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Ultrametricity, frustration and the graph colouring problem

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Abstract. Using techniques of numerical taxonomy we study ultrametricity in the planar graph colouring problem with three and four colours. Evidence of a non-trivial hierarchical organisation is given for the case $q=3$. For $q=4$ we find a simpler ultrametricity with only equilateral triangles of side length $d \simeq 0.77$. This example shows that lack of frustration does not rule out ultrametricity completely although it appears in a rather trivial way.

1. Introduction

Recent developments in the mean-field theory of spin glasses have shown that the distribution of local minima in configuration space has several interesting properties (Mézard *et al* 1984). Particularly relevant are the ultrametricity of the pure states and a non-self-averaging order parameter of the Sherrington-Kirkpatrick (SK) model of spin glasses.

New concepts and tools, originally developed in the statistical mechanics of disordered systems can be used in the study of complex optimisation problems.

What these problems have in common is frustration and disorder, properties which are known to lead to a rich structure of minima of the free energy. Kirkpatrick and Toulouse (1985) studied the travelling salesman problem and they found that the quasi-optimal solutions are organised hierarchically (see also Sourlas 1986).

Which are the properties responsible for ultrametricity is still an open question. Since frustration is a common property of systems which have been found to be ultrametric it is interesting to study problems which differ only in the presence of frustration. An example of this is provided by the graph colouring problem (GCP) (Bouchard and Le Doussal 1986).

The GCP with q colours consists of painting the N vertices of a graph in such a way that the number of links connecting vertices with the same colours is minimised. For $q \geqslant 4$ it is always possible to perform a perfect painting which means that there is no frustration. On the other hand for $q=3$ the system is frustrated and in general the optimal solutions will have links connecting vertices painted with the same colours.

If ultrametricity holds, previous experience shows that it becomes exact only when the size of the system becomes larger. Indeed the replica calculations for the SK model were done in the thermodynamic limit and also the numerical simulations show an improvement of ultrametricity as the size N is increased (Bhatt *et al* 1984, Parga *et al* 1984, Parga 1987).

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Since for graphs with a finite number of vertices we expect only an approximate ultrametricity we need ways to measure the departure from a true ultrametric organisation of the optimal solutions. The technique we used is borrowed from biological taxonomy (Sokal *et al* 1963) which was already proposed for physical systems by Parga (1987) and Rammal *et al* (1985). Given a set of optimal paintings the method constructs two different ultrametrics which should coincide as the graphs become large. The difference of these ultrametrics is measured by calculating magnitudes describing the structure of the associated hierarchical trees (Parga 1987). Alternatively an ultrametricity degree $\mathscr{D}$ can be defined (Rammal *et al* 1985).

A different taxonomic analysis of the GCP was previously performed by Bouchaud and Le Doussal (1986) who measured the ultrametricity degree $\mathscr{D}$. However they omitted the analysis in N restricting themselves to $N=25$. We also think that our way to measure ultrametricity describes better the structure of the hierarchical trees. Besides, an error in that reference in the evaluation of the degree $\mathscr{D}$ for the crucial case $q=3$ makes it desirable to have an independent analysis of the problem. We found $\mathscr{D}=0.61$ instead of the value $\mathscr{D}=0.06$ quoted by those authors†.

This paper is organised as follows. In § 2 we describe the problem and introduce several definitions. In § 3 we present our results for the probability distribution $P(d)$ of distances between quasi-optimal states and the ultrametricity tests. We also include our analysis with N and we show how ultrametricity is spoiled as worse quasi-optimal solutions are included.

Finally we present also a criterion to determine when the method can be applied and the conclusions.

2. Definitions

2.1. *The model*

The cost function for a configuration $S=\{S_i\}$ where $S_i=1,2,\ldots,q$ is the colour of the ith vertex is

$$F(S)=\sum_{(i,j)}\delta_{S_i,S_j} \tag{1}$$

where (i,j) runs over all the links of the graph.

To find the N_s states of lowest F we start with a random configuration and accept only changes that decrease the cost function. The improvements of the configurations are made in an iterative form. In each step all the vertices are painted with the least-used colour in the neighbouring ones. We consider only planar graphs with a mean connectivity $C\simeq 5$ generated in such a way that no solution with $F=0$ exists for $q=3$. These planar graphs were generated according with the algorithm described by Fisher and Wing (1966). An analysis of this technique shows that all planar graphs have the same probability of appearing. For each one we found $N_s=200$ different solutions with $F=0$ for $q=4$ (in this case a perfect colouring is always possible). For $q=3$ we obtained $N_s=200$ solutions for each graph for $N=25$ (we considered five graphs), and $N_s=50$ for $N=50$ and 70. We took $F=F_0$, where F_0 is as small as possible for a given connectivity and number of vertices. For the last two values of N we considered two graphs for each one. For the best solutions we found $F_0=5$, 6 for $N=25$, $F_0=7$, 9 for $N=50$, and $F_0=10$, 12 for $N=70$.

† After checking their calculations the authors of that work agreed with our estimation of $\mathscr{D}$.

2.2. Ultrametricity

A metric space is said to be ultrametric if any three points α, β, γ satisfy the following inequality:

$$d(\alpha, \beta) \leqslant \max\{d(\alpha, \gamma), d(\beta, \gamma)\}. \tag{2}$$

Since ultrametricity is not an exact property for finite N, the distance between two categories of the hierarchy is not well defined and there is no unique way to associate a tree with the data (Rammal *et al* 1986). Two simple techniques have been designed to deal with cases where ultrametricity is not exact; these are the single-linkage and complete-linkage clustering (Sokal *et al* 1963). They correspond respectively to taking the distance between categories as the minimum or the maximum between any member of one category and any member of the other. In this way two new matrix distances $d^<$ and $d^>$ between the N_s elements of the set of solutions are obtained.

To compare the two procedures we use the probability $f(\omega, d)$ of having a cluster of weight ω when the tree is cut at a scale d, and all the states have the same weight $1/N_s$. The distribution of cluster weights $\omega_I = n_I/N_s$ at scale d, where n_I is the number of states in the cluster I, is

$$f(\omega, d) = \sum_I \delta(\omega_I - \omega) \tag{3}$$

and its moments are given by

$$M_k(d) = \overline{\frac{1}{N_s^k} \sum_I n_I^k} \tag{4}$$

where the bar denotes the average over the graphs.

Notice that the $M_k(d)$ are the probability that the k states are in the same cluster in particular (Mézard *et al* 1984)

$$M_2(d) = y(d). \tag{5}$$

Another relevant quantity is the distribution of distances

$$P(d) = \frac{1}{N_s^2} \sum_{\alpha,\beta} \delta(d^{\alpha\beta} - d) \tag{6}$$

where $d^{\alpha\beta}$ is the distance between the quasi-optimal solutions α, β.

In the same way we evaluate the pair distributions

$$P^<(d) = \frac{1}{(N_s)^2} \sum_{\alpha,\beta=1}^{N_s} \delta(d^<_{\alpha\beta} - d) \tag{7}$$

$$P^>(d) = \frac{1}{(N_s)^2} \sum_{\alpha,\beta=1}^{N_s} \delta(d^>_{\alpha\beta} - d) \tag{8}$$

for the two ultrametrics defined previously.

It is also usual to define the quantity

$$Y(d) = \int_0^d P(x)\, \mathrm{d}x \tag{9}$$

and

$$y(d) = \overline{Y(d)}. \tag{10}$$

Notice that results only make sense when the tree is studied at a scale d where both distributions have a substantial overlap.

3. Numerical results

The distance between two solutions α, β is defined as the fraction of vertices with different colours, i.e.

$$d(\alpha, \beta) = \frac{1}{N} \sum_{i=1}^{N} (1 - \delta_{\alpha_i, \beta_i}). \tag{11}$$

The numerical results are based upon several samples of various sizes $N = 25$, 50, 55, 60, 70.

The results for $P(d)$ are exhibited in figures 1 and 2. In figure 1 we show $P(d)$ for the case $q = 3$, $N = 25$ and $N_s = 14$, 50. Notice that the spread in $P(d)$ does not change much with N_s. This is contrary to what happens with the SK model of spin glasses with equal weights (Parga 1987). This is because the number of optimal solutions in the GCP is always larger than the number of lowest-energy states of the SK model. Here, all the solutions included in $P(d)$ have the same value of F_0. For different values of N the behaviour of $P(d)$ is similar, having the same tail and peak.

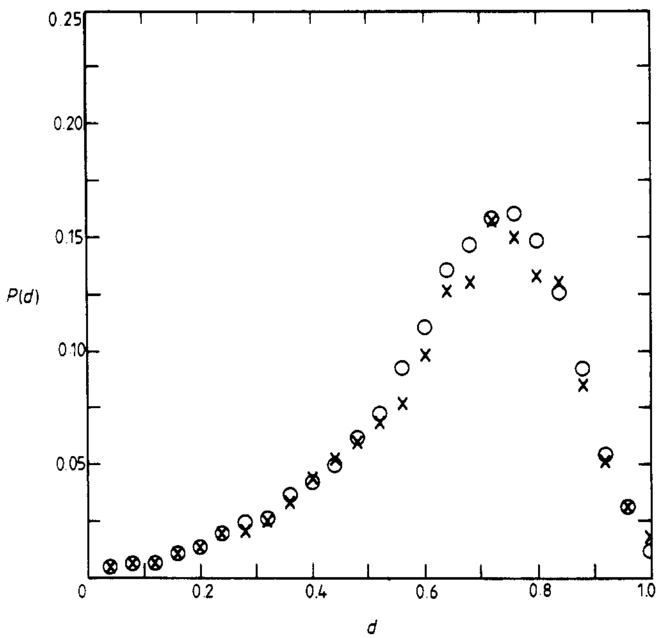

Figure 1. $P(d)$ for the case $q = 3$ and $N = 25$. The curves correspond to $N_s = 14$ (×) and $N_s = 50$ (○).

In figure 2 we show $P(d)$ for the case $q = 4$, $N_s = 14$ and $N = 25$, 70. Although not shown in this figure the behaviour is similar for different values of N_s. However it differs from the case $q = 3$ in that $P(d)$ changes with N, becoming narrower and peaked at about $d \simeq 0.77$ as N increases. The distributions do not include the self-distance contributions.

Comparing $P^<$ and $P^>$ for different values of N for the case $q = 3$ we checked that there is a range of d between 0.4–0.6 where these distributions overlap. This means that we can apply the taxonomic analysis for this range of values of d.

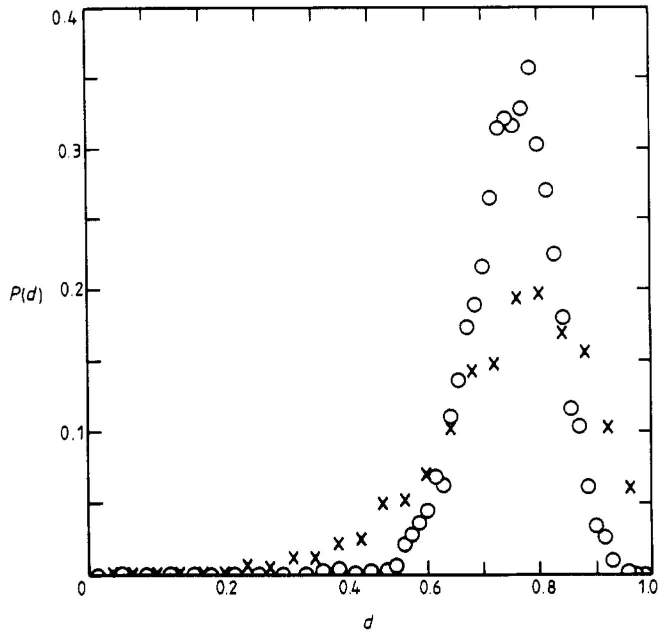

Figure 2. $P(d)$ for the case $q = 4$ and $N_s = 14$. The curves correspond to $N = 25$ (×) and $N = 70$ (○).

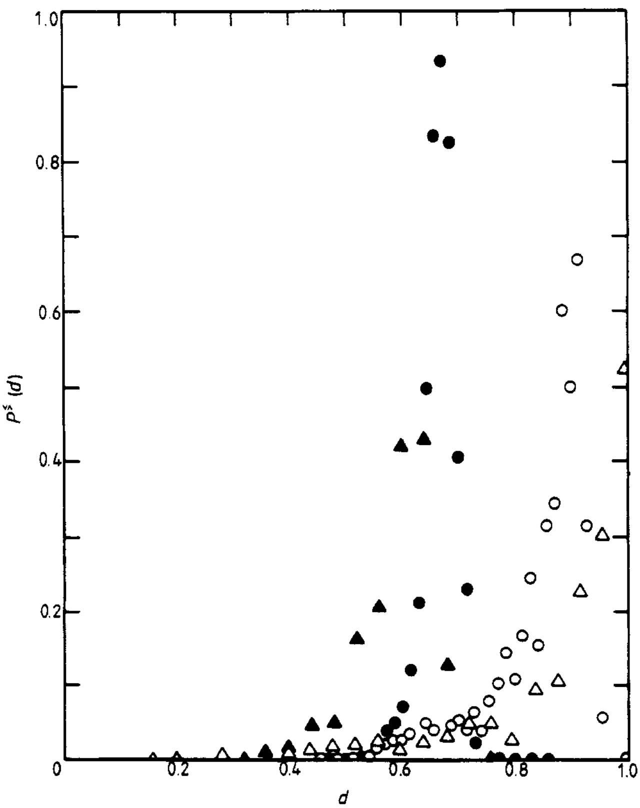

Figure 3. Pairwise distribution for the case $q = 4$, and $N_s = 14$. For $N = 25$, $P^<$ (▲) and $P^>$ (△). For $N = 70$, $P^<$ (●) and $P^>$ (○).

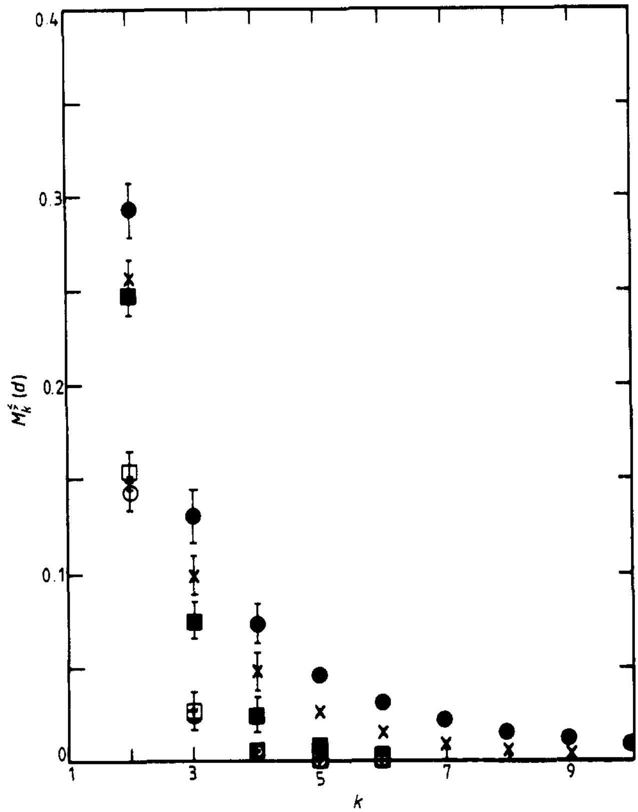

Figure 4. The first moments of the cluster weight distribution at the scale $d = 0.4$ for the case $q = 3$ and $N_s = 14$, calculated with the single- and complete-linkage procedures: for $N = 25$: single linkage (●) and complete linkage (○); $N = 50$: single linkage (×) and complete linkage (+); $N = 70$: single linkage (■) and complete linkage (□). We have included error bars only where they are greater than the size of the data points.

In figure 3 we show $P^<$ and $P^>$ for $N = 25$, 70 with $q = 4$. Here these distributions overlap in a very narrow interval where they take very small values.

As we already said, we calculated the cluster weight distributions $f^<$ and $f^>$ corresponding to the single- and complete-linkage procedures respectively. Once obtained we evaluated their moments $M_k^<(d)$ and $M_k^>(d)$ using (4).

In figure 4 we show the first moments for $q = 3$ and $N_s = 14$. Here $N = 25$, 50, 70 for both the single- and complete-linkage techniques. The tree was cut at a scale $d = 0.4$. Notice that the difference between the two procedures tends to decrease as N increases. This figure is to be compared with figure 7 of Parga (1987) where the moments are calculated for a model ultrametric by construction and for the SK model. In all these cases they show a similar behaviour. Although we chose $d = 0.4$ analogous results still hold for any other value of d in the range of interest.

As pointed out by Rammal *et al* (1985), when the number of considered solutions increases, ultrametricity tends to disappear. This is clear in figure 5 where we plot the moments for $q = 3$, $N = 25$, 50, 70 and $N_s = 50$ at the same scale $d = 0.4$. Figures 4 and 5 are based on the same graphs. One can see that the differences between the

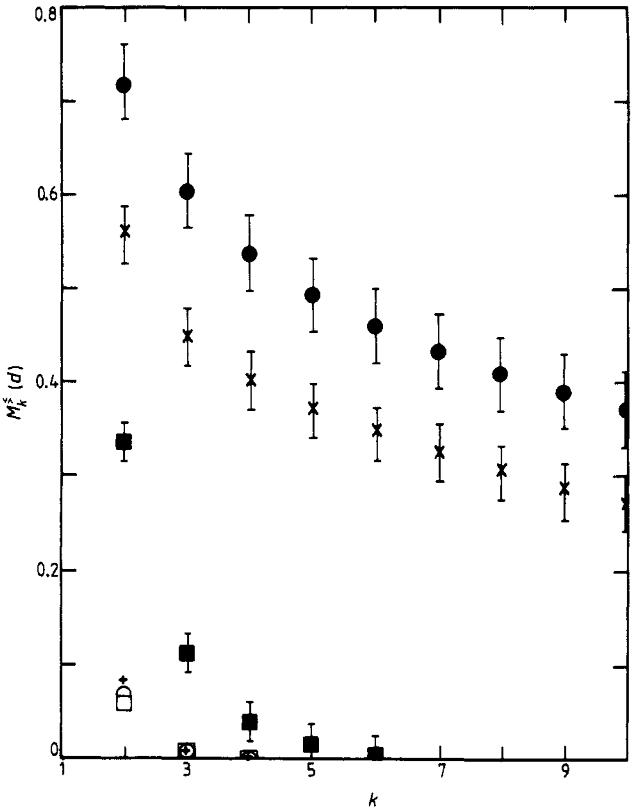

Figure 5. Same as figure 4 with $N_s = 50$. Error bars are treated as in figure 4.

single- and complete-linkage procedures are, for the three values of N, larger than those of figure 4.

Once the moments are found it is interesting to compare $M_2^<$ and $M_2^>$ with the direct calculation of $y(d)$ based on $P(d)$. Figure 6 compares y, $M_2^<$ and $M_2^>$ for $q = 3$, $N_s = 14$ for several values of N. The difference between these quantities tends to decrease with N. Let us notice that y approaches the single-linkage prediction as N increases. This is also similar to what occurs for the simple ultrametric model treated by Parga (1987). It is also in agreement with the fact that as ultrametricity improves with increasing N the single-linkage procedure yields the optimal ultrametric.

It should be remarked that this ultrametricity test was done with the lowest state we could find. Choosing a set of solutions with a larger F the test would not be positive. Ultrametricity depends strongly on the detailed structure of the quasi-optimal states. Figure 7 exhibits the moments calculated with the single- and complete-linkage techniques for sets of solutions which are slightly less optimal than the best ones we have. Here $N = 55, 70$ with $N_s = 14$ at the scale $d = 0.5$. We took solutions with $F_0 = 8$, 9 for $N = 55$ (the best solutions we found have $F_0 = 7$) and $F_0 = 11, 14$ for $N = 70$. Comparing with figure 4 we see that the data of figure 7 have a behaviour with N which is opposite to that followed by an ultrametric set.

We now discuss the connection between ultrametricity and frustration. In order to clarify this point the results for $q = 3$ should be compared with those for $q = 4$.

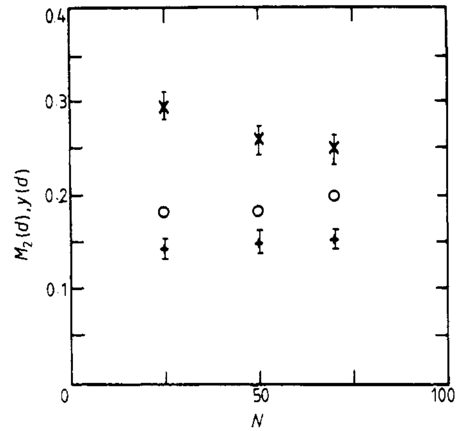

Figure 6. Comparison of $M_2^<$, $M_2^>$ and $y(d)$ at the scale $d = 0.4$ as a function of N for the case $q = 3$, $N_s = 14$. $M_2^<$ (×), $M_2^>$ (+), $y(d)$ (○). Error bars are treated as in figure 4.

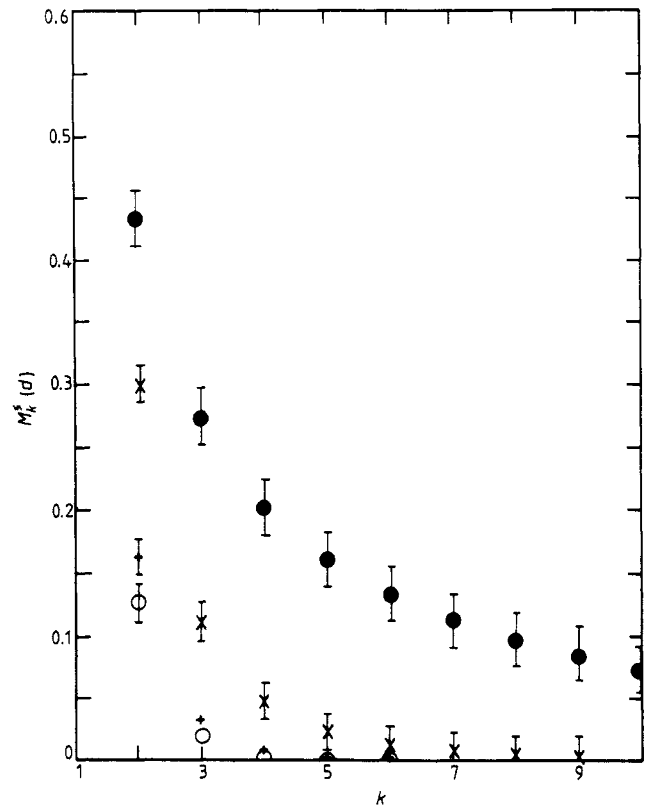

Figure 7. The moments $M_k(d)$ for $q = 3$ at a scale $d = 0.5$ calculated with the single- and complete-linkage procedures, using slightly less optimal solutions. For $N = 55$: single linkage (×) and complete linkage (+); $N = 70$ single linkage (●) and complete linkage (○). Error bars are treated as in figure 4.

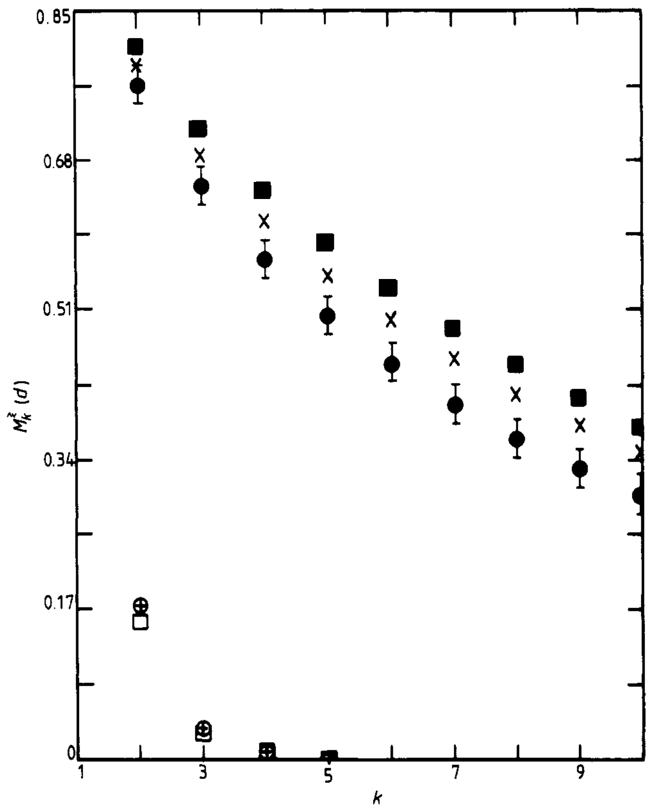

Figure 8. The moments $M_k(d)$ at a scale $d = 0.7$ for the case $q = 4$ and $N_s = 14$. For $N = 25$: single linkage (●) and complete linkage (○); $N = 50$: single linkage (×) and complete linkage (+); $N = 70$: single linkage (■) and complete linkage (□). Error bars are treated as in figure 4.

Comparing the distributions in figure 3, we see that the overlap between all of them is negligible. Indeed there is no range of d where the method can be applied for the case $q = 4$. An example of a wrong application is shown in figure 8, where we plot the moments $M_k^{>}$ and $M_k^{<}$. The tree was cut at a scale $d = 0.7$ and contrary to what happened in figure 4 the difference between the two procedures tends to increase with N indicating lack of ultrametricity. Nevertheless studying the behaviour of $P^{<}$ and $P^{>}$ with N (figure 3), we see that they become closer as N is increased. This means that for the case $q = 4$ a more simple hierarchical structure exists, one in which all the states are at the same distance between them.

To conclude, we have analysed the relevance of frustration for the ultrametricity of the set of quasi-optimal solutions of the GCP. For the frustrated case there are clear signs of the existence of ultrametricity with both equilateral and isosceles triangles present. For the unfrustrated case ultrametricity is still a property of the system but now there are only equilateral triangles.

This behaviour can be understood; for the unfrustrated case it is very easy to obtain zero energy solutions and these are not correlated. They are essentially random four-colour configurations. An average overlap of 0.25 is then expected in agreement with the value $d \simeq 0.77$ found in figure 2. This argument can also be used for more than four colours; in this case the peak of the distance distribution appears at $d = 1 - 1/q$. We have checked this explicitly for $q = 5$ and we found $d \simeq 0.8$ as expected.

References

Bhatt R and Young A 1986 *J. Magnet. Mater.* **54** 191
Bouchaud J and Le Doussal P 1986 *Europhys. Lett.* **1** 91
Fisher G and Wing O 1966 *IEEE Trans. Circuit Theory* **CT-13** 154
Kirkpatrick S and Toulouse G 1985 *J. Physique* **46** 1227
Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M A 1984 *J. Physique* **45** 843
Parga N 1987 *J. Physique* **48** 499
Parga N, Parisi G and Virasoro M A 1984 *J. Physique Lett.* **45** 1063
Rammal R, Angles d'Auriac J and Doucat B 1985 *J. Physique Lett.* **46** L945
Rammal R, Toulouse G and Virasoro M 1986 *Rev. Mod. Phys.* **58** 765
Sokal R R and Sneath P 1963 *Principles of Numerical Taxonomy* (San Francisco: Freeman)
Sourlas S 1986 *Europhys. Lett.* **2** 919