Applying the Concept of Partially Ordered Sets on the Ranking of Near-Shore Sediments by a Battery of Tests

Rainer Brüggemann,*,† Efraim Halfon,‡ Gerhard Welzl,§ Kristina Voigt,§ and Christian E. W. Steinberg†

Institute of Freshwater Ecology and Inland Fisheries, Müggelseedamm 310, D-12587 Berlin, Germany, Biology Department, McMaster University, Hamilton, Ontario, Canada, and GSF - National Research Center for Environment and Health, Institute for Biomathematics and Biometry, D-85764 Neuherberg, Germany

Received June 5, 2000

When a ranking of some objects (chemicals, geographical sites, river sections, etc.) by a multicriteria analysis is of concern, then it is often difficult to find a common scale among the criteria, and therefore even the simple sorting process is performed by applying additional constraints, just to get a ranking index. However such additional constraints, often arising from normative considerations, are controversially discussed. The theory of partially ordered sets and its graphical representation (Hasse diagrams) does not need such additional information just to sort the objects. Here, the approach of using partially ordered sets is described by applying it to a battery of tests, developed by Dutka et al. In our analysis we found the following: (1) The dimension analysis of partially ordered sets suggests that, at least in the case of the 55 analyzed samples and the evaluation by the scores, developed by Dutka et al., there is a considerable redundancy with respect to ranking. The visualization of the sediment sites can be performed within a two-dimensional grid. (2) Information, obtained from the structure of the Hasse diagram: For example six classes of sediment sites have high priority, and each class exhibits a different pattern of results. (3) Loss of information, when an aggregation of test results is used in order to guarantee complete comparability among all objects. A relation between information drawn from the graphic and the uncertainty of ranking after using an aggregation is given. (4) The sensitivity analysis identifies one test as most important, namely the test for Fecal Coliforms/ *Escherichia coli*. This means that the ranking of samples is heavily influenced by the results of this specific test.

1. INTRODUCTION

Hasse diagrams have been used to rank chemicals according to environmental hazards (see ref 2 for a recent review). At the basis of the Hasse diagram technique (HDT) is the assumption that we can perform a ranking while avoiding the use of an ordering index. Hasse diagrams not only present information on the ranking but, most important, also show whether the criteria, characterizing the objects, lead to ambiguities in the ranking. For example, an object might be ranked higher according to one criterion but lower according to another. These two objects are not ordered because their data are "contradictory". This ambiguity is hidden when we use an index for ranking, i.e., if we aggregate the results of the battery of tests to only one quantity (an index function) but is immediately evident by the presence or absence of lines in a Hasse diagram. [Sometimes we also write "test battery" or simply "battery".] Therefore, the HDT is very appropriate for a comparative evaluation of polluted or degraded sites, when a multicriterial assessment by a battery of tests is in mind. In this paper however, the ecotoxicological test battery and its results are not of primary concern (a detailed discussion can be found in refs 1 and 3), but we investigate new methods to extract further information from Hasse diagrams. These are as follows: (1) the dimension of Hasse diagrams with respect to visualization of the ranking results. (2) Sets of samples, with specific test reactions, i.e., (2a) priority sites and (2b) sites, having a specific pattern of test results in common. We call this kind of result from Hasse diagrams "structural information". (3) The loss of information, which appears, when an aggregation of test results is used, and (4) the so-called matrix **W**, that quantifies the influence of criteria on ranking (sensitivity analysis).

* Corresponding author phone: +49 (30) 64181-665 or 662; e-mail: Brg@IGB-Berlin.de.

† Institute of Freshwater Ecology and Inland Fisheries.

‡ McMaster University

§ GSF - National Research Center for Environment and Health, Institute for Biomathematics and Biometry.

2. METHODS

The so-called Hasse diagram technique is explained in several publications (see for example ref 3). For the sake of convenience of the reader we briefly repeat some facts.

Criteria include both quantitative and qualitative properties.

An *attribute* is a numerical quantity logically related to a criterion. We denote these attributes as q_1, q_2, ..., q_n. It is convenient to denote the full attribute set as A. A **family** of $L := 2^n - 1$ attribute sets is considered in our analysis, namely the **power set** of A without the empty set. Each subset of attributes is denoted by A_i, with $A_i \subseteq A$, and is used to perform a sensitivity analysis (see later).

10.1021/ci000055k CCC: $20.00
Published on Web 05/15/2001

The concept "*tuple*" generalizes from the following: pair of data, triple of data. We avoid the concept "vector", because the properties of a linear space are not needed.

Data are the numerical values corresponding to each criterion by which a given object is characterized.

An *object* is the item of interest. Each object, x, is characterized by a tuple of data ($q(x) = (q_1(x), q_2(x),..., q_n(x))$). The set of *m* objects is called *E*. We also write the following: an object x is an *element* of a set. Objects are ranked graphically by Hasse diagrams, applying an order relation (see below). The cardinality operator "card" acts on finite sets, and the result is the number of elements of sets. For example, when the object set *E* contains *m* objects, then card $E = m$.

Order relation: Two objects $x,y \in E$ are characterized by the tuples $(q_1(x), q_2(x),...,q_n(x)$ and $(q_1(y),q_2(y),...,q_n(y))$. We say x and y are *comparable*, if $q_i(x) \leq q_i(y)$ or $q_i(y) \leq q_i(x)$, for all $i = 1,2,..,n$. If $q_i(x) \leq q_i(y)$ for **all** i, then we write $x \leq y$. If $q_i(x) \leq q_i(y)$ **not** for all i, i.e., if there exists at least one i* with $q_{i*}(x) > q_{i*}(y)$ and one i** with $q_{i**}(x) < q_{i**}(y)$, then the two objects x,y are *incomparable* (with respect to the considered set of attributes). In that case we write $x \,||\, y$. The demand "for all" to set up an order relation we call the *generality principle*. Sets equipped with an order relation are called *p*artially *o*rdered *sets* (posets). A *total order* is a set, whose order relation leads to complete comparability, i.e., each object is comparable with each other.

Equivalent objects in Hasse diagrams:[4,5] Different objects that have the same data with respect to a given set of attributes. They are elements of an equivalence class with the equivalence relation, R, "equality of the characterizing tuples". Often it is useful to study the partially ordered set of equivalence classes (E/R, the "quotient set" under R) instead of *E* and to select one object as a *representative* of its equivalence class.

A *case* is a shorthand notation for an analysis by Hasse diagrams of *m* objects and with a defined attribute set A_i. Thus, we call a given set of attributes used for a comparative evaluation an *information basis*, (abbreviation: *IB*), to express the importance of the selection of the attributes for rankings: By the order relation the set *IB* induces a poset and a Hasse diagram, respectively, as its visualization. Therefore we write specifically (*E*,*IB*). Sometimes we also write (*E*,*A*) or (E,A_i) if specific attribute combinations must be indicated.

An *aggregation* is a method to assign to a vectorial quantity a scalar: The tuple $(q_1,q_2,..,q_n) \in IR^n$ (n-dimensional space of attributes) is mapped onto a scalar $\Gamma \in IR$ (a one-dimensional space). In evaluation studies this map often is realized by weighted sums, i.e.

$$\Gamma = \Sigma g_i * q_i \; (i=1,...,n), \quad g_i \geq 0: \text{weights} \qquad (1)$$

Generally an aggregation may be formulated as a monotonic, differentiable function f of $q_1,q_2,..,q_n$.

Transitivity: Order relations have to fulfill certain mathematical axioms. One of them is the transitivity. Transitivity expresses that for $a,b,c \in E/R$ the relation $a \leq b$, $b \leq c$ implies $a \leq c$.

Hasse diagrams visualize the order relations of posets in the plane. Lines due to transitivity are omitted. Hasse diagrams are oriented acyclic graphs (digraphs); instead of drawing arrows, indicating that object a is "greater" than object b, the object a is located above b in the plane. As ordinary graphs Hasse diagrams are triangle free. A digraph consists of a set E/R of objects (exactly: classes) drawn as small circles or small rectangles. A line in the Hasse diagram indicates that the two objects connected by that line are "comparable" with each other.

Crossing of lines: When a Hasse diagram is drawn in the plane and straight lines connecting comparable objects cross another although there is no element of the poset at intersection point, a crossing of lines still appears. Note that some experience is needed to minimize the number of such crossings. In general cases not all crossings can be avoided.

Maximal elements, "max" $\in E/R$: There is no $x \in E/R$ with $x \geq$ max.

Minimal elements, "min" $\in E/R$: There is no $x \in E/R$ with $x \leq$ min.

Isolated elements, "iso" $\in E/R$: elements which are maximal and minimal elements at the same time.

If there is only one maximal/minimal element, then this is called *greatest/least* element.

Key elements: Substructures within a Hasse diagram, i.e., relations among objects as well as the importance of criteria in ranking are investigated with the help of key elements. Any object of the poset (*E*,*IB*) can be chosen as a starting point to begin the analysis and is then called a "key element". For convenience, all chosen key elements form a set *K*, a subset of *E*. Note that for this kind of analysis we refer to *E* not to E/R. The reason is that we aim to study the effect of different attributes. When different cases are examined, then different quotient sets would arise. We want to avoid cumbersome notations.

The *successor set* of a key element $k \in E$ is the set of *all* objects $y \in E$ for which $y \neq k$ and $y \leq k$. The set of all successors of key element k is denoted as $G(k)$. [Note the similar concept of "down-sets" and order ideals generated by some elements in ref 6). We also write "$G(k)$ is *generated* by object k." $G(k) \cup \{k\}$ is a principal order ideal.] The properties of the successor set $G(k)$ and its relation with successor sets of other key elements are first used to analyze the structure of a Hasse diagram, but later they will be used to perform the sensitivity analysis.

Relations between elements of posets: To investigate the global structure of the relations between any two elements of the posets, we perform this analysis mathematically. This structural relation might be hidden within the geometrical representation of the Hasse diagram. Often one is interested in the number of objects which have common properties compared to two key elements. Therefore, we introduce the symmetrical matrix **D**, whose entries are calculated from the cardinalities of all intersections of pairs of successor sets.

$$D_{ij} := \text{card}\,[G(i) \cap G(j)] \quad i,j \in E \qquad (2)$$

[A generalization may be $D(K) := \text{card}\,[\cap G(k)]$, $k \in K$; however, for practical purposes the binary relation (eq 2) seems to be sufficient.] The values of D_{ij} (note that a crude upper bound is card $E - 1$ and card $E/R - 1$, respectively) are mostly useful to identify two objects which have either

Table 1. Scores of Five Test Battery Results for Representatives of the Equivalence Classes of E/R

identifier	FC	CP	CH	MT	GT
1	2	0	0	4	0
2	1	0	0	2	0
3	2	0	0	2	0
4	3	0	0	0	0
5	3	3	2	0	0
7	2	0	0	8	0
9	1	0	0	6	2
11	1	0	0	0	0
12	3	0	0	2	0
14	1	0	0	8	0
17	3	0	0	6	0
18	1	0	0	2	4
23	1	0	0	0	4
25	4	0	0	0	0
27	5	0	0	0	0
31	4	5	4	0	0
32	3	0	0	8	0
91	2	0	0	0	0
92	3	0	0	4	0
95	3	5	2	6	0

many common or only very few common successors. Another and more useful concept is that of the number of "local" contradictions of a class $x \in E/R$: U(x), which is the number of classes $y \in E/R$, with $y \neq x$, y||x:

$$U(x) = [\text{card } E'(x)] \text{ with } E'(x) = \{y \in E/R:\ y \neq x, y||x\} \quad (3)$$

Note that U(x) has an upper bound, namely card E/R -1.

3. RESULTS

3.1. Sediment Samples of Lake Ontario as Object Set and the Tests of the Battery as Information Base. A battery of tests developed by Dutka et al.[1] to test the sediments of near-shore sites of Lake Ontario (Canadian part) is used to exemplify the definitions and some results of HDT. In Lake Ontario 55 sediment samples were tested, thus, the set E contains 55 objects. Dutka et al. classified their results and used discrete scores instead of the measured (raw) data. For our analysis we took their classification. Therefore, instead of the symbol q_i for the ith attribute we use s_i for the score of the ith test of the battery. Five tests are combined to form a battery: (1) Fecal Coliforms "FC", [FC is an indicator designed to control the health state of the sediments.]. (2) Coprostanol "CP", (3) Cholesterol "CH" [CP and CH are indicators of loadings by fecals], (4) Microtox tests "MT", and (5) Genotoxicity tests "GT" [MT and GT describe some kind of acute toxicity and the potential for cancerogenicity, respectively (Table 1).].

By scoring the data many equivalence classes (in fact 20) arise. It is convenient to refer only to these classes by specifying a representative for each class, i.e., besides the sensitivity study we apply the concept of quotient sets. With the specific equivalence relation R_5 meaning equality in all **five** scores s_{FC}, s_{CP}, s_{CH}, s_{MT}, and s_{GT}, the following sediment samples are equivalent (Table 2), and the quotient set is denoted as E/R_5.

The information base of the battery of tests is $IB := \{s_{FC}, s_{CP}, s_{CH}, s_{MT}, s_{GT}\}$. The partial ordering of the samples arises as explained in section 2. The visualization of the partial order by a Hasse diagram is shown in Figure 1.

3.2. Dimension Analysis (Task 1). Posets can be characterized by several numbers. One of these is the dimension of a poset, **dim (E/R,*IB*)** which is the minimum number of total orders needed to represent the original poset. Instead of explaining, what "represent" means, another more restricted definition is given, which is operationally tractable: If a Hasse diagram (eventually fictitiously supplied by a greatest and least element) can be drawn in the plane without any crossings of lines, then it can be embedded into a two-dimensional grid[8] and then dim(E/R, *IB*) = 2. Once the dimension d of a poset is found with d < card *IB*, then corresponding many new latent ordering variables l_1, l_2,..., l_d can be used to form the same Hasse diagrams as found by the original attributes. I.e. the same ranking must be possible by a *lower* number of latent ordering variables and a redundancy within the battery of original attributes is possible. However, the numerical relation between the original attributes and the latent ordering variables may be very difficult to be found and, if, then hard to interpret (as is often the case in principle component analysis too).

Here, the poset (E/R, $\{s_{FC}, s_{CP}, s_{CH}, s_{MT}, s_{GT}\}$) could be drawn without any crossings of lines; therefore, the dimension of this poset is two (see Figure 1). Correspondingly, the poset (E/R_5,*IB*) can also be visualized by a two-dimensional grid as is shown in Figure 2.

Both visualizations have their own advantages:

Structures within a Hasse diagram, for example successor sets or sets of samples separated from others by incomparabilities, can be more easily discovered by a representation like that of Figure 1.

In multivariate statistics the reduction of data is typically performed by principal components analysis or by multidimensional scaling. These methods preserve the distance between objects optimally. When order relations are the essential aspect to be preserved in the data analysis, the optimal result is a visualization of the sediment sites within a two-dimensional grid.

Some further remarks with respect to the representation within a two-dimensional grid should be given:

- Some scores of the test battery are additionally shown. From them the values of the scores of other objects can be estimated or exactly calculated. For example, for class 17, FC must have the value 3, because the lower object 92 and the higher object 95 have $s_{FC} = 3$. The value of CP must be 0 because $s_{CP}(32) = 0$, which is the lowest value. Similarly $s_{CH}(17) = 0$ and $s_{GT}(17) = 0$, whereas for $s_{MT}(17)$ only the interval $4 \leq s_{MT}(17) \leq 8$ can be predicted from the knowledge of the neighbors in the Hasse diagram.
- Most important: The grid can be thought of as being a coordinate system, with one axis of a latent order variable l_1 and another by l_2, according to dim(E/R_5,*IB*) = 2. By these two latent ordering variables, each class $\in E/R_5$ can be characterized by a pair, which represents correctly the order relations (important for ranking) but which is clearly not unique with respect to a numerical representation. Table 3 gives some examples.
- The interpretation of the latent variables l_1 and l_2 is supported by checking the configurations within the two-dimensional grid in terms of its a priori content (variables FC, CP, CH, MT, GT). A clear correlation can be detected between FC and the latent variable l_1 and also between GT

Table 2. Equivalence Classes and Their Battery of Tests Pattern[a]

equivalence class	FC	CP	CH	MT	GT	remark
{**2**,8}	1	0	0	2	0	
{**4**,6,10,13,19,21,22,29,30,48,94}	3	0	0	0	0	
{**11**,16,40,41,42,43,44,45}	1	0	0	0	0	the best class (i.e.: the least element)
{15,**92**}	3	0	0	4	0	
{**17**,35}	3	0	0	6	0	
{20,24,26,28,34,37,39,49,50,51,**91**,93}	2	0	0	0	0	
{**23**,60}	1	0	0	0	4	
{**27**,33,46,47}	5	0	0	0	0	one of the priority classes

[a] Number of sites in bold letters are later used as representatives for the whole equivalence class.

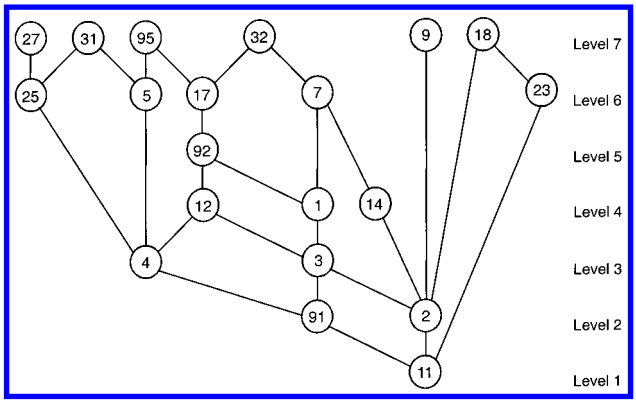

Figure 1. The comparative evaluation of samples from Lake Ontario, as generated by the EDP-program WHASSE. Note, that the quotient set and representatives (i.e. objects belonging to an equivalence class and representing all others of that class) are shown. The partitioning of E/R_5 into subsets, horizontal arranged, the level, is useful for referring to the Hasse diagram and therefore included, albeit we actually do not use them.

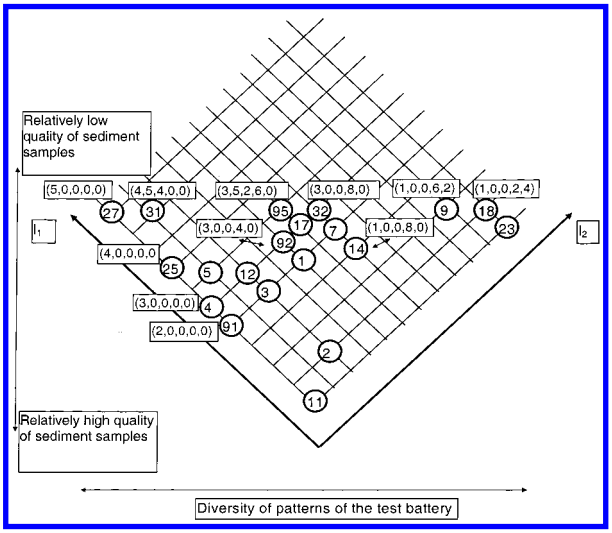

Figure 2. Visualization of the ranking result of the sediment samples of Lake Ontario after dimension analysis.

and the latent variable l_2. Sometimes these variables FC and GT with primary meaning are called *polar* items. The other variables accentuate the possibility of discrimination in a nonlinear manner. Therefore, in a qualitative sense, the ranking of the sediment sites of the Lake Ontario seems to be mainly determined by a hygienic and an ecotoxicological component.

- Some objects could be embedded into the grid in alternative ways. However, the order theoretical information, namely the comparabilities and incomparabilities are maintained. (This can be easily proved by verifying that the Hasse diagram induced by five attributes is isomorphic to that, induced by the two latent variables.)

Table 3. Order Theoretical Classification of Representatives Found in Figure 2

representative	l_1	l_2	remark
11	0	0	least element
91	4	0	
3	4	2	
17	5	5	
9	2	10	maximal element

- In principle, a representation in a two-dimensional plane can also be found applying statistical software, especially the module POSAC (Partially Ordered Scalogram Analysis with Coordinates, SYSTAT 9).[7] If the dimension of a poset is two, POSAC may find a two-dimensional representation with the same partial ordering structure as the original data. In general POSAC finds the optimal solution in terms of the "coefficient of correct representation". This parameter specifies the proportion of pairs, whose comparability and incomparability relations are correctly represented. A new version of POSAC allows processing in higher dimensions, but an exact embedding in order theoretical dimension analysis seems to be difficult.

3.2. Structural Information (Task 2). (a) Priority elements are the maximal and isolated elements, which can be easily found by inspection of Figure 1. We find six equivalence classes of samples of high priority. The representatives are as follows: sample 27, 31, 95, 32, 9, 18. Each of these maximal elements represents a class corresponding to R_5. For example the object 27 represents the class {27, 33, 46, 47}. For the other nontrivial classes see Table 2.

The object 27 is worse than site 25, and site 25 is worse than site 4. These statements can be repeated until the relatively best sample, 11, is reached. Sample 31 is also considered as a priority element; however, there are other reasons as for example for sample 27. Here the first three tests indicate a high activity. If we had a common scale for FC and for the other two tests CP and CH, then sample 27 might be not as hazardous considered as sample 31. However the difference of 1 point (in the score of 27 in comparison to that of 31) *may* represent a critical status.

(b) Some successor sets of maximal elements are of specific interest, namely those which have zeros within their tuple. Because of the generality principle all successors have to have at least the same zeros. Therefore subsets of E/R can be found, which can be characterized by *templates*: A tuple of some key element "k" is written as a combination of the signs "*" and "0". The sign "0" indicates that the lowest and the sign "*" that any other value of a test is

Table 4. Partitioning of the Set of Samples

name of the subset	representatives of the subset	common template	generating key elements	no. of "0's" [a]
FC	4,11,25,27,91	(*,0,0,0,0)	27	4
FC_MT	1,2,3,7,12,14,17,32,92	(*,0,0,*,0)	32	3
FC_MT_GT	9,18,23	(*,0,0,*,*)[b])	9, 18	2
FC_CH_CP	5,31	(*,*,*,0,0)[b])	31	2
"95"	95	(*,*,*,*,0)	95	1

[a] The number of "0's" defines the order, by which the subsets are formed. [b] The intersection of the two successor sets is contained in that of $G(27)$.

actually present. Then

$$\text{for all } x \in G(k) \text{ the number of "0's" of their templates can only increase proceeding downward in a Hasse diagram and for all } x \in (G(k) \cap G(k')) \text{ all "0" of k and k', respectively, are present in the template of x} \quad (4)$$

The evaluation of eq 4 is very simple, if q_i are discrete variables. With the help of the concepts of templates a partitioning of the set E/R can be performed. Begin with the maximal elements, k. Select that key element which has the largest number of "0's" in its template and gather all successors. Then the key element together with its successors form the first subset. Continue this procedure till the set E/R is exhausted. Some care is needed, when there is more than one key element with the same number of "0's". If the template is the same, then unify the subsets; if this is not the case then (a) if $G(k) \cap G(k') \subseteq G(k^*)$, and the number of zeros in the template of k* is greater than that of k (and by supposition of k'), then the elements of $G(k) \cap G(k') \subseteq E/R$ are already assigned to the class of the pattern of k* and (b) if $G(k) \cap G(k') \not\subset G(k^*)$, then the elements of $G(k) \cap G(k')$ form a new template and consequently a new class of a specific pattern.

By application of eq 4 in the case of our battery of tests we arrive at the following result: First to gain familiarity with the concept of templates we discuss an example: A maximal element with zeros in their scores is to be selected. For example the key element 32 may be considered as represented by the template (*,0,0,*,0). Now all successors of 32 must have at least the same pattern of zeros as object 32. The other tests may have decreased values, including zero. Let us now consider the intersection of G(32) and G(31). Their templates are as follows: (*,0,0,*,0) and (*,*,*,0,0). Then the template for all objects of $G(32) \cap G(31)$ must have the form (*,0,0,0,0). For all common successors of the objects 32 and 31 s_{FC} may have values greater 0, whereas we know that s_i (i = CP,CH,MT,GT) *must* be 0. The representatives of $G(32) \cap G(31)$ are 4, 91, and 11. For these samples we therefore know their templates and thus their qualitative loading pattern without using (lengthy and boring) tables.

By applying eq 4 and the procedure explained above (namely beginning with a maximal element with the largest number of zeros as key element and proceed until E/R_5 is exhausted) a partitioning of the set of samples is suggested (Table 4).

Finally according to Table 4 the set E can be partitioned into

$$E = FC \oplus FC\_MT\_GT \oplus FC\_MT \oplus FC\_CH\_CP \oplus \{\mathbf{95}\}$$

which is considered as a main result of task 2b. (The abbreviations arise from those tests, which are switched on for at least the maximal elements). The symbol $\oplus$ means a union of disjunctive sets.]

3.3. Aggregation Procedure (Task 3). (a) The role of a contradictory pair: Let be $q_1, q_2, ..., q_n$ the n results of the battery containing n tests. Often an overall aggregation is performed by calculating a weighted sum (eq 1). If there is a contradiction between two tested objects, for example, two sediment sites a and b, then $\Gamma(a) > \Gamma(b)$ or $\Gamma(b) \geq \Gamma(a)$ depending on the weights, whereas for comparable pairs of sites from a $\geq$ b always $\Gamma(a) \geq \Gamma(b)$ follows. The advantage of HDT is based on the fact that there is no need to find an aggregation procedure to perform a ranking.

(b) Rankings in dependence of local incomparabilities: Objects with a large local incomparability are very sensitive with respect to the selection of weights in forming an ordering index like eq 1 or with respect to the particular form of the function f.

Let Γ be ordered like $\Gamma(a) < \Gamma(b) <....< \Gamma(x)$, then we say object a has (with respect to Γ) the rank 1, object b the rank 2, etc. The rank of an object x is denoted as Rk(x). Equivalent objects get the same rank. Consider now different tuples of weights, $(g_1,g_2,..,g_n)$, for example, motivated by different environmental protection goals, then the ranks (of a, b, c given by Γ) change in dependence of such tuples. An object x may get its maximum rank Rk_{max} for a specific selection of g_i-values and its minimum rank Rk_{min} for another one. If we define the *var*iability of Rk with respect to the specific selection of an aggregation function by $var(x) := Rk_{max}(x) - Rk_{min}(x)$, then it can be shown by the help of the concept of linear extensions (see ref 8) that

$$var(x) \leq U(x) \quad (5)$$

The inequality 5 demonstrates the loss of qualitative insights into the set of objects, if a battery of tests is used, but an ordering index like that calculated by eq 1 is applied. Furthermore it can be shown by a counterexample that for weighted sums, like eq 1, the equality in eq 5 does not hold.[9]

We apply the considerations above to the ranking of the samples of Lake Ontario:

The sample 9 may serve as an example: sample 9 cannot be compared with many other equivalence classes. For example $D_{9,32}$ (based on the quotient set E/R_5) is only 2, $U(9) = 17$. Indeed for sample 9 note the following pattern: high score for MT and a medium value for GT. This is a singular property, which leads to only few objects comparable with sample 9. Especially the local incomparabilities indicate a high potential for a wrong ranking based on aggregation procedures, like Γ of eq 1, because $var(9) \leq 17$, i.e., the rank of sample 9 may vary almost over the whole range of possible rank values: If there is a consensus, that MT is not as important as the other tests, and its score will get a low weight in eq 1. In consequence the sample 9 would be ranked very low (however still worse than sample 2 and

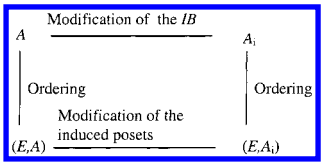

Figure 3. Comparison of attribute sets by studying the corresponding induced posets.

sample 11). If however, MT would have a high weight, then the sample 9 may be located on the top of any total order.

3.4. Sensitivity Analysis of the Ranking (Task 4). The ranking of the objects is sensitive to the set of attributes. To quantify the importance of an attribute on ranking the basic idea is to compare posets obtained by different attribute sets with each other. To compare posets means that an appropriate metric must be found, by which the distance between any two posets can be calculated. There are many possibilities to define distances (see ref 10). The concept of principal successor sets is our starting point. The notation of successor set must be expanded to include all the actual combinations of attributes. Within the generalization of having a family of attribute sets *the successor set depends not only on the key element but also on which attributes are used.* Therefore the following notation $G(k,A)$ or $G(k,A_i)$ is used, where G is the successor set, k denotes some arbitrary chosen key element, A is the full set of attributes, and A_i is a subset of attributes, $A_i \subseteq A$. Schematically the procedure can be shown as follows (Figure 3):

We quantify the dissimilarity between two posets (E,A_i), (E,A_j) with respect to a given key element k by counting the elements of the symmetrized difference between two successor sets as follows:

$$W(k,A_i,A_j) := \text{card}\{[G(k,A_i)\backslash G(k,A_j)]\cup[G(k,A_j)\backslash G(k,A_i)]\} = \text{card}[G(k,A_i)\cup G(k,A_j)]\backslash[G(k,A_i)\cap G(k,A_j)] \quad (6)$$

[Note once again that each attribute set induces a new equivalence relation; therefore, the analysis is related on (E,A_i) instead of $(E/R,A_i)$.] For a given key element, two Hasse diagrams (given by two arbitrary sets of attributes) are more dissimilar, the more the successor sets $G(k,A_i)$ and $G(k,A_j)$ differ. We note

$$W(k,A_i,A_j) \geq 0 \text{ and } W(k,A_i,A_j) = W(k,A_j,A_i) \quad (7)$$

The square matrix, denoted by $\mathbf{W}(k)$ has $L = 2^n - 1$ columns and rows, respectively, and has two properties: the "additivity principle" and the "consistency principle".

The additivity principle is as follows: Let $A_1 \subseteq A_2 \subseteq A_3 \ldots \subseteq A_v$ then it can be easily proved that

$$W(k,A_v,A_1) = \Sigma\, W(k,A_r,A_{r-1}) \; r=2,\ldots v \quad (8)$$

The "consistency equation" is as follows: Let be $A_1 \cup A_2 = A_3$ then

$$W(k,A_1,A_2) = W(k,A_1,A_3) + W(k,A_2,A_3) \quad (9)$$

The additivity equation (eq 8), for example, expresses that the distance between the posets (E,A_v) and (E,A_1) is a sum of stepwise distances. Equations 8 and 9 are computationally useful.

The matrix $\mathbf{W}$ is the key for the sensitivity analysis of ranking: This large but symmetrical matrix needs not always be analyzed in its entirety because we are only interested in some few attribute sets. The sensitivity analysis of the criteria used in ranking can be performed with the following steps:

(1) Since we are interested only in comparisons of the full attribute set A with subsets A_i, only one row of the matrix $\mathbf{W}$ is of interest: $W(k,A,A)$, $W(k,A,A_1)$, ..., $W(k,A,A_p)$.

(2) To see the influence of attributes on a Hasse diagram we compare the posets obtained by A with those obtained by the attribute sets with only n-1 attributes. Therefore the effect of dropping exactly one attribute is given by the remaining n entries of the first row, $W(k,A,A_1)$, ..., $W(k,A,A_n)$ (compare Figure 3). Note that the enumerations of the subset A_i are as follows: $A_i = \{q_1, \ldots, q_{i-1}, q_{i+1}, \ldots, q_n\}$, $A_1 = \{q_2, \ldots, q_n\}$,..., $A_n = \{q_1, \ldots, q_{n-1}\}$

(3) The remaining n matrix elements of step (2) are put together to form a "sensitivity tuple" of the key element k, $\sigma(k) := [W(k,A,A_1), \ldots W(k,A,A_n)]$.

(4) $\sigma(k)$ can also be written as $[\sigma_1, \ldots, \sigma_n]$. The larger σ_i the larger is the symmetrized difference between $G(k,A)$ and $G(k,A_i)$ and correspondingly the larger the influence of attribute q_i on the position of key element k within the Hasse diagram under A.

(5) The matrix $\mathbf{W}(k)$ depends on the selection of the key element k. If however, more objects are to be analyzed we generalize as follows

$$W(K,A_i,A_j) = \Sigma W(k,A_i,A_j) \; k \in K \subseteq E$$

where K is any set of key elements, in a shorter notation $\mathbf{W}(K) = \Sigma\, \mathbf{W}(k)$. $\mathbf{W}(K)$ quantifies the effect of modifying the attribute set (i) to a key element or (ii), for example, to priority elements, or finally (iii) to the whole set E.

(6) *All* objects are selected as key elements. Therefore instead of $\mathbf{W}(k)$, $\mathbf{W}(E)$ is to be investigated. $\mathbf{W}(E)$ is the total matrix of the set E. We note that a crude upper limit of $\mathbf{W}(E,A_i,A_j)$ can be found simply by comparing a poset of m solely noncomparable elements with a poset where all m elements are equivalent to each other. Together with eq 7

$$0 \leq W(E,A_i,A_j) \leq m\,(m\text{-}1) \quad (10)$$

(7) $W(E)$ is used as a measure of sensitivity of a ranking with respect to the attributes used. Accordingly we suggest to quantify the sensitivity by

$$\sigma_i := W(E,A,A_i) \; 1 \leq i \leq n$$

with the enumeration scheme of step 2.

For our example the matrix $\mathbf{W}$ has the following values (Table 5)

From this matrix the sensitivities are as follows:

$$\sigma(FC) = 795,\ \sigma(CP) = \sigma(CH) = 0,\ \sigma(MT) = 360 \text{ and } \sigma(GT) = 124$$

Therefore the test "FC" is the most important one within the attribute set containing five tests. The tests CP and CH

Table 5. Values of the Matrix **W** for Different Combinations of Attributes

W	case 0	case 1	case 2	case 3	case 4	case 5
case 0	0	795	0	0	360	124
case 1		0	795	795	1155	919
case 2			0	0	360	124
case 3				0	360	124
case 4					0	484
case 5						0

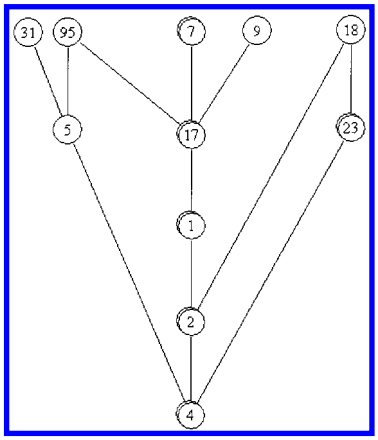

Figure 4. Fifty-five samples evaluated with the test battery of Dutka, except the test for FC. The double circles indicate nontrivial equivalence classes, i.e., equivalence classes with more than one object.

do not have any influence on the order of the theoretical structure of the set of samples, i.e., does not influence the priority of the sites. Their low sensitivity is also found by Dutka et al., who established a regression model between the two quantities. Note that this conclusion refers to the classified values of the battery of tests. Therefore the result with respect to FC should be carefully examined: The high sensitivity may be induced by the scoring process.

Figure 4 shows the Hasse diagram (generated by the EDP-program, WHASSE therefore drawn in its standard format: circles, and each object as high as possible in the drawing plane). [EDP-program WHASSE is available for testing and noncommercial purposes from the first author. For more information the e-mail address is given: BRG@IGB-BERLIN.DE.]

As can easily be seen, there are dramatic changes.

4. DISCUSSION AND CONCLUSION

The battery of tests approach helps to evaluate objects using different criteria simultaneously. [Note that the idea of interpreting chemical aspects as basical multicriterial and thence analyzable in terms of posets is also advocated in refs 11 and 12. More information about posets in chemistry can be found in a recent specific issue of *Match*.[13]] The decision of which sites are "good" or "bad", i.e., the sorting process is more difficult the larger the number of samples and especially the larger the number of tests, since there is more information that can be used to differentiate among the tested objects. This, in turn, leads to difficulties for ranking, because the complexity of a well designed battery is being lost, if in order to compare the tested objects, a ranking index is constructed (e.g. eq 1). The presentation by a Hasse diagram avoids the arbitrariness in constructing a ranking index. Applying concepts of partially ordered sets must not be performed in isolation. All results depend on the data representation used. Here we wanted to demonstrate the HDT extending the results of Dutka et al.[1] Therefore we did not need statistical analyses. However, generally, the appropriate data representation is of much concern (see ref 14 for a very interesting probabilistic concept). The use of cluster analysis and principal component analysis may be helpful in obtaining a statistically relevant data representation and in avoiding insignificant numerical differences of the attributes, which in turn would lead to insignificant comparabilities and incomparabilities and thus to very complex Hasse diagrams.

A combination of Hasse diagram techniques and explorative statistical methods could be a very promising approach for future tasks in environmental sciences. Approaches in this respect were followed on the pollution of regions in Germany with heavy metals[15] and on the contents of environmental databases.[16]

The main advantage of a ranking by HDT is that it can be performed without any normative constraints. HDT simply sorts the objects without any additional information. Beyond sorting, many conclusions can be drawn from Hasse diagrams because they represent a well-defined mathematical structure. Summarizing the following recommendations can be given:

- If the battery of tests is used to test many objects, perform a cluster analysis to get rather numerically robust results. Instead of the measured results for each object use some characteristic values of the cluster (mean values or some other quantities, describing a cluster center).
- Apply HDT to look for priority objects, to identify objects or subsets with characteristic patterns (in mathematical terminology: find "order ideals"), or to select sequences (in order theoretical terminology: "chains") of objects.
- Perform a dimension analysis to estimate the redundancy of the test system and a sensitivity study to identify important or less important attributes. The rationale for the importance of each attribute cannot be drawn from the HDT; here the scientific background is needed: What are the characteristics for all the tested objects, are there any internal correlations among the attributes?
- If an aggregation is done, as for example by eq 1, then note that the weights may have an important influence on the ranking results via Γ if objects have a high degree of incomparability. i.e., to calculate the U(x)-values and estimate the quantity var(x).

REFERENCES AND NOTES

(1) Dutka, B. J.; Walsh, K.; Kwan, K. K.; El Shaarawi, A.; Liu, D. L.; Thompson, K. Priority site selection from degraded areas based on microbial and toxicant screening tests. *Water Pollut. Res. J. Can.* **1986**, *21(2)*, 267−282.

(2) Brüggemann, R. In *Proceedings of the Workshop on Order Theoretical Tools in Environmental Sciences;* Berichte des IGB, Institut für Gewässerökologie und Binnenfischerei: Berlin, 1998; Heft 6, Sonderheft I, pp 1−9.

(3) Brüggemann, R.; Halfon, E. Comparative Analysis of Nearshore Contaminated Sites in Lake Ontario: Ranking for Environmental Hazard. *J. Environ. Sci. Health* **1997**, *A32(1)*, 277−292.

(4) Brüggemann, R.; Oberemm, A.; Steinberg, C. Ranking of Aquatic Effect Tests Using Hasse Diagrams. *Toxicol. Environ. Chem.* **1997**, *63*, 125−139.

(5) Brüggemann, R.; Bartel, H.-G. A Theoretical Concept to Rank Environmentally Significant Chemicals. *J. Chem. Inf. Comput. Sci* **1999**, 39, 211−217.

(6) Davey, B. A.; Priestley, H. A. *Introduction to Lattices and Order;* Cambridge University Press: Cambridge, 1990.
(7) Systat Program; SPSS Inc.; 2000; http://www.spss.com/software/science/SYSTAT/. See, also: Borg, I.; Shye, S. *Facet Theory − Form and Content;* Sage Publications: Thousand Oaks, CA, 1995.
(8) Trotter, W. T. *Combinatorics and Partially Ordered Sets Dimension Theory*; John Hopkins Series in the Mathematical Science; The J. Hopkins University Press: Baltimore, 1991.
(9) Luther, B. Ph.D. Thesis, 2000; in preparation.
(10) Monjardet, B. Metrics on partially ordered sets − a survey. *Discrete Mathematics* **1981**, *35*, 173−184.
(11) Klein, D. J.; Babic, D. Partial Orderings in Chemistry. *J. Chem. Inf. Comput. Sc.* **1997**, *37*, 656−671.
(12) Klein, D. J. Similarity and Dissimilarity in Posets. *J. Math. Chem.* **1995**, *18*, 321−348.
(13) Partial Orderings in Chemistry. In *Match;* Klein, D. J., Brickmann, J., Eds.; 2000; pp 1−290.
(14) Sørensen, P. B.; Mogensen, B. B.; Carlsen, L.; Thomsen, M. The Influence on Partial Order Ranking from Input Parameter Uncertainty − Definition of a Robustness Parameter. *Chemosphere* **2000**, 595−600.
(15) Welzl, G.; Voigt, K.; Rediske, G. In *Proceedings of the Workshop on Order Theoretical Tools in Environmental Sciences;* Berichte des IGB, Institut für Gewässerökologie und Binnenfischerei: Berlin, 1998; Heft 6, Sonderheft I, pp 101−110.
(16) Voigt, K.; Welzl, G.; Rediske, G. In *Proceedings of the 20th Annual National Online Meeting*; Williams, M., E., Ed.; Information Today Inc.: Medford, NJ, 1999; pp 487−497.

CI000055K