately imply that the zero-temperature entropy of the spin-glass is 0. Our results strongly suggest that this is so. We have not been able rigorously to prove this because we lack sufficient control on the finite-N effects.

Our results have other interesting applications as well. The traveling salesman problem (TSP) and other combinatorial optimization problems have been studied as spin-glasses. The TSP is the problem of finding the shortest tour visiting each of n cities once, given a matrix of distances between them. In the TSP a tour is said to be λ-opt if it cannot be shortened by interchange of λ links.[6] Evidence has been presented[7] that the 2-opt tours and the 3-opt tours are ultrametrically organized. Again a polynomial bound would be interesting as it is generally believed that there are exponentially many 2-opt tours.[6]

In 1982 Hopfield[8] proposed a "neural network" model in which, by a sculpting of the energy landscape of spin-glasses, it is possible to store content-addressable memories. Recently, Parga and Virasoro[9] have proposed a model to use the natural ultrametric structure of spin-glasses for hierarchical memory storage. The question of capacity, which is not addressed in Ref. 9, is generally considered crucial in memory models.

With these motivations we have studied embeddings of ultrametric structures in larger metric spaces and found bounds on their size, and also embedding algorithms in several cases. We present our methods more fully elsewhere[10]; here we will state some results and stress the physical consequences.

Definition 1.—An ultrametric space is a metric space (X,d) which satisfies

$$d(x,z) \leq \max[d(x,y),d(y,z)]. \quad (1)$$

Equivalently every triangle (x,y,z) is isosceles with the third side shorter than or equal to the other two. In Ref. 4, for instance, it is shown that the canonical example of such a space is a branching tree, as in Fig. 1, where the points of the space are nodes at the bottom of the tree, and the distance between any two points is the height that one must ascend up the tree in order to reach a common predecessor.

Let (E,d) be a metric space. Let $X \subset E$ such that with the induced metric, X is ultrametric. We ask, what is the maximal size of X? We have studied this problem for (a) subsets (A_i), $i=1,\ldots,k$, of an N-set with metric

$$d(A_i,A_j) = \max(|A_i|,|A_j|) - |A_i \cap A_j|;$$

(b) N-dimensional hypercube, i.e., (0,1) or (1,−1)

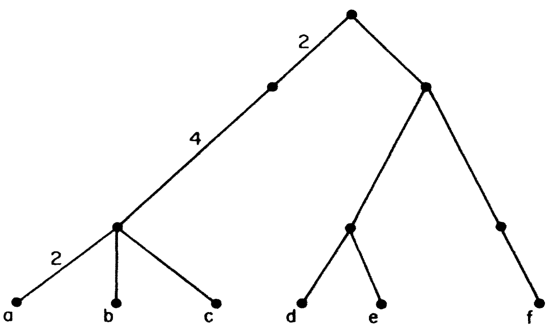

FIG. 1. Typical tree. The points of the space are the bottom nodes labeled a–f. For example $d(a,b)=2$, $d(c,e)=8$, $d(d,f)=6$.

vectors of length N with the Hamming distance d_H; and (c) R^N with the Euclidian distance d_E.

Theorem 1: In (a), (b), and (c), $|X| \leq N+1$. Moreover this bound can be attained.

In Ref. 10 we prove this theorem. Here we sketch the proof in case (b). The other cases are similar.

Consider a maximal set $X_1, \ldots, X_k$ of $(1,-1)$ vectors in R^N having an ultrametric structure for the Hamming distance d_H. Form the $k \times N$ matrix having X_j for its jth row. Let B be the $k \times k$ matrix $B = AA^t = (b_{ij})$. Obviously $\operatorname{rank} B \leq N$. Moreover $b_{ij} = N - 2d_H(X_i, X_j)$. A careful study of B shows that $\operatorname{rank} B \geq k-1$. Therefore $k \leq N+1$.

The upper bound is obtained by the following construction:

$$X_1 = -1, 1, 1, 1, \ldots, 1,$$

$$X_2 = 1, -1, 1, 1, 1, \ldots, 1,$$

$$\vdots$$

$$X_N = 1, 1, \ldots, 1, -1,$$

$$X_{N+1} = -1, -1, -1, \ldots, -1.$$

One might conjecture that for trees with a rich branching structure this bound could be lowered significantly. Yet in Ref. 10 we show a construction of trees with constant arity (branching number) l and size $\geq N(l-1)/l^2$. More generally, we give constructions of ultrametric sets on the hypercube for any tree for which an ultrametric set exists. It is possible that these constructions can be improved to yield the ultrametric set of minimal dimension for any tree.

In the replica-symmetry-breaking model[2] for the infinite-range spin-glass,[1] the equilibrium states are vectors whose ith component is m_i, the magnetization of the ith site. In Refs. 3 and 4 it is shown that under the Euclidian metric, any triangle among these states satisfies condition (1) with probability 1. We would like a polynomial bound on the number of states in order to show that there is no contribution to the zero-temperature entropy. Theorem 1 in case (c) will yield this if we can extend it to bound the case where a small set of triangles violates ultrametricity. This motivates the following definition.

Let (Y,d) be a finite metric space of cardinality k. Let $T(Y)$ be the set of triangles in Y and $T'(Y)$ be the subset of those triangles violating condition (1). $|T(Y)| = \binom{k}{3}$. Similarly consider (Y_k, d) a sequence of finite metric spaces of cardinality k, for arbitrarily large integers k.

Definition 2.—(Y_k,d) is almost ultrametric if and only if

$$\lim_{k\to\infty} |T'(Y_k)|/|T(Y_k)| = 0.$$

(Y,d) is q-almost ultrametric if and only if $|T'(Y)| \leq \binom{k}{3} k^{-q}$ for $3 \geq q > 0$.

The union of any ultrametric set of size $O(N)$ on the N-hypercube with its mirror image comprises an example of an almost-ultrametric set. In Ref. 10 we prove the following theorem, for Y taken from one of cases (a), (b), or (c).

Theorem 2: If (Y,d) is q-almost ultrametric then $|Y| \leq (\frac{3}{2}\sqrt{3}N)^{2/q}$.

This theorem is proved by application of a theorem of Spencer[11] to show that there is an exactly ultrametric subset of Y of size at least $(2/3\sqrt{3})k^{q/2}+1$. Theorem 1 then yields the result.

In Ref. 7 experimental evidence was presented that the 2-opt tours in the traveling salesman problem are ultrametrically organized. It is generally expected that there will be an exponential number of these.[6] It would be very interesting if there were only a polynomial number, as this might form the basis for an effective algorithm.[12] If one considers a tour on n cities as a subset of rank n of the $\binom{n}{2}$ set of links and uses the metric of case (a), Theorem 1 bounds the largest ultrametric set of tours by $\binom{n}{2}$. Theorem 2 indicates a polynomial bound on the size of any set of tours which is q-almost ultrametric. The metric of case (a) is the appropriate metric and was used in Ref. 7.

Definition 3.—(Y,d) is ϵ-ultrametric if and only if for every triple (e_1,e_2,e_3) of distinct points of Y we can find a triple (a_1,a_2,a_3) of points in a fixed ultrametric set (X,d) such that $e_i \in B(a_i,\epsilon)$ for $i=1,2,3$, where $B(a_i,\epsilon)$ is the ball of radius ϵ around a_i.

In Ref. 9 structures which seem to be $\sqrt{N}$-ultrametric on the hypercube in our definition are considered. These may be exponential in size.[10]

In conclusion, we have stated theorems bounding the size of ultrametric structures. These strongly suggest that there is no contribution to the entropy of the Sherrington-Kirkpatrick spin-glass from the multiplicity of equilibrium states in the thermodynamic limit. We have not quite proven that there is no such contribution to the entropy as we do not understand the exact nature of corrections to ultrametricity which occur in the replica-symmetry-breaking model for finite N. One possibility is that a small fraction of the triangles violate ultrametricity (almost ultrametric), in which case we have shown strong bounds. Another possibility is that all the triangles violate ultrametricity by a small amount (ϵ-ultrametric). This question deserves further study. In any case the single spin-flip metastable states (known to be exponentially numerous[13] are at most ϵ-ultrametric since their deviations from ultrametricity reflect both the deviations of the equilibrium states from ultrametricity and the spread of the metastable states from the equilibrium states.

Further, it is true for any instance of the traveling salesman problem either that there are a polynomial number of 2-opt tours or that these tours are not q-almost ultrametric for any finite q. In our opinion, the 2-opt tours are most likely analogous not to the equilibrium states of the spin-glass, but rather to the metastable states. The computational evidence probably indicates an underlying (quasi)ultrametric structure, corresponding to the equilibrium states.

Finally, large enough structures can be constructed to encourage ultrametric memory models, even for the case of exact ultrametric trees with a rich branching structure [since one only expects to store $O(N)$ states in any spin-glass]. Our constructions of embeddings on the hypercube of general trees may be useful in this regard.

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