MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **67** (2012) 731-744

ISSN 0340 - 6253

Antichains in Partial Order, Example: Pollution in a German Region by Lead, Cadmium, Zinc and Sulfur in the Herb Layer

Rainer Bruggemann[1) and Kristina Voigt[2)

1) Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Department Ecohydrology, Berlin, Müggelseedamm 310, 12587 Berlin, Germany, E-mail: brg_home@web.de

2) Helmholtz Center Munich, Institute of Biomathematics and Biometry, Ingolstaedter Landstr. 1, 85764 Neuherberg, Germany, kvoigt@helmholtz-muenchen.de

(Received July 4,2011)

Abstract

Simple elements of partial order theory turned out to be useful tools when rankings are needed. Here we show, how a subset of objects, mutually incomparable (called an antichain) can be further analyzed. There is a surprising relation to extremal graph theory, namely an application of the famous theorem of Turan.

As example, we analyze the partially ordered sets of regions in the South - West of Germany, where the characterizing attributes are discretized concentrations of Lead, Cadmium, Zinc and Sulfur in the herb layer.

1. Introduction

In multi-indicator systems, the concept of partially ordered sets is a useful tool in many different fields of research, see the following, certainly not complete list (sequenced after the years): Randic, 1978, Ruch and Gutman, 1979, Bartel, 1994, 1995, Klein, 1995, Klöpffer and Volkwein, 1995, Galassi et al., 1996, Klein and Babic, 1997, Luther and Gnauck, 2002, Pavan and Todeschini, 2004, Castro et al., 2005, Sørensen et al., 2006, Bruggemann and Voigt, 2008, Duchowicz et al., 2008, Newlin and Patil, 2010, Bruggemann and Patil, 2010, Todeschini, 2011, Tsakovski and Simeonov, 2011). Partially ordered sets (posets) can also be considered as a first step in evaluation and decision finding. However, the analysis of posets for decision making is usually only seen as a preprocessing step, because in general, partially ordered sets do not allow a unique ranking (which is of interest for its own right, see for example Bruggemann and Carlsen, 2011, or De Loof et al., 2011).

In our example, regions in Baden-Wuerttemberg, South-West of Germany were selected and monitored with respect to concentrations of the chemical elements Pb, Cd, Zn and S in the herb layer. This multi-indicator system with regions as objects and concentrations of the four chemical elements as indicators (syn.: attributes) raises the questions: 1) How can we get information about the pollution status? and 2) What can be said about geochemical relations? For example does an increase in pollution with respect to one pollutant always imply the increase of another pollutant?

The first step to get answers is the visualization of the poset by a Hasse diagram. There are many references available which show examples of the analysis of Hasse diagrams, see e.g. Bruggemann et al., 2001, books such as Bruggemann and Patil, 2011 and special issues of journals such as MATCH Commun.Math.Comput.Chem 42, 2000 (Klein and Brickmann, 2000).

According to the used software (PyHasse, see for instance Voigt et al., 2010) Hasse diagrams are arranged in the way that the < - relation between two objects x and y ($x < y$) is geometrically represented by a position of y above the position of x and by a line or a sequence of lines connecting x with y. Hasse diagrams are directed graphs without cycles and if arranged in the given way, mostly analyzed in a vertical manner (increasing pollution, increasing toxicity, etc.). The horizontal dimension is often of less interest, especially if a linear order is wanted in order to find decisions. In that sense unfortunately the concept of incomparability is seen as an obstacle rather than as a means to "see where an object is and why it is, where it is" (Bruggemann and Patil, 2011).

We began to study this horizontal component of a Hasse diagram in Bruggemann and Voigt, 2011 where we more closely analyzed separated subsets. Here we turn back to more elementary parts of incomparability, namely to antichains, A famous result about antichains is the Dilworth theorem (Priestley and Davey, 1990, Crawley and Dilworth, 1973), which relates the number of elements in the maximum antichain with the number of chains (for definitions, see below). Some studies about antichains can also be found in Trotter, 1992, such as the concept of "alternating cycles" and the problem of finding the dimension of posets which is immediately related to the presence of antichains. However, so far to our knowledge the appearance of antichains obtained from data matrices has not found much interest in the literature. For example, in Ivanciuc and Klein 2004 the leading idea is to find approximations of order preserving maps, relating chemical structures/reactions and their partial order with chemical data such as toxicity or bioaccumulation. Incomparability is then seen rather as a relaxation in this task than of interest for its own right.

Our paper is organized as follows:

Section 2: Basic definitions and presentation of the example

Section 3: Countings in antichains

Section 4: Conclusions and outlook.

2. Basic material and the example of pollutionof a german state

2.1 Basic definitions

Partially ordered sets: Let G be a set of objects, characterized by some attributes $q_1,\dots,q_m$. Then we call $(G, \leq)$ a partially ordered set, as follows:

$x,y \in G, x < y :\Leftrightarrow \; q_i(x) \leq q_i(y)$ for all i=1,...,m, and there is at least one index i^* for which the strict inequality $q_{i^*}(x) < q_{i^*}(y)$ holds.

(1)

A pair $x,y \in G$, for which neither $x = y$, nor $x < y$, nor $y < x$ can be found, is called incomparable and symbolized by $x \,||\, y$.

The set of attributes, used in (1) is called an information base, abbreviated as IB.

Notation: Let $IB' \subseteq IB$, then $x <_{IB'} y$, x is less than y with respect to the attributes of IB'.

<u>Chain</u>: A subset $G' \subseteq G$ is called a chain, when all elements of G' can be ordered.

<u>Antichain</u>: A subset $G' \subseteq G$ is called an antichain, when no two elements of G' are ordered, i.e. for all $(x,y) \in G'^2$ follows: $x||y$.

The analysis of chains (“vertical analysis of Hasse diagrams”) is most often of more interest, as chains can be seen as an interim result of ranking. Antichains are of less interest, albeit they are the obvious indication that different quantities cannot necessarily be measured on one scale, i.e. they are incommensurable. The question is: What can we deduce from the appearance of antichains with respect to the objects and with respect to the attributes? A first attempt toward an answer is given in this paper.

2.2 Example

When the number of objects is small enough, then we can draw a little bar diagram, indicating the values of $q_i \in IB$ of the corresponding object. We call this kind of special drawing an “intelligent Hasse diagram”. In Figure 1 we see the “intelligent Hasse diagram” with respect to the pollution of the German state Baden-Wuerttemberg by Pb, Cd, Zn and S, especially in the target herb layer. The herb layer is thought of as indicator of local and medium-ranged transport processes. The German state Baden-Wuerttemberg was thought of as divided into 60 regions and at representative sites the concentrations (in mg/kg dry mass) in different targets were measured. Here we discretized the concentrations and obtained scores as follows:

(i) Corresponding to the recommendations of the Environmental Protection Agency of Baden-Wuerttemberg we selected three classes for Pb, Cd and Zn and two classes for S.

(ii) The range of data was correspondingly divided into intervals of equal length

(iii) The intervals were enumerated increasingly by 0,1,..

(iv) If a concentration c of a region x falls into the interval $I_s = [c_{min}^{(s)}, c_{max}^{(s)})$ then region x got the score s.The concentrations $c_{min}^{(s)}$ and $c_{max}^{(s)}$ define the borders of the sth interval.

Due to the replacement of quantities, continuous in concept by scores we obtained many equivalence classes. Hence we, finally are studying 14 representatives labeled by numbers such as 18, 35, etc.. (Figure 1).

The Hasse diagram, shown in Figure 1, gives a series of useful information, namely:

1. the pollution status of each region
2. geochemical aspects
3. identification of chains (in a messy Hasse diagram this task is done by the module chain4.py)
4. identification of antichains

It may be useful to explain Figure 1 in some more detail:

The general degree of pollution increases starting from the bottom of the diagram and proceeding upwards. However the kind of pollution differs. From the point of view of human health or ecotoxicity the combined effect of Pb together with S, or of Pb and Cd may differ, even if both pollutions have the same intensity (compare object (region) “22” with the scores Pb = 1, S = 1 and “45” with the scores Pb = 1, Cd = 1). As long as there exists no generally accepted common scale to calculate the combined effect, it is wise, to keep such elements of G separated, i.e. to avoid compensation due to the averaging process in many decision support systems. Several chains can be detected in the Hasse diagram. For example:

“30” < “17” < “22” < “14” < “57”.

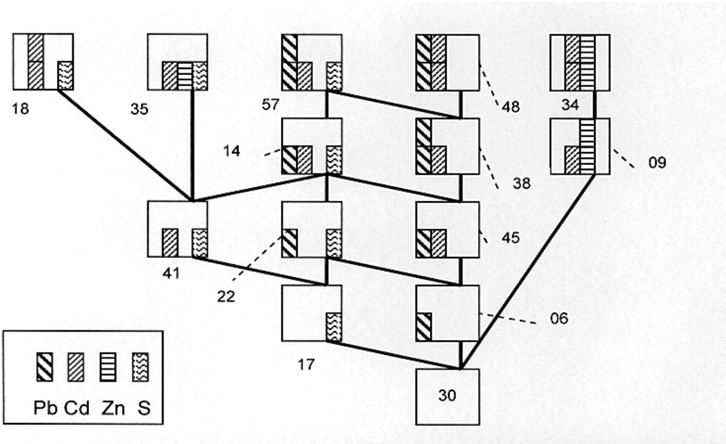

Figure 1. –Partial ordering of the regions of Baden-Wuerttemberg (see text). Modified after Bruggemann et al. 1999

Such chains show that an increase of one attribute does not imply a decrease of another one. In the chain considered the scores of Pb and Cd are simultaneously increasing, starting at “30” and finally ending up in “57”.

The analysis of the Hasse diagram in Figure 1 leads us to the discussion of one of the different facets of incomparability, namely of separated subsets such as {09,34} vs {06,17,41,22,45,14,38,18,35,57,48} (Bruggemann and Voigt, 2011). Another facet of incomparability is the appearance of antichains, For example G' = {18, 34, 35, 48, 57}. The elements of G' also are maximal elements and therefore of special interest. What can be said about G', which seems to be without any structure? This question motivates, what we will discuss in more detail in the next section.

3. Antichains and their analysis

3.1 Some additional notations

For the sake of generality we write $q_1,..,q_m$ for the attributes and $x_1,...,x_n$ for the objects. If we specify two objects or two attributes, then we write x, y (objects) or q, p (attributes).
The following subsets are of interest:

$A(G') = \{(x_i,x_j), i < j$ for all $x_i, x_j \in G' \subseteq G\}$

$Q(IB') = \{(q_i, q_j), i < j$ for all $q_i, q_j \in IB' \subseteq IB\}$

As the incomparability relation is symmetric, any exchange of the indices does not affect the incomparability. We call *S(IB')* a complete graph on IB' with the vertex set *IB'* and the edge set $\{\{q_i, q_j\}\}: q_i, q_j \in IB', q_i \neq q_j\}$. Note, the symbol *S* is motivated from the concept of a "simplex".

Furthermore we define:

$AC(G', IB') \subseteq \{(x_i, x_j) \in A(G'), x_i ||_{IB'} x_j\}$.

From Figure 1, we selected G'={18, 35, 57, 48, 34} and see that this subset forms an antichain, leading to the set of object pairs, $AC(G',IB)=\{(18,35), (18,57),...,(48,34)\}$. The question now is: Take a pair $(x,y) \in AC(G',IB)$. Which attribute pair $(q,p) \in Q(IB)$ keeps the incomparability $x||y$?

We introduce the matrix *ACM* (from AntiChain Matrix). Let $(x,y) \in AC(G')$ be a row and $(q,p) \in Q(IB')$ a column of this matrix which is only completely defined if *G'* and *IB'* are also indicated. We, however refer in the following in all cases to *G'* and *IB'* so that the notation can be simplified. Then:

$$ACM(x,y),(q,p) = \begin{cases} 1 & \text{if } x||_{(q,p)}\, y \\ 0 & else \end{cases} \tag{2}$$

We call *RAC(x,y)* the rowsum of *ACM* concerning the row of *(x,y)*, and *CAC(q,p)* the columnsum of *ACM*, concerning the column *(q,p)*. Any objectpair *(x,y)* can be characterized by *RAC(x,y)* and any attribute pair *(q,p)* can be characterized by *CAC(q,p)*. These numbers can given a contextual interpretation as follows:

The larger *RAC(x,y)* the more severe its status as an incomparable object pair, because in many combinations of attributes an incomparability $x||_{(q,p)}\, y$ appears. Similarly we can interpret *CAC(q,p)* as describing the importance of a certain attribute pair for being responsible for the incomparabilities of $(x,y) \in AC$.

Finally it is useful to introduce *Sred(x,y)* ("Reduced complete graph") as that graph, where the vertices are the elements of *IB'* and a vertex *q* is connected with vertex *p* if and only if

$ACM(x,y),(q,p) = 1$.

3.2 Normalization of *RAC* and *CAC*

For comparison purposes (for example to compare different antichains in one poset, or the same subset of objects forming antichains in different posets) it is wise, to normalize the row- and columnsums of *ACM*. Let $m'=|IB'|$ and $n'=|G'|$. Then clearly $m'*(m'-1)/2$ and $n'*(n'-1)/2$ are upper bounds.

We define:

$$cac(q,p) := CAC(q,p)/[n'*(n'-1)/2] \tag{3}$$

To prepare the next step, namely the normalization of *RAC*, we define:

Transitive triples of attribute pairs: Three attribute pairs are transitively closed, if the pairs consist of three attributes, which form a triangle in *S(IB')*. (4)

The three attribute pairs $(q_1,q_2),(q_1,q_3),(q_1,q_4)$ are not a transitive triple of pairs. Their representation as a graph *Sred(x,y)* would be a star with q_1 in the center. Similarly $(q_1,q_2),(q_2,q_3),(q_1,q_4)$ is not transitively closed. The representation *Sred(x,y)* is a bifurcation free tree with q_4 at the one, and q_3 at the other end. However $(q_i,q_j),(q_j,q_k),(q_k,q_i)$ form a transitive triple of attribute pairs.

Observation:

In *ACM*, given one object pair *(x,y)* the columns of pairs forming a transitive triple cannot have simultaneously three entries 1.

Proof:

Let us select x,y and let us assume $x \,||_{(q1,q2)}$, $x||_{(q1,q3)}$ and $x||_{(q2,q3)}y$. The three attribute pairs form a transitively closed triple.Then $x \,||_{(q1,q2)}\, y$ can without restriction of generality be written as $x>_{q1} y$ and $x<_{q2} y$. Consider now q_1 and q_3, concerning the incomparability $x \,||_{(q1,q3)}\, y$. We already know: $x >_{q1} y$, hence it must be valid $x<_{q3} y$. Finally concerning the supposed incomparability $x \,||_{(q2,q3)}\, y$: With respect to q_2 we know: $x <_{q2} y$, with respect to q_3 we know: $x <_{q3} y$. Hence $x <_{(q2,q3)} y$. Therefore within a transitive triple of attribute pairs not all three attribute pairs can lead to an incomparability for x,y.

Corollary:

Following the observation above, the graph with maximal number of edges for a selected pair $(x,y) \in AC$ cannot be a complete graph, because this graph cannot contain triangles.

Therefore, the maximal number of edges of the graph *Sred(x,y)* is governed by a theorem of extremal graph theory, the theorem of Turan (Harary,1974). The maximal number of edges in a triangle - free graph, i.e. of incomparabilities and hence the maximum number of rowsums of *ACM* is:

$$u_{\max} = \left\lfloor \frac{m'^2}{4} \right\rfloor \tag{5}$$

where the brackets indicate that the greatest integer is to be taken being less than or equal $m'^2/4$. In the case of four attributes any cycle with four edges and valences 2 is a candidate for an allowed graph of attributes maximizing the rowsum.

Hence the correct normalization of rowsums is as follows:

$$rac(x,y) := RAC(x,y)/u_{\max} \tag{6}$$

If, for example $|IB|=4$ and $x,y \in AC(G',IB)$ then the corresponding simplex would be a tetrahedron, whereas the graph *S(x,y)* following (5) is a circle with four vertices.

Remark 1:

A similar derivation in order to determine the maximal number of edges, in a graph whose vertices are the objects of an antichain is not possible, because $x||_{(qi,qj} |y$ does not imply which relations are valid for $x||_{(qi,qj)}\, z$ or $y\; ||_{(qi,qj)}\, z$. Hence the upper limit of importance of a given attribute pair (q_i,q_j) is just $n'*(n'-1)/2$, with $n'=|G'|$.

Remark 2:

Corresponding to the arguments used in the proof of the observation every $2n+1$ circle of attribute pairs cannot simultaneously lead to entries 1 of the *ACM*. As, however we are interested in a lower upper bound of *RAC* the exclusion of any $2n+1$-circle ($n>1$) is here of minor interest.

3.3 Application

The needed calculations are performed by means of the software package PyHasse. This software package was and is currently developed by the first author and contains now 60 programs, all written in Python (which motivates us to write “Py”Hasse). PyHasse is designed for an ordinal analysis of data matrices. In Figure 2 the graphical user interface of antichain6Excel.py is shown.

The module antichain6Excel.py delivers a series of results, which are shown after pressing the corresponding button. For example, after selecting the Excel-Sheet with the data of pollution of Baden-Wuerttemberg, a Hasse diagram pops up (not shown) and pressing “Calc antichain statistics” a window like that, shown in Figure 2 (bottom) can be examined. After selection of the data matrix an entry box opens, where the elements of an antichain can be read in.

Usually a bar diagram representing the *rac*- and *cac*-values, resp. is wanted. Therefore this specific module has an interface to Excel, so results can be immediately visualized using the professional software of Excel (Figure 3).

Examining Figure 3, one sees that the object pairs [48, 35] (slight notation change because of technicalities in the PyHasse program) and [57, 34] are incomparable independent which of the attribute pairs is selected. So we conclude that these two object pairs are incomparable ”to a high degree”. Any subset of *IB* down to a pair of attributes will lead to incomparability of these two object pairs. Another object pair, such as for example [18,35] has a low degree (namely of above 0.2 and less 0.4). Therefore it can be expected that deleting columns from the data matrix (for example for performing a sensitivity study) the pair [18,35] becomes comparable.

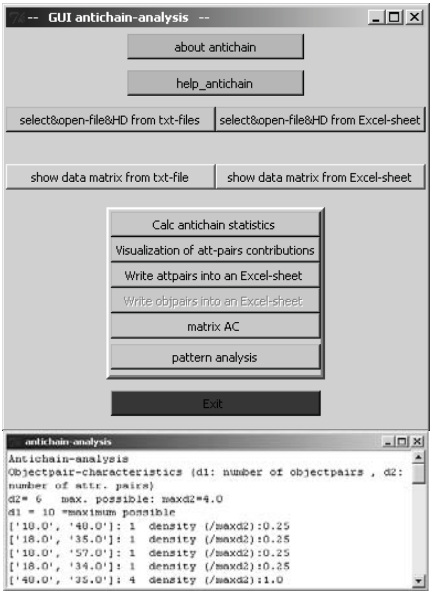

Figure 2: Top: Graphical user interface of PyHasse, module (program) antichain6Excel.py. Bottom: one of the results windows (see text)

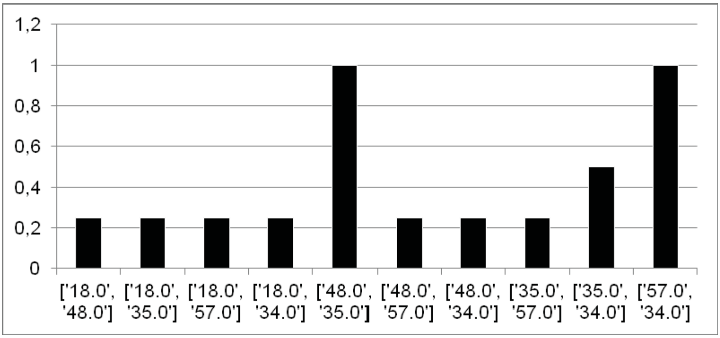

Figure 3: *rac* for the different object pairs.

Figure 3 shows the aggregated state, i.e. the rowsums. In Table 1, the matrix *ACM* and the rowsums *RAC* are shown, where the individual contributions of each attribute pair and object pair can be inspected.

Table 1: Antichain matrix (*ACM(IB,G')*) allowing a detailed investigation of an antichain

	[Pb, Cd]	[Pb, Zn]	[Pb, S]	[Cd, Zn]	[Cd, S]	[Zn, S]	RAC
[18, 48]	0	0	1	0	0	0	1
[18, 35]	0	0	0	1	0	0	1
[18, 57]	1	0	0	0	0	0	1
[18, 34]	0	0	0	0	0	1	1
[48, 35]	0	1	1	1	1	0	4
[48, 57]	0	0	0	0	1	0	1
[48, 34]	0	1	0	0	0	0	1
[35, 57]	0	1	0	0	0	0	1
[35, 34]	0	0	0	0	1	1	2
[57, 34]	1	1	0	0	1	1	4

In Figure 4 some graphs, *Sred(x,y)*, derived from *S(IB)* are shown:

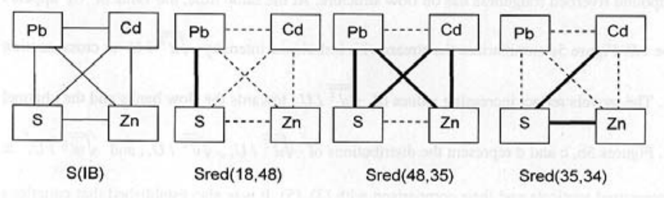

Figure 4: Graphs *S(IB)* and *Sred(x,y)*. Bold lines, realized for a given object pair.

These graphs are useful, because we can see how far attributes are crucial for maintaining an incomparability: If for example [18, 48] is selected, then both attributes Pb and S are crucial.

Without one of these two, object 18 will be comparable to object 48. In [35, 34] we see that elimination of the attribute S (sulfur in the herb layer) would imply a comparability for 34 with 35. Hence the analysis of the graphs *Sred(x,y)* supports a local sensitivity analysis. "Local" because only a pair $(x,y) \in AC(G',IB)$ is of concern. A further evaluation of the matrix *ACM* by Formal Concept Analysis (see for example Bartel, 1994, 1995) seems to be promising but is out of the scope of this paper.

Similarly we can check the role of attribute pairs (Figure 5):

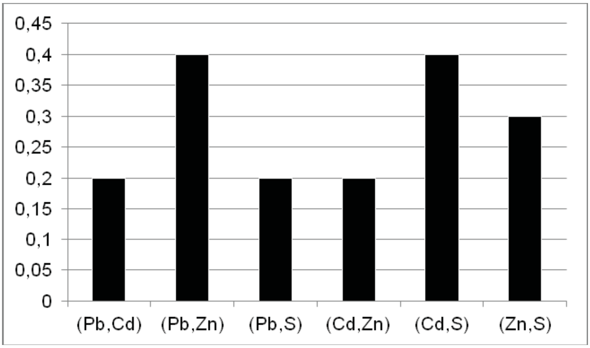

Figure 5: *cac* for the different attribute pairs of the selected antichain.

The tendency to generate incomparable pairs is greatest for (Pb,Zn) and (Cd,S) then (Zn,S) . followed by the other possible attribute pairs.

4. Conclusion and outlook

The representation of partial orders by Hasse diagrams is a helpful tool to discuss topics for which a ranking is considered as important. Many conclusions can be directly drawn from the graphical scheme.

Especially useful is the presentation of the order theoretical relations as "intelligent Hasse diagram" (see Figure 1), but also the possibility to look at chains within the partially ordered set. Consequently the new software package PyHasse provides several tools for the identification of chains (see chain4.py) and for statistical characterizations (as in antichain6Excel.py). When partial order is applied, then very often not a linear order arises but incomparabilities appear. If not a complete ranking is the only purpose of the study then the partial order itself motivates to perform some simple, albeit useful, explorative statistics as demonstrated in section 3. The analysis of properties of the antichain matrix (*ACM*) and of its column- *CAC* and rowsums, *RAC* is at its very beginning. We show that even an antichain has a certain kind of structure, namely the pairs $(x,y) \in AC(G',IB')$ derived from an antichain as well as the pairs $(q,p) \in Q(IB)$ can be differentiated and that the need of normalization leads to the consideration of graphs such as *Sred(x,y)* which must be trianglefree.

Future work has to focus on the following questions: How can the graph *Sred(x,y)* be characterized in terms of concepts of graph theory? How can a (valued) graph be characterized, which is thought of as a result of summing over all contributions of *ACM* for a given column, i.e. when scanning through all $(x,y) \in AC$? Furthermore: When, as it is the case in our example, only two object pairs are strongly incomparable, what can be said for the decision making process? Furthermore, which implication has the exclusion of $2n+1$ circles in *Sred(x,y)*?

The paper of Annoni et al., 2011 has shown that the analysis of posets in terms of *G'* or *IB'* does not give the full insight, as numerical values of the attributes for the different objects also play an important role. For example the object pair [48,35] has *rac*=1, however, a slight deviation of the numerical values may completely change the result. A corresponding variance based sensitivity study should be performed in the near future.

References

Annoni, P., R. Bruggemann, A. Saltelli, Partial order investigation of multiple indicator systems using variance-based sensitivity analysis, *Env. Mod. Soft.* **26** (2011) 950–958.

Bartel, H. G., Formalbegriffsanalytische Untersuchung ausgewählter Aromatizitätskriterien. *MATCH Commun. Math. Comput. Chem*. **30** (1994) 9–35.

Bartel, H. G., Formale Begriffsanalyse und Materialkunde: Zur Archäometrie altägyptischer glasartiger Produkte, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 27–46.

Bruggemann, R., S. Pudenz, K. Voigt, A. Kaune, K. Kreimes, An algebraic/graphical tool to compare ecosystems with respect to their pollution. IV: Comparative regional analysis by Boolean arithmetics, *Chemosphere* **38** (1999) 2263–2279.

Bruggemann, R., E. Halfon, G. Welzl, K. Voigt, C. Steinberg, Applying the concept of partially ordered sets on the ranking of near-shore sediments by a battery of tests, *J. Chem. Inf. Comp. Sci.* **41** (2001) 918–925.

Bruggemann, R., K. Voigt, Basic principles of Hasse diagram technique in chemistry, *Comb. Chem. High Throughput Screen.* **11** (2008) 756–769.

Bruggemann, R., G. P. Patil, Multicriteria prioritization and partial order in environmental sciences, *Environ. Ecol. Stat.* **17** (2010) 383–410.

Bruggemann, R., L. Carlsen, An improved estimation of averaged ranks of partial orders, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 383–414.

Bruggemann, R., G. P. Patil. *Ranking and Prioritization for Multi-indicator Systems. Introduction to Partial Order Applications*, Springer, New York, (2011) in press .

Bruggemann, R., K. Voigt, A new tool to analyze partially ordered sets – Application: Ranking of polychlorinated biphenyls and alkanes/alkenes in river Main, Germany, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 231–251.

Castro, E. A., F. M. Fernandez, P. R. Duchowicz, QSPR modeling of the enthalpy of formation based on partial order ranking, *J. Math. Chem.* **37** (2005) 433–441.

Crawley, P., R. P. Dilworth, *Algebraic Theory of Lattice Theory*, Prentice-Hall, Englewood Cliffs, 1973.

Davey, B. A., H. A. Priestley, *Introduction to Lattices and Order*, Cambridge Univ. Press, Cambridge, 1990.

De Loof, K., B. De Baets, H. De Meyer, Approximation of average ranks in posets, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 219–229.

Duchowicz, P. R., M. G. Vitale, E. A. Castro, Partial order ranking for the aqueous toxicity of aromatic mixtures, *J. Math. Chem.* **44** (2008) 541–549.

Galassi, S., A. Provini, E. Halfon, Risk assessment for pesticides and their metabolites in water, *Intern. J. Environ. Anal. Chem.* **65** (1996) 331–344.

Harary, F., *Graphentheorie*, R. Oldenbourg-Verlag, München, 1974.

Ivanciuc, T., D. J. Klein, Parameter-free structure-property correlation via progressive reaction posets for substituted benzenes, *J. Chem. Inf. Comp. Sci.* **44** (2004) 610–617.

Klein, D. J., Similarity and dissimilarity in posets, *J. Math. Chem.* **18** (1995) 321–348.

Klein, D. J., D. Babic, Partial orderings in chemistry, *J. Chem. Inf. Comp. Sci.* **37** (1997) 656–671.

Klein, D. J., J. Brickmann (Eds.), Partial orderings in chemistry, *MATCH Commun. Math. Comput. Chem.* **42** (2000) 1–290.

Klöpffer, W., S. Volkwein, Bilanzbewertung im Rahmen der Ökobilanz, in: Thom'e-Kozmiensky, K. Joachim (Eds.), *Management der Kreislaufwirtschaft*, EF-Verlag für Energie- und Umwelttechnik GmbH, 1995, pp. 336–340.

Luther, B., A. Gnauck, The relevance of cluster methods to priority objects, in: K. Voigt, G. Welzl (Eds.), *Order Theoretical Tools in Environmental Sciences - Order Theory (Hasse diagram technique) Meets Multivariate Statistics-*, Shaker–Verlag, Aachen, 2002, pp. 141–157.

Newlin, J., G. P. Patil, Application of partial order to stream channel assessment at bridge infrastructure for mitigation management, *Environ. Ecol. Stat.* **17** (2010) 437–454.

Pavan, M., R. Todeschini, New indices for analysing partial ranking diagrams, *Anal. Chim. Acta* **515** (2004) 167–181.

Randic, M., Graph–theoretical analysis of structure–property and structure–activity correlations, *Int. J. Quant. Chem.* **5** (1978) 245–255.

Ruch, E., I. Gutman, The branching extent of graphs, *J. Combin. – Inf. Sys. Sci.* **4** (1979) 285–295.

Sørensen, P. B., D. Lerche, M. Thomsen, Developing decision support based on field data and partial order theory, in: R. Brüggemann, L. Carlsen (Eds.), *Partial Order in Environmental Sciences and Chemistry*, Springer–Verlag, Berlin, 2006, pp. 260–283.

Todeschini, R., The j-index: A new bibliometric index and multivariate comparisons between other indices, *Scientometrics* **87** (2011) 621–639.

Trotter, W. T., *Combinatorics and Partially Ordered Sets Dimension Theory*, Johns Hopkins Univ. Press, Baltimore, 1992.

Tsakovski, S., V. Simeonov, Hasse diagram technique as exploratory tool in sediment pollution assessment, *J. Chemom.*, in press.

Voigt, K., R. Bruggemann, H. Scherb, H. Shen, K. H. Schramm, Evaluating the relationship between chemical exposure and cryptorchidism by discrete mathematical method using PyHasse software, *Env. Model. Soft.* **25** (2010) 1801–1812.