

# **Ranking of Polluted Regions in South West Germany Based on a Multi-indicator System**

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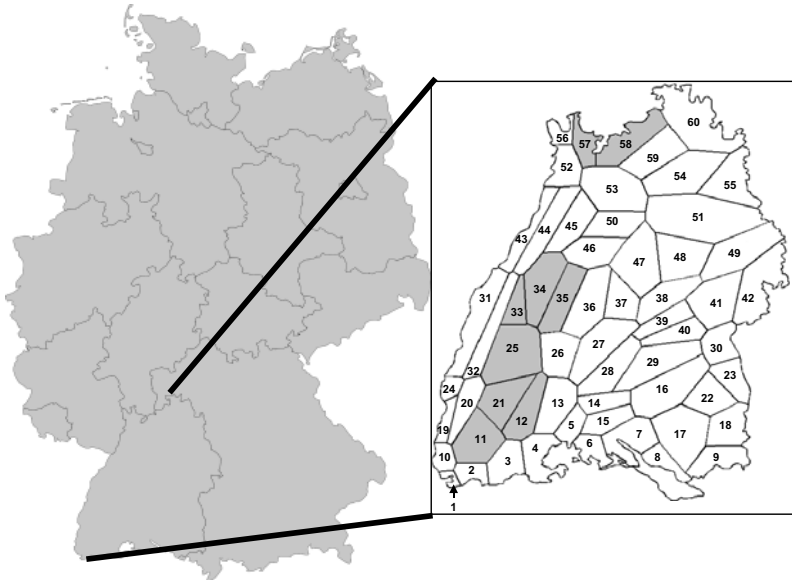
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## **Abstract**

Multi-indicator systems are of increasing importance in every field of science, corresponding to the complexity of objects to be ranked. Here we apply multi-indicator systems in order to describe and characterize the pollution in the South-West of Germany by the metals Lead, Pb, Cadmium, Cd, Zinc, Zn and Sulfur, S. We demonstrate the need of a preprocessing of data, before an analysis towards ranking is possible or meaningful. The univariate clustering method after Ward is applied and analyzed with respect to its robustness by a “soft bootstrapping procedure”. We show that without the need of numerically aggregated indicators (which may insert a high degree of subjectivism into the analysis) or without performing more complex operations (as in traditional Decision Support Systems such as e.g. PROMETHEE) we can obtain relative orders of regions corresponding to their pollution load. In our example we discuss the pollution by chemicals elements in two biological targets.

## 1 Monitoring Pollution

For monitoring of pollution, the south-west German state of Baden-Wuerttemberg is divided into 60 regions by the Environmental Protection Agency of Baden-Wuerttemberg (EPA) (Fig. 1). The regions are defined by their most homogeneous natural and geological environments, with the minority with granitic underground (Bruggemann et al. 1998, 1999, 2003; Luther et al., 2000).



**Figure 1:** Location of the state of Baden-Wuerttemberg, Germany, and its division into 60 regions. In the inset map, the grey regions show different geology (granitic rock) from the remainder of the white regions (limestone and other geological formations).

For monitoring pollution caused by four important chemical elements, the EPA of Baden Wuerttemberg selected different targets: for instance (i) herb layer (Ks: German “Krautschicht”) and (ii) epiphytic mosses (Ms). Results of the monitoring of these targets then form the basis of a priority list to reduce pollution.

In the study presented here, we consider pollution by Pb, Cd, Zn and S, in the herb layer and the epiphytic mosses. These elements are of particular interest because they affect the environment and human health in many ways, and in a wide range of temporal sequences,

corresponding to different transport paths and reaction networks within the environment. The problem is how to obtain from this multi-indicator system a ranking, i.e. a meaningful partially ordered set of regions.

The chemical elements Pb, Cd and Zn were monitored in the herb layer and in the epiphytic mosses. In the herb layer additionally sulfur concentrations were measured. Thus there were 7 parameters by which the pollution was quantitatively described (each is described by the two letter code for the vegetation, followed by the code for the element): KsPb, KsCd, KsZn, and KsS, and MsPb, MsCd, and MsZn (Table 1).

**Table 1:** Data matrix with measured data of pollution by chemical elements in two targets, the herb layer (Ks) and in the epiphytic mosses (Ms). Because of some missing data only 58 regions remain.

Region	KsPb	KsCd	KsZn	KsS	MsPb	MsCd	MsZn
1	1	0.04	21	1540	21.7	0.396	76.2
2	0.7	0.14	27	1770	12.9	0.351	68.7
3	0.8	0.14	31	1710	13.34	0.468	47.5
4	0.8	0.02	26	1790	10.87	0.294	34.1
5	1.1	0.1	32	1990	14.13	0.424	45.2
6	1	0.07	29	1750	11.1	0.207	31
7	1.2	0.09	28	1600	14.4	0.304	41
8	1.5	0.07	27	1750	19.8	0.361	55
9	0.09	0.2	850	580	17.5	0.309	45.4
10	1	0.03	29	1780	13.35	0.527	62.2
11	0.9	0.08	27	1720	23.4	0.43	63.1
12	0.16	0.23	910	1460	9.78	0.213	39.9
13	0.18	0.18	1160	350	14.4	0.276	48.2
14	1	0.17	34	1830	12.04	0.591	41.4
15	0.9	0.1	24	1670	13.7	0.362	43.2
16	1	0.12	32	1520	13.4	0.36	50.5
17	0.6	0.06	36	1820	12.77	0.295	63.4

18	0.5	0.43	28	4030	11.3	0.346	46.7
19	0.8	0.01	18	4030	11.33	0.384	83.9
20	1.5	0.14	32	1730	16.2	0.324	58.4
21	0.06	0.24	830	620	14	0.474	63.6
22	1	0.03	28	2150	14.5	0.312	41.3
23	1.1	0.04	42	2000	17.1	0.265	56
24	1.7	0.18	39	1740	13.7	0.254	56.7
25	0.9	0.09	35	1460	18.4	0.592	74.9
26	0.8	0.05	19	1620	12.16	0.262	43.9
27	0.1	0.12	26	1600	14.3	0.364	54.4
28	0.9	0.05	34	1670	11.5	0.277	36.1
29	0.6	0.14	27	1680	9.22	0.404	29.5
30	0.8	0.08	27	1610	14.25	0.347	52.8
31	1.1	0.15	28	1740	22.5	0.423	49.6
32	1.2	0.03	35	1820	18.6	0.434	81.2
33	0.16	0.26	800	530	51	0.54	84.8
34	0.14	0.39	950	400	17.8	0.409	62
35	0.08	0.24	720	1960	30.1	0.475	102
36	1.2	0.05	31	1570	12.9	0.352	38.6
37	0.6	0.12	33	1580	13.1	0.338	47.3
38	1.7	0.18	34	1720	16.1	0.313	49.7
39	1	0.1	38	1740	16.7	0.417	40.9
40	0.7	0.06	34	1770	11.2	0.367	12.3
41	0.7	0.17	39	1840	11.22	0.54	43.2
42	0.7	0.1	33	1690	10.74	0.491	63
43	0.5	0.11	39	4030	11.92	0.265	89.5
44	0.8	0.08	38	1800	16.9	0.282	56.7

45	1.5	0.17	45	1780	17.3	0.433	48.8
46	0.8	0.09	33	1680	15.1	0.333	74
47	1.1	0.11	25	1650	21.3	0.419	135
48	2.3	0.42	33	1600	23.5	0.682	72.3
49	0.8	0.11	37	1680	9.6	0.337	49.6
50	1.4	0.13	29	1730	17.8	0.308	142
51	0.8	0.14	22	1640	19.2	0.489	55.1
52	2	0.23	36	4030	22.4	0.379	57.2
53	1	0.12	36	1750	16.9	0.403	46.3
54	0.7	0.1	26	1750	9.08	0.285	42.6
56	1	0.11	34	1970	40.2	0.631	118
57	1.7	0.15	39	1850	19.4	0.402	57.4
58	1	0.11	28	1980	11.65	0.244	47.3
59	1.3	0.13	26	1470	17.4	0.554	50.2
60	1	0.2	32	2160	14.8	0.368	54.4

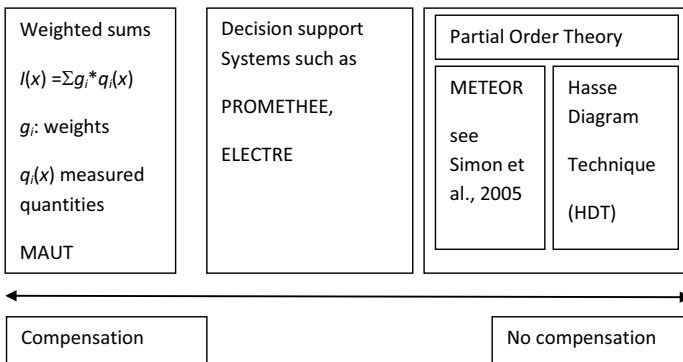
In this paper we discuss the problem of ranking by statistical and order theoretical methods. Our approach presents: the problem of ranking within a multi-indicator system, principles of partial order, data preprocessing by cluster analysis, results of statistical and order theoretical methods, a summary and a critical discussion.

## **2 Ranking within Multi-indicator Systems**

There are many methods to obtaining a ranking on the basis of a multi-indicator system. Most of these methods aim at a definition of a scalar (univariate) ranking index. Beside the simple process of defining a weighted sum of the parameter values (see for example MAUT, Schneeweiss, 1991), many more sophisticated methods are often considered such as PROMETHEE and ELECTRE (Brans and Vincke, 1985, Roy, 1990). A recent overview is given by Huang et al., 2011.

Following Munda, 2008 and Munda and Nardo, 2008, different decision support methods should be characterized by the degree of compensation: When a weighted sum is used as aggregation method, then compensation (in our example of pollution in Baden-Wuerttemberg) means that a region can get a ranking indicating a good state, even though good (i.e. low concentrations) values in some chemical elements can mask the potentially dangerous value of one single other chemical element. This compensation effect is generally unwanted. Nevertheless the use of weighted sums is widespread, because of their simplicity and transparency. For example, weighted sums play an important role in the European Communities monitoring of the progress of innovation in different European member states (Nardo, 2008, Annoni and Kozovska, 2010, Cherchye et al. 2010, N.N. 2009, Falbo et al., 2010, Fattore, 2010). The crucial problem of finding appropriate weights by which the parameter values are combined in the weighted sum, has been studied in a robustness approach (Annoni and Kozovska, 2010) and by fuzzy concepts (Annoni et al., 2008, Fattore, 2008, Yager 1988). Nevertheless the main disadvantage of weighted sum is the compensation.

Discrete mathematics, especially partial order theory, provides a very simple non-compensatory method (Figure 2) (see Annoni and Bruggemann, 2009, Bruggemann et al., 2001, Bruggemann and Voigt, 2008, Bruggemann and Patil, 2010, 2011, Carlsen, 2008, Sørensen et al., 2003, Tsakovski and Simeonov, 2008, Bruggemann, Carlsen, 2012). Therefore we apply the method of partially ordered sets in this study, which in turn needs a careful preprocessing of data.



**Figure 2:** The degree of compensation as a scale to characterize different methods of evaluating multi-indicator systems (see text).

## 3 Methods

### 3.1 Overview

There is considerable interest in combining the two theoretical aspects of clustering and ordering. Recently, Owsinski (2011) has proposed a unifying approach based on formal mathematical programming schemes, which is applicable to both clustering and ordering (see also Owsinski (2012)). The algorithms, however, are computationally difficult and here we prefer a two step procedure. Firstly a preprocessing of data is proposed in order to secondly obtain a partial order which is to be analyzed.

### 3.2 Basics of partial order theory

In our context, a set of objects  $X$  is to be examined. The elements of  $X$  are the regions of Baden- Wuerttemberg, and each element of  $X$  is characterized by a tuple of indicators  $q(x) = (q_1(x), q_2(x), \dots, q_m(x))$ . In the present study,  $m = 7$ , corresponding to the seven indicators of pollution. We give  $X$  a binary structure, namely that of a partial order as follows:

$x, y \in X: x < y$  if and only if  $q(x) < q(y)$ , i.e.

if and only if  $q_i(x) < q_i(y)$  for all  $i = 1, \dots, m$  (1)

The relationship (1) among elements of  $X$ , the objects, leads to partially ordered sets. Although this relationship is simple, its evaluation is difficult and needs software support. There are many possibilities to endow a set with relations such that this set gets the structure of a partially ordered set. The decisive point to speak of partially ordered sets is that the relations have to obey the following axioms (reflexivity (an object can be compared with itself), antisymmetry (if an object  $x$  is better than object  $y$  then the statement object  $y$  is better than object  $x$  implies  $x = y$ ) and transitivity ( $x < y$  and  $y < z$  then  $x < z$ )). Eq. (1) as one of the relations to obtain partially ordered sets fulfills the above mentioned axioms and has the advantage of avoiding a mingling and hence a compensation of indicator values  $q_i(x)$  in order to get a ranking index. In chemistry, other useful realizations of partial order can be found, see e.g. Klein and Brickmann, 2000, Ruch, 1975, Ruch and Gutman, 1979, Restrepo and Klein, 2011, Klein and Ivanciuc, 2006 or Randic 1990. If  $q(x) < q(y)$  we say that  $x$  and  $y$  can be compared and that  $x$  is "less"  $y$ . If  $q_i(x) < q_i(y)$  for some  $i$  and  $q_j(x) > q_j(y)$  for some other  $j$ , then  $x$  and  $y$  cannot be compared. Then,

the pair  $(x, y)$  is a pair of incomparable objects, the technical notation is:  $x \parallel y$ . Such an incomparability always indicates that any aggregation of indicator values is crucial, depending on external information.

For evaluation purposes, the partial order concept of a “chain” is important. A chain is a subset  $X'$  of  $X$ , such that for all elements of  $X'$  a sequence  $x_1 < x_2 < x_3 < \dots < x_{|X'|}$  can be found.  $|X'|$  denotes the number of elements in  $X'$ . Hence the more chains we can find and the longer the chains are, the more important is the result for evaluation purposes. The reason is that these sequences do not depend on any subjective information, i.e. they are purely based on the data matrix which finally is used.

An antichain is a subset  $X'$ , where for no pair  $(x, y)$ ,  $x, y \in X'$  a  $<$ -relation can be found. Antichains are important because the priority elements are almost every time elements of an antichain. In the case studied here, regions which are in an antichain and do not have an upper neighbor in the Hasse diagram are called maximal elements and are of special interest, because these regions need as first an environmental improvement.

In the Hasse Diagram Technique (HDT) the partially ordered set (often denoted by  $(X, \leq)$ ) depends on the selected indicators and their values. Therefore we write  $(X, IB)$ , where  $IB$  is the “information base” (Bruggemann and Voigt, 1995), which is the set of indicators (or attributes), to indicate that the set  $X$  is partially ordered due to eq. (1). The HDT is an ordinal method, the detailed metric information is lost, and only the ordinal information is retained. Therefore one of the most crucial methodological tasks in HDT is how to preprocess data which are continuous in concept. We apply a cluster analysis for any single indicator with the aim of determining: (i) the number of clusters, and (ii) where to set the border between two neighboring clusters (see below, to understand why we can speak of “neighboring clusters”).

### **3.3 Statistical methods**

#### ***Univariate clustering***

Usually cluster analysis is considered as a multivariate statistical method. The main aim of clustering is a rigorous reduction of the size of the dataset, without losing the essential information. Indeed, the clustering tasks can be solved for a large number of objects.



Well-known cluster analysis techniques such as the partitional  $K$ -means and the hierarchical Ward's method are based on minimization of the sum of squares criterion (Bartel et al. 2003, Luther et al. 2000, Mucha 1992, Mucha 2002). Clustering requires some measures of pairwise distance on the multivariate space. Unfortunately, distances are often dependent on the scales of the variables. In applications, this can become a crucial point. To avoid this problem the data is usually standardized before doing multivariate cluster analysis. More information on data preparation by standardization, in an application of cluster analysis to ecology, is given by Mucha et al. (2002).

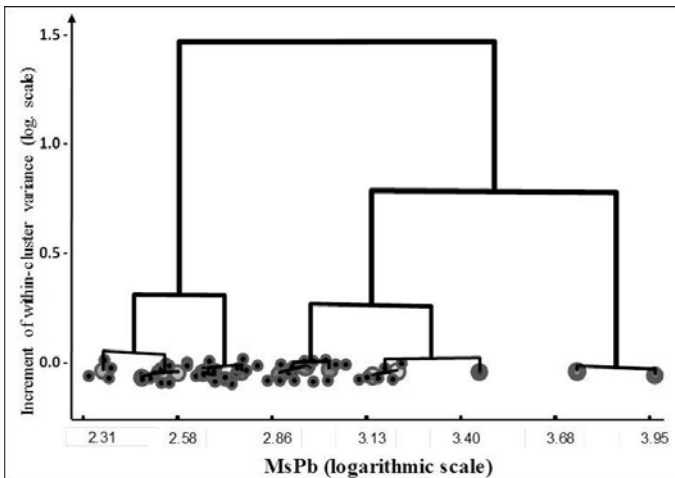
In the present paper, we propose a data preprocessing step based on univariate cluster analysis accompanied by a special bootstrap validation. The aims are to objectify and automate the determination of categories for each single indicator (variable) when data is continuous. That is, in the present study,  $m = 7$  univariate clusterings are necessary. Generally, a categorization (down-grading in the scale) of a quantitative variable is often referred as data binning.

Our approach of univariate cluster analysis results in a categorization of quantitative data where the number of categories (clusters) is validated by automatic resampling techniques. In order to find homogeneous clusters (i.e., intervals in the univariate case) in the sense of minimizing the within-cluster variances, we choose the hierarchical Ward's method because it investigates numerous partitions at the same time, and usually provides a unique result. The hierarchical cluster analysis contrasts with the partitional cluster analysis such as the iterative  $K$ -means method (Steinhaus 1956, MacQueen 1967), where the result depends on both the initial partition used as the starting point, and on the number of clusters that has to be fixed in advance. For explanation purposes (and without loss of generality), we will consider the indicator MsPb (lead in epiphytic mosses) in more detail in the present paper.

Of course, there are other appropriate cluster analysis methods that can be used for solving the task of binning. Beside our favorite Ward's method looking for clusters of similar volumes we recommend also the "generalized" Ward's method that can find clusters of different volumes (for details, see Mucha 2009).

**Technical procedure, Ward's method**

Starting from a matrix of pairwise squared Euclidean distances ( $d_{ih}$ ) between any two observations  $i$  and  $h$ , Ward's method merges in a stepwise manner those two clusters that result in a minimum increment of within-cluster variance (for details, see Mucha et al., 2002). In the first step, the within-cluster sum of squares  $w\{i, h\}$  of two objects  $i$  and  $h$  is simply  $w\{i, h\} = m_i m_h / (m_i + m_h) d_{ih}$ . Usually, and as it is in the present application, the masses  $m_i$  and  $m_h$  are equal to 1. However, when starting with already aggregated data, the mass of an object equals the cardinality of the observations that it presents, i.e., the mass is a positive number 1,2,3,... At the end of the agglomeration procedure, Ward's hierarchical cluster analysis method presents a hierarchy of nested partitions that can be visualized in a dendrogram (Figure 3). By cutting the tree at a certain level of increment of within-cluster variance (at the ordinate in Figure 3), one gets a partition into  $K$  clusters ( $K= 2, 3, 4, \dots$ ). Thus, in one run, many partitions are obtained simultaneously. The aim of our proposed data preprocessing step is to determine  $K$  categories (i.e.  $K$  clusters) on the ordinal scale. In other words, we apply univariate clustering, based on a quantitative original indicator, in order to obtain a new ordinal indicator with a range of  $K$  categories. The choice of an appropriate  $K$  is the main problem in clustering. Therefore, for each variable, we performed clustering accompanied by special bootstrap validation.



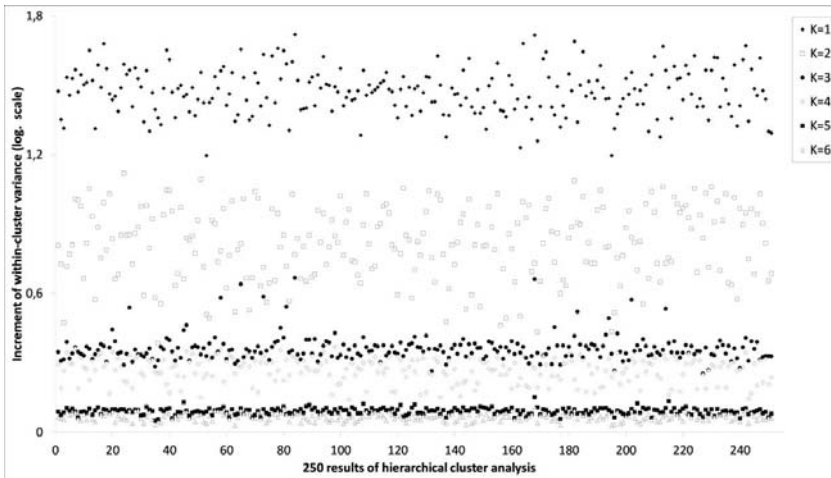
**Figure 3:** An ordered dendrogram (Mucha et al. 2005) where the horizontal coordinate of the regions are their values of MsPb (lead in the epiphytic moss, see data matrix in Table 1). The points are jittered slightly in the opposite direction to reduce overlap.

### ***Bootstrapping***

Efron's (1979) bootstrap approach is resampling taken with replacement from the original data. Concretely, the original bootstrap technique can be formulated by choosing the following weights of objects:  $m_i = l$ , if object  $i$  is drawn  $l$  times, and  $m_i = 0$ , otherwise. Here it is supposed that originally  $m_i = 1$  with  $i = 1, 2, \dots, n$ . In clustering, the so-called sub-sampling (i.e., resampling taken without replacement from the original data) is another approach (see Hartigan (1969)):  $m_i = 1$ , if object  $i$  is drawn randomly, and  $m_i = 0$ , otherwise. Here we recommend another bootstrap method, called soft bootstrapping in the following, that consists of random change of the original masses  $m_i = 1$  to some degree. This resampling scheme of assigning randomized masses  $m_i > 0$  (under the constraint that the total sum of masses equals  $n$ ) is especially appropriate for a small sample size because no object is excluded from the bootstrap sample. Ward's clustering is performed for every bootstrap sample. Such a result is called a bootstrap clustering. As the final result of the simulations, the validated number of clusters  $K$  will become the number of categories.

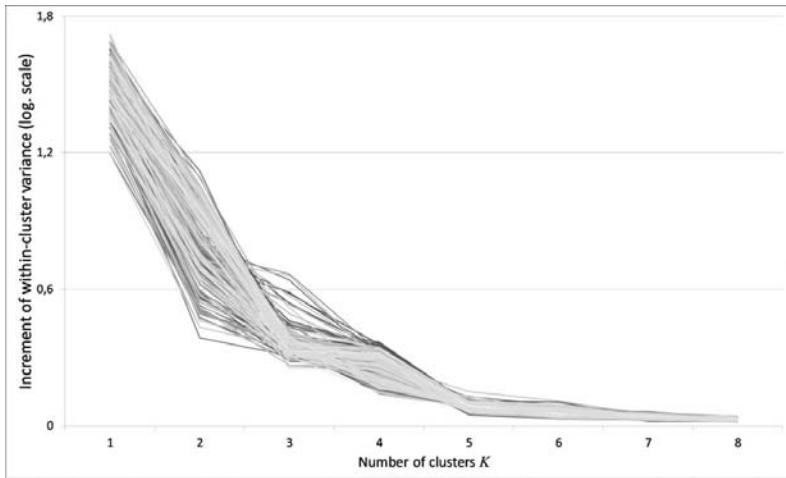
Let us look at the results of simulations for the indicator MsPb in detail. Figure 3 shows the result of Ward's method based on the original sample. We refer to it later on as the original clustering. Because of outliers in MsPb a logarithmic transformation of the data was done. There is a total order of the regions in the univariate case (see the locations of the regions at the abscissa). The terminal nodes of the tree correspond to the (logarithmic) values of MsPb of these regions. By cutting the tree by a horizontal line at a high distance level such as 1 one gets a partition into  $K=2$  clusters. Furthermore, by cutting at a middle distance level such as 0.5, the result is a partition into  $K=3$  clusters.

However, the key question remains: how many clusters (categories) should be selected? And, what are stable clusters from a statistical point of view? The original clustering has to be confirmed and reproduced in face of random perturbations of the data set by resampling methods as mentioned above. Hennig (2007) pointed out: "An important aspect of cluster validity is stability. Stability means that a meaningful valid cluster shouldn't disappear



**Figure 4:** The distance levels of the original clustering (at left) and 250 bootstrap clusterings by Ward’s method. A point on the abscissa reflects one result of a cluster analysis: The corresponding distance levels of amalgamation of clusters are located above the point parallel to the ordinate.

easily if the data set is changed in a non-essential way.” Bootstrapping and some alternative resampling methods are recommended for validation of the original clustering. Thus, cluster analysis of a random drawn sample of the data should lead to similar results. The results of many Ward’s clusterings for the indicator MsPb are visualized in Figures 4 and 5, and show the distance levels for different number of clusters. Usually, Figure 5 is used for a so-called scree-test about the number of clusters. In addition to the original clustering, there are 250 bootstrap clusterings based on random generated masses  $m_i$  coming from the interval around 1:  $[0.25, 1.75]$ , i.e.  $m_i = 1 + (1.5 r_i - 0.75)$  is a randomized mass of object  $i$ , where  $r_i \in [0,1]$  is a random generated uniform number. To assess the stability of the original clustering with respect to a new bootstrap clustering, a similarity measure between two cluster analysis results is needed.



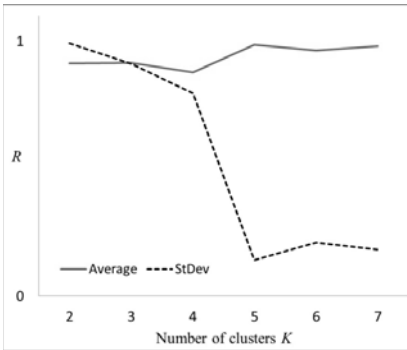
**Figure 5:** Distance levels of clusterings by Ward's method versus the number of clusters. Each line represents one clustering. This is another view of the results presented in Fig. 4.

### *Measures of cluster stability*

Some measures of cluster stability are based on the comparison of pairs of observations (objects) concerning their class membership of two partitions. Examples are the Rand index  $R^* = (a + d) / (n(n-1)/2)$  (Rand 1971) and the adjusted Rand index  $R$  (Hubert and Arabie 1985). The number of objects is denoted by  $n$ ,  $a$  is the number of pairs of objects placed together in both partitions,  $d$  is the number of pairs placed in different clusters in both partitions. Simply, in the numerator, one counts the pairwise matches of objects that are “good” in the sense of similarity between the two partitions, and this is done with regard to the total number of pairwise matches in the denominator. The adjusted Rand index  $R$  is the preferred index for determining the number of clusters. It is obtained by some additional adjustments, for details see Hubert and Arabie 1985.

Additionally, these measures can be easily determined on the basis of the confusion matrix (pivot table) that is obtained by crossing two partitions. Such a confusion matrix has two key benefits: it simplifies the computation of  $R$  and it is the basis for similarity measures between individual clusters of different partitions (see below). For an introduction in this topic and for further details, see Mucha, 2009. In our example, concerning the regional pollution, soft bootstrapping is applied. At this juncture, a reasonable amount of randomness is added to the original mass  $m_i$  of object (region)  $i$ . The number of clusters (categories) is estimated based on the adjusted Rand index  $R$ . For the decision about the number of clusters, the mean of 250  $R$  values is used (see Figure 6). Other well-known indices measure the similarity between two sets (clusters)  $E$  and  $F$  such as the Jaccard index  $\gamma(E,F) = |E \cap F| / |E \cup F|$  and the Dice index  $\tau(E,F) = 2|E \cap F| / (|E| + |F|)$ . The two indices evaluate the stability of individual clusters. By repeating resampling techniques many times, one gets many values of similarity by comparing the original clustering with many bootstrap clusterings (Figure 6).

**Figure 6:** Mean and standard deviation of the adjusted Rand index  $R$  versus the number of clusters  $K$ . Herein, for reasons of comparison the standard deviation is multiplied by 4. It decreases strongly between four and five clusters. The final decision for  $K=5$  clusters is motivated by both the maximum mean value and the minimum standard deviation (and its strong decrease) that are obtained from 250  $R$  values resulting from 250 bootstrap clusterings.

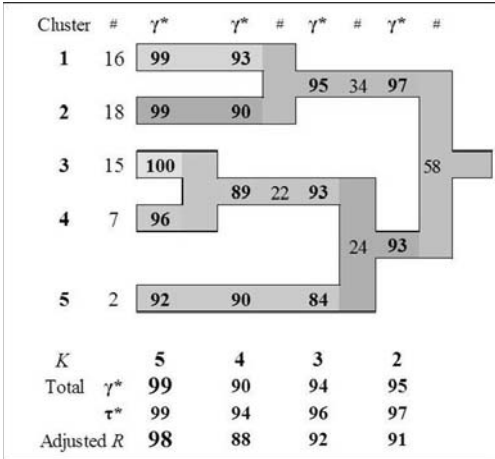


The main results of the bootstrap validation are shown as an “informative dendrogram” (Figure 7). Usually, a dendrogram summarizes graphically a hierarchical clustering (as shown in Figure 3). However, additional information is presented in an

informative dendrogram about the stability of the clusters, and the number of regions of the clusters (shown below the symbol #). The averaged Jaccard measure  $\gamma^*$  is the mean value of 250 Jaccard values  $\gamma$ . It is used to evaluate the stability of every cluster. It is difficult to determine an appropriate threshold by which a cluster is considered stable. Let us look at the partition into five clusters in Figure 7. Here cluster 3 (comprising 15 regions) is the most stable cluster, and has reached the highest level ( $=0.9961$ ) near the maximum Jaccard

value of 1 (i.e., 100%). In contrast, cluster 5 (comprising only two regions) is the least stable cluster. It has a Jaccard measure  $\gamma^*$  of only 0.9173 (i.e., approximately 92%).

**Figure 7:** An “informative dendrogram” that contains the results of validation of stability for each cluster (the tree at the top with Jaccard index in bold) and for the whole clustering (partition) into 2, 3, 4, and 5 clusters. At the bottom, the values of Jaccard and Dice are



pooled values of the corresponding estimates of the clusters above. All these values and the adjusted Rand index  $R$  are in %. Below the symbol # the number of regions in each cluster is indicated. For example: Going from right to left, the 58 MsPb values are divided in two clusters of 34 and 24 objects, respectively.

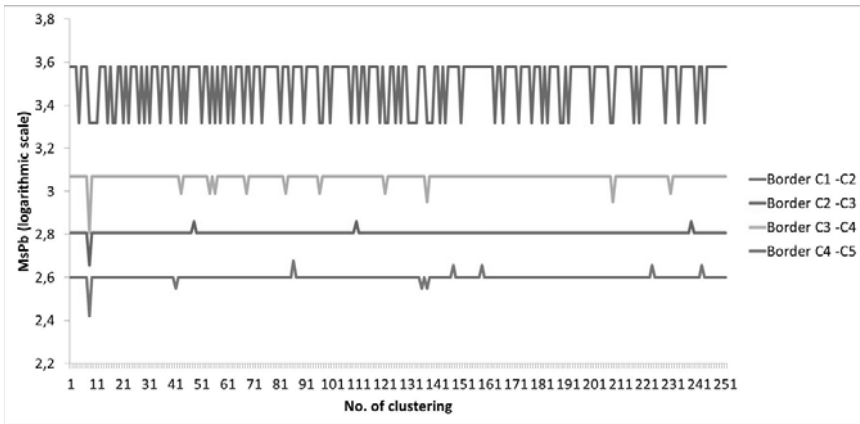
The numerical values at the bottom of Figure 7 can be used for decisions about the number of clusters. For instance, the total Jaccard measure is obtained by

averaging all Jaccard-stability values of individual clusters of a partition. The partition into  $K=5$  clusters is the most stable one because it has a total Jaccard index of 0.99 (i.e., 99%). Therefore, in our example, 5 clusters (categories) are assessed as the most stable result also by all other of the applied indexes. This is also in agreement with the so-called scree-test of the distance levels (see Figure 5). Cluster  $C_1$  becomes value (category) 1, cluster  $C_2$  becomes 2 and so forth. There is automatically a total order in the set of the clusters with  $C_{k-1} < C_k$  because the Ward procedure and the bootstrapping are applied on the single quantitative indicator MsPb.

### ***Borders of the clusters***

The concept “border between two clusters” comes into play when an object  $i$  being member of cluster  $C_1$  could almost equivalently be an element of cluster  $C_2$ . Then object  $i$  crosses the border between  $C_1$  and  $C_2$ . It is clear that here topological argumentation could be established, see Restrepo et al., 2005 and 2006; Restrepo and Mesa, 2011, where boundaries and inner elements of a cluster are rigorously defined. Beyond this the similarity of tree-graphs is an important concept to deepen the concept of “borders of

clusters”, see Restrepo et al., 2007. These theoretical investigations based on topological concepts will be of high interest in the future. Here, the border between two clusters (intervals)  $C_{k-1}$  and  $C_k$  is simply defined as the mean of the maximum value of  $C_{k-1}$  and the minimum value of  $C_k$ , and we can investigate the stability of the borders themselves based on bootstrap simulations (Figure 8).



**Figure 8:** Variation of the borders of several bootstrap clusterings into  $K=5$  clusters.

Figure 8 visualizes the variability of the borders between the neighboring clusters for all 251 clusterings into 5 clusters. The border between  $C_2$  and  $C_3$  is the most stable one: it is shifted only four times out of 250 runs. However, not in all cases such a stable result can be obtained: Consider the border between cluster  $C_4$  and  $C_5$ . Evidently it switches between two extrema. The reason is that  $C_5$  has only a small size (see Figure 3 at the right hand side: The cluster consisting of the two regions 33 and 56, respectively). Obviously, these two regions seem to be outliers of the indicator MsPb, see Table 1. The uncertainty with respect to the border of  $C_4$ - $C_5$  can be boiled down to the question, should region 56 get the ordinal value of 4 (standard) or 5 concerning the indicator MsPb.



**Result of the preprocessing by cluster analysis**

Table 2 contains the within-cluster averages of the data preprocessing step performed for all 7 indicators of the multi-indicator system. For this purpose, each of the original quantitative variables is transformed into an ordinal variable by applying univariate cluster analysis including validation by bootstrapping (as described above in detail for the indicator MsPb).

**Table 2:** Within-cluster averages

Class	MsPb	MsCd	MsZn	KsPb	KsCd	KsZn	KsS
1	10.92	0.24	28.6	0.12	0.04	20.0	520.0
2	13.84	0.30	45.1	0.74	0.1	27.0	1 600.0
3	17.71	0.35	58.3	1.06	0.13	34.0	1 769.0
4	23.56	0.42	78.4	1.54	0.18	40.0	2 030.0
5	45.60	0.50	110.0	2.15	0.24	822.0	4030
6		0.62	138.5		0.43	1 160.0	
<b>Total</b>	<b>16.30</b>	<b>0.38</b>	<b>58.2</b>	<b>0.92</b>	<b>0.13</b>	<b>119.0</b>	<b>1 812.0</b>

As a byproduct of the simulations, the univariate assessment of the importance of variables can be figured out: It is based on how likely it is that the underlying distribution is heterogeneous with several different populations. The univariate cluster analysis delivers a decomposition of the indicators due to the heterogeneity of their variances. The more modes in its density an indicator has the more important it is. So, an additional result of clustering can be the estimates of weights of indicators (this can be the subject to future investigations, see also section 5 of this paper).

## 4 Final Results

### 4.1 Summarizing Ward’s cluster method

After applying the statistical methods explained in section 3.3, the clusters and their borders are derived. In performing the cluster analysis, the separation in modes for some indicators is best visualized when an order preserving transformation is performed. Such

an order-preserving transformation,  $f$ , is a transformation of the indicators, such that in terms of the original attributes for any two objects  $a < b$  we find  $f(a) < f(b)$ . The indicators are now as follows (Table 3).

**Table 3:** Summarizing the preprocessing steps to obtain the final indicators  
 Second column: transformation of the original data, third column: The results of cluster analysis

Indicator	Trans-formation	Number of discrete values	Interpretation
MsPb	log	5	Pb in epiphytic mosses
MsCd	–	6	Cd in epiphytic mosses
MsZn	–	6	Zn in epiphytic mosses
KsPb	–	5	Pb in herb layer
KsCd	–	6	Cd in herb layer
KsZn	log	6	Zn in herb layer
KsS	–	6	S in herb layer

## 4.2 Analysis by partial order concepts

Three aspects are now considered: (i) comparison of the preprocessing versus original data matrix, (ii) discussing the results of the partial order concept in terms of evaluation of the polluted regions, and (iii) uncertainty of assigning the value 4 or 5 of MsPb for region 57.

### *(i) Comparison of the preprocessed data matrix versus the original data matrix*

The objective is to describe the pollution of the different Baden-Wuerttemberg regions, and to visualize this by a Hasse diagram, based on eq. (1). Therefore the effect of preprocessing must be measured by partial order theory concepts. In Table 4 we compare the number of possible comparisons (i.e. how many pairs  $x < y$  can be found), the number of incomparable pairs (i.e. how many pairs  $x \parallel y$  can be found), and the maximal length of the chains (length of maximum chain) in each partially ordered set. As each comparison allows a decision about the status of the two regions, the tripling of the number of comparisons brought about by a using a preprocessed data matrix, shows the great value of this approach for evaluation purposes.

**Table 4:** Comparison of the preprocessed and the original data matrix according to partial order theory

Method for the data matrix	Number of comparisons	Number of incomparable pairs	Length of the maximum chain
original	125	1,528	3
preprocessed	324	1,329	7

As equivalences do not appear, an increase in the number of comparisons is accompanied by a decrease of the number of incomparable pairs. The high number of incomparable pairs (in comparison to the number of comparable pairs) indicates, how frequently an averaging process to get a scalar ranking index would be crucial for a possible compensation. The preprocessing reduces those incomparabilities arising from small numerical data differences. The marked increase in the maximum length of a chain after pre-processing of the data shows that now a ranking at maximum among 6 regions is possible, (in comparison to among only three regions with the original data matrix).

**(ii) The Hasse diagram of the preprocessed data matrix is shown in Figure 9.**

*Maximal, minimal elements, chains:*

The items of particular interest in the Hasse diagram (Figure 9) are:

- 17 maximal elements (representing the regions with the worst pattern of pollution). They can be found in Figure 9 as those elements, which have no upper neighbor.
- 10 minimal elements (4, 6, 9, 12, 13, 21, 26, 27, 28, 29, 27,) which are regions of least pollution and which can be found from Figure 9 as those elements which have now lower neighbor. See for example region 6. From this element there are no lines to lower neighbors.
- Two chains as example:  
 chain no: 10 (start: 26, endpoint: 57) count of elements: 6: 26, 15, 30, 59, 20, 57,  
 chain no: 2 (start: 26, endpoint 48) count of elements: 6: 26, 15, 30, 46, 25, 48,
- Following the lines upwards one may end at different regions. Starting from region 26 (which is one of the minimal elements), one will stop once for example in region

57, and once in e.g. region 48. Evidently, the values of all of the 7 indicators do not decrease. However, the values of the 7 indicators change in different pollution profiles: In case of region 57, the main increase in pollution is due to MsPb (75% of the total possible range), MsCd (80%), whereas for region 48 which is the endpoint of another chain (also starting from region 26,) the main increase is due to MsPb(75%) , MsCd(100%) , KsPb(75%), KsCd(100%).

*Sensitivity:*

The impact of each attribute, i.e. of KsPb, KsCd,..., MsZn on the structure of the poset is

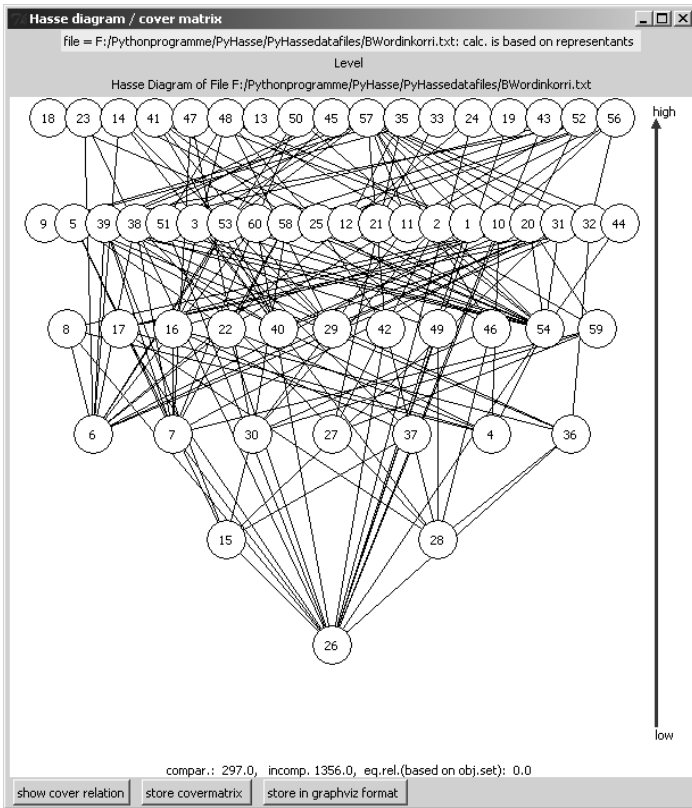
$$\text{MsPb} < \text{MsZn} = \text{KsPb} < \text{KsCd} < \text{MsCd} < \text{KsS} < \text{KsZn}$$

(For details, see Bruggemann et al., 2001, Voigt et al, 2011.)

Within the three most important attributes the herb layer appears two times and the target epiphytic mosses once. Hence the time and cost intensive monitoring of both, herb layer and epiphytic mosses seems to be justified. The chemical element Pb either found in epiphytic mosses, MsPb, or in the herb layer Ks does not have much impact on the poset. The chemical element Zn in the herb layer is striking as it has a high influence on the structure of the partial order, based on the 7 attributes. Elimination of this column (KsZn) from the data matrix leads to a poset which has only 10 maximal elements. Elimination of the first attribute (MsPb) from the data matrix leads to a poset with the same number of maximal elements, 17, i.e. has obviously less influence on the structure of the poset.

*Antichain:*

The 17 maximal objects in Figure 9 form an antichain, we call this set simply MAX. The pairs of attributes which imply the incomparability between any two regions of MAX can be counted, for details see Bruggemann and Voigt, 2012. For example the pair MsPb, MsZn implies rarely an incomparability among the elements of MAX, whereas MsZn, KsCd imply in almost 50% of all incomparable pairs made of elements of MAX an incomparability. In Table 5 the relative contribution, “density”, of each possible attribute pair is shown. A density of 1 means that the corresponding attribute pair leads to an incomparability among all possible pairs, made of elements of MAX.



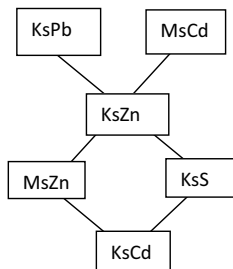
**Figure 9:** Hasse diagram of the 58 regions in Baden-Wuerttemberg, characterized by 7 indicators of pollution, after preprocessing. PyHasse software (free available from the first author) was used in constructing this Hasse diagram. The regions are located in six horizontal levels according to an increasing pollution from the bottom to the top

**Table 5:** Density of attribute pairs, such as ['MsPb', 'MsCd'] based on the 136 possible pairs of regions, taken from MAX

Attribute pair	density	Attribute pair	density
['MsPb', 'MsCd']	0.22	['MsZn', 'KsPb']	0.26
['MsPb', 'MsZn']	0.15	['MsZn', 'KsCd']	0.49
['MsPb', 'KsPb']	0.25	['MsZn', 'KsZn']	0.45
['MsPb', 'KsCd']	0.32	['MsZn', 'KsS']	0.35

['MsPb', 'KsZn']	0.3	['KsPb', 'KsCd']	0.34
['MsPb', 'KsS']	0.46	['KsPb', 'KsZn']	0.48
['MsCd', 'MsZn']	0.34	['KsPb', 'KsS']	0.38
['MsCd', 'KsPb']	0.34	['KsCd', 'KsZn']	0.28
['MsCd', 'KsCd']	0.27	['KsCd', 'KsS']	0.43
['MsCd', 'KsZn']	0.4	['KsZn', 'KsS']	0.45
['MsCd', 'KsS']	0.47		

A graph can be obtained, with the attributes as vertices and edges if the two elements of a pair have densities  $\geq$  limit (here we arbitrarily select 0.4 as limit), Figure 10.



**Figure 10:** Which attribute pairs are mainly responsible for the incomparabilities among the 136 pairs of regions, taken from MAX.

In the graph (Figure 10) MsZn and KsCd are connected by an edge, because these two attributes have the density 0.49 and lead to conflicts in almost 50% of all 136 pairs of regions, taken from MAX (Table 4). There is no connection between MsZn and KsS, because the density is only 0.35. From the six edges, corresponding to densities  $\geq$  0.4 three edges refer to attributes with different targets (herb layer and epiphytic mosses) (one of them with the same chemical element, Zn) and three edges appear, where the incomparability is not induced by concentrations in different targets but only by concentrations of different elements in the same target, i.e. in the herb layer.

*(iii) Effect of data uncertainty for region 57 due to the pollution parameter MsPb*

In terms of partial order theory, an object is characterized by (i) its position, (ii) the regions to which it is order-theoretically adjacent, and (iii) the number of incomparabilities it has. When considering all these properties, there are no differences whether or not the attribute MsPb is assigned a value of 4 or 5. Hence the assignment within the cluster analysis for this single uncertain case has no consequence in partial order theory.

## **5 Summary and Discussion**

More and more multi-indicator systems are used, due to the complexity of the phenomena to be ranked and it is good policy for the sake of transparency to keep the valuable information inherent in each indicator separated. The HDT is the technique by which this can be achieved (see Bruggemann, Carlsen, 2012).

We have shown how a partially ordered set can be analyzed, where the Hasse diagram is an important tool. The identification of chains may be considered as the most important question. In practical applications, the appearance of incomparabilities is considered as uncomfortable, even as a reason not to apply partial order methods. Although nowadays many methods are available to deal with antichains, any further research is welcomed. We have only shown an example, how the list of maximal elements can be further studied; a systematic procedure is far beyond the focus of this paper. The obvious next question is, which attribute pair is specifically contributing to a selected pair of regions. One possible method would be to analyse tripartite graphs, as shown in Bruggemann and Voigt, 2011.

One of the main problems in HDT is the notion of “relevant” numerical differences among the data. The preprocessing based on univariate Ward’s cluster analysis is a promising approach. An alternative already published is fuzzy partial order (Annoni et al., 2008, De Loof et al, 2012, Bruggemann et al., 2012), however beside some technical questions the problem appears to be how to defuzzify, and which membership-value should be used to get crisp results? Therefore we recommend using univariate clustering as a preprocessing step, despite the disadvantage that the procedure is not yet integrated in the PyHasse software.

There is considerable scientific, statistical interest in the impact of attributes, and the realized values within an object set, on the structure of the partial order and hence on the ranking. Recently Annoni et al., 2011 presented a new approach. There is a technique to

get *a priori* information about the influence of attributes in the univariate cluster analysis; as more modes in the univariate density are taken into regard, the more differentiating will be the discretized attribute, and the greater the probability to induce incomparabilities. The interplay of the number of modes taken from the univariate cluster analysis, and the resulting sensitivity of a partial order with respect to attributes, is an important task for future work.

Finally we draw the readers attention to the fact that partial order theory is able to provide a ranking of all objects (i.e. not only those in chains), without finding, for example, the weights of the attributes in weighted sums by means of some deeper theoretical considerations (see for instance Winkler, 1982 and an interesting application by Carlsen et al., 2002, Carlsen 2008). The immediate application of Winkler's concept of averaged ranks is computationally extremely hard, as the complexity of the needed calculation goes with  $|\mathcal{X}|!$ . Even if the elegant lattice theoretical approach (see De Loof et al., 2006, 2008) is applied, the number of objects should not exceed 50 (see Bruggemann and Carlsen, 2011). Developments may include a) sampling techniques (see Bublely and Dyer, 1999, Lerche et al., 2003, Sørensen and Lerche, 2002., and b) approximations (see Bruggemann et al., 2004, 2005 and Bruggemann and Carlsen, 2011). A new approach for deriving rankings is based on the concept of probability of  $x > y$  or  $x < y$  (concept of mutual ranking probability, see Bruggemann and Voigt, 2006) given  $x \parallel y$  (De Loof et al., 2011).

Even if composite indicators are constructed the ranking due to partial order may be useful for comparisons and to identify where weights play a crucial role (see for instance Bruggemann et al., 2008). So, the theory of partial order in its variant as HDT may become a valuable instrument in all those cases where ranking is of interest and where multi-indicator systems are needed to deal with the inherent complexity of the objects to be ranked. Especially environmental pollution is highly complex as not only different chemicals are to be considered also different targets.

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