

On the Efficiency and Sensitivity of a Pyramidal Classification Algorithm

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Abstract

In this paper we propose a Pyramidal Classification Algorithm, which together with an appropriate aggregation index produces an indexed pseudo-hierarchy (in the strict sense) without inversions nor crossings. The computer implementation of the algorithm makes it possible to carry out some simulation tests by Monte Carlo methods in order to study the efficiency and sensitivity of the pyramidal methods of the Maximum, Minimum and UPGMA. The results shown in this paper may help to choose between the three classification methods proposed, in order to obtain the classification that best fits the original structure of the population, provided we have an *a priori* information concerning this structure.

Keywords: Pyramidal classification methods, aggregation index, pseudo-hierarchy, Robinsonian dissimilarity, Monte Carlo evaluation, overlapping clusters

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1 Introduction

Ultrametric trees are the most studied representations using discrete models. The aim of this class of models is to produce a family of partitions that can be interpreted as a set of “natural” classifications of a given population.

Pyramidal trees, introduced by E. Diday, are a logical generalization of ultrametric trees. In the pyramidal model, each classification is given by a set of overlapping clusters, instead of a partition. The pyramidal representation being less restrictive, it is closer to the initial structure of the population than in the hierarchical case. Bertrand and Diday [BD85], Diday [Did86b, Did86a], Durand [Dur86, Dur88], Durand and Fichet [DF88] have studied some interesting topics about this pyramidal structures, also called pseudo-hierarchical structures.

The aim of the pyramidal representation methods is to detect the presence of a pseudo-hierarchical structure on a given population Ω , starting from a dissimilarity matrix on this population. The process that has this aim consists of transforming the initial dissimilarity into a Robinsonian dissimilarity by means of a pyramidal clustering procedure; this Robinsonian dissimilarity obtained is equivalent to an indexed pseudo-hierarchy.

Diday, inspired by the agglomerative hierarchical classification algorithms, proposes (see [Did86b]) an agglomerative pyramidal classification algorithm which is adapted to the peculiar characteristics of the pyramidal structures; among these we can point out the fact that each group can have up to two predecessors, as well as the existence of a total order on the population to be classified which is compatible with the pseudo-hierarchy. In general, this algorithm produces indexed pseudo-hierarchies in a wide sense, which may present inversion problems. In our work we propose a modification of Diday’s algorithm that makes possible the construction of an indexed pseudo-hierarchy in the strict sense and *without inversion problems*. So the algorithm described in this paper produces simpler pseudo-hierarchies than Diday’s one. This new algorithm, which we call **PIRAM**, was introduced in [CGA95]. We think that the new features of our algorithm will facilitate the application of the pyramidal classification methods in real problems.

In applied problems it is necessary to measure the fitting between the pseudo-hierarchical structure obtained by using some algorithm and the initial structure of the population. This fitting can be measured by comparing the dissimilarity δ , associated with the initial structure, and the dissimilarity d , associated with the structure produced by the algorithm.¹ This comparison can be made by using a number of different approaches (see [Gor96]). In this paper we will concentrate on the analysis of the behaviour of the following coefficients:

- The γ -Goodman-Kruskal coefficient defined in [GK54] as

$$\gamma = \frac{(S_+ - S_-)}{(S_+ + S_-)},$$

where S_+ , S_- are the number of pairs of couples $\{i, j\}$, $\{r, s\}$ with $(d_{ij} - d_{rs})(\delta_{ij} - \delta_{rs}) > 0$, or < 0 respectively (concordant resp. discordant pairs); This coefficient is interpreted in [Bak74] in the following way:

¹The distance d between two individuals in the pseudo-hierarchy is the level at which both individuals join the same cluster; this kind of distances are sometimes called *threshold* distances.

γ = probability of consistent ranking- probability of inconsistent ranking.

A modification of this coefficient was used in [Hub74] to implement a *stopping rule* (see [Gor96]).

- The cophenetic correlation coefficient defined in [SR62] as

$$\rho = \frac{Cov(d, \delta)}{\sigma(d)\sigma(\delta)}.$$

Furthermore, the computer implementation of the algorithm **PIRAM** (see [GCA94a], [GCA94b] and [GC96]), called **PIRAM1.0**, has allowed us to compare the pyramidal and the “classical” hierarchical classification methods (see [CGA95]). We have also compared three different pyramidal methods – *Maximum*, *Minimum*, and *UPGMA*– associated with three different ways of defining the distance between clusters (*aggregation index*). In this paper we present the simulation tests by Monte Carlo methods produced in order to study the efficiency and sensitivity of these pyramidal methods in an empirical way and in terms of the expected mean value of the γ and ρ coefficients (see [CA95a] and [CGA96]).

2 Pyramidal models

In this section we will introduce some concepts related to pyramidal models, such as Robinsonian dissimilarity and pseudo-hierarchy.

Given a dissimilarity d , defined on a finite set Ω , we will call it a **Robinsonian dissimilarity** if it is a symmetric dissimilarity such that there exists a total order \leq_{Ω} on Ω , such that

$$\max\{d(\omega_i, \omega_j), d(\omega_j, \omega_k)\} \leq d(\omega_i, \omega_k)$$

for any $\omega_i, \omega_j, \omega_k \in \Omega$ such that $\omega_i \leq_{\Omega} \omega_j \leq_{\Omega} \omega_k$. From this definition it is easy to see that any ultrametric dissimilarity is also a Robinsonian dissimilarity (see [Did86b]).

Given a finite set Ω and $\mathbf{P} \in Pow(\Omega)$, we will say that \mathbf{P} is a **pseudo-hierarchy**, if it satisfies the following properties:

P.1 $\Omega \in \mathbf{P}$.

P.2 for all $\omega \in \Omega$, $\{\omega\} \in \mathbf{P}$.

P.3 for all $h, h' \in \mathbf{P}$, $h \cap h' = \emptyset$ or $h \cap h' \in \mathbf{P}$.

P.4 There exists a pre-order $\leq_{\mathbf{P}}$ on Ω such that every $h \in \mathbf{P}$ is an interval with respect to $\leq_{\mathbf{P}}$. We say that $\leq_{\mathbf{P}}$ is an order **compatible** with \mathbf{P} .

Note that $\mathbf{P} \in Pow(\Omega)$ is a hierarchy if it satisfies [P.1], [P.2] and the following properties:

P.5 for all $h, h' \in \mathbf{P}$, $h \cap h' \in \{\emptyset, h, h'\}$.

P.6 For all $h \in \mathbf{P}$, $\cup\{h' \in \mathbf{P} : h' \subseteq h\} \in \{h, \emptyset\}$.

Since, given a hierarchy, there is always an order on the population compatible with it, we can conclude that a hierarchy is a pseudo-hierarchy (see [Did86b]). See also [GS94] for a deeper analysis of the relations between ultrametric dissimilarities, Robinsonian dissimilarities, hierarchies and pyramids.

Given two groups of a pseudo-hierarchy, h and h' , we say that h' is a **predecessor** of h when $h \subset h'$ and there is no other group p in the pseudo-hierarchy such that $h \subset p \subset h'$. It can be proved that any group in a pseudo-hierarchy can have up to two predecessors, while in a hierarchy every group has only one predecessor (see [Cap93]).

Given \mathbf{P} as a pseudo-hierarchy on Ω , a function $i : \mathbf{P} \mapsto \mathbb{R}^+$, such that for all $\omega \in \Omega$, $i(\{\omega\}) = 0$ and for all $h, h' \in \mathbf{P}$, if $h \subseteq h'$ then $i(h) \leq i(h')$, is called an **index** associated with \mathbf{P} , and the pair (\mathbf{P}, i) is called an **indexed pseudo-hierarchy**. If, in addition, the function i verifies that for all $h, h' \in \mathbf{P}$, if $h \subset h'$ then $i(h) < i(h')$, we will say that (\mathbf{P}, i) is an **indexed pseudo-hierarchy in the strict sense**. The elements in a pseudo-hierarchy will be called **groups** of the pseudo-hierarchy, and if a pseudo-hierarchy is indexed, the value of the index over each group will be called **index of the group**.

If (\mathbf{P}, i) is an indexed pseudo-hierarchy on Ω , the **dissimilarity associated with (\mathbf{P}, i)** is defined as the threshold distance, i.e.,

$$d(\omega_1, \omega_2) = i(h)$$

where h is the smallest (with respect to the inclusion relation) $h \in \mathbf{P}$ such that $\omega_1 \in h$ and $\omega_2 \in h$ (see [Cap93]).

The relationship between Robinsonian dissimilarities and pseudo-hierarchies is studied, among others, in [Did86a] and in [CA95b] where the following results can be found:

Theorem 2.1 *If (\mathbf{P}, i) is an indexed pseudo-hierarchy on Ω , then the dissimilarity associated with (\mathbf{P}, i) is a Robinsonian dissimilarity. ■*

Remark 2.1 *Every Robinsonian dissimilarity determines an indexed pseudo-hierarchy, which is unique, so we can conclude that there exists a natural bijection between the set of indexed pseudo-hierarchies and the set of Robinsonian dissimilarities on a set Ω .*

The type of overlapping clustering associated with an indexed pseudo-hierarchy can be represented graphically in a pyramid-like shape by using a type of connex graphs called **pyramidal trees** (for this reason sometimes we write *pyramid* for *pseudo-hierarchy*). The visual representation of Indexed Hierarchies is provided by the well known *dendrograms*. Let us see some examples

Example 2.1 Let $\Omega = \{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5\}$, with $\omega_1 \leq \omega_2 \leq \omega_3 \leq \omega_4 \leq \omega_5$. Let

$$\mathbf{P} = \{ \{\omega_1\}, \dots, \{\omega_5\}, \{\omega_2, \omega_3\}, \{\omega_3, \omega_4\}, \{\omega_1, \omega_2, \omega_3\}, \{\omega_3, \omega_4, \omega_5\}, \\ \{\omega_2, \omega_3, \omega_4\}, \{\omega_2, \omega_3, \omega_4, \omega_5\}, \{\omega_1, \omega_2, \omega_3, \omega_4\}, \Omega \};$$

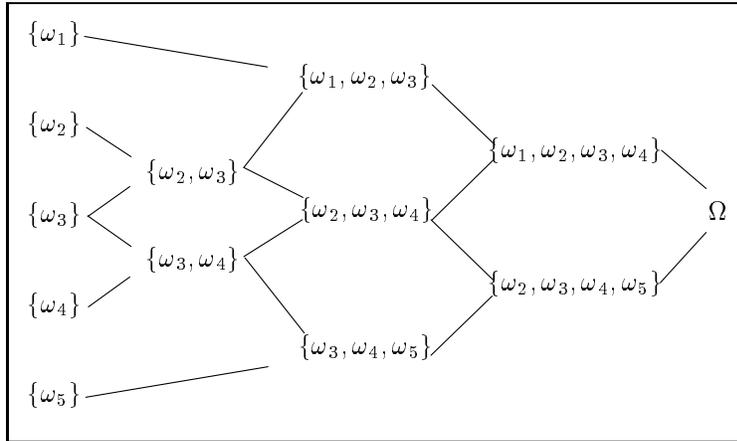
if we define

$$\begin{array}{ll} i(\{\omega_j\}) = 0, \text{ for } j \in \{1, \dots, 5\} & i(\{\omega_2, \omega_3, \omega_4\}) = 5 \\ i(\{\omega_2, \omega_3\}) = 2 & i(\{\omega_2, \omega_3, \omega_4, \omega_5\}) = 5 \\ i(\{\omega_3, \omega_4\}) = 2.5 & i(\{\omega_1, \omega_2, \omega_3, \omega_4\}) = 6 \\ i(\{\omega_1, \omega_2, \omega_3\}) = 3 & i(\Omega) = 7 \\ i(\{\omega_3, \omega_4, \omega_5\}) = 4, & \end{array}$$

then \mathbf{P} is an indexed pseudo-hierarchy.

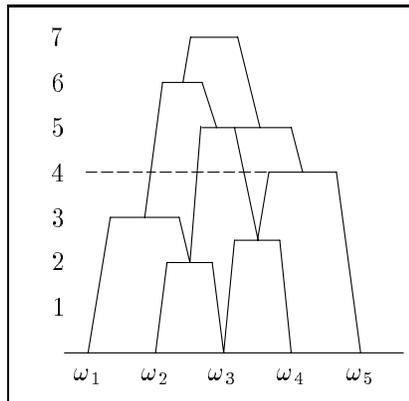
If we start from the singletons, $\{\omega_1\}, \dots, \{\omega_5\}$ and we determine their successive predecessors, we obtain the graphical representation of the pseudo-hierarchy displayed in Figure 1, and a representation of the indexed pseudo-hierarchy (\mathbf{P}, i) displayed in a pyramidal form in Figure 2. ■

Figure 1: A pseudo-hierarchy



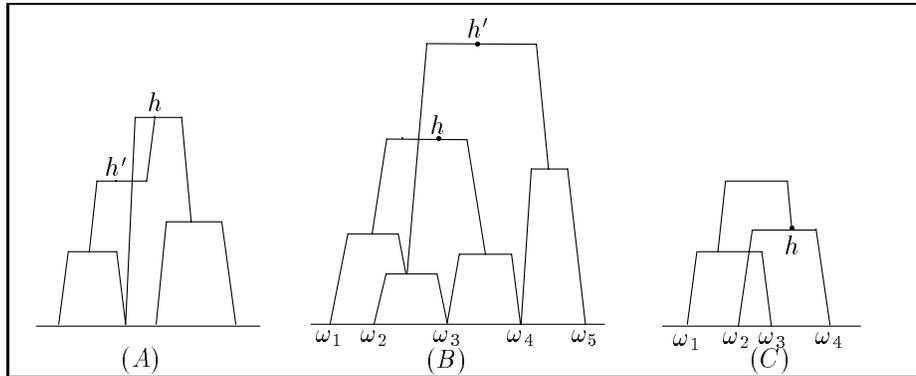
Example 2.2 Note that, if we proceed as in the hierarchical case, the pyramidal classification obtained from the pyramidal tree shown in Figure 2 at level 4, and which correspond to the vertical lines crossed by the horizontal line drawn at that level, are the following: $\{\omega_1, \omega_2, \omega_3\}, \{\omega_2, \omega_3\}, \{\omega_3, \omega_4\}, \{\omega_3, \omega_4, \omega_5\}$, which, obviously, is a set of overlapping clusters. ■

Figure 2: Pyramidal graph of the pseudo-hierarchy of Example 2.1



We introduce now two concepts: a function $f : \mathbf{P} \mapsto R^+$ on a pseudo-hierarchy \mathbf{P} presents an **inversion** if there exist $h, h' \in \mathbf{P}$ such that $h \subset h'$ and $f(h) > f(h')$. An order \leq on Ω originates a **crossing** over a set $\mathbf{P} \in \text{Pow}(\Omega)$ either if there exists a group $h \in \mathbf{P}$ which is not an interval with respect to this order or there exist groups $h, h' \in \mathbf{P}$ such that $h \cap h' \neq \emptyset$ and $h \cap h' \notin \mathbf{P}$. Examples of pyramidal-like shapes that present inversion or crossings are displayed in Figure 3. Note that due to its definition, the index of a pseudo-hierarchy cannot present inversions and an order compatible with a pseudo-hierarchy cannot present crossings. Nevertheless, these concepts which, in fact, are implicit in the definition of a pseudo-hierarchy, should be considered in the process of generating pseudo-hierarchies from dissimilarity matrices.

Figure 3: (A) Inversion: $h \subset h'$ and $i(h') < i(h)$; (B) Crossing: $h \cap h' = (\omega_2, \omega_3, \omega_4) \neq \emptyset$ but $h \cap h' \notin \mathbf{P}$; (C) $h = (\omega_2, \omega_4) \in \mathbf{P}$ is not an interval w.r.t. the order associated with the pseudo-hierarchy.



3 PIRAM, a Pyramidal Classification Algorithm

Let $\Omega = \{\omega_1, \dots, \omega_n\}$ be a finite set and let δ_0 be a dissimilarity defined on the individuals of Ω . Like in the agglomerative hierarchical case, the algorithm we present builds a sequence of levels in such a way that the $(i + 1)$ -th level is obtained by joining two groups among the groups obtained at the i -th level. In order to compute the distance between groups, an aggregation index should be chosen. Since the two groups joined may overlap, additional conditions should be stated to build up an order on Ω which is intended to be compatible with the final pseudo-hierarchy. The process will continue until all the individuals of the population belong to a single group.

So, after having fixed the function f in (1), the algorithm of pyramidal classification **PIRAM** described hereinafter produces

- a sequence R_0, \dots, R_m , each R_i being a set of overlapping classes of elements of Ω , in such a way that $\mathbf{P} = \cup R_i$ is a pseudo-hierarchy;
- a sequence of dissimilarities $\delta_0, \delta_1, \dots, \delta_m$, each δ_i defined on the set R_i ;

- a sequence $\leq_0, \leq_1, \dots, \leq_m = \leq_{\mathbf{P}}$ of partial linear orders on the set Ω such that $\leq_{\mathbf{P}}$ is a total order on Ω , every $h \in R_i$ is an interval with respect to \leq_i , and \leq_{i+1} extends \leq_i , i.e., if $\omega_j \leq_i \omega_k$ then $\omega_j \leq_{i+1} \omega_k$;
- an increasing sequence of real numbers r_0, \dots, r_m which will correspond with the range of the index associated with the pseudo-hierarchy \mathbf{P} .

Note that the existence of an order compatible with the pseudo-hierarchy \mathbf{P} makes it possible to interpret the groups of \mathbf{P} as $\leq_{\mathbf{P}}$ -intervals and, in fact, each of its groups can be displayed as a sequence of distinct elements of Ω . So, when merging two groups, the set-theoretical operation “join” can be seen as a certain kind of concatenation operation between sequences. So we will consider the following operation:

If $h_i = (\alpha_1, \dots, \alpha_n) \in \Omega^n$ and $h_j = (\beta_1, \dots, \beta_l) \in \Omega^l$ then

$$h_i + h_j = \begin{cases} (\alpha_1, \dots, \alpha_n, \beta_1, \dots, \beta_l) & \text{if } h_i \cap h_j = \emptyset \\ (\alpha_1, \dots, \alpha_n, \beta_k, \dots, \beta_l) & \text{if } h_j = (\alpha_s, \dots, \alpha_n, \beta_k, \dots, \beta_l) \text{ and} \\ & (\alpha_1, \dots, \alpha_{s-1}) \cap h_j = \emptyset \\ \text{not defined} & \text{in any other case} \end{cases}$$

We describe now the steps of the algorithm:

- A1.** The procedure starts with the set $R_0 = \{\{\omega_1\}, \dots, \{\omega_n\}\}$, and the dissimilarity δ_0 . Let $r_0 = 0$ and let \leq_0 be the partial order defined by $\omega_i \leq_0 \omega_j$ iff $i = j$. For any $\omega \in \Omega$ we define $i(\{\omega\}) = 0$.

Given $R_{k-1}, \delta_{k-1}, \leq_{k-1}$ and r_{k-1} , we consider $i_k = r_{k-1}$ and

- A2.** We choose a pair $(h_i, h_j) \in R_{k-1}^2$ such that $\delta_{k-1}(h_i, h_j) = i_k$ and it satisfies the following conditions

A2.1 $h_i + h_j$ is defined.

A2.2 there is no other pair (h_i^*, h_j^*) such that $h_i \subset h_i^*, h_j \subset h_j^*$ and $\delta_{k-1}(h_i^*, h_j^*) = i_k$.

A2.3 there is a partial linear order on Ω , \leq_k , such that all the elements in $R_{k-1} \cup \{h_i + h_j\}$ are intervals with respect to \leq_k and such that \leq_k extends \leq_{k-1} .

- A2'** If no pair satisfies A2.1, A2.2 and A2.3 then we set $a = i_k$ and we consider a new value of $i_k := \min\{\delta_{k-1}(h_r, h_s) : \delta_{k-1}(h_r, h_s) > a, h_r, h_s \in R_{k-1}\}$ and we go back to step **A2**.

- A3.** Assume that the pair (h_i, h_j) chosen in step **A2** satisfies conditions A2.1, A2.2, and A2.3. We say that h_i and h_j have been **joined**. We define $h_{n+k} = h_i + h_j$, $i(h_{n+k}) = i(h_i + h_j) = \delta_{k-1}(h_i, h_j)$ and $r_k = \delta_{k-1}(h_i, h_j)$.

To build the set R_k we consider the set $R_k^* = R_{k-1} \cup \{h_i + h_j\}$ and

A3.1 we delete h_i from R_k^* , if h_i has been joined twice;

A3.2 we delete h_j from R_k^* , if h_j has been joined twice;

A3.3 we delete from R_k^* all those elements h_r in R_{k-1} such that $i(h_r) = i(h_i + h_j)$.

A3.4 we delete from R_k^* all those elements h_r in R_{k-1} such that $h_r \subset h_i + h_j$ and h_r contains none of the extrema of $h_i + h_j$ (see Figure 4).

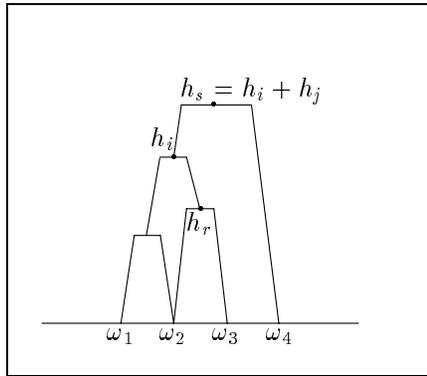
Finally, a new dissimilarity δ_k is defined between the groups of the set R_k in the following way:

$$\delta_k(h, h') = \begin{cases} 0 & \text{if } h \cap h' \in \{h, h'\} \\ \delta_{k-1}(h, h') & \text{if } h, h' \in R_{k-1} \\ \max\{f(\delta_{k-1}(h, h_i), \delta_{k-1}(h, h_j), \dots), i(h')\} & \text{if } h' = h_{n+k} = h_i + h_j \end{cases} \quad (1)$$

where f is the function that determines the pyramidal method used, and which has to be the same within all the process. Usually (see [KR90]) we consider $f = \max$ (**Maximum Method** which yields the **complete link pyramidal method**) or $f = \min$ (**Minimum Method** which yields the **single link pyramidal method**) or $f = UPGMA$ (**UPGMA method**, see [SM58]).

A4. Steps A.2 and A.3 are iterated until $h_i + h_j$ contains all the elements of Ω .

Figure 4: Step A3.4. The extrema of h_s are ω_1 and ω_4 ; the extrema of h_r are ω_2 and ω_3 ; $h_j = \{\omega_4\}$.



Note that by conditions A3.1 and A3.2 each group in the pseudo-hierarchy can only be joined twice. Thus each group can have at most two predecessors.

Conditions A2.2 and A3.3 are the basic points which differentiate our algorithm from Diday's one. Thanks to these conditions, the algorithm becomes faster and the pseudo-hierarchy produced is indexed in the strict sense as shown in [CGA95]. In addition, as we will see in Theorem 3.1, the pseudo-hierarchy built by the algorithm introduced does not present inversions nor crossings, and therefore the inversion problems of Diday's algorithm are solved.

Theorem 3.1 ([CGA95]) *The algorithm PIRAM of pyramidal classification, together with the clustering index defined in (1), builds an indexed pseudo-hierarchy without crossings nor inversions.*

Proof: It is straightforward to see that this pyramidal classification algorithm builds an indexed pseudo-hierarchy. The proof is similar to the proof that Diday's algorithm also builds an indexed pseudo-hierarchy (see [Did86b, Did86a]), and will be omitted here.

Due to condition A2.3, the order $\leq_{\mathbf{P}}$ is a total order on Ω such that all the elements of the pseudo-hierarchy are intervals with respect to this order. Due to condition A3.4, the group h_r , which is deleted from R_k^* , will never be joined in a posterior step of the algorithm. This two facts make the pseudo-hierarchy crossings-free, that is, the resulting indexed pseudo-hierarchy will not present crossings (see Figure 4).

Concerning inversion, by **A2'**, the definition of $\delta_k(h, h')$ in (1)² and the use of the sequence r_0, \dots, r_m , the pseudo-hierarchy will also be inversion-free. ■

From this algorithm we have developed a system for pyramidal classification (called **PIRAM1.0**) such that, starting from the number of individuals to classify and a matrix containing the dissimilarities between them, the system classifies individuals by the Minimum, Maximum and UPGMA methods, giving as an output an indexed pseudo-hierarchy in the strict sense, and the corresponding pyramidal tree. As fitting measurements between the pyramidal structure obtained and the initial structure of population, the correlation coefficient ρ and the γ coefficient of Goodman-Kruskal are calculated, both defined between the pyramidal dissimilarity obtained and the initial dissimilarity.

4 Monte Carlo evaluation of the pyramidal classification methods.

Based on the algorithm **PIRAM** and on the corresponding computer system **PIRAM1.0**, several Monte Carlo simulation tests have been performed. The goal is to assess in an empirical way the efficiency and sensitivity of the Minimum, Maximum and UPGMA pyramidal methods in regaining the pyramidal structure underlying in the initial data, always in terms of the expected mean value of the γ and ρ coefficients. In this study we follow the methodology introduced by F. B. Baker in [Bak74] to compare two hierarchical procedures but with several modifications other than the obvious difference between the structures considered. The main differences are the following: a) the “noises” added to the initial dissimilarities follow a normal distribution instead of being of the form $R_b K X$ where R_b is the basal value, K is an *a priori* constant and X is a random number $-1 \leq X \leq 1$; and b) we compare the “initial” and the “final” dissimilarities but we also compare the “perturbed” dissimilarity with the “final” dissimilarity. This latter comparison makes it possible to evaluate the behaviour of the algorithm when studying arbitrary structures and to compare the spread of the distribution of the coefficients in the general case and for certain particular cases.

In the simulation tests, populations of $n = 4, 5, 6, 10, 16, 20$ individuals have been considered. For each of these populations, we have fixed two dissimilarities, $\delta_{\mathbf{P}}(n)$ and $\delta_{\mathbf{E}}(n)$. While the dissimilarities $\delta_{\mathbf{P}}(n)$ are chosen to be strictly Robinsonian, corresponding to strictly pyramidal structures, the dissimilarities $\delta_{\mathbf{E}}(n)$ are chosen to be chained ultrametric. These dissimilarities are called *basal dissimilarities* and are displayed in Appendix A. Let $\sigma_{\mathbf{P}}(n)$ and $\sigma_{\mathbf{E}}(n)$ be the standard deviation of the corresponding dissimilarities. Next, we have perturbed 10,000 times each of the basal dissimilarities $\delta_B(n)$, $B \in \{\mathbf{P}, \mathbf{E}\}$ with three random variables $\epsilon^k(n, i) \sim N(0, \sigma_B^k(n))$ for $k \in \{l, m, h\}$ such that

²note that by this definition $\delta_k(h, h_{n+k}) \geq i(h_{n+k})$

$\sigma_B^l(n) = \sigma_B(n)/3$, $\sigma_B^m(n) = \sigma_B(n)$ and $\sigma_B^h(n) = 3\sigma_B(n)$. In this way $\sigma_B^k(n)$ becomes a measure of the distortion degree (error level) introduced in the basal structures ($k = l$: (l)ow, $k = m$ (m)edium, $k = h$ (h)igh) and we obtain, for each basal dissimilarity and each $i \leq 10,000$, three new dissimilarities $\delta_B^k(n, i) = \delta_B(n) + \epsilon^k(n, i)$ with $k \in \{l, m, h\}$, $B \in \{\mathbf{P}, \mathbf{E}\}$, called *perturbed dissimilarities*.

From the perturbed dissimilarities, and by using the system **PIRAM1.0**, we compute the dissimilarities associated with the pyramidal structure obtained by using the method of the Maximum ($d_B^k(MAX, n, i)$), Minimum ($d_B^k(MIN, n, i)$) and UPGMA ($d_B^k(UPGMA, n, i)$). Finally, the obtained Robinsonian dissimilarity is compared with both the *perturbed* and the *basal* dissimilarities. See Figure 12 for a graphical display of the whole process. We have called test *S1* the test in which the basal dissimilarities are strictly Robinsonian and test *S2* the test in which the basal dissimilarities are enchainned ultrametric. The results obtained in test *S1* are shown in Tables 1 and 3 and the ones obtained in test *S2* in Tables 2 and 4.

5 Results and conclusions

Next we discuss the empirical results of the tests *S1* and *S2* reported in see Appendix C and based in 10,000 samples for each n .

Concerning sensitivity to data errors of the pyramidal classification methods, we should study the influence of small variations of the initial dissimilarities on the pyramidal structure obtained through the algorithm. As a first approach we can state that for each value of n , for each level of perturbation and each basal dissimilarity, as the distortion level increases the value of the coefficients M_γ and M_ρ decrease and the value of S_γ and S_ρ increase.

Concerning the efficiency of the methods considered, if the original structure of the population is strictly pyramidal, when looking at the comparison Basal/Final (Table 1), we can observe that the values of γ and ρ obtained for the Maximum method are higher than for any other method. In addition, the values of the standard deviation of the coefficients are also smaller for the Maximum method, independently of the number of individuals and of the perturbation level considered, as can be seen in the following table, that summarizes the behaviour of the coefficients for each error level and each method:

Error level	Coefficient	Methods		
		Maximum	UPGMA	Minimum
low	M_γ	≈ 0.99	≈ 0.75	≈ 0.6
	S_γ	≈ 0.02	≈ 0.1	≈ 0.1
medium	M_γ	0.85→0.90	≈ 0.75	≈ 0.6
	S_γ	0.05→0.17	≈ 0.1	≈ 0.1
high	M_γ	0.37→0.45	0.28→0.34	0.16→0.36
	S_γ	0.39 → 0.13	0.37 → 0.14	0.37 → 0.10

Concerning the average value for M_ρ and S_ρ , at the low error level the value of M_ρ is 0.99 and the value of S_ρ is 0.01 for the Maximum method, while for the other two methods the values of M_ρ are smaller and the values of S_ρ greater (roughly 0.09). At the medium error level the values of M_ρ for the Maximum method are 10% lower than the corresponding to the low error level and the

values of S_ρ are 10% higher; for the other two methods the values of M_ρ are considerably less and the values of M_ρ are slightly higher than for the Maximum case. At the high error level, the values of M_ρ are less than at the low error level and the values of S_ρ tend to be very high. So we can conclude that the Maximum method produces better results and more homogeneous. Concerning sensitivity to data errors, the Maximum method is the least sensitive; even at the medium error level it regains the initial structure yielding “good” values for the coefficients. The UPGMA method is more sensitive to data error, but at the high error level it is similar to the Maximum method. The Minimum method exhibits some difficulties in regaining the initial structure and so it is more sensitive to data errors.

Thus, from an empirical point of view we can state that if the initial structure of the population is strictly pseudo-hierarchical (not a hierarchy), the pyramidal method of the Maximum regains the pseudo-hierarchical structure underlying in the initial data in a better way than the other two methods and it is the least sensitive to the introduction of noise in the original data, so it will produce a better classification; the Minimum method is the most sensitive to data errors and the classification produced by this method will less resemble the initial structure than the classification produced by any of the other methods.

If the structure of the population is ultrametric enchainned the values of γ and ρ obtained for the Minimum method are higher than the ones obtained by the other methods, as can be seen in the following table, that summarizes the results displayed in Table 2.

Error level	Coefficient	Methods		
		Maximum	UPGMA	Minimum
low	M_γ	0.97	0.98	0.98
	S_γ	0.02	0.02	0.02
medium	M_γ	0.63→0.91	0.79 → 0.93	0.83 → 0.93
	S_γ	0.06→0.19	0.06→0.19	0.06→0.19
high	M_γ	0.21→0.48	0.35 →0.45	0.42 → 0.49
	S_γ	0.40 → 0.12	0.56→0.16	0.56 → 0.14

We should note that although the range of values and the maximum values of M_γ are similar for the three methods, the values of M_γ decrease at a faster rate for the UPGMA method than did for the Minimum method, and faster for the Maximum method than for the UPGMA. In addition, the minimum value of the coefficients is smaller for the Maximum case than for the UPGMA and smaller for the UPGMA than for the Minimum. The Minimum method yields stable and homogeneous values for the low and medium error level, while at the high perturbation level the values are stable, with small deviations. So, in this case we can see that the Minimum method exhibits less sensitivity, and that a significant decrease of the values of M_γ and M_ρ and a significant increment of S_γ and S_ρ is only obtained when the error level is high. For instance, we can observe that for the Minimum method the value of M_γ decreases a 14% when we go from the low error level to the medium error level, while in the other two cases this coefficient decreases a 17% for the UPGMA method and a 30% for the Maximum case.

Finally, we can conclude that if the structure of the initial data is enchainned ultrametric, the Minimum method yields a better classification of the population. Thus in this case the most efficient method is the Minimum one. This

method is also the least sensitive to data errors. These results follow from a more general result, proved in [CGA95], which states that the Minimum pyramidal method and the Hierarchical Minimum method are the same, and, as it is well known, the last one tends to produce enchainned ultrametric structures.

Concerning the relation Perturbed/Final, the differences between the coefficients M_γ and M_ρ increase as n grows, M_γ being lower than M_ρ . Analyzing the values of the coefficient for each of the methods, we can see that for the Maximum method the values of M_γ in the strictly pyramidal case are quite lower than the corresponding values of M_ρ .

In addition, the simulation tests performed and the results obtained make it possible to draw some conclusions concerning the independence of our algorithm with respect to the initial structure of the population. Note that when the error level is high, we can consider that the perturbed dissimilarities have been generated randomly from normal distributions. In this case we can observe that the results of Tables 3 and 4 are very similar, independently of the initial structure of the data (for the Maximum method the difference between the values of γ and ρ for the cases enchainned and strictly pyramidal and the highest error level is, at the most of 0.02); also, the standard deviations are quite small, so we can conclude that the algorithm is independent of the initial structure of the population. Besides, the low values of σ suggest that the results obtained when comparing the initial and the final dissimilarities are significant, because of the concentration of the values of the coefficients around their mean value. So, we can conclude that, although some methods are better for certain initial structures, the algorithm exhibits an uniform behaviour.

At the low and medium error level, the Maximum method yields better results than the other two methods, independently of the basal structure considered. By examining the two extremal cases we can see that if the basal structure is enchainned, up to medium perturbation on the data, the methods produce similar results; for the strictly pyramidal basal structure, the maximum yields very good values while the other are worse. From these facts and the previous discussion we can conclude that if we have *a priori* information concerning the structure of the population, indicating that the structure is enchainned, then the best method we can use is the Minimum one. In absence of this kind of information or with information suggesting any other basal structure, the Maximum method will produce better results.

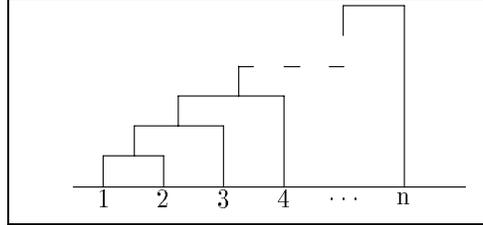
A Basal Dissimilarities used in tests S1 and S2

A.1 Enchained dissimilarities (Test S1)

Figure 5: $\delta_{\mathbf{E}}(n)$; $\sigma_{\mathbf{E}}(4) = 0.74$, $\sigma_{\mathbf{E}}(5) = 0.1$, $\sigma_{\mathbf{E}}(6) = 1.25$, $\sigma_{\mathbf{E}}(10) = 2.21$, $\sigma_{\mathbf{E}}(16) = 3.63$, $\sigma_{\mathbf{E}}(20) = 4.64$

$$\begin{pmatrix} 0 & 11 & \dots & \dots & n+9 \\ & 0 & 12 & \dots & n+9 \\ & & \dots & \dots & \dots \\ & & & 0 & n+9 \\ & & & & 0 \end{pmatrix}$$

$$n \in \{4, 5, 6, 10, 16, 20\}$$



A.2 Strictly Robinsonian dissimilarities (Test S2)

Figure 6: $\delta_{\mathbf{P}}(4)$; $\sigma_{\mathbf{P}}(4) = 1.37$

$$\begin{pmatrix} 0 & 11 & 14 & 14 \\ & 0 & 12 & 14 \\ & & 0 & 11 \\ & & & 0 \end{pmatrix}$$

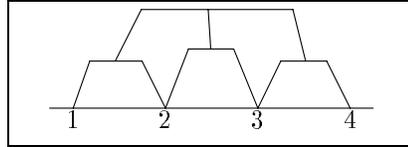


Figure 7: $\delta_{\mathbf{P}}(5)$; $\sigma_{\mathbf{P}}(5) = 1.56$

$$\begin{pmatrix} 0 & 11 & 14 & 15 & 15 \\ & 0 & 12 & 15 & 15 \\ & & 0 & 11 & 14 \\ & & & 0 & 13 \\ & & & & 0 \end{pmatrix}$$

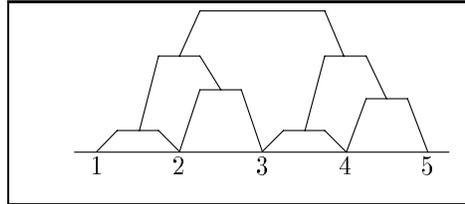


Figure 8: $\delta_{\mathbf{P}}(6)$; $\sigma_{\mathbf{P}}(6) = 1.5$

$$\begin{pmatrix} 0 & 12 & 13 & 15 & 15 & 15 \\ & 0 & 11 & 15 & 15 & 15 \\ & & 0 & 11 & 14 & 14 \\ & & & 0 & 12 & 14 \\ & & & & 0 & 12 \\ & & & & & 0 \end{pmatrix}$$

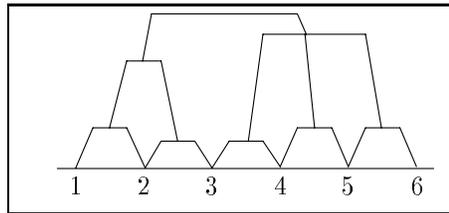


Figure 9: $\delta_{\mathbf{P}}(10); \sigma_{\mathbf{P}}(10) = 1.7$

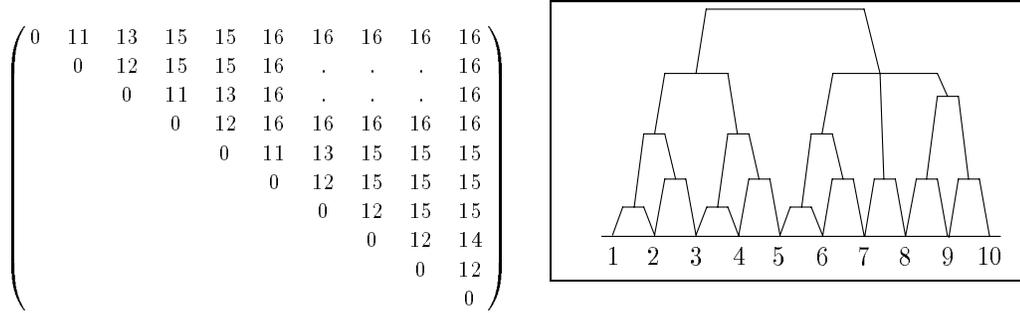


Figure 10: $\delta_{\mathbf{P}}(16); \sigma_{\mathbf{P}}(16) = 2.43$

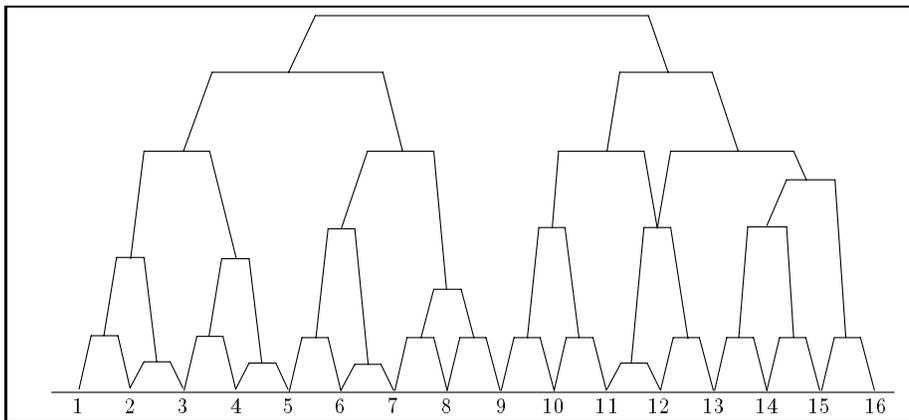
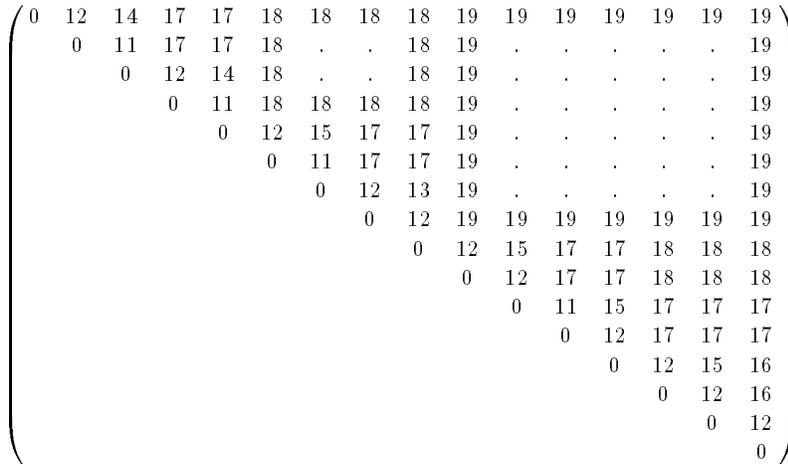
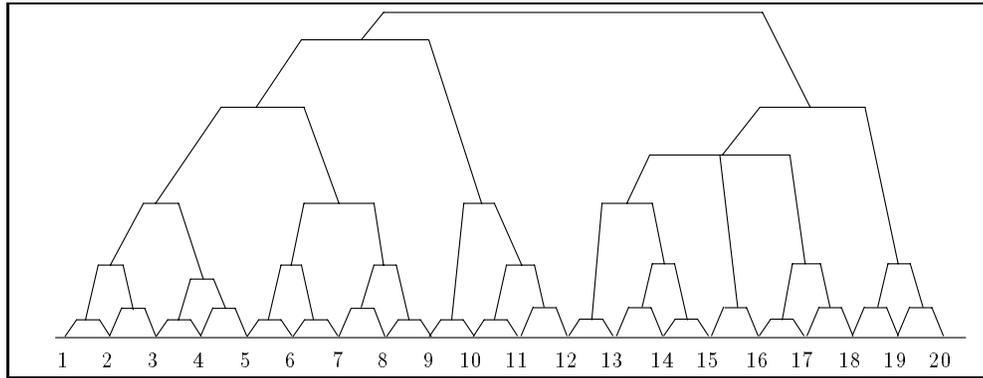


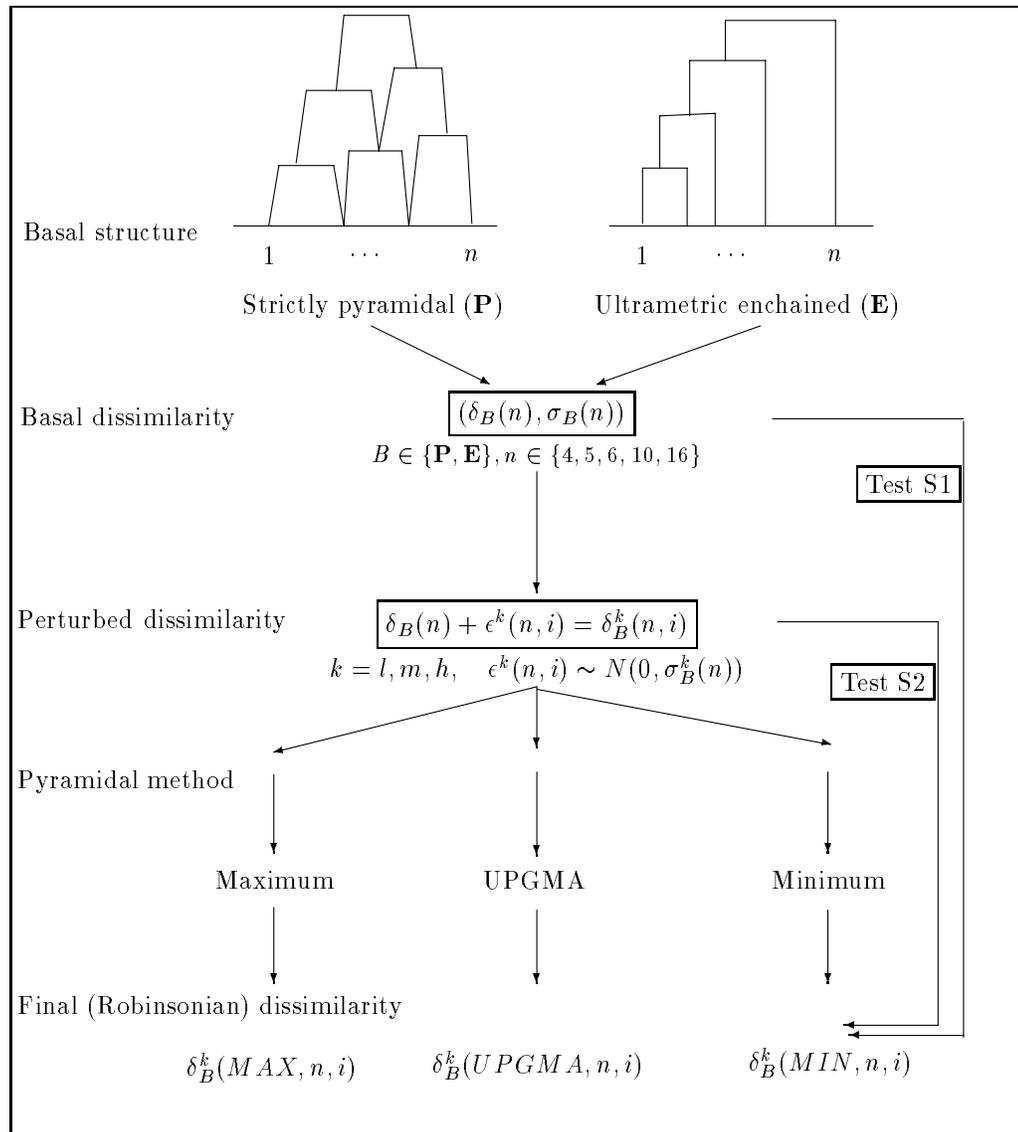
Figure 11: $\delta_{\mathbf{P}}(20)$; $\sigma_{\mathbf{P}}(20) = 2.4$

0	11	14	15	15	17	17	17	17	18	18	18	19	19	19	19	19	19	19	19
	0	12	15	15	17	.	.	17	18	18	18	19	19
		0	11	13	17	.	.	17	18	18	18	19	19
			0	12	17	17	17	17	18	18	18	19	19
				0	11	14	15	15	18	18	18	19	19
					0	11	15	18	18	18	18	19	19
						0	12	14	18	18	18	19	19
							0	11	18	18	18	19	19
								0	11	15	15	19	19
									0	11	14	19	19
										0	12	19	19	19	19	19	19	19	19
											0	11	15	15	16	16	16	17	17
												0	12	14	16	16	16	17	17
													0	11	16	16	16	17	17
														0	12	16	16	17	17
															0	11	14	17	17
																0	12	17	17
																	0	12	14
																		0	12
																			0



B The simulation process

Figure 12: Tests S1 and S2



C Tables

Means (M_X) and standard deviations (S_X) of the values of the coefficients γ and ρ calculated between the basal or perturbed dissimilarities and the final (Robinsonian) dissimilarity obtained by the methods of the Maximum, Minimum and UPGMA.

Table 1: Basal dissimilarity: **Strictly Robinsonian**; Comparison **Basal-Final**

n	σ_k^n	Maximum				UPGMA				Minimum			
		M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ
4	l	1.00	0.03	0.99	0.01	0.99	0.07	0.87	0.06	0.99	0.07	0.82	0.07
	m	0.88	0.17	0.87	0.13	0.79	0.28	0.68	0.22	0.81	0.28	0.65	0.20
	h	0.45	0.42	0.46	0.39	0.34	0.45	0.33	0.37	0.36	0.47	0.33	0.37
5	l	0.99	0.02	0.98	0.01	0.73	0.13	0.81	0.09	0.63	0.04	0.67	0.09
	m	0.83	0.17	0.87	0.11	0.61	0.18	0.65	0.17	0.60	0.17	0.60	0.14
	h	0.38	0.31	0.44	0.31	0.31	0.32	0.34	0.30	0.31	0.32	0.33	0.30
6	l	0.99	0.02	0.98	0.01	0.49	0.14	0.52	0.10	0.45	0.10	0.47	0.06
	m	0.85	0.14	0.88	0.10	0.53	0.17	0.56	0.14	0.48	0.14	0.49	0.10
	h	0.37	0.27	0.43	0.27	0.28	0.26	0.31	0.24	0.27	0.24	0.29	0.22
10	l	0.99	0.01	0.98	0.01	0.76	0.10	0.77	0.07	0.59	0.16	0.64	0.08
	m	0.87	0.08	0.66	0.15	0.68	0.10	0.52	0.17	0.56	0.10	0.57	0.11
	h	0.40	0.19	0.29	0.21	0.33	0.18	0.22	0.18	0.27	0.16	0.25	0.18
16	l	0.98	0.01	0.98	0.08	0.77	0.05	0.59	0.16	0.62	0.08	0.63	0.06
	m	0.90	0.05	0.73	0.11	0.74	0.06	0.56	0.16	0.60	0.09	0.57	0.08
	h	0.41	0.14	0.29	0.18	0.37	0.14	0.18	0.13	0.27	0.12	0.25	0.10
20	l	0.98	0.01	0.99	0.00	0.78	0.07	0.80	0.04	0.53	0.15	0.61	0.09
	m	0.85	0.10	0.91	0.05	0.72	0.10	0.76	0.06	0.54	0.17	0.60	0.09
	h	0.26	0.15	0.38	0.13	0.28	0.18	0.36	0.14	0.16	0.11	0.25	0.10

Table 2: Basal dissimilarity: **Enchained**; Comparison **Basal-Final**

n	σ_k^n	Maximum				UPGMA				Minimum			
		M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ
4	l	0.95	0.07	0.99	0.01	0.84	0.13	0.88	0.06	0.99	0.05	0.83	0.07
	m	0.95	0.07	0.97	0.05	0.79	0.17	0.78	0.17	0.88	0.19	0.76	0.16
	h	0.95	0.07	0.95	0.07	0.76	0.20	0.73	0.20	0.79	0.21	0.73	0.19
5	l	0.96	0.04	0.99	0.01	0.66	0.16	0.82	0.09	0.55	0.10	0.67	0.10
	m	0.89	0.09	0.95	0.05	0.62	0.18	0.71	0.16	0.61	0.19	0.68	0.16
	h	0.84	0.10	0.89	0.08	0.64	0.18	0.68	0.18	0.65	0.19	0.67	0.17
6	l	0.94	0.04	0.99	0.01	0.44	0.14	0.54	0.11	0.42	0.11	0.5	0.07
	m	0.85	0.08	0.93	0.05	0.53	0.17	0.63	0.15	0.51	0.17	0.59	0.13
	h	0.75	0.10	0.84	0.08	0.56	0.15	0.64	0.15	0.54	0.16	0.61	0.14
10	l	0.84	0.04	0.98	0.01	0.62	0.10	0.76	0.07	0.49	0.16	0.65	0.08
	m	0.67	0.08	0.86	0.05	0.50	0.11	0.67	0.09	0.43	0.13	0.60	0.10
	h	0.50	0.08	0.70	0.07	0.40	0.10	0.55	0.11	0.33	0.12	0.50	0.12
16	l	0.78	0.04	0.98	0.01	0.61	0.08	0.76	0.05	0.48	0.15	0.64	0.08
	m	0.57	0.07	0.84	0.03	0.47	0.07	0.68	0.06	0.38	0.11	0.59	0.08
	h	0.34	0.06	0.59	0.05	0.30	0.06	0.48	0.07	0.22	0.07	0.41	0.09
20	l	0.80	0.04	0.98	0.00	0.63	0.07	0.78	0.04	0.44	0.15	0.62	0.08
	m	0.58	0.06	0.83	0.03	0.49	0.07	0.68	0.05	0.38	0.12	0.58	0.08
	h	0.28	0.05	0.54	0.05	0.26	0.06	0.45	0.06	0.18	0.06	0.37	0.08

Table 3: Basal dissimilarity: **Strictly Robinsonian**; Comparison **Perturbed-Final**

n	σ_k^n	Maximum				UPGMA				Minimum			
		M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ
4	l	1.00	0.00	0.98	0.01	1.00	0.00	0.99	0.01	1.00	0.00	0.99	0.01
	m	0.91	0.15	0.89	0.09	0.93	0.19	0.93	0.10	0.93	0.19	0.93	0.10
	h	0.48	0.40	0.49	0.37	0.42	0.56	0.47	0.50	0.42	0.56	0.47	0.49
5	l	1.00	0.00	0.98	0.01	1.00	0.00	0.99	0.01	1.00	0.00	0.99	0.01
	m	0.85	0.14	0.88	0.08	0.90	0.17	0.92	0.08	0.91	0.17	0.92	0.08
	h	0.42	0.30	0.47	0.29	0.43	0.42	0.47	0.39	0.44	0.43	0.48	0.38
6	l	1.00	0.01	0.98	0.01	1.00	0.00	0.99	0.01	1.00	0.00	0.99	0.01
	m	0.82	0.12	0.87	0.07	0.89	0.15	0.91	0.08	0.89	0.16	0.92	0.07
	h	0.38	0.25	0.44	0.26	0.42	0.35	0.47	0.34	0.44	0.37	0.48	0.34
10	l	0.96	0.02	0.98	0.01	0.99	0.03	0.99	0.01	0.99	0.02	0.99	0.00
	m	0.73	0.10	0.84	0.07	0.84	0.11	0.91	0.05	0.86	0.10	0.92	0.04
	h	0.30	0.17	0.38	0.18	0.39	0.24	0.46	0.23	0.45	0.24	0.53	0.23
16	l	0.94	0.02	0.98	0.01	0.97	0.03	0.99	0.00	0.98	0.03	0.99	0.00
	m	0.66	0.11	0.79	0.09	0.80	0.08	0.90	0.04	0.83	0.08	0.92	0.03
	h	0.23	0.14	0.31	0.14	0.35	0.18	0.44	0.18	0.46	0.17	0.56	0.17
20	l	0.93	0.02	0.98	0.01	0.96	0.03	0.99	0.00	0.97	0.02	0.99	0.00
	m	0.63	0.11	0.77	0.09	0.79	0.07	0.90	0.04	0.83	0.06	0.93	0.02
	h	0.21	0.12	0.29	0.12	0.35	0.16	0.43	0.16	0.49	0.14	0.60	0.14

Table 4: Basal dissimilarity: **Enchained**; Comparison **Perturbed-Final**

n	σ_k^n	Maximum				UPGMA				Minimum			
		M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ	M_γ	S_γ	M_ρ	S_ρ
4	l	1.00	0.00	1.00	0.00	1.00	0.00	0.99	0.01	1.00	0.00	0.99	0.01
	m	0.99	0.04	0.98	0.03	0.93	0.14	0.90	0.09	0.93	0.13	0.90	0.90
	h	0.96	0.07	0.96	0.06	0.78	0.21	0.75	0.19	0.79	0.21	0.75	0.18
5	l	0.98	0.02	0.99	0.01	1.00	0.01	0.98	0.01	1.00	0.00	0.98	0.01
	m	0.94	0.07	0.97	0.03	0.86	0.13	0.88	0.08	0.86	0.13	0.88	0.07
	h	0.86	0.09	0.91	0.08	0.65	0.18	0.70	0.16	0.66	0.19	0.69	0.16
6	l	0.97	0.02	0.99	0.01	1.00	0.01	0.98	0.01	1.00	0.01	0.98	0.01
	m	0.88	0.07	0.94	0.04	0.81	0.11	0.87	0.07	0.81	0.11	0.86	0.07
	h	0.77	0.10	0.86	0.08	0.58	0.15	0.67	0.14	0.57	0.16	0.65	0.15
10	l	0.93	0.02	0.98	0.01	0.95	0.03	0.97	0.01	0.96	0.02	0.98	0.01
	m	0.74	0.07	0.88	0.04	0.72	0.07	0.84	0.05	0.71	0.07	0.84	0.04
	h	0.53	0.09	0.71	0.08	0.44	0.10	0.58	0.10	0.41	0.11	0.56	0.10
16	l	0.89	0.02	0.97	0.01	0.91	0.02	0.97	0.00	0.91	0.02	0.97	0.00
	m	0.63	0.08	0.81	0.06	0.66	0.05	0.82	0.04	0.66	0.04	0.82	0.03
	h	0.36	0.07	0.58	0.06	0.35	0.07	0.52	0.07	0.32	0.07	0.48	0.08
20	l	0.88	0.02	0.97	0.01	0.90	0.02	0.97	0.00	0.90	0.01	0.97	0.00
	m	0.59	0.08	0.78	0.06	0.65	0.04	0.81	0.03	0.64	0.03	0.82	0.02
	h	0.31	0.06	0.53	0.05	0.32	0.07	0.50	0.06	0.30	0.06	0.45	0.07

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