MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **73** (2015) 277-302

ISSN 0340 - 6253

Incomparable - What Now, III. Incomparabilities, Elucidated by a Simple Version of ELECTRE III and a Fuzzy Partial Order Approach

Rainer Bruggemann[1], Lars Carlsen[2]

[1] *Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Dept. Ecohydrology, Mueggelseedamm 310, D-12587 Berlin-Friedrichshagen, Germany*

[2] *Awareness Center Linkøpingvej 35, Trekroner, DK-4000 Roskilde, Denmark*

(Received October 29, 2014)

ABSTRACT

Decision making is to an increasing extent supported by multi-criteria decision analysis (MCDA) software. Especially when a ranking of objects (chemicals, geographical units, nations, strategies etc) is wanted, an initial step is the development of a multi-indicator system (MIS). One of the famous MCDA concepts to obtain a ranking from MIS is realized in the series of ELECTRE-algorithms. The major task of decision support systems is to obtain a total order. On the other hand, an evaluation of MIS by partial order leads to directed graphs, where objects often are not connected, i.e., not being comparable with each other. In the partial order terminology this relation is called 'incomparability'. Partial order does a priori not lead to a total order, which is most often seen as a severe disadvantage. The reason for incomparabilities among objects can be traced back either to conceptual conflicts, or simply to small, even minute data differences. The software ELECTRE III (and others of the ELECTRE family) takes care for these latter cases by a set of parameters beyond the data matrix and functions describing the degree of user preferences. In that sense ELECTRE III can be (and is) seen as a fuzzy method. In partial order theory fuzzy concepts can be inferred too. The present study compares the results of ELECTRE (simplified) and of fuzzy partial order theory. As an example a group of environmentally hazardous chemicals is selected. It turns out that the concept of fuzzy posets provides an effective instrument to reduce the number of incomparabilities, without the need of additional parameters beyond those of the data matrix as is the case in ELECTRE III.

1 Introduction

The hazard exerted by substances which are persistent (P), bioaccumulating (B) and toxic (T) can be described by three indicators, associated with P, B and T (see e.g. [1]). Application of these three indicators simultaneously shows that, e.g., DDT is more hazardous than DDD.

However, the same indicators also show that DDT and ALD cannot be compared (see for details [2]). The main problem is that often the ranking aim cannot directly be expressed by one indicator. Within the above mentioned example: There is no single indicator, measurable or as outcome of mathematical simulation models, expressing “the” hazard. Instead many indicators are needed as a proxy to approach the ranking as in the case mentioned above. Therefore the expression multi-indicator system (MIS) becomes somewhat popular, to indicate the multivariate character of the ranking [3].

Often a set of indicators allows not only a ranking but also, because of an induced metric, to obtain an impression of how far one object is better (which in the present study means less hazardous) than another one. However, the true art is how to get the indicators. In the example of Failed States 12 indicators were derived [4]. There is typically a great effort of knowledge to obtain these indicators. A mathematical mapping to get a one-dimensional scalar, just to be used as a ranking indicator [5] is not only hiding all the background information but also has the effect of an often unwanted compensation [6]. In the case of the Failed States, the composite indicator is generated by a simple addition of the values for the 12 single indicators [4].

In natural sciences much information can be obtained as measurable quantities or quantities which can be calculated by reliable mathematical simulation models. For example in environmental chemistry much information about molecular macroscopic properties are derived from QSAR models (see e.g. [7]) or about transport properties and residence times are derived by deterministic mathematical models, such as GREAT_ER [8, 9] or EUSES [10-12]. The framework of EUSES [10, 11] is accepted by the relevant authorities of EU, to calculate the needed information. However, the system EUSES is complicated to use due to the high number of input parameters needed [11, 12].

In this paper the focus is on environmental chemicals, pesticides, which are so powerful in the battle to reduce hunger, but are now due to their hazardous environmental- and human health properties banned by the Stockholm Convention [13]. Although these chemicals are under strict regulation, an illegal use is wide spread and once brought into the environment the long life time of these substances implies serious concern [14].

The present paper's intention is a methodological one. Hence, in many fields it turns out that partial order applied on MIS can be useful [3]. Nevertheless, a typical outcome of poset-theory is the so-called incomparability as for example the two chemicals DDT and ALD, mentioned above. Incomparability means that a unique ranking cannot be found for all objects and most multi-criteria decision analysis tools focus at deriving a single ranking scalar, i.e., incomparability is no longer of concern. We here analyze incomparability specifically when the indicators of a MIS have a metric.

In continuing the series about incomparabilities in partially ordered sets (posets), see [2, 15, 16] we ask how concepts of multivariate statistics, such as cluster analysis, fuzzy theory or famous multi-criteria decision tools such as ELECTRE [17-21] interact with or compare to partial order methodology. The issue of cluster analysis and partial order has recently been discussed [15] and shall not be further considered here.

Imagine a MIS with k indicators. Based on these indicators r objects are to be ranked by MCDA-methods. Within the conventional machinery of decision support systems, such as ELECTRE III [17-21] objects would be brought into a linear order by means of a series of additional parameters. Thus, ELECTRE III needs parameters evaluating

- the degree of indifference
- the degree of significance
- the veto-parameters
- weights (for details, see below).

How these parameters are used to eventually get the important credibility matrix s(x,y) will be sketched in section 2.3.

The objective of the present study is to compare ELECTRE III (considered by [17] as a fuzzy tool and implemented in PyHasse (see below) in a simplified manner, see sect. 2.3) with fuzzy partially ordered sets, both methods being applied to the data set previously investigated by [1]. We conclude the paper by a similarity analysis and critical summary, where the question

as to how far additional parameters beyond the set of selected indicators is helpful or not in the light of fuzzy poset theory.

2 Materials and Methods

2.1 Environmental chemistry

Sailaukhanuly et al. [1] published a study about persistent organic chemicals, where a multi-indicator system (MIS) consisting of persistence, bioaccumulation and toxicity (PBT-criteria) as the single indicators was investigated. They show that in general simple concepts of partial order theory can give insights into the possible rankings without the use data and information pieces beyond the data matrix (of measured or simulated values). A central role plays the graphical visualization of partially ordered sets by Hasse diagrams displaying much useful information (see for instance [4]). However - as discussed above - the presence of incomparabilities most often is considered as a drawback in decision support, which often causes the preference of other decision support systems such as PROMETHEE [22] or the ELECTRE family [17-21].

Table 1 shows the column-wise [0,1]-normalized data (see [4]) of 12 pesticides (r , the number of objects = 12). The idea is, to rank the chemicals due to their hazard, which as mentioned above is not directly measurable.

Before the MIS (consisting of three elementary indicators) is discussed in more details, some basic definitions are needed to understand the example.

2.2 Basic definitions of the theory of partially ordered sets

Partial order relations can be obtained in many different ways. Even, if the partial order is to be defined to deal with a data matrix we can still define different partial order relations among objects.

Let X be the finite set of objects, and IB the set of indicators q_i, (i = 1, … ,$|IB|$) then we define:

$x,y \in X$: $x \le y : \Leftrightarrow q_i(x) \le q_i(y)$ for all $q_i \in IB$, (1)

Eq. 1 represents a partial order P, which we often denote as $P = (X, IB)$ to indicate the interaction between the order relation and the set of indicators. The set X together with the partial order structure is called a partially ordered set.

Many other realizations of partial orders may not be based on Eq. 1, therefore the partial orders based on Eq. 1 are considered as outcome of the so-called Hasse Diagram Technique (HDT).

Table 1: Normalized (column-wise) data matrix (rounded to three decimals) of 12 pesticides (PBT-substances) included in the Sailaukhanuly study [1]

Pesticide	Pers	BioA	Tox
DDT	0.084	1.000	1.000
DDE	0.009	0.856	0.160
DDD	0.099	0.679	0.171
MEC	0.027	0.339	0.101
ALD	0.263	0.852	0.627
DIE	0.293	0.383	0.041
HCL	0.428	0.480	0.104
CHL	1.000	0.751	0.212
LIN	0.027	0.000	0.000
HCB	0.057	0.574	0.187
PCN	0.054	0.180	0.028
PCP	0.012	0.354	0.010

Some notational remarks are given for the convenience of the reader, albeit these basic concepts can be found in many references; see for instance [2, 3, 15, 16].

a. Objects, for which $x \leq y$ or $x \geq y$ are called comparable, in sign $x \perp y$. A set of objects for which only $x \perp y$ holds can be completely ordered or (syn.) ranked.

b. Objects, for which Eq. 1 does not hold, are called incomparable. When object x is incomparable with y, it is denoted $x \parallel y$. In reference to the starting point of this analysis, i.e., the MIS, incomparability indicates a conflict in data, because there is at least one indicator for which $x > y$, and another, for which $y > x$.

c. Objects for which $q_i(x) = q_i(y)$ for all $i = 1,..,k$ are called equivalent. The usual elaboration of the partial order is based on representative elements of the equivalence classes and the information about the equivalence classes is retained as background material. An equivalence class consisting of more than one element is called nontrivial. A measure , introduced quantifying the extent of (nontrivial) equivalence classes is:

$$K = \Sigma N_i*(N_i-1) \quad (2)$$

N_i being the elements in the ith equivalence class. Singletons do not contribute to the sum.

As at the same time for $r = |X|$ it is valid $r = \Sigma N_i$, it can be easily shown by the method of maximizing functions under additional constraints (sometimes called method of Lagrange), see for example [23] that an equal population of the equivalence classes (i.e. $N_1=N_2=... >1$) maximizes K. Hence K is a considered as a good measure to quantify the role of equivalence classes, especially when the number of nontrivial equivalence classes is the same for different variants, as will be discussed later. In the following the defining equations are thought of as taken from a set without equivalent elements.

d. The set $U(x, P)$ denotes the set of incomparable elements. Thus, $U(x, P) = \{y \in X: y \parallel x \text{ in } P\}$

e. Priority elements

1. Isolated elements $Iso(X, P) = \{x: x \in X, \text{ there is no } y \in X, \text{ such that } x \perp y\}$ (3)
2. Maximal elements $Max(X,P) = \{x: x \in X, \text{ there is no } y \in X, \text{ such that } y > x\}$ (4)
3. Minimal elements $Min(X,P) = \{x: x \in X, \text{ there is no } y \in X, \text{ such that } y < x\}$ (5)

Isolated, minimal and maximal elements are of general interest as they are the extreme objects. Often a ranking is performed just to find the top- and bottom elements.

f. Chains: Let $C \subseteq X$, if all x, y $\in C$ obey (1) then C is called a chain. (6)

g. Antichain (AC): Let $AC \subseteq X$, if for all x, y $\in AC$ is valid x ‖ y,
then AC is called an antichain (7)
Chains are subsets of objects for which a complete ranking can be obtained, without the need of an aggregation of indicators to a one-dimensional ranking scalar ("vertical analysis of the Hasse diagram technique).
Antichains are of interest, because here conflicting objects are displayed. Usually one is interested in the indicators which cause the conflict, see [24].

h. A weak order is a binary relation, which is reflexive, complete, and transitive in contrast to a total order that further requires antisymmetry. Because antisymmetry in not required, a sequence of objects may have ties, such as the weak ordered set {a, b, c, d} may be represented as a < b ≅ c < d.

i. Matchings of two posets: Let x, y ∈ X. Let $\therefore$ be a symbol for the relation between x and y, i.e. $\therefore$ may be taken from the set {<, >, ‖, ≅}. When two posets are to be compared, it can be done by checking x $\therefore_1$ y for the first and x $\therefore_2$ y for the second poset. There are 16 different combinations such as <<, <>, ><, ‖< , etc. possible. These 16 combinations are called matchings which can be condensed to five typical outcomes, such as "isotone" (<< or >>), "antitone" (<> or ><), etc. (see below). See for further details [3]. A simple method to determine the proximity of two posets is to count coincident matchings when all objects of X are mutually compared in poset 1 and in poset 2.

2.3 Basic remarks concerning fuzzy posets and ELECTRE III

Fuzzy posets

The core of fuzzy posets is that the <-relation is replaced by a fuzzy inclusion relation, by a matrix of subsethoods SH(x, y) describing as to how far x < y. The needed approach is described by [25] is given as follows: Once again any logical difficulty is avoided, when it is assumed that the scaling level of indicators is a metric one. Then the fuzzy subsethood SH(x, y) between x and y is:

$$SH(x,y) := \frac{\sum_{i=1}^{k} \min(q_i(x), q_i(y))}{\sum_{i=1}^{k} q_i(x)} \text{ , m number of indicators} \qquad (8)$$

If the nominator equals 0 then SH(x, y) is set to 1.

The resulting matrix *SH* among all pairs of objects does not necessarily describe a partial order. There are several steps necessary (see [25-28]) to get a matrix R_{pre} which fulfills the axioms of a partial order relation. As usual, one of the central steps (as in any fuzzy approach) is the final defuzzification. After the defuzzification the resulting matrix has only entries 0 and 1 according to a user determined *α-cut* (Eq. 9).

The entries of matrix R_{pre} are called $r_{i,j} \in (0,1]$ (in former publications also α). These entries describe the subsethood (near 0, no subsethood, near 1 almost a complete subsethood). Eq. 9 describes the role of the user given *α-cut*, by which a crisp matrix R is obtained.

$$R_{i,j} = \begin{cases} 1 if \ \ r_{i,j} \geq \alpha - cut \\ 0 \qquad otherwise \end{cases} \qquad (9)$$

Lowering/enlarging the α-cut means that larger/smaller data differences are tolerated to get equivalence classes. The list of the entries of R_{pre} ordered for increasing values is helpful information for the user to find his α-cut. By incorporating objects into equivalence classes the number of x ⊥ y -, as well as of x ∥ y - relations is reduced. By applying the fuzzy poset concept the main interest is in the reduction of the incomparability relations. A direct relation of the α-cuts to the numerical noise in data is not possible. Therefore other attempts as a fuzzy-like Monte-Carlo-simulation [29] or hierarchical cluster analysis [15] are of interest. The methodological advantage of the fuzzy poset concept is that tolerating or not of numerical differences is not necessarily related to the statistical concept of noise.

ELECTRE III

As PROMETHEE [22], ELECTRE III is a MCDA-method aiming at a one dimensional scalar, by which a ranking of the objects can be performed. ELECTRE III is one method out of a family of methods, known as “ELECTRE family”. There are numerous descriptions of ELECTRE III (and its variants) [6, 18, 19] may serve as selected references on this theme. Important in the context of this paper is the brief discussion of the parameters of ELECTRE III. An elaborate description can be found in [20].

1. Indifference: Numerical differences of indicator values may be considered as irrelevant. They are considered as irrelevant when the absolute difference of indicators is less than a certain limit, which can be specifically selected for each indicator and for each object (within the simplified ELECTRE-module of PyHasse the relation to the objects is suppressed);

   thus, indifferent if: $q_i(x) - q_i(y) \leq g_i(y),\ i = 1,...,k$ (10)

   which means that with respect to the i^{th} indicator the two objects x and y are equivalent: $x \cong y$.
2. Significance: A preference between two objects can be clearly stated, when the absolute difference of indicator values exceeds a certain limit. This limit can be selected separately for each indicator and for each object (once again in PyHasse the dependency on objects is suppressed). Indicator values larger than the indifference and less than the significance level are mapped linearly onto a new scale. The significance degree ($p_i(y)$ is given as

   $q_i(x) - q_i(y) > p_i(y),\ i = 1,...k$ (11)

   then with respect to the considered indicator q_i, the object x is to be preferred over y, i.e. $x > y$.

   When the difference of the i^{th} indicator for x and y is less the significance level $p_i(y)$, then a linear interpolation is performed, when the concordance $c_i(x,y)$ is to be calculated.

3. With help of (1) and (2) a concordance $c_i(x,y)$ is defined, which describes the preference of x over y with respect to the i[th] indicator.

$$c_i(x,y) := \begin{cases} 1 & if \quad q_i(x) \geq q_i(y) - g_i(y) \\ \dfrac{q_i(x) - q_i(y) + p_i(x)}{p_i(x) - g_i(x)} & if \quad q_i(x) \geq q_i(y) - p_i(x) \\ 0 & otherwise \end{cases} \tag{12}$$

By introducing the weights w_i the concordance index $c(x,y)$ is found:

$$c(x,y) = \frac{\sum_{i=1,..k} w_i \cdot c_i(x,y)}{\sum_{i=1,..k} w_i} \tag{13}$$

4. By the steps 1-3 the degree of the preference of object x over y, $c(x, y)$, or the degree of the preference of object y over x, $c(y, x)$, can be stated. In ELECTRE III a discordance is defined, to express as to how far the preference y over x can outbalance that of the preference x over y. In order to describe the discordance a new parameter, the parameter veto, v_i, is introduced. The veto depends on the indicator actually considered and the object. As in the steps 1-2 the dependence of the parameters $veto_i$ on objects is suppressed.

$$d_i(x,y) = \begin{cases} 1 & if \; q_i(y) - q_i(x) > v_i(x) \\ \dfrac{q_i(y) - q_i(x) - p_i(x)}{v_i(x) - p_i(x)} & if \; q_i(y) < q_i(x) + p_i(x) \\ 0 & otherwise \end{cases} \tag{14}$$

When there is an indicator, which favors y over x strongly, then the discordance gets its maximal value. In other cases a linear interpolation with the minimal value = 0 is applied to calculate the discordance indicator.

5. Weights: To get the final outcome the scaled preferences are combined by means of weights. The weights are associated with each single indicator. Due to [6] the

unwanted compensation effect is somewhat reduced in ELECTRE III in comparison to the compensation effect when linear weighted sums are considered.

6. Concordance index $c_i(x, y)$ and discordance indices $d_i(x, y)$ are combined to obtain the credibility index $s(x, y)$ which varies in the range [0,1]. The value $s(x, y) = 1$ expresses a strict preference of x over y , taken all significance, indifference, weights, and veto-values into account. In that sense ELECTRE III is a fuzzy method, as values less 1 are possible too.

$$s(x,y) := c(x,y) \cdot \prod_{i \in D} \frac{1 - d_i(x,y)}{1 - c(x,y)} \qquad (15)$$

$$i \notin D, \; then : s(x,y) = c(x,y)$$

The set D is the set of indicators. where $d_i(x, y) > c(x, y)$.
When $d_i(x, y)$ gets it maximal value for all i, then the role of the veto is, to overrule $c(x,y)$ because then $s(x, y) = 0$.

7. From the matrix $s(x,y)$ the row- and column sums can be calculated. The row sum expresses the dominance of x over y, whereas the column sum the dominance of y over x is expressing, i.e. the sub-dominance of x in comparison to y. The final matrix is in ELECTRE III analyzed by a stepwise selection process which ends up in a ranking index. Here, instead the dominance and sub-dominance vectors Dom, Sub are calculated. Most often dominance and subdominance do not lead to conflicts. Hence, if x is very dominant over y, then y is very weakly dominant over x. However, in some times conflicts appear, therefore both vectors correctly oriented, for example Dom(x), S':= max(Sub) - Sub(x), can be considered as an ELECTRE-MIS system and can once again analyzed by a partial order. In the following, the MIS evaluated by fuzzy partial order is compared with the two-indicator system Dom(x), S'(x) as the outcome of ELECTRE III.

2.4 Software PyHasse

Based on the free available interpreter programming language Python (Python vs 2.6), the first author developed a software package, called PyHasse. "Py" stands for Python, and "Hasse" stands for the mathematician Helmut Hasse, who made Hasse diagrams and partial order popular [30]. PyHasse now includes more than 100 specialized programs (see [31]). In the future PyHasse will be available in two versions: A package, including some selected (simplified) modules, which will be accessible through the Internet (and which are based on Python 3.4), and a version, considered now as an expert version, containing all modules, but only available on request and dispatched by compact discs. Both PyHasse variants will be developed further according to actual tasks and demands.

2.5 Hasse diagram and some results of the PBT-substances

Application of Eq. 1 leads to a poset that can be visualized by the Hasse diagram is shown in Fig. 1.

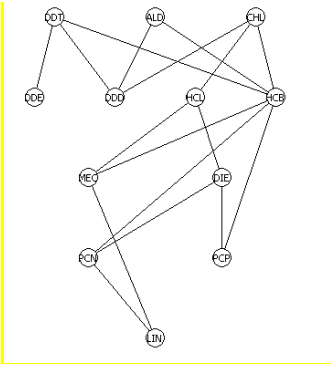

Figure 1. Hasse diagram of the 12 PBT-substances [1]. Indicators are Persistence, Bioaccumulation and Toxicity (PyHasse software).

In [2,15] details were presented, which can be drawn from the inspection of Fig. 1. In graph-theoretical terms the Hasse diagram has a structure, see for example the subset {DDT, DDE, ALD, DDD} which has no order theoretical connection with {HCL, DIE}, whereas the set {DDE,DDD} has no order theoretical connection to {HCB, HCL, MEC, DIE, PCN, PCP, LIN} i.e. to almost all others. It is important to note that any decision support system mapping the set of indicators onto one ranking index will lose this specific information as the only

graph-theoretical structure is that of a single chain. We note that the count of incomparabilities of the poset, visualized in Fig. 1 equals 31.

Evaluation, as presented here, is based on data, even of different scaling levels. However, when indicators have the same scaling level (implying a metric) as it is the case in the study discussed here, it is justified to classify data conflicts, where the numerical data differences are small as non-existent. In contrast one may search for data profiles which are strikingly deviating from the others.

3 View into incomparabilities

3.1 Fuzzy partial order

The data of Sailakhanauly [1] are columnwise normalized, while the fuzzy analysis is performed with the module fuzzyHD16_1.py of PyHasse. The mathematical background is explained in [28]. In Table 2 the entries of the matrix R_{pre},i.e., the matrix elements $r_{i,j}$, sorted for increasing values, are shown. For the defuzzification to get a crisp partial order these data can be helpful to select appropriate α-cuts. For example, different *α-cuts*, taken from an interval between two subsequent values of the matrix elements of R_{pre} will not lead to different partially ordered sets. On the other hand at intervals of subsequent matrix entries, which are very small only a careful selection of an *α-cut* will render a relevant result.

Table 2: Values of the R_{pre}-matrix, $r_{i,j}$ see section 2.3, ordered for increasing values.

0.102	0.537	0.572	0.586	0.625	0.67	0.704	0.708	0.75	0.771
0.783	0.819	0.838	0.871	0.877	0.897	0.898	0.911	0.941	0.959
0.96	0.962	0.969	0.988	0.993	0.997	1.0			

We first perform a defuzzification at α-cut = 0.9 which means that 10 values of R_{pre}, those > 0.9, gets the value 1. By this selection we are close to the original data, i.e., even relatively small numerical differences are not ignored (Fig. 2), nevertheless it cannot be expected that the original Hasse diagram (Fig.1) will be obtained, applying Eq. 1 directly on the (normalized) data.

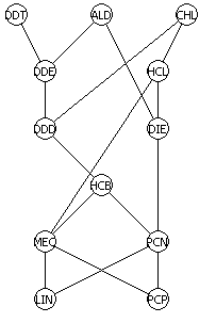

Figure 2. Hasse diagram based on the defuzzification at 0.9;
no nontrivial equivalence classes, i.e., K = 0 (Eq. 2).
Note, there is an artificial overlap of edge (PCP, DIE)
and the vertex PCN. In reality PCN ‖ PCP.

In comparison to the Hasse diagram shown in Fig. 1 the number of incomparabilities is reduced (now 17 incomparable pairs of representative elements), the graph gets a more "slim" appearance, with now 6 levels. It is further noted that now DDE and DDD are comparable to many other chemicals. A further relaxation (Fig. 3) by selecting the α-cut at 0.75 (more or equal than 19 entries of R_{pre} will become the value 1) leads to some nontrivial equivalence classes.

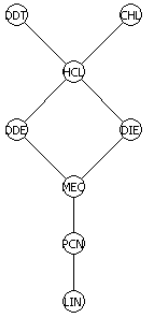

Figure 3. Defuzzification at 0.75. Nontrivial equivalence classes:
[DDT, ALD], [DDE, DDD, HCB], [MEC, PCP]. *K*=10 (Eq. 2)

In Fig. 3 the partial order based on the representative elements has only two incomparabilities. Hence it can be seen that the fuzzy concept is an efficient method to reduce incomparabilities, without forcing them to disappear, as in most MCDA-methods. Now, the chemicals DDE (and DDD as an element of the equivalence class, represented by DDT) are only incomparable with DIE.

An even further relaxation to a defuzzification *at* α*-cut* = 0.7 leads to a total order LIN < PCN < MEC < DDE < DIE < DDT < CHL within the set of representative elements. With respect to the complete set X the obtained sequence is a weak order, because there are nontrivial equivalence classes: [DDT, ALD], [DDE, DDD, HCB], [MEC, PCP], [DIE, HCL].

Defuzzification at 0.6 leads to a weak order with respect to the set X: LIN < PCN < MEC ≅ PCP < DDE ≅ DDD ≅ DIE ≅ HCL ≅ HCB < DDT ≅ ALD ≅ CHL, K = 28 (Eq. 2).

As can be seen by inspecting Figures 2 and 3 the number of incomparabilities is drastically reduced, when *the* α*-cut* is decreased. When α*-cut* gets values such as 0.7 or 0.6 even no incomparability appears, we get weak orders, related to the object set X.

3.2 Application of ELECTRE III

The PyHasse module applied for this part of the study is electresimpl6_3.py
We selected the following parameters:

- indifference level for all three indicators: 0.1
- significance level for all three indicators 0.2
- veto-level for all three indicators: 0.2
- weights: 0.33,0.33,0.34, e.g., virtually equal for the three indicators

Starting from the columnwise normalized data matrix of [1] the result is shown in Fig. 4.

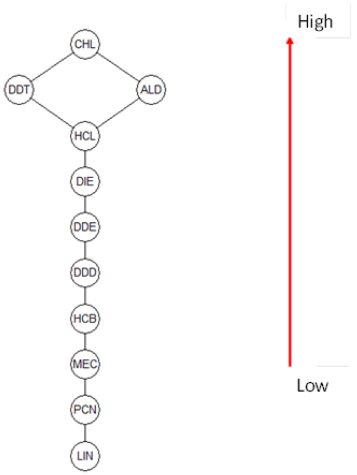

Figure 4. Result of a simplified version of ELECTRE III.
Nontrivial equivalence class: [MEC, PCP]

3.3 Proximity analysis

The theoretical basis of the proximity analysis is briefly explained in section 2.2 and in more detail in [3]. An application on human health can be found in [32].

The software package PyHasse offers several modules to perform the proximity analysis, here the module similarity10_1.py. The results of the proximity analysis among the posets a) ELECTRE III and b) three outcomes of the fuzzy poset method are shown in Table 3. As mentioned in sect. 2.2 the results are in terms of the condensed quantities isotone, antitone, indifferent (not to be confused with indifference in ELECTRE III), weak isotone and equivalent. There are by r*(r-1), r being the number of chemicals (here: r = 12) relations possible, when all possible object pairs are considered (i.e. DDE, DDD) as well as (DDD, DDE)).

The overall proximity is the sum of isotone and weak isotone, divided by the total number of possible relations, i.e., 12*11/2 = 66. (The consideration of (x,y) and (y,x) bears no new information with respect to the proximity calculation, therefore only r*(r-1)/2 comparisons are needed and counted as isotone, antitone, etc.)

Table 3: Contribution to the five characteristics of similarity.

	α-*cut* = 0.9	α-*cut* = 0.75	α-*cut* = 0.6
overall proximity	0.742	0.909	0.985
incomparabilities, based on the object set	17	5	0
Count of nontrivial equivalence classes	0	3	3
K (Eq. 2)	0	19	28
isotone, matchings such as: >>, <<	48	56	52
antitone, matchings such as: ><,<>	0	0	0
weak isotone, matchings such as: >=, <=,…	1	3	12
indifferent, matchings such as: ‖>, ‖<,…	17	6	1
equivalent, matching: ==	0	1	1

4 Discussion

4.1 Fuzzy posets as substitute for ELECTRE?

First of all it can be seen that there are no conflicts in the order-relations. That means there is no contribution to antitone; it cannot be happen that the outcome of ELECTRE states x > y, whereas the outcome of fuzzy partial order states x < y.

The above described overall proximity (*isotone*+*weak isotone*)/(*r**(*r*-1)/2) is only a measure for a first orientation. As can be seen (Table 3) this number, not surprisingly, increases with decreasing α-*cut*. Decreasing α-*cuts* are causing larger and larger equivalence classes, until finally the chemicals are all in one equivalence class. Hence, the overall proximity unambiguously tends toward the value 1. More differentiated information is the contribution to isotone. Here it can be seen that this contribution does not increase with decreasing α-*cuts*. Instead isotone is reduced, when α-*cut* = 0.6, because too many equivalences in the fuzzy poset appear. Consequently, taken these three α-cuts, the best coincidence is obtained, where isotone gets its maximum. Here the maximum among the three cases is found at α-*cut* = 0.75. The overall proximity is still > 0.9 which is considered as a good coincidence between the

MCDA-method ‘ELECTRE’ and the fuzzy-poset method. The inspection of Table 3 shows clearly that only the parameter (in fact the only parameter) *α-cut* was varied in the case of the fuzzy-poset method, whereas ELECTRE allows the variation of the 12 parameters (cf. section 3.2). It is completely clear that for example extreme weighting schemes, which may often be pretty subjective, which favors one indicator on the expense of the other two, a good counter-part could not be found in the fuzzy-poset - method, as by the very definition, the attributes cannot combined by weights in an obvious and simple manner.

Hence, a fair comparison of ELECTRE with fuzzy posets needs at least equal weights, which still leaves 9 parameters that potentially could be varied (cf. 3.2). Due to the same reasons, a differentiation of one parameter type, say for example ‘indifference’ with the indicators is not appropriate. Thus, in fact ELECTRE III, in order to be compared with fuzzy-poset-methods can only be varied, taking the same different values of indifference, significance and veto for any indicator, i.e., three parameters.
In a future study further combinations in the sense described here will be studied. However, this is outside the scope of the present study.

We may now pose the question: Is the possibility to model decision situations by three parameters better than that given by the fuzzy-poset method, where only one parameter, *α-cut*, can be varied? Unambiguously, the answer is bivalent. When an appropriate statistical analysis can be performed leading to an idea about what indifference and significance and veto should be, then ELECTRE is clearly a model, where this knowledge can be modeled. Thus, in such case a decision based on ELECTRE has a firm basis. Otherwise, any reduction of arbitrariness should be an important aspect. In that sense the fuzzy partial order method offers possibilities, which should be applied, when the (statistical) background knowledge is poor. In [33, 34] suggestions are made how to find an optimal *α-cut*, nevertheless here still much research is needed.

4.2 Is the concept of partial order still needed in order to perform MCDA?

The above discussion (Section 3) was devoted to reduce the role of incomparability in different ways.

Applying ELECTRE III , albeit in a simplified version most of the objects could be given a certain rank (see Fig. 4). Although Roy [35] makes clear that the graph theoretical representation of the partial order is an important step within the ELECTRE-family and although PROMETHEE I ends with a partial order [19], the main purpose of MCDA-methods is to "squeeze out" a total order in order to facilitate or at least support decision making.

So, why partial order, where incomparabilities will appear?
Even if we could argue that many MCDA methods require a high scaling (quantitative) level, whereas partial order in general is not restricted on indicators having a high or the same scaling level, we cannot use this argument in the study presented here, as we here have quantitative data, which allow defining distances etc. So we can sharpen the question to 'Do we need partial order when the entries of the data matrix are quantitative data?' We will argue 'yes'. The point of view by partial order is that of an analysis of an evaluation. We want to see the conflicts, and then to analyze them, we want to see the chains, which display objectively (at least if the data matrix is objectively designed) total orders of subsets of X. We want to see and understand why an object to be evaluated has a position in terms of a vertical (rank oriented view) as well in terms of a horizontal evolution (conflict oriented view). This kind of twofold, but intertwined view is also typical for the well-known method of POSAC, [36-38] which in our eyes [39] should attract much more interest within the MCDA-scene.

When the poset's visualization by a Hasse diagram is not helpful, because of the multitude of lines, then the aspect of why is an object located where it is can be investigated by

- applying navigation tools
- applying cluster analysis (hierarchical or e.g. kmeans [15])
- applying fuzzy concepts as explained here.

If the Hasse diagram is not helpful, because the fraction of incomparable pairs is overwhelming, then it is helpful to

- check the data matrix as explained by [40], especially check as to how far too much information is paralyzing the decision.
- sort out criteria whose indicators lead to conflicts with respect to all objects (problem of the correct orientation) ,
- perform partial order analyses with classes of criteria
- or apply METEOR (see [3, 41,42] to trace back where weights are crucial in getting the final total order.

4.3 Need of parameters in evaluation

4.3.1 Non-fuzzy-methods

Basically the Hasse diagram technique (HDT) does not need any parameters, once a data matrix is designed. As in statistical applications, where confidence limits are to be preselected by the user, in HDT limits must be defined to get further insights. So further analyses need parameters as explained in Table 4.

Table 4: Parameters useful for procedures beyond HDT

Parameter	Tasks	Module of PyHasse	Remarks	References
f	control of distances	incompposet	"pecularity of data profiie"	[2]
Δ	control of the numerical differences of incomparable objects	scan_incomp	"Which object pair and which indicator pair have a conflict $\geq\Delta$	[2]
cut-level	hierarchical cluster analysis	dendrogram4	determines which partition can be selected and hence which transversale can be defined	[15]

4.3.2 Method of Fuzzy-posets

This method, which specifically intends to avoid hard yes/no - decisions with respect to x < y, x = y, or x>y, needs the parameter α-*cut*, which can be interpreted as degree of exactness, to which the data can be attributed. So if α-*cut* = 0, then any numerical value is unimportant, whereas if α-*cut* = 1, any known digit is of importance and is mapped into the position of objects in a Hasse diagram. In any case there is a single parameter governing the output of the PyHasse module. In contrast the MCDA tools (for a review, see [6, 19]) starting from a given evaluation matrix (data matrix) needs many parameters:

- weights (as for example in PROMETHEE,ELECTRE, weighted sums)
- parameters determining the form of local preference functions (PROMETHEE)
- parameters describing indifference, significance, veto and credibility. (ELECTRE)

Hence HDT is not only parameter free (in the sense of does not require a distribution characteristic) but also 'economical' with respect to parameters.

4.4 How do we locate HDT with respect to MCDA and conventional multivariate statistics

First of all, HDT is pretty new in comparison to the both other methods. MCDA goes back to Borda and Condorcet 18th century [6], statistics has its roots with Laplace in the 18th century too, albeit cluster analysis and principal component analysis have remarkable younger birthdays (whenever it is possible to date these techniques). Partial order was firstly investigated by Dedekind, who called partially ordered sets "dieder-gruppen" (German). Birkhoff and Hasse made partial order popular [31, 43]. Patil and Taillie seem to be the first which apply Eq. 1 to get data-driven posets [45,46]. Halfon applied Eq. 1 to environmental chemical [47] and even earlier to a classification of mathematical transport and behavior models [48]. In Halfon's papers the evaluation aspect was in the focus. Ranking as a tool to evaluate objects is clearly the main result in many MCDA-methods, whereas ranking is not in the focus of conventional multivariate statistics, albeit they are very helpful to deduce evaluations. See instance Lindgren, [49] who applied PCA to derive a ranking of chemicals. As in MCDA the concept of incomparability does not play a role, it can be observed "on the fly" but is not an aim per se. Hence, from the point of view of HDT, Hasse diagrams, which

are complete orders (i.e. all objects are in a chain) allow a quick evaluation but do not have metric information. In Hasse diagrams where antichains are dominant such that no direct conclusion is available the questions should arise:

- Are the indicators well selected and adequate concerning the problem?
- Are numerical differences important, even if they are small?

An answer on both questions with “no” means that the design of the MIS should be improved. Most informative are those Hasse diagrams which incorporate chains as well as some incomparabilities. In that case we are talking about a “structure “ of the Hasse diagram and only in that case methods as described here can be applied in a meaningful manner. So we see HDT as an increasing field in the intersection of multivariate statistics and MCDA-methods, where the ranking and the indicators in their role for a ranking can be studied.

5 Conclusions and Outlook

In this paper the huge space of parameters to be applied on ELECTRE III was drastically reduced by

1. letting the indifference, significance and veto-parameters being independent on the indicator values of the objects and
2. let all parameters of the four types (indifference, significance, veto, weights) being the same or almost the same for all indicators

It is clear that by this procedure of defining the ELECTRE parameters we lose all possibly important freedoms to model a decision problem. Instead this paper is focused on the role of the α-*cuts* and on the question as to how far the fuzzy posets are not in contradiction to the ELECTRE III results. Not surprisingly that defuzzification was the best, which lets only five incomparabilities and only few nontrivial equivalence classes. It can be stated that if no preferences among the indicators are formulated (equal significances, indifferences, veto-values, weights) then the fuzzy poset approach is able to reproduce the order relations found by ELECTRE III.

Nevertheless two main questions remain open:

1. Can we relate the *α-cuts* with certain statistical measures of uncertainty or noise? and
2. What happens if the restrictions 1. and 2. are relaxed?

As already mentioned, it is the very nature of the partial order approach not to need to define preferences among the indicators. So the question is not, how good can the fuzzy approach model the ELECTRE approaches, but at which parameter - constellation of ELECTRE III the fuzzy approach taking all indicators into account will fail (measured by an properly defined quantity).

References

[1] Y. Sailaukhanuly, A. Zhakupbekova, F. Amutova, L. Carlsen, On the ranking of chemicals based on their PBT characteristics: Comparison of different ranking methodologies using selected POPs as an illustrative example, *Chemosphere* **90** (2013) 112–117.

[2] R. Bruggemann, L. Carlsen, Incomparable – What now I? *MATCH Commun. Math. Comput. Chem*. **71** (2014) 699–714.

[3] R. Bruggemann, G. P. Patil, *Ranking and Prioritization for Multi-indicator Systems - Introduction to Partial Order Applications*, Springer, New York, 2011.

[4] L. Carlsen, R. Bruggemann, An analysis of the "failed states index" by partial order methodology, *J. Soc. Struc*. **14** (2013) 1–31.

[5] P.Annoni, R. Bruggemann, L. Carlsen, A multidimensional view on poverty in the european union by partial order theory, *J. Appl. Stat.*, in press.

[6] G. Munda, *Social Multi–Criteria Evaluation for a Sustainable Economy*, Springer–Verlag, Berlin, 2008.

[7] M. T. D. Cronin, D. J. Livingstone, *Predicting Chemical Toxicity and Fate*, CRC Press, New York, 2004.

[8] D. Showanek, K. Fox, M. Holt, R. Schroder, V. Koch, G. Cassani, M. Matthies, G. Boeije, P. Vanrolleghem, A. Young, G. Morris, C. Gandolfi, T. C. J. Feijtel, GREAT-ER: a new tool for management and risk assessment of chemicals in river basins - Contribution to GREAT-ER #10, *Wat. Sci. Tech.* **43** (2001) 179–185.

[9] J. Klasmeier, M. Matthies, Georeferenzierte Expositionsmodellierung in Flussgebieten, in: J. Wittmann, D. K. Maretis (Eds.), *Simulation in Umwelt- und Geowissenschaften, Workshop Osnabrück 2003*, Shaker-Verlag, Aachen, 2003, pp 95–107.

[10] European Union System for the Evaluation of Substances 2.0 (EUSES 2.0). Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands (RIVM Report no. 601900005). J. P. A. Lijzen, M. G. J. Rikken (Eds.), Available via the European Chemicals Bureau, http://ecb.jrc.it, 2004.

[11] F. A. M. Verdonck, G. Boeije, V. Vandenberghe, M. Comber, W. de Wolf, T. Feijtel, M. Holt, V. Koch, A. Lecloux, A. Siebel–Sauer, P. A. Vanrolleghem, A rule–based screening environmental risk assessment. Tool derived from EUSES, *Chemosphere* **58** (2005) 1169–1176.

[12] V. Berding, S. Schwartz, M. Matthies, Visualisation of the complexity of EUSES, ESPR–*Environ. Sci. Pollut. Res*. **6** (1999) 37–43.

[13] Stockholm Convention http://chm.pops.int/Home/tabid/2121/language/en-GB/Default.aspx (accessed Nov. 2014).

[14] J. Vijgen, C. Egenhofer, Obsolete (lethal) Pesticides, A ticking time bomb and why we have to act now. http://www.ihpa.info/docs/library/reports/timeBomb_Obsolete_Pesticides.pdf (see also http://www.ihpa.info/) (accessed Nov. 2014).

[15] R. Bruggemann, L. Carlsen, Incomparable: what now II? Absorption of incomparabilities by a cluster method, *Qual. Quant.*, in press.

[16] L. Carlsen, R. Bruggemann, O. Kenessova, E. Erzhigitov, Evaluation of analytical performance based on partial order methodology, *Talanta* **132** (2015) 285–293.

[17] B. Roy, Electre III: Un Algorithme de Classements fonde sur une representation floue des Preferences En Presence de Criteres Multiples, *Cahiers du Centre d'Etudes de Recherche Operationelle* **20** (1972) 32–43.

[18] B. Roy, D. Bouyssou, Comparison of two decision-aid models applied to a nuclear power plant siting example. *Eur. J. Oper. Res.* **25** (1986) 200–215.

[19] J. Figueira, S. Greco, M. Ehrgott, *Multiple Criteria Decision Analysis, State of the Art Surveys*, Springer, Boston, 2005.

[20] J. Borken, Umweltindikatoren als ein Instrument der Technikfolgenabschätzung - Selektion, Aggregation und multikriterielle Bewertung am Beispiel des Verkehrs. Fakultät für Angewandte Wissenschaften. Universität Freiburg/Breisgau. PhD-Thesis, 2005, 153 pp.

[21] A. Colorni, M. Paruccini, B. Roy, *A-MCD-A, Aide Multi Critere a la Decision, Multiple Criteria Decision Aiding*, JRC European Commission, Ispra, 2001.

[22] J. P. Brans, P. H. Vincke, A preference ranking organisation method (The PROMETHEE method for multiple criteria decision - making), *Manag. Sci.* **31** (1985) 647–656.

[23] J. N. Bronstein, K. A. Semendjajew, Taschenbuch der Mathematik, B. G. Teubner, Stuttgart, 1991.

[24] R. Bruggemann, K. Voigt, Antichains in partial order, example: pollution in a German region by lead, cadmium, zinc and sulfur in the herb layer, *MATCH Commun. Math. Comput. Chem*. **67** (2012) 731–744.

[25] B. Kosko, Neural Networks and Fuzzy Systems - A dynamical Systems approach to Machine Learning. Pentice Hall, London, 1992.

[26] B. De Baets, H. De Meyer, On the existence and construction of T-transitive closures. *Inf. Sci.* **152** (2003) 167–179.

[27] B. Van de Walle, B. De Baets, K.C. Kersebaum, Fuzzy multi-criteria analysis of cutting techniques in a nuclear dismantling project, *Fuzzy Sets Sys.* **74** (1995) 115–126.

[28] R. Bruggemann, A. Kerber, G. Restrepo, Ranking objects using fuzzy orders, with an application to refrigerants, *MATCH Commun. Math. Comput. Chem*. **66** (2011) 581–603.

[29] R. Wieland, R. Bruggemann, Hasse diagram technique and Monte Carlo simulations, *MATCH Commun. Math. Comput. Chem*. **70** (2013) 45–59.

[30] H. Hasse, *Vorlesungen über Klassenkörpertheorie*, Physica-Verlag, Marburg, 1967.

[31] R. Bruggemann, L. Carlsen, K. Voigt, R. Wieland, PyHasse software for partial order analysis: Scientific background and description of selected modules, in: R. Bruggemann, L. Carlsen, J. Wittmann (eds.), *Multi-indicator Systems and Modelling in Partial Order*, Springer, New York, 2014, pp. 389–423.

[32] K. Voigt, 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. Modell. Softw.* **25** (1010) 1801–1812.

[33] K. De Loof, M. Rademaker, R. Bruggemann, H. De Meyer, G. Restrepo, B. De Baets, Order theoretical tools to support risk assessment of chemicals, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 213–230.

[34] P. Annoni, P., M. Fattore, R. Bruggemann, A multi-criteria fuzzy approach for analyzing poverty structure, *Stat. Appl.* (2011) 7–30.

[35] B. Roy, The outranking approach and the foundations of the ELECTRE methods, in: C. A. Bana e Costa (Ed.), *Readings in Multiple Criteria Decision Aid*, Springer–Verlag, Berlin, 1990, pp. 155–183.

[36] S. Shye, R. Amar, Partial-order scalogram analysis by base coordinates and lattice mapping of the items by their scalogram roles, in: D. Canter (Ed.), *Facet Theory: Approaches to Social Research*, Springer-Verlag, New York, 1985, pp. 277–298.

[37] S. Shye, Facet theory, in: T. Husen, T. N. Postlethwaite (Eds.), *International Encyclopedia of Education*, Pergamon Press, Oxford, 1994, pp. 2213–2219.

[38] I. Borg, S. Shye, *Facet Theory - Form and Content*, Sage Publ., Thousand Oaks, 1995.

[39] R. Bruggemann, L. Carlsen, Multi-criteria decision analyses. Viewing MCDA in terms of both process and aggregation methods: Some thoughts, motivated by the paper of Huang, Keisler and Linkov, *Sci. Tot. Environ*. **42** (2012) 5293–5295.

[40] G. P. Patil, W. L. Myers, R. Bruggemann, multivariate data sets for inference of order: Some considerations and explorations, in: R. Brüggemann, L. Carlsen, J. Wittmann (Eds.), *Multi-indicator Systems and Modelling in Partial Order*, Springer, New York, 2013, pp. 13–45.

[41] U. Simon, R. Bruggemann, S. Pudenz, Aspects of decision support in water management - example Berlin and Potsdam (Germany) II - improvement of management strategies, *Wat. Res*. **38** (2004) 4085–4092.

[42] U. Simon, R. Bruggemann, S. Mey, S. Pudenz, METEOR - application of a decision support tool based on discrete mathematics, *MATCH Commun. Math. Comput. Chem*. **54** (2005) 623–642.

[43] G. Birkhoff, *Lattice theory*, Providence, Rhode Island, 1984.

[44] M. G. Reggiani, F. E. Marchetti, On assessing model adequacy, *IEEE Trans. Sys. Man Cyber*. **5** (1975) 322–330.

[45] G. P. Patil, C. Taillie, Ecological diversity: concepts, indices and applications, in: The Biometric Society, Proceedings of the 9th Biometric Conference, Volume II; Boston, August 22-27, 1976. The Biometric Society, Boston, 1976, pp. 383–411.

[46] G. P. Patil, C. Taillie, Diversity as a concept and its measurement, *J. Am. Stat. Assoc*. **77** (1982) 548–561.

[47] E. Halfon, M. G. Reggiani, On ranking chemicals for environmental hazard, *Environ. Sci. Technol*. **20** (1986) 1173–1179.

[48] E. Halfon, Is there a best model structure ? I: Modelling the fate of a toxic substance in a lake, *Ecol. Modell*. **20** (1983) 135–152.

[49] F. Lindgren, L. Eriksson, S. Hellberg, J. Jonsson, M. Sjöström, S. Wold, A strategy for ranking environmentally occurring chemicals: Part IV: Development of chemical model systems for characterization of halogenated aliphatic hydrocarbons, *Quant. Struct. Act. Relat*. **10** (1991) 36–42.