Aggregation patterns in hierarchy/proximity spaces

André Kretzschmar^{1,*}, Samuel Soubeyrand¹ and Nicolas Desassis²

¹ INRA, Unité Biostatistique et Processus Spatiaux, Agroparc, F-84914 Avignon, France

² MERE project, INRIA/INRA, UMR INRA/SupAgro Analyse des Systèmes et Biométrie, 2
place Viala, F-34060 Montpellier, France

* Corresponding author: andre.kretzschmar@avignon.inra.fr – FAX : +33(0)432722182

Abstract

The classical approaches for modelling spatial structures address aggregation through a set of distributional hypotheses. They require a large number of data and the definition of a spatial distance for the characterization of spatial correlations. When only scarce abundance data and no Euclidean distance are available, we propose a method to explore the structuring patterns by the association of a hierarchical/proximity description of the space under study (units formed by subunits) and a multiple permutation test battery capturing the similarity between units (permutation being applied at subunits or units level). No Euclidean distances being available among the elements of a hierarchical level, proximity will be used instead of distance and will be defined by the structural relationships of units or subunits. The multiple test aims to assess different types of structuring, determined either by occupancy or by abundance or by both, at unit or subunit level.

We address the relevancy of this approach with a simulation study where samples, formed by ordered subunits and units, are designed to exhibit the different types of structuring. The method is also illustrated with a case study (distribution of aphids on

Citrus branches). It results from this application a decomposition of the complexity of pattern structuring and the evidence, for a single species in its natural environment, to develop diverse types of pattern structuring. Additionally to their direct implications, the results of the test battery may provide valuable preliminary hypotheses and could serve as a constraining context for the next step of modelling.

Keywords

density singularity ; permutation tests ; simulation studies ; aggregate scale ; aggregation patterns ; complexity decomposition.

1 Introduction

1.1 Capturing aggregation characteristics

Biological populations present spatial patterns which could be regarded as signatures of population dynamics responding to environmental heterogeneity (Levin, 1992) and to limitation in spatial connectivity and dispersal. According to this general statement, characterising the patterns can help to identify settlement strategies of populations in their environments (Grimm *et al.*, 2005; Wiegand *et al.*, 2003).

Presently, under different names (“clustering”, “structuring”, “spatial structures or patterns”, “aggregation”, etc...), spatial structurings are described using different approaches with specific adaptations to each case study (see, for instance : Tilman *et al.*, 1996; Perry *et al.*, 2002; Johst *et al.*, 2002; Keitt *et al.*, 2002; Gilbert *et al.*, 2003; Inouye, 2005, Conlisk *et al.*, 2007).

Such a variety of approaches points out the difficulty of characterising how living beings exhibit spatial structuring and leads to take into account that structuring of populations should not be studied out of the context of specific populations strategies and out of environmental spatial organisation. But efficient models of these strategies in order to provide comprehensive representation of structuring patterns are “far to be

1 reached” (Baddeley, 2008). As a mid step study, it is nevertheless possible to focus on
2 the complexity of patterns and to expect that the decomposition of this complexity leads
3 to elaborate realistic and accurate models of population dynamics.

4 The future modeling we have in mind will reflect the population strategy of colo-
5 nization; in this case, aggregation would be regarded in a spatio-temporal perspective.
6 The difficulty to directly cope with such a modeling leads us to apply a pattern-oriented
7 modeling approach (Grimm *et al.*, 2005; Wiegand *et al.*, 2003). The question is then to
8 define the pattern characteristics (also called summary statistics) which will allow the
9 analyst to point out the main components of colonization strategies. In other words, we
10 aim to capture the different scales and hierarchical levels at which structuring can be
11 depicted (Bar Hen and Picard, 2007).

12 1.2 Aggregation in hierarchy/proximity spaces

13 Classical methods used for studying aggregation are standardly applied for physical
14 spaces with Euclidean distances; e.g. variogram, auto-covariance, Moran’s index plotted
15 against distance (Chilès and Delfiner 1999; Cressie, 1991), deviance from complete spatial
16 randomness (CSR), *K*-function (Diggle, 2003; Illian *et al.*, 2008).

17 However, situations arise where a distance cannot be defined in a univocal manner.
18 Consider a tree attacked by aphids for example, how to define a distance between aphids
19 settled on leaves carried by shoots nested in branches? Do we use the Euclidean distance
20 in the 3D space? Do we use a distance measured (in meters or number of leaves) along
21 shoots and branches? In such a situation, instead of defining a distance *stricto sensu*, we
22 propose to characterize aggregation by resorting to the more robust notions of hierarchy
23 and proximity.

24 The hierarchy attached to a given portion of space (a piece of branch for example)
25 is defined when, in this space, it is possible to identify several units, each of one being
26 divided into sub-units. For example : leaves are nested in shoots, shoots are nested in
27 branches. When no Euclidean distances are available among the elements of a hierarchi-
28 cal level, proximity will be used instead of distance and will be defined by the structural

relationships of units or sub-units ; for example, leaves are ordered in a shoot, shoots are ordered in a branch; see Fig. 1.

(Figure 1 about here)

This hierarchy/proximity scheme is shared by many data sets in population ecology (Virtanen *et al.*, 1996 , Henderson *et al.*, 2002; Oddou *et al.*, 2004; Laine and Hansky, 2006; Soubeyrand *et al.*, 2007a, 2007b, 2008b). Note that the proximity can be a temporal proximity. For instance, consider a set of habitats for a given species and suppose that the abundance is measured annually at the end of the growing season in each habitat; in this case, the annual observations are the units, the units are ordered in time, and the subunits are the habitats (see Laine and Hanski, 2006, for such a data set).

To sum up the problem, we aim to characterize aggregation in hierarchical spaces (i) which contain subunits nested in units, (ii) where a relation of proximity between units exists (not necessarily between subunits) and (iii) where population abundance is measured at the subunit level. It has to be noted that in a space made of many levels of hierarchy, aggregation can be studied at different scales by applying, to different couples of levels, the procedure here proposed.

In the above defined hierarchy/proximity spaces, aggregation is considered in two ways. First, a spatial pattern is regarded with a binary filter: each subunit is weighed either by the value 0 or the value 1 describing a status (absence or presence of a species, abundance less or greater than a given threshold). Thus, aggregation is a non-randomness in occupancy. Second, abundance is studied as a quantitative variable and aggregation is due to abundance singularities among the subunits which are occupied. Unoccupied subunits are excluded at this step because if not, a non-randomness in abundance can be only due to a non-randomness in occupancy. Doing so, we aim to filter out the patterns related with occupancy.

Both forms of non-randomness and their combinations are illustrated by Fig. 2. Third, aggregation in occupancy and/or in abundance can take place at various scales in the sampled space (within a unit, over several units —how many?). In addition, aggregation can be modulated because of the irregularity or fragmentation of the space.

1 Here, we are concerned by the variation in the number of subunits per unit.

2 (Figure 2 about here)

3 1.3 Analysing aggregation with a multiple test procedure

4 The detection and characterisation of non-randomness and the determination of the scale
5 of objects on which non-randomness is based require the choice of appropriate statistical
6 tools. To meet this aim, we characterise a spatial pattern observed on a hierarchical
7 space by its multivariate response to a set of permutation tests (Manly, 1997) made at
8 various scales. The set of tests is diverse enough to tackle non-randomness in occupancy,
9 non-randomness in abundance, and variation in scale of aggregation. Using permutations
10 allows us to account for the irregularity (or fragmentation) of the space. The method
11 allows us to capture the possible complexity of aggregation.

12 In what follows, we present the multiple test procedure and apply it on simulated
13 data and real data. Carrying out the procedure for simulated data shows what mul-
14 tivariate responses to the test battery are obtained with diverse forms of aggregation.
15 The real data describes spatial patterns of aphids in branches sampled on citrus trees.
16 Each branch contains 10 ordered shoots and each shoot contains a varying number of
17 leaves on which aphids were counted. The application of the method to this data set
18 allows us to decompose the complexity of aphid aggregation. For the sake of clarity,
19 we built the method and applied it when the proximity between units is just a mat-
20 ter of order (shoots are distributed (ordered) on a 1D line, i.e. the branch). However,
21 at the end of this communication, we consider the application of the method in more
22 complex configurations. In addition, we discuss the decomposition of complex forms of
23 aggregation.

2 Methods : Multiple test procedure

2.1 From density singularities to randomness hypotheses

Although the definition of an aggregate is as diverse as the object to which it is applied, it is commonly accepted that aggregation is associated to singularities (unexpected high values) among a density field. A density singularity reflects a departure from a null hypothesis which governs, in our context, (i) what are the abundances of individuals in the subunits and (ii) how these abundances are structured in the space. Under the complete spatial randomness (CSR) hypothesis, a classical null hypothesis in spatial statistics (Diggle, 2003, Illian *et al.*, 2008), individuals are settled independently and uniformly on leaves; consequently, the numbers of individuals in subunits are drawn from independent Poisson distributions with a common expected value.

This hypothesis is particularly strong and it can be relevant to consider lighter null hypotheses under which, for instance, the abundances are not Poissonian and/or the subunits are not equally suitable to settlement of individuals. Using other null hypotheses prevent us to detect aggregates which are not interesting in our context (e.g. aggregates at the subunit scale). The reasons why an aggregate should be detected as such depend on the phenomena investigated and questions of interest. Three null hypotheses of Partial Spatial Randomness were considered. They are not defined through a settlement process as the CSR hypothesis is, but through permutations of space pieces with their numbers of individuals. The permutations (Manly, 1997) allow us to preserve the marginal distribution of individual abundances without making any distribution assumption such as the Poisson one made under the CSR hypothesis. Specific choices for the nature and the size of the permuted space allow us to focus on different types of aggregates (non-randomness in occupancy, in abundance, and at given scales). Notice again that we consider spaces made of units, themselves made of subunits. The three null hypotheses that we propose are defined as follows.

- H_{01} : the observed pattern of occupancy (individual presence/absence) conforms with the distribution of patterns obtained when all the subunits are permuted (see

Fig. 3, top). Under this hypothesis, the probability of presence of individuals in a subunit is independent of the occupancy pattern around it. In other words, there is no spatial structure in the subunit occupancy pattern.

- H_{02} : the observed pattern of abundances conforms with the distribution of patterns obtained when only the occupied subunits are permuted (see Fig. 3, centre). Under this hypothesis, abundances are not spatially structured on the subset of occupied subunits irrespectively to the spatial pattern corresponding to H_{01} . This hypothesis will be tested to investigate the abundance pattern conditional on the occupancy pattern.
- H_{03} : the observed pattern of abundances conforms with the distribution of patterns obtained when the units are permuted (see Fig. 3, bottom). Under this assumption, abundances are not structured at the scale of several units irrespectively to the spatial pattern corresponding to H_{01} and H_{02} for a single unit.

Departures from H_{01} or H_{02} can reflect similarity between close subunits, and a departure from H_{03} can reflect a similarity between close units.

(Figure 3 about here)

2.2 Statistics and tests

In the previous paragraph, we defined null hypotheses with the aim to detect the existence of specific types of aggregates. We now provide statistics which were used to test if the observed patterns conform or not with the patterns obtained by permutations under the null hypotheses.

We used statistics measuring the similarity between neighbour subunits or units in the zone where an aggregate is searched for. Additionally, in order to capture the size which characterizes a given aggregate, the test was sequentially applied to groups of units, called uplets, corresponding to increasing numbers n of close units.

For the sake of simplicity, we assume in the following that the units are distributed in a space along one dimension. Thus, the proximity relationship between units simplifies

into an order relationship. The case of several dimensions is discussed at the end of this article. When units are ordered, a n -uplet is a group of n successive units. In a space of q units, the number of 2-uplets is $q - 1$, the number of 3-uplets is $q - 2$ and so on.

The test statistics is defined here. Consider a pattern of individuals observed on a space made of q ordered units in which are nested various numbers of subunits. Let n be a fixed uplet size. Let A_{nk} denote the set of abundances (counts) or occupancies (binary indices 0/1 for absence/presence) measured in subunits belonging to the k -th uplet of size n ($1 \leq k \leq K_n$ where K_n is the number of n -uplets). Let μ_{nk} and σ_{nk}^2 denote, respectively, the sample mean and the sample variance based on A_{nk} . The test statistic S_n is the mean-variance pair corresponding to the maximum mean over the K_n n -uplets

$$S_n = (\mu_{nk^*}, \sigma_{nk^*}^2) \quad \text{with} \quad k^* = \operatorname{argmax}_{1 \leq k \leq K_n} \mu_{nk}.$$

Figure 4 illustrates the computation of S_n for an hypothetical space with four units and observed at the scale of abundances in subunits. A similar computation can be performed when the space is observed at the scale of occupancies in subunits or at the scale of abundances in units.

(Figure 4 about here)

With the statistic S_n , we focused on the n -uplet with the highest abundance of individuals (using the maximum mean) and we look at its homogeneity (using the variance); an homogeneous uplet with a high abundance may reflect an aggregate. So, S_n characterises what could be the aggregate at the scale of n -units. The following procedure based on permutations allows us to determine the significance of this potential aggregate (if there is an aggregate at any uplet size n , then there is aggregation in the pattern under study).

For any uplet size, each of the three null hypotheses can be tested as follows. The mean-variance statistic proposed above is computed for the observed pattern and for 5000 permuted patterns obtained under the null hypothesis. This yields a cloud of points (one observed point plus 5000 so-called permuted points) spread in the mean-variance plane (see Fig. 5). The presence of an aggregate in the observed pattern should result in a

1 point significantly aside from the permuted points. A p-value is then computed in order
2 to measure the departure of the observed point from the simulated distribution. For
3 each point j (the observed point $j = 0$ and the 5000 permuted points $j = 1, \dots, 5000$),
4 one computes the number N_j of points in its surrounding. The surrounding is defined
5 by a rectangle whose centre is the point under consideration and whose dimensions are
6 one fifth of the maximum horizontal and vertical amplitudes of the point cloud (different
7 values were tried for defining the surrounding of a point and one fifth was selected as
8 a value providing both power and stability in the tests). The rectangle defining the
9 surrounding of the observed point is drawn on Fig. 5. The p-value of the test is then
10 the proportion of permuted points for which N_j is less or equal than N_0 :

$$\frac{1}{5000} \sum_{j=1}^{5000} \delta(N_j \leq N_0),$$

11 where $\delta(N_j \leq N_0) = 1$ if $N_j \leq N_0$ and zero otherwise. The test is one-tailed because we
12 aim to only detect the points which are aside from the cloud.

13 (Figure 5 about here)

14 Assume that N different sizes of uplets are taken into consideration, as there are three
15 null hypotheses, a set of $3 \times N$ p-values describes a studied pattern. Thus, a pattern has a
16 signature in a $3N$ -dimensional space allowing (i) the identification of density singularities
17 that we associated with aggregates, and (ii) the differentiation between various types and
18 sizes of density singularities.

19 3 Results

20 3.1 Simulation methods

21 In order to assess the pertinence of the tests proposed here, a simulation study has been
22 performed. Four types of simulated samples have been built expected to reject specific
23 null hypotheses. They were achieved (see Appendix) by combining three layers: (i) a
24 hierarchical space $\mathbb{E}$, (ii) a structure in occupancy $O : \mathbb{E} \rightarrow \{0, 1\}$ defined over $\mathbb{E}$ and

1 with value zero or one, and (iii) a structure in abundance $A : \mathbb{E} \rightarrow \mathbb{N}$ defined over $\mathbb{E}$ and
2 with integer values.

3 • An OA -sample, structured in occupancy and abundance, was obtained by multi-
4 plying the two structures O and A (i.e. the abundance at any subunit e in $\mathbb{E}$ is
5 $O(e) * A(e)$).

6 • An O -sample, structured in occupancy only, was obtained by multiplying O and a
7 random permutation of A .

8 • An A -sample, structured in abundance only, was obtained by multiplying A and a
9 random permutation of O .

10 • A $\emptyset$ -sample, with no structure, was obtained by multiplying a random permutation
11 of O and a random permutation of A .

12 For each of this type, 100 samples have been simulated and then, each of them was
13 submitted to the three test battery. Fig. 6 (four top panels) illustrates the types of
14 patterns which are obtained.

15 (Figure 6 about here)

16 3.2 Multiple test results

17 For each type of simulated samples, the counts of samples (among 100) with p-values
18 less than 0.05 are provided for the three hypotheses and the nine uplet-sizes. If the null
19 hypothesis is satisfied, five tests among 100 are expected to be rejected. A star marks the
20 counts which are significantly higher than this value, with the risk of 0.05 (the binomial
21 distribution $B(100, 0.05)$ was used to assess the significance).

22 (Table 1 about here)

23 As general results, it is pointed out :

24 • the multiple test provided the right description of the type of structuring which
25 have been simulated (see Tab. 1): in general, H_{01} and H_{02} are rejected simultane-

- 1 ously for OA -samples, H_{01} is rejected for O -samples, H_{02} is rejected for A -samples
2 and neither H_{01} nor H_{02} are rejected for $\emptyset$ -samples.
- 3 • additionally, it is to be noticed that, in all types, H_{03} is never rejected. We face
4 here a lack of power when testing H_{03} . By permuting only ten units, we were
5 not able to detect medium scale aggregates as shown in Fig. 6 (top right) where
6 two dense aggregates have been nevertheless simulated. To better understand this
7 particular problem, samples with *LARGE* aggregates (a single aggregate covering
8 about five units) have been simulated (see Fig. 6, bottom). As shown in Table 1,
9 H_{03} is rejected for 4- or 5-uplets. However the lack of power is still noticeable (H_{03}
10 is rejected only 15 and 23 times over 100 for, respectively, 4- and 5-uplets).
- 11 • in Tab. 1, the frequencies of test rejections decrease with uplet size for H_{01} (OA -
12 and O -samples) and H_{02} (OA - and A -samples). This decreasing trend reflects that
13 small and medium scale aggregates have been simulated in these samples. When
14 large aggregate samples are simulated, another trend is seen: the frequencies of
15 rejection of H_{01} and H_{03} first increase and then decrease; the frequency of rejection
16 of H_{02} is first constant and then decreases.
- 17 • Tab. 1 does not provide the association between hypotheses which would allow us
18 to depict, for example, that aggregates in occupancy are always associated with
19 aggregates in abundance or, on the contrary, that these two types of aggregates are
20 never on the same space. To study such associations, we can consider the trivariate
21 responses to the test of (H_{01}, H_{02}, H_{03}) . Instead of looking to these responses for each
22 n -uplet, we summarized information over the n -uplets: for instance, the response
23 $(1,0,0)$ is obtained for a sample for which H_{01} is rejected for at least one n -uplet
24 and H_{02} and H_{03} are not rejected for any n -uplet. Thus, a synthetic description is
25 obtained by the distribution of these responses on a cube : at the different corners
26 of this cube representation, are given the percentage of samples which reject one,
27 two or three null hypotheses (Fig. 7).
- 28 The cube for $\emptyset$ -samples (Fig. 7, top left) provides the expected distribution of

the trivariate responses when no structuring patterns are simulated together with marginal confidence intervals obtained by parametric bootstrap (Efron and Tibshirani, 1993). The four other cubes in Fig. 7 clearly show other distributions in accordance with the specific characteristics of each type of simulations. Regarding the associations between the hypotheses, we clearly see on the cube of *OA*-samples that H_{01} and H_{02} are mainly rejected together (aggregates in occupancy and abundance are detected on the same spaces); in contrast, the situation in the case study is more complicated: there are a significant number of spaces with both types of aggregates and significant numbers of spaces with only one type (occupancy or abundance).

To summarize, the multiple test can be regarded as able to detect various types and sizes of aggregates. It works as a relevant descriptor of the structuring patterns observed on hierarchy/proximity schemes and leads finally to the decomposition of the complexity of the observed patterns.

(Figure 7 about here)

3.3 Case study

Aphid spatial patterns were observed on branches of *Citrus* trees located in Corsica (France). Each observed branch consisted of 10 successive shoots (their order being known); each shoot was formed by different numbers of leaves varying between 1 and 20. On each leaf, aphids were counted at the end of shoot growing period (beginning of June and beginning of September). As no informations are available on the orientation of each shoot, the data describing a branch are simplified into an incomplete grid (Fig. 8) satisfying the hierarchy/proximity scheme introduced above: each branch is a sample, shoots are ordered units, leaves are subunits and each subunit is weighted by the number of aphids attached.

(Figure 8 about here)

1 3.3.1 Types and scales of the aggregates

2 Table 2 shows that aggregation in occupancy occurs at small and medium scales and,
3 at less extent at large scales. In contrast aggregation in abundance only occurs at small
4 scales. And no aggregation extending over several shoot is detected, which may result
5 from a lack of statistical power when H_{03} is tested. It has to be noticed that the null
6 hypotheses are less often rejected than in the simulation study; this could depict that
7 these natural branches leads to less simple structuring patterns than those simulated
8 above.

9 (Table 2 about here)

10 3.3.2 Associations of aggregate types

11 Even if, as shown above, H_{01} and H_{02} are both rejected, Fig. 9 of the cube representation
12 of the multiple test leads to a trivariate response distribution which is significantly
13 different from the distribution for *OA*-samples. Indeed, H_{01} and H_{02} are often rejected
14 alone, contrarily to what was observed for *OA*-samples. Aggregations in occupancy and
15 in abundance are not always associated and can occur in distinct spaces. Thus, in the
16 collection of observed branches, the complexity of aggregation figures is larger than the
17 one produced by the simulation study: there seems to be several categories of branches
18 in regards to aggregation (see Fig. 8). The future of this study would be to understand
19 the specific features which explain this complexity.

20 (Figure 9 about here)

21 4 Discussion & Conclusion

22 4.1 Analysing aggregation without Euclidean distance

23 In the literature, two major approaches have been explored to deal with aggregation. The
24 first one is based on indices of variance between distant locations and aims to characterize
25 aggregation in maps of individual abundances. Examples of tools corresponding to this
26 approach are the variogram, the auto-covariance and the Moran's indice plotted against

distance (Chilès and Delfiner 1999; Cressie, 1991). Note that indices of variance such as the F_{ST} statistic also exist for analyzing spatial structuring in genetic maps (Epperson, 2003), but in this communication our interest is restricted to demographic data, that is to say occupancy and abundance data.

The second approach is based on deviance from complete spatial randomness (CSR), and aims to characterize aggregation in patterns of points, the points being the locations of (groups of) individuals. Most of the corresponding tools use the intensity function of points and functions of the inter-event distances as the K -function (Diggle, 2003, Illian *et al.*, 2008). For example, a variation in the intensity or an excess of short inter-point distances will be interpreted as signs of aggregation. Note that it is possible to look at deviances from spatial randomness in the context of an inhomogeneous intensity (Brix *et al.*, 2001); in this case the aim is to study a sort of double clustering structure.

In this article, we have presented a multiple test of aggregation which aims to overcome the absence of classical distance measurements required by the standard methods described above. Instead of distance we have described the space by two “dimensions” : proximity and hierarchy so to capture explicit spatial structuring. These two components allow us to give a framework for understanding the “similarity” between different locations in a given space and the multiple test carries the possibility to decompose the similarity following its strictly spatial component (also called “occupancy” in the paper) and its abundance component. It is usual to address structuring pattern by the discrepancy of one observed sample from the Complete Spatial Randomness (CSR) hypothesis (Diggle, 2003). The reference to CSR limits the approach of structuring patterns because it is an extreme case of “no pattern” and because it is adapted to global structuring patterns. When the CSR is taken as null hypothesis to test aggregation in the simulated sample presented here, almost 100% of the sample are rejecting the null hypothesis. Additionally, it is relevant to consider that all locations of the space are not available to the presence of the populations under study. A Partial Spatial Randomness (PSR) has been approached by using permutation tests. The characterisation of structuring relies then of the resistance to permutation, i.e. the fact that the observed sample is located

1 outside the cluster of the permuted samples in a given space of parameters.

2 Finally, each dimension of the multiple test realizes either the similarity component
3 responsible of the structuring (occupancy or abundance) or the hierarchical scale at
4 which takes place the structuring. The finer the hierarchical scale, the more precise the
5 scale at which aggregation is detected. The hierarchy has been defined here at the uplet
6 scale and by the hierarchical level from sub-units to units.

7 The simulation study has shown the applicability of the multiple test and has allowed
8 us to clarify the properties and the limits of this approach.

9 4.2 Decomposing the complexity of aggregation

10 The multiple test in the framework of PSR reference leads to a pertinent decomposition
11 of the complexity of structuring modes. As each of the test step provide a vision of
12 structuring, the multiple test procedure enlightens a multiple structuring which leads to
13 a better understanding of how the final spatial structure is built, with a dominance of
14 occupancy characteristics or of the abundance properties and at which uplet scale (or
15 hierarchical level) the structuring pattern is relevant to be considered. If the complexity
16 of patterns does not allow to identify individually the patterns or the aggregate itself,
17 the multiple test provides an evaluation of the dimension at which aggregates could be
18 detected. In absence of distance criteria and with no constraint on the model for marginal
19 distribution of the individual characteristics, the multiple procedure is a guide to focus
20 on the dimension at which the structuring pattern should be modelled. Additionally,
21 in giving the different hypotheses which are rejected by a given spatialized population
22 sample, it attests to the constraints to be followed in the modelling approaches to be
23 developed.

24 We have already noticed in the introduction that aggregation can be analysed in
25 hierarchical spaces involving a large number of levels while only two have been considered
26 in the case study presented above. In the former case questions about self-similarity
27 arise: Is aggregation present at every level? Is it the same type of aggregation which
28 is observed? Fractal methods are currently used to bring responses to such questions

(Ferrandino 2004; Mandelbrot 1977; Storch *et al* 2008) but in any case they require the definition of a distance. Without distance but with the notion of proximity as defined in our approach, we could investigate the questions about self-similarity.

It is to be noticed that, in this study, the units are ordered on a one-dimensional axis. This limitation, which works in the case study, could be overcome by a more complex definition of the relationships between units. The procedure in itself would not be modified or invalidated by a more complex definition of spatial proximity as the neighbourhood systems proposed in Rue and Held (2005); it could be even considered that it is a property of this approach to allow to account for spatial complexity by the way of the definition of hierarchy/proximity structure.

4.3 Ecological perspectives

The main results in the case study on aphids may be linked to ecological processes given rise to the observed patterns. For example, the existence at a significant level of the four types of patterns ($\emptyset$, O , A and OA) could illustrate the diversity in the results of the interaction between the aphid dynamics and the irregularity of the spatial structure of the host plant. The small aggregates in abundance (A aggregates) could be linked with the reproduction component of the aphid dynamics which occurs at a very local scale (foundation effect due to the few reproductive females). The aggregates in occupancy (O aggregates), which are larger than the A -ones, could be linked with the dispersal ability of offsprings.

These qualitative links which are made between our results and the ecological processes could be strengthened:

- by spatiotemporal surveys (the reproductions, the migrations, the formation of aggregates would be followed with time) and/or
- by a model selection approach (selecting a model of the population dynamics which gives rise to the same type of patterns than the observed ones).

Regarding the second point, we mentioned in the introduction the difficulty of construct-

ing a model for aphid structuring patterns because of their complexity. The present study should be valuable in this perspective in providing assumptions for the constraints to be incorporated in the model fitting procedure (Grimm *et al.*, 2005; , Wiegand *et al.* 2003) using minimum contrast estimation (Dacunha-Castelle and Duflo, 1982 ; Soubeyrand *et al.*, 2008a) or approximate Bayesian computation (Beaumont *et al.*, 2002).

A last remark to emphasize that the method explored in this paper and the results of such approach do not depend by any way on the type of biological components (defining the space as well as the individuals). It is indeed possible to generalize this procedure, the quality of which relies essentially on (i) the pertinent choice of null hypotheses of the multiple test in order to capture specificities of the strategies which individuals spread and on (ii) the suitability of the hierarchical description to account for the specificity of the space under study, both being the premisses of more accurate models based on times series. It is to be noticed that the hierarchy considered in this article (leaf, branch) can be extended in the range of levels considered (cell, leaf, branch, tree, orchard; see Soubeyrand *et al* 2007c) and even exported to other contexts, e.g. administrative hierarchical structures in human epidemiological surveys (Henderson *et al* 2002) and insect dynamics surveys (Soubeyrand *et al* 2009).

Acknowledgments

The data which were used here in the case study have been collected by INRA, Unité ROSE, 400 route des Chappes, 06903 Sophia Antipolis, France. We warmly thank L. Lapchin and R. Boll for introducing us to these data and for the fruitful discussions about aggregation in aphids ecology. We are also very grateful to the colleagues at Biostatistics and Spatial Processes laboratory for their availability and comments about this work.

Appendix

OA -, O -, A - and $\emptyset$ -samples were simulated by combining three layers defined in this appendix. R programs (lines starting with $>$) show how the layers were obtained and combined.

Layer one: the hierarchical space $\mathbb{E}$ was made of 10 units. Each unit was composed of a random number of subunits drawn in a uniform counting distribution ranging from 5 to 25.

```
> ns=10      # number of shoots
> nlmin=5    # minimum number of leaves per shoot
> nlmax=25   # maximum number of leaves per shoot
> E=NULL
> for(i in 1:ns) E=rbind(E,cbind(i,1:sample(nlmin:nlmax,1)))
```

Layer two: the occupancy structure $O : \mathbb{E} \rightarrow \{0, 1\}$ was defined as the excursion set of a Gaussian random process (Lantuéjoul, 2002): that is to say for all $e \in \mathbb{E}$, $O(e)$ equals one if $Z(e) > 0$ and zero else, where $Z : \mathbb{E} \rightarrow \mathbb{R}$ denotes the Gaussian process defined over $\mathbb{E}$ and with values in $\mathbb{R}$. To obtain aggregated “ones” and aggregated “zeros”, a Gaussian auto-correlation function was used to simulate the Gaussian process (Chilès and Delfiner, 1999).

```
> sc=0.2    # scaling parameter governing proximity of subunits
>           # in the case of occupancy
> D=sqrt(outer(E[,1],E[,1],''-'' )^2+outer(sc*E[,2],sc*E[,2],''-'' )^2)
>           # distance matrix
> Zmean=0.2  # mean of the underlying Gaussian process Z
> Zvar=0.5   # variance of the underlying Gaussian process Z
> Z=mvrnorm(1,rep(Zmean,nrow(E)),Zvar*exp(-D^2))
>           # mvrnorm() is available in the MASS library
> O=(Z>0)
```

Layer three: the abundance structure $A : \mathbb{E} \rightarrow \mathbb{N}$ was based on a doubly stochastic random process (Diggle, 2003): A log-Gaussian random process $Y : \mathbb{E} \rightarrow \mathbb{R}_+$ with a Gaussian auto-correlation function was first simulated; Then, the abundance $A(e)$ in

1 subunit $e \in \mathbb{E}$ was drawn from a Poisson distribution with mean value $Y(e)$ to which
2 the value one is added (to avoid null abundances). The spatial structuring of Y allowed
3 us to get a spatially structured abundance process A . Remark: This model can also be
4 written in the framework of spatial generalized linear mixed models (Diggle *et al.* 1998).

```
5 > sc=0.05 # scaling parameter governing proximity of subunits
6 > # in the case of abundance
7 > D=sqrt(outer(E[,1],E[,1],''-'' )^2+outer(sc*E[,2],sc*E[,2],''-'' )^2)
8 > Ym=c(-1,0) # range for the mean of the Gaussian process Y
9 > Yvar=5 # variance of the Gaussian process Y
10 > Y=exp(mvrnorm(1,rep(runif(1,Ym[1],Ym[2]),nrow(E)),Yvar*exp(-D^2)))
11 > A=1+rpois(length(Y),Y)
```

12 Then, the three layers are combined as follows to get the four sorts of samples
13 presented in the simulation study.

```
14 > OApattern=0*A # sample structured in occupancy and abundance
15 > Opattern=0*sample(A) # sample structured in occupancy
16 > Apattern=sample(0)*A # sample structured in abundance
17 > NOpattern=sample(0)*sample(A) # unstructured sample
```

18 References

- 19 Baddeley, A., 2008. Analysing spatial point patterns in R. Workshop notes. CSIRO eds.
20 <http://www.csiro.au/resources/pf16h.html>
- 21 Bar-Hen, A. and Picard, N., 2007. Simulation study of dissimilarity between point pro-
22 cess. Computational Statistics, 21; 487-507.
- 23 Beaumont, M. A., Zhang, W. and Balding, D. J., 2002. Approximate Bayesian Compu-
24 tation in Population Genetics. Genetics, 162; 2025-2035.
- 25 Brix, A., Senoussi, R., Couteron, P. and Chadœuf, J., 2001. Assessing Goodness of Fit
26 of Spatially Inhomogeneous Poisson Processes. Biometrika, 88; 487-497.
- 27 Chambers, J. M., Freeny, A. and Heiberger, R. M., 1992. Analysis of variance; designed
28 experiments. In: J. M. Chambers and T. J. Hastie (editors), Statistical Models in S.

- 1 Wadsworth and Brooks/Cole, Pacific Grove, pp.145-194
- 2 Chilès, J.-P. and Delfiner, P., 1999. Geostatistics. Modeling Spatial Uncertainty. Wiley,
- 3 New York, 695 pp.
- 4 Conlisk, E., Bloxham, M., Conlisk, J., Enquist, B. and Harte, J., 2007. A new class of
- 5 models of spatial distribution. Ecological Monography, 77 (2); 269:284.
- 6 Cressie, N. A. C., 1991. Statistics for Spatial Data. Wiley, New York, 900 pp.
- 7 Dacunha-Castelle, D. and Duflo M., 1982. Probabilités et statistiques, tome 2, Problèmes
- 8 à temps mobile. Masson, Paris, 286 pp.
- 9 Diggle, P. J., 2003. Statistical Analysis of Spatial Point Patterns (2nd ed.), Academic
- 10 Press, New York, 159 pp.
- 11 Diggle, P. J., Tawn, J. A. and Moyeed, R. A., 1998. Model-based geostatistics. Applied
- 12 Statistics, 47; 299-350.
- 13 Efron, B. and Tibshirani, R. J., 1993. An introduction to the bootstrap. Chapman &
- 14 Hall. New York, 436 pp.
- 15 Epperson, B. K., 2003. Geographical genetics. Princeton University Press, 369 pp.
- 16 Ferrandino, F.J., 2004. Analytical and Theoretical Plant Pathology Measuring Spatial
- 17 Aggregation in Binary Epidemics: Correlative Analysis and the Advantage of Fractal-
- 18 Based Sampling. Phytopathology 94: 1215-1227.
- 19 Gilbert, M., Fielding, N., Evans, H.F. and Gregoire, J.-C., 2003. Spatial pattern of invad-
- 20 ing *Dendroctonus micans* (Coleoptera : Scolytidae) populations in the United Kingdom.
- 21 Can. J. For. Res., 33(4); 712:725
- 22 Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W. M., Railsback, S. F., Thulke,
- 23 H.-H., Weiner, J., Wiegand, T. and DeAngelis, D. L., 2005. Pattern-oriented modeling of
- 24 agent-based complex systems : lesson for ecology. Science, 310; 987-991
- 25 Henderson, R., Shimakura, S. and Gorst, D.; 2002. Modeling spatial variation in
- 26 leukemia survival data. Journal of the American Statistical Association, 97; 965-972.
- 27 Illian, J., Penttinen, A., Stoyan, H. and Stoyan, D., 2008. Statistical Analysis and Mod-
- 28 elling of Spatial Point Patterns. Wiley, New York.
- 29 Inouye, B. D., 2005. Scaling up from local competition to regional coexistence across

- 1 two scales of spatial heterogeneity : insect larvae in the fruits of *Apeiba membranacea* .
- 2 Oecologia, 145; 188-196.
- 3 Johst, K., Brandl, R., Eber, S., 2002. Metapopulations persistence in dynamic land-
- 4 scapes : the role of dispersal distance. Oikos, 98; 263-270.
- 5 Keitt, T.H., Bjørnstad, O., Dixon, P.M. and Citron-Pousty, S., 2002. Accounting for spa-
- 6 tial pattern when modeling organism-environment interactions. Ecography, 25; 616-625.
- 7 Laine, A.-L. and Hanski, I., 2006. Large-scale spatial dynamics of specialist plant
- 8 pathogen. Journal of Ecology, 94; 217-226.
- 9 Lantuéjoul, C., 2002. Geostatistical Simulation, Models and Algorithms. Springer,
- 10 Berlin, 256 pp.
- 11 Levin, S., 1992. The problem of pattern and scale in ecology. Ecology, 73(6); 1943-1967
- 12 Mandelbrot, B.B., 1977. The Fractal Geometry of Nature. Freeman, San Francisco.
- 13 Manly, B.F.J., 1997. Randomization, bootstrap and Monte Carlo methods in Biology.
- 14 (2nd ed.), Chapman and Hall, London, 281 pp.
- 15 Oddou-Muratorio, S., Demesure-Musch, B., Pelissier, R. and Gouyon, P.-H., 2004. Im-
- 16 pacts of gene flows and logging history on the local genetic structure of a scattered tree
- 17 species *Sorbus torminalis* L. Crantz. Molecular Ecology, 13; 3689-3702.
- 18 Perry, J.N., Liebhold, A.M., Rosenberg, M.S., Miriti, J., Jakomulska, A. and Citron-
- 19 Pousty, S., 2002. Illustrations and guidelines for selecting statistical methods for quan-
- 20 tifying spatial pattern in ecological data. Ecography, 25; 578-600.
- 21 Rue, H. and Held, L., 2005. Gaussian markov random fields. Theory and applications.
- 22 Chapman and Hall, New York, 263 pp.
- 23 Soubeyrand, S., Enjalbert, J., Sanchez, A. and Sache, I., 2007a. Anisotropy, in density
- 24 and in distance, of the dispersal of yellow rust of wheat: Experiments in large field plots
- 25 and estimation. Phytopathology, 97; 1315-1324.
- 26 Soubeyrand, S., Sache, I., Lannou, C. and Chadœuf, J., 2007b. A frailty model to assess
- 27 plant disease spread from individual count data. Journal of Data Science, 5; 67-83.
- 28 Soubeyrand, S., Thébaud, G. and Chadœuf, J., 2007c. Accounting for biological vari-
- 29 ability and sampling scale: a multi-scale approach to building epidemic models. Journal

- 1 of the Royal Society Interface 4: 985-997.
- 2 Soubeyrand, S., Carpentier, F., Desassis, N. and Chadœuf, J., 2008a. Incorporating a
- 3 contrast in the Bayesian formula: What consequences for the MAP estimator and the
- 4 posterior distribution? Applications in spatial statistics. arXiv:0804.4780v1
- 5 Soubeyrand, S., Held, L. Höhle, M. and Sache, I., 2008b. Modelling the spread in space
- 6 and time of an airborne plant disease. Applied Statistics, 57; 253-272.
- 7 Soubeyrand, S., Neuvonen, S. and Penttinen, A., 2009. Mechanical-statistical modelling
- 8 in ecology: from outbreak detections to pest dynamics. Bulletin of Mathematical Biol-
- 9 ogy 71: 318-338.
- 10 Storch, D., Scaronizling, A.L., Reif, J., Polechová, J., Scaronizlingová, E. and Gaston,
- 11 K.J., 2008. The quest for a null model for macroecological patterns: geometry of species
- 12 distributions at multiple spatial scales. Ecological Letters 11: 771-784.
- 13 Tilman, D. and Kareiva, P., 1996. Spatial Ecology: The Role of Space in Population
- 14 Dynamics and Interspecific Interactions. Princeton Univ. Press, Princeton, 368 pp.
- 15 Virtanen, T., Neuvonen, S., Nikula, A., Varama, M. and Niemelä, P., 1996. Climate
- 16 change and the risks of *Neodiprion sertifer* outbreaks on Scots pine. Silva Fennica, 30;
- 17 169-177.
- 18 Wiegand, T., Jeltsch, F., Hanski, I. and Grimm, V., 2003. Using pattern-oriented
- 19 modeling for revealing hidden information: a key for reconciling ecological theory and
- 20 application. Oikos, 100; 209-222.

1 Table 1

Types	Hypotheses	n-uplets								
		n=1	n=2	n=3	n=4	n=5	n=6	n=7	n=8	n=9
<i>OA</i>	Freq $H_{01} \leq 0.05$	63*	69*	69*	60*	51*	51*	48*	42*	43*
	Freq $H_{02} \leq 0.05$	70*	68*	57*	56*	46*	36*	32*	18*	7
	Freq $H_{03} \leq 0.05$	0	1	3	5	4	5	6	2	1
<i>O</i>	Freq $H_{01} \leq 0.05$	63*	68*	69*	60*	52*	52*	49*	42*	42*
	Freq $H_{02} \leq 0.05$	4	5	4	8	7	8	8	5	5
	Freq $H_{03} \leq 0.05$	0	4	3	1	4	5	5	4	2
<i>A</i>	Freq $H_{01} \leq 0.05$	9	5	4	3	7	4	6	3	5
	Freq $H_{02} \leq 0.05$	56*	60*	57*	49*	49*	31*	30*	13*	7
	Freq $H_{03} \leq 0.05$	0	1	2	5	4	3	2	4	3
$\emptyset$	Freq $H_{01} \leq 0.05$	3	4	5	3	3	1	6	6	4
	Freq $H_{02} \leq 0.05$	4	7	4	3	5	7	5	4	3
	Freq $H_{03} \leq 0.05$	0	3	1	2	3	3	6	4	1
<i>LARGE</i>	Freq $H_{01} \leq 0.05$	33*	53*	65*	69*	64*	59*	42*	31*	24*
	Freq $H_{02} \leq 0.05$	96*	95*	91*	93*	94*	86*	82*	69*	31*
	Freq $H_{03} \leq 0.05$	0	1	3	15*	23*	2	0	1	0

Table 1: Number of *OA*-, *O*-, *A*- and $\emptyset$ -samples and of *LARGE* aggregate samples, the p-value of which are ≤ 0.05 at increasing size of uplet, for the three different null hypotheses. * : significancy at the level of 5% by comparison with a draw in $B(100, 0.05)$.

1 Table 2

Type	n-uplet	n=1	n=2	n=3	n=4	n=5	n=6	n=7	n=8	n=9
Branches	Freq $H_{01} \leq 0.05$	33*	31*	30*	28*	34*	23*	16*	14*	10*
	Freq $H_{02} \leq 0.05$	24*	20*	15*	12*	11*	6	5	2	0
	Freq $H_{03} \leq 0.05$	0	2	3	5	3	2	3	1	4

Table 2: Percentage of branches the p-value of which are ≤ 0.05 at increasing size of uplet, for the three different null hypotheses. * : significancy at the level of 5% by comparison with a draw in $B(160, 0.05)$.

1 List of Figures

587	1	Hierarchical spaces made of subunits (dots) nested in units (thin lines	
588		on the left and rectangles on the right). Proximities between units are	
589		indicated by the thick segments. Remark: degrees of proximity between	
590		subunits can be defined on the left (this scheme may represent the system	
591		leaves-shoots-branch) but not necessarily on the right (this scheme may	
592		represent the system branch-tree-orchard).	26
593	2	Typical ways of aggregation in occupancy (filled squares on the 2D grid)	
594		and/or abundance (red tall bars for high values; yellow small bars for low	
595		values). a: no aggregation; b: aggregation in abundance; c: aggregation	
596		in occupancy; d: aggregation in abundance and occupancy.	27
597	3	Examples of permutations applied to an occupancy pattern at the subunit	
598		level (top), to an abundance pattern at the subunit level (centre) and to	
599		an abundance pattern at the unit level (bottom).	28
600	4	Decomposition of an hypothetical space with four units into the three	
601		2-uplets and computation of the test statistics $S_n, n = 2$	29
602	5	Observed statistic $S_n = (\mu_{nk^*}, \sigma_{nk^*}^2)$ for a given pattern of a given space	
603		(large dot) and statistics computed for 5,000 permuted patterns (small	
604		dots). The rectangle centred around the observed statistic defines its	
605		surrounding used in the computation of the test p-value.	30
606	6	Schematic images of $\emptyset$ -, OA -, O -, A - and $LARGE$ -samples (red circle :	
607		occupied subunits, sizes proportional to the abundances indicated with	
608		black numbers; green diamond : unoccupied subunits)	31

- 609 7 Cube decomposition of the multiple test results for $\emptyset$ -, OA -, O -, A - and
610 *LARGE*-samples. In the multiple test procedure, three hypotheses with
611 two modalities (0=accepted: H_{0i} and 1=rejected: $\bar{H}_{0i}$) are tested and
612 eight different trivariate responses are expected ((0,0,0), (1,0,0), (0,1,0),
613 (0,0,1), (1,1,0), (1,0,1), (0,1,1) and (1,1,1)). On the cube representation
614 each direction carries one hypothesis and each corner carries one trivariate
615 response. The number at each corner gives the percentage of samples for
616 which the respective trivariate response is obtained. 32
- 617 8 Schematic images of four real branches (the construction of the schematic
618 images is explained in Fig. ??). The four branches have been chosen
619 because they respond differently to the multiple test and correspond to
620 the four types defined in the simulation study : $\emptyset$ -branch = no one of the
621 three hypotheses rejected; OA -branch = H_{01} and H_{02} are both rejected;
622 O -branch = H_{01} only is rejected; A -branch = H_{02} only is rejected. 33
- 623 9 Cube decomposition of the multiple test results for the real branches. The
624 construction of the cube is explained in Fig. ?? 34

Figure 1: Hierarchical spaces made of subunits (dots) nested in units (thin lines on the left and rectangles on the right). Proximities between units are indicated by the thick segments. Remark: degrees of proximity between subunits can be defined on the left (this scheme may represent the system leaves-shoots-branch) but not necessarily on the right (this scheme may represent the system branch-tree-orchard).

Figure 2: Typical ways of aggregation in occupancy (filled squares on the 2D grid) and/or abundance (red tall bars for high values; yellow small bars for low values). a: no aggregation; b: aggregation in abundance; c: aggregation in occupancy; d: aggregation in abundance and occupancy.

Figure 3: Examples of permutations applied to an occupancy pattern at the subunit level (top), to an abundance pattern at the subunit level (centre) and to an abundance pattern at the unit level (bottom).

Figure 4: Decomposition of an hypothetical space with four units into the three 2-uplets and computation of the test statistics S_n , $n = 2$.

Figure 5: Observed statistic $S_n = (\mu_{nk^*}, \sigma_{nk^*}^2)$ for a given pattern of a given space (large dot) and statistics computed for 5,000 permuted patterns (small dots). The rectangle centred around the observed statistic defines its surrounding used in the computation of the test p-value.

Figure 6: Schematic images of $\emptyset$ -, OA-, O-, A- and LARGE-samples (red circle : occupied subunits, sizes proportional to the abundances indicated with black numbers; green diamond : unoccupied subunits) .

Figure 7: Cube decomposition of the multiple test results for $\emptyset$ -, OA-, O-, A- and LARGE-samples. In the multiple test procedure, three hypotheses with two modalities (0=accepted: H_{0i} and 1=rejected: $\bar{H}_{0i}$) are tested and eight different trivariate responses are expected ((0,0,0), (1,0,0), (0,1,0), (0,0,1), (1,1,0), (1,0,1), (0,1,1) and (1,1,1)). On the cube representation each direction carries one hypothesis and each corner carries one trivariate response. The number at each corner gives the percentage of samples for which the respective trivariate response is obtained.

Comment citer ce document :

Kretzschmar, A., Soubeyrand, S., Desassis, N. (2010). Aggregation patterns in hierarchy/proximity spaces. Ecological Complexity, 7 (1), 21-31. , DOI : 10.1016/j.ecocom.2009.03.012

Figure 8: Schematic images of four real branches (the construction of the schematic images is explained in Fig. 6). The four branches have been chosen because they respond differently to the multiple test and correspond to the four types defined in the simulation study : $\emptyset$ -branch = no one of the three hypotheses rejected; OA -branch = H_{01} and H_{02} are both rejected; O -branch = H_{01} only is rejected; A -branch = H_{02} only is rejected.

Figure 9: Cube decomposition of the multiple test results for the real branches. The construction of the cube is explained in Fig. 7.