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Hasse Diagram Technique and Monte Carlo Simulations

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Abstract

Monte Carlo simulations are well known within risk assessments; similarly there is some interest in applying simple elements of partial order theory in the field of decision analysis, ranking and evaluation. Much criticism concerning the application of partial order to data matrices originates from the translation of even small numerical differences of data into instances of partial order theory. It is mainly the appearance of incomparabilities that is often seen as being a disadvantage, especially when the data differences are considered irrelevant for ranking purposes. Several attempts to improve this situation have already been reported in the literature. The most effective approach to date is the fuzzy approach which, however, also has its disadvantages. For this reason, in this paper we combine Monte Carlo simulations with instances of partial order theory, namely the concept of dominance and separability of subsets into partially ordered sets. The example is taken from a well-known set of data, namely High Production Volume Chemicals (HPVC).

1 Introduction

There are around 100,000 chemicals on the market, many of which may be hazardous to the environment. A typical question that arises is: how can we decide which chemicals require special attention (see for instance [13])? One possibility is to rank chemicals

according to the hazard they pose to the environment. The problem is that there is no measurable quantity to describe "hazard to the environment". Instead, the practice is to select indicators that describe aspects of the environmental hazard. Therefore, the first step taken before chemicals can be ranked is to define indicators to suit the ranking purpose. The next step is to quantify the indicators such that a data matrix can ultimately built up combining the chemicals and the indicators. The columns of this matrix are defined by the indicators and the rows are associated with the corresponding chemical. The ranking of chemicals involves the analysis of a multi-indicator system [3, 4], which in turn necessitates an analysis of a data matrix with respect to the purpose of the ranking. Many techniques have been developed to tackle multi-indicator systems; famous examples are PROMETHEE [2] and ELECTRE [11]. Whereas these multi-criteria decision analysis (MCDA) tools are quite sophisticated, assigning a tuple of indicator values to a scalar, other methods such as weighted sums are very simple and are therefore often preferred over MCDA tools due to their transparency. In contrast to these MCDA methods, partial order keeps the indicator values separate (i.e. not numerically combined), meaning there is no compensation - an unwanted side-effect of MCDA tools [10]). The price, however, is that not all objects can be compared with all others; they are - in technical terms - incomparable.

Whether comparable or incomparable objects appear depends on the numerical values of the indicators. When the indicators are continuous in concept, then the problem is often that numerical differences within a single indicator seem to be irrelevant for the ranking purpose. The idea therefore arose [6, 8, 12] to apply fuzzy concepts. Van de Walle applied Kosko's subsethood measure, which combines the different indicators numerically. Although this internal aggregation (see below) assigns a scalar for each pair of objects, the structure of a partial order is maintained. Indeed, instead of the original data matrix a relational matrix arises, which leads to a family of partially ordered sets, ready for final analysis.

In this paper, we suggest a method following the basic idea of the Hasse diagram technique (HDT) [4]), which keeps the indicators separate and which extracts as much information as possible from the partial order relations. Our manuscript is organized in the following manner.

After summarizing Kosko's approach (see [6] for details) we introduce the method, which basically uses the concept of dominance and separability matrices [15]) (subsection 2.3); in the next subsection (section 2.4) we discuss the computer technical realization. Subsection 2.5 presents a simple fictitious example and the data matrix of a real case. The method is exemplified in section 3. We start off by using simple matrices of fictitious

objects for demonstration and then proceed to apply the method to the set of High Production Volume Chemicals (HPVC) from the EINECS list [14]. This set was also used to compare MCDA methods with the partial order concept, i.e. with HDT [9], and to demonstrate the variance-based sensitivity approach [1]. Finally we summarize our results in section 4 and discuss the method critically in section 4 and conclude the paper in section 5.

2 Method

2.1 Idea

Dominance and separability matrices, as introduced by Restrepo and Bruggemann, 2008 [15] are means to order disjoint classes of objects. In the following we call the ordered set of indicator values of an object x a "profile". When the profile is perturbed by Monte Carlo simulation, each new profile, denoted as $q(x^{rd})$, obtained from that of a given object x belongs to that object. We can therefore define classes by gathering all perturbed indicator value profiles that belong to certain objects and, instead of examining the order relations among the objects, we can discuss the dominance values of pairs of classes. When there is a criss-cross of profiles of objects x and y, caused by only small numerical differences, the dominance of x over y with respect to a subset of indicators is quite often similar to that of y over x. This fact can be used to define equivalence classes (complete set of indicators) and thus to find a new relational graph. More often, however, we find a dominance of x over y, and vice versa, only with respect to single indicators, which we will call "noise equivalence" (abbrev.: noise equiv.); see below for details. This idea is specified in the 'Theory' subsection. In the "Kosko-approach" subsection we summarize Kosko's widely used method to obtain fuzzy partial orders.

2.2 Kosko-approach

The idea behind Kosko's approach is to replace the order relation $x < y$ with a fuzzy subsethood, $SH(x, y)$. The subsethood matrix $SH(x, y)$ does not necessarily fulfill the axioms of a partial order. However, as shown in [7], there is an iterative method to obtain an approximate matrix that can be interpreted as a matrix describing a quasi order. After extracting the equivalence relations, a reduced matrix is obtained, which is the relational matrix of a strict partial order, [4]. The core of this approach is $SH(x, y)$, which is defined as:

$$SH(x,y) = \begin{cases} \dfrac{\sum_i min(q(x,i), q(y,i))}{\sum_i q(x,i)} & : \quad \sum_i q(x,i) \neq 0 \\ 1 & : \quad otherwise \end{cases} \tag{1}$$

The two summations of indicator values $q(x,i)$ (value of the ith indicator of object x) contrast with the idea of the Hasse diagram technique, which keeps the indicators (even if considered dimensionless by an appropriate normalization) separate (i.e. not numerically combined) for as long as possible in order to trace back the effect of each indicator to the ranking of objects. Although Kosko's approach works well and is able to reproduce the partial order by a crisp evaluation of the indicator values, we think that the numerical combination as in $SH(x,y)$ is a point that must be considered inconsistent.

2.3 Theory

Let X be the set of objects $x \in X$, $q(x)$ its tuple of indicator values and IB the set of indicators (information base). Let $q(x^{rd})$ be the tuple of values of x, randomly changed, given a certain distribution function D.

Let p be the parameters describing D and n the number of Monte Carlo simulations that change $q(x)$ into n tuples, called $q(x^{rd})$. We consider the map:

$$f : q(x) \rightarrow RD(x), with : RD(x) = \{q(x^{rd})\} \tag{2}$$

Formally we assign to each tuple $q(x^{rd})$ an object x^{rd} and consider the set $X(x,n) = \{x^{rd}\}$, obtained after n MC simulations. Thus, we install a one-to-one map:

$$X(x,n) \rightarrow RD(x) \tag{3}$$

We assume that p and n is the same $\forall x \in X$. Then instead of $|X|$ objects we have a set of $|X| * n$ objects called $X(n)$. $X(n)$ can be considered as a disjoint sum of $X(x,n)$. $X(n) = X(x_1,n) + X(x_2,n) + ... + X(x_t,n) = |X|$.

Instead of analyzing the order relations among $x \in X$ we analyze the set of three quantities, see [15]:

$$Dom(X(x_i,n), X(x_j,n)) \text{ , } Dom(X(x_j,n), X(x_i,n)) \text{ and } Sep(X(x_i,n), X(x_j,n))$$

We use the following abbreviations

$$d_{ij} = |\{(x_i^{rd}, x_j^{rd}) : x_i^{rd} \in X(x_i,n), x_j^{rd} \in X(x_j,n), x_i^{rd} > x_j^{rd}\}|$$

$$d_{ji} = |\{(x_i^{rd}, x_j^{rd}) : x_i^{rd} \in X(x_i, n), x_j^{rd} \in X(x_j, n), x_i^{rd} < x_j^{rd}\}|$$

$$s_{ij} = |\{(x_i^{rd}, x_j^{rd}) : x_i^{rd} \in X(x_i, n), x_j^{rd} \in X(x_j, n), x_i^{rd} \| x_j^{rd}\}|$$

and call d_{ij} the dominance of $X(x_i, n)$ over $X(x_j, n)$ and s_{ij} the separability between $X(x_i, n)$ and $X(x_j, n)$. Our main interest and the computational basis here is the analysis of d_{ij}. The main idea is to analyze dominance and separability as function of e.g. noise (see section 2.4) instead of realizations of simulation $X(x_i, n)$. From this point of view, a directed graph $G(\epsilon)$ can be defined as follows: set of vertices $= x \in X$ and a set of arrows $i \to j = \{x_i \in X, x_j \in X, i \neq j, \text{ with } d_{ij}/n > \epsilon\}$.

To avoid cumbersome notations and if no confusion is possible, we simply write $Dom(x, y)$ instead of $Dom(X(x, n), X(y, n))$.

The graph $G(\epsilon)$ may contain cycles, depending on the selection of ϵ and can sometimes be interpreted as a poset, similarly to the case shown by [15] with dominance among classes found for X when $\epsilon \geq 0.5$. At the moment, however, the basic result is $G(\epsilon)$ without assuming the additional structure of a poset. Therefore we present both the network corresponding to $G(\epsilon)$ and - if possible - the Hasse diagram as the visualization of the poset (see section 3.2).

Assume the following situation:

- $x < y$ with respect to an indicator set IB_1 of indicators with small numerical differences and
- $x > y$ with respect to the residual set IB_2 of indicators, albeit with large numerical differences.

Then $Dom(X(x, n), X(y, n)) \gg Dom(X(y, n), X(x, n))$ because the small numerical differences with respect to IB_1 are often leveled out by noise. When $Dom(X(x, n), X(y, n)) > \epsilon > Dom(X(y, n), X(x, n))$, the crisp graph $G(\epsilon)$ will have an arrow $x \to y$. We call this situation the noise equivalent: objects are considered equivalent with respect to IB_1. Hence incomparabilities caused by slight numerical differences of at least one indicator can be enriched due to the Monte Carlo simulation.

2.4 Implementation

The implementation (fuzzy.py) is a proof of the concept implementation written in Python[1] using the python modules: numpy[2] (numerical package like Matlab), networkX[3] (a package for creating, manipulating, and studying the structure, dynamics, and functions of complex networks) and matplotlib[4] for graphical visualization. Furthermore, software graphviz [17] is applied to draw the Hasse diagrams. Fuzzy.py as open source software can be downloaded from http://www.zalf.de.

The implementation uses the same probability parameters for all q_i. In case of uniform distribution, the noise can be (and is realized in the actual implementation) defined as: $noise = p/100.0 * u(-1,1) * (max(q_i) - min(q_i))$, where $u(-1,1)$ is a uniform distributed random number between (-1,1), $max(q_i)$ is the maximum value of q_i in the data sample, and $min(q_i)$ is the minimum value of q_i. This means the noise is a percentage of the range of each q_i. Other formulations of uniform noise are possible, too. In other words: The statistical data uncertainty is described by distribution functions and by there appropriate parameters such as p in the special case of uniform distribution as actually selected.

The code fuzzy.py is written in an object-oriented programming style. The code consists of three main classes (sit, compare_sit, hassegraph) and a number of additional general functions. The class "sit" stores the x, $q(x)$ and the probability distribution (uniform and triangular are already implemented, other distributions can easily be inserted) that includes its parameters. $X(n,x) = \{x^{rd}\}$ is created dynamically during the simulation. Based on "sit" the class "compare_sit", is responsible for simulation and data storage.
Matrices $Dom(X(x_i,n), X(x_j,n))$, $Dom(X(x_j,n), X(x_i,n))$ and
$Sep(X(x_i,n), X(x_j,n))$ are calculated during the simulation. The simulation itself is based on numpy, where the creation of random values according to the selected probability distribution is particularly useful. Dominance can be visualized (see below) using the "make_graph_matrix(dom,eps)" function.

The class "hassegraph" is used to build and visualize a partial order. Modules networkX and matplotlib are used for visualization. The methods of networkX have been proven to be powerful enough to visualize $G(\epsilon)$, whereas graphviz visualizes the transitive-reduced digraph, i.e. the Hasse diagram (HD).

[1] http://www.python.org/
[2] http://numpy.scipy.org/
[3] http://networkx.lanl.gov/
[4] http://matplotlib.sourceforge.net/

2.5 Data sets

Two artificial data sets with three objects a, b, c and two attributes[5] q_1 and q_2 (Table: 1, 2) are used to illustrate the method:

sit	q_1	q_2
a	1.0	1.0
b	3.0	3.0
c	3.0	2.0

Table 1. Artificial data set1

sit	q_1	q_2
a	1.0	1.0
b	3.0	3.0
c	4.0	2.0

Table 2. Artificial data set2

Data set1 has the crisp order: $a < c < b$; data set2 has a crisp partial order: $a < b$ and $a < c$ but also the $b \parallel c$ relation, $\parallel$ being the symbos for incomparability.

Alternatively to this artificial data set, a more realistic data set HPVC (Table 3) is used to show how the HD is changed according to the method suggested here.

$HPVC$	chemical name	PV	Tox	$Accum$	$Persist$
CNB	1-Chloro-4-Nitrobenzene	4	78.5	2.6	99.8
NA	4-Nitroaniline	2	45	1.4	100
NP	4-Nitrophenol	1	73	1.9	99.9
ATR	Atrazine	2	75.7	2.5	99.5
CHL	Chlormequat chlorid	2	0	-2.2	99
DIA	Diazinon	1	77.4	3.3	100
DIM	Dimethoate	2	72.5	0.7	100
LIN	Ethofumesate	1	69	2.7	99.6
GLY	Glyphosphate	2	28	0.002	99.7
ISO	Isoproturon	2	77	2.5	70
MAL	Malathion	3	79.96	2.7	0
THI	Thiram	2	79.7	1.7	100

Table 3. Real life data set of 12 HPVC chemicals

The indicators PV, Tox, $Accum$ and $Persist$ describe the environmental impact of substances. In particular, PV is a score with values taken from 1,2,3,4 as follows:

[5] we use "attribute" in this paper when the meaning is not important

- 1 : 5000 - 10000 tpa (ton per annum)
- 2 : 10000 - 50000 tpa
- 3 : 50000 - 100000 tpa
- 4 : 100000 - 500000 tpa

Tox is an indicator derived from acute toxicity for fish LC_{50} (correspondig to [14]). In order to obtain the same orientation of the indicator (a high value indicates a high hazard) $Tox = max(LC_{50}) - LC_{50}$. The well known n-octanol-water partition coefficient (in logarithmic form) is used to measure accumulation, i.e. $Accum = \log(Kow)$. $Persist$, a measure of persistence, is derived from the biodegradation intensity, BD, measured in percentage of degradation per day. As before, we require a reorientation as follows: $Persist = max(BD) - BD$. This data matrix combines indicators that are continuous in concept, such as Tox, $Acccum$ and $Persist$, and discrete, such as PV. A crisp analysis by partial order theory would interpret, for instance, $Tox(LIN) = 2.7$ and $Tox(ISO) = 2.5$ as different values. In our approach, these are such small differences (in comparison to the whole range of values $\in [0, 79.96]$) that they can be modeled as irrelevant.

3 Results

3.1 Fictitious example

Data set1 was used to show the change in Dom and Sep according to $q_2(c) = 2.0 + 0.1 * delta$ for $delta \in \{0, 1, 2, ..., 17, 18, 19\}$. At the beginning of the simulation we have $a < c < b$. During the simulation there is a range where $b \approx c$, i.e. where both $Dom(X(b, n), X(c, n))$ and $Dom(X(c, n), X(b, n)) > \epsilon$. For the sake of simplicity, we call this range the "fuzzy range". At the end of the simulation there should be $c > b$, as the following Figure 1 shows.

$Sep(b, c)$ is nearly constant during the simulation. In any case, the matrix entries $Dom(c, b) + Dom(b, c) + Sep(b, c) = 1.0$ see [15]. Figure 1 shows that $delta \in \{0, 1, 2, 3, 4, 5, 6, 7\} \rightarrow Dom(c, b) < Dom(b, c)$, indicating a preference of b over c; $delta \in [8, 12] \rightarrow b \approx c$ is the fuzzy range and $delta \geq 12 \rightarrow Dom(c, b) \gg Dom(b, c)$.

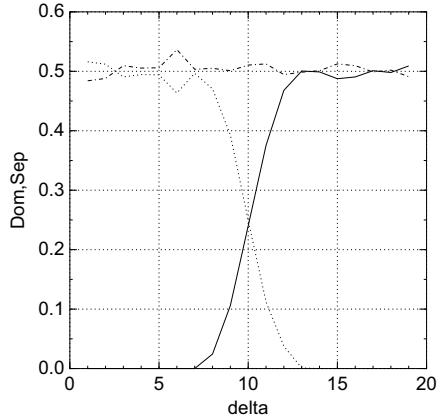

Figure 1. Data set 1: $Dom(c,b)p10$ (solid) versus $Dom(b,c)p10$ (dotted), p10: 10% random noise and $Sep(b,c)$ (dashed).

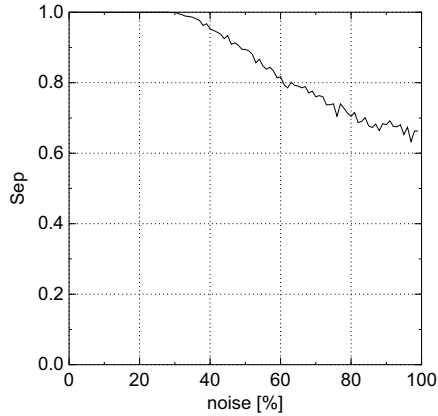

Figure 2. Data set 2: $Sep(b,c)$ as function of noise

The artificial data set2 has no clear preference as b and c are incomparable. Figure 2 shows the result of the simulation. $Sep(b,c)$ starts at 1.0 when the noise is low $< 20\%$ and begins to decrease. Very high noise makes the data set comparable to some degree. On the other hand, even with 80% noise $Dom(c,b) = 0.1075$ and $Dom(b,c) = 0.188$ are small compared to $Sep(b,c) = 0.7045$. Hence objects c and b remain incomparable. In other words, incomparabilities caused by small numerical differences can be leveled out, such that large numerical differences dictate the behavior of a pair of objects as a function

of noise, i.e. they are decisive whether or not a greater relation or an incomparability appears.

3.2 Structure analysis

The Python program was used to analyze and visualize the HPVC dataset. The user can change ϵ and $p \in (0..1)$ to get an overview. Figure 3 shows the original data structure ($p = 0$) and Figure 4 demonstrates the enrichment due to ($p = 0.05$).

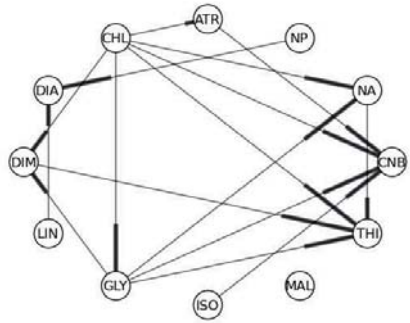

Figure 3. Original data structure, $G(\epsilon)$, applying networkX, the thickened part of the line indicates the orientation of the edge

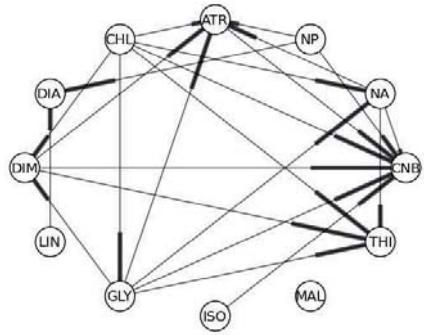

Figure 4. Enriched structure, $G(\epsilon)$ (networkX): $p = 0.05$ and $\epsilon = 0.2$

The analysis by networkX is designed to prove that the concept allows fast simulation at the cost of structural analysis. The output is a directed graph (without loops) but not an HD. To transform this directed graph, direct paths between nodes $path_{i \to j}$ have to

be removed additionally if there exists an alternative path: $path_{i\to\ldots\to j}$ which is just the transitive reduction. When the directed graph is transitively reduced, the resulting HD looks more informative.

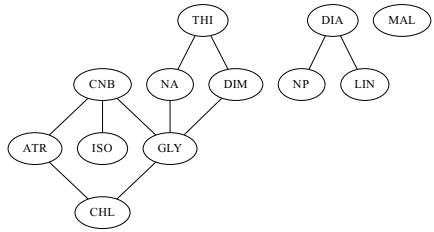

Figure 5. Original HD, applying graphviz [17]

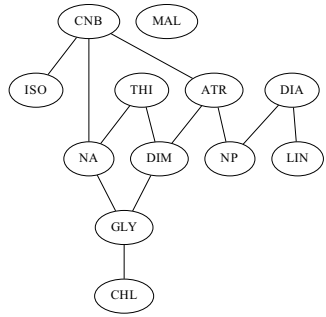

Figure 6. HD after simulation ($p = 0.05$ and $\epsilon = 0.2$)

The result of the Monte Carlo simulation is a new partial order, visualized as a HD. The original HD is shown in Figure 5; Figure 6 shows the simulated HD ($p = 0.05$ and $\epsilon = 0.2$). Note that, for the sake of clarity (avoiding crossing of lines by tools of graphviz), we do not use the drawing standards here as in the usual HDT. The most striking aspect is that there are three graph-theoretical components in the original HD. However, in the simulated HD there are only two graph-theoretical components, one of which is an isolated element (Malathion, MAL). The oriented edge $ATR \to NP$ i.e. there are new comparabilities. The maximum and minimum elements in both graphs are the same, and MAL remains an isolated element. However, there are new paths in the simulated HD: $\{CNB \to NA,\ ATR \to DIM,\ ATR \to GLY,\ ATR \to NA,\ ATR \to NP\}$ i.e. there are new comparabilities. The strength of these new connections is larger than $\epsilon = 0.2$. The enrichment facilitates a comparison between chemicals: for instance, in the original HD,

atrazine (ATR) had one successor (CHL) and one predecessor (CNB); in the modified HD, ATR has five successors (DIM, GLY, NA, NP and CHL) and keeps its predecessor.

As the example of HPVC is quite often used in theoretical studies and hence often contextually discussed, it should be sufficient here to explain the fact that $\{DIA, NP, LIN\}$ is a separate subset [5] with respect to the other two components (unconnected parts of the HD). In [5] the use of a tripartite graph was introduced to study the separateness of two object subsets. Here, however, a look at the rather small data matrix shows that the separation is mainly caused by a low PV for $\{DIA, NP, LIN\}$ and a larger value of $log(Kow)$ as an indicator of the accumulation tendency, whereas many of the main subset $\{THI, CNB, NA$,...,$CHL\}$ has lower values of $log(Kow)$ and larger values for the production volume. The remaining incomparabilities are caused by PV and $Persist$. Nevertheless, as Figure 6 shows, the numerical differences are small enough for a Monte Carlo simulation to create additional comparabilities.

Table 4 shows the new paths in greater detail:

Additional links	$Accum$	PV	Tox	$Persist$
$ATR \rightarrow DIM$	$>$	$=$	$>$	noise-equiv
$ATR \rightarrow GLY$	$>$	$=$	$>$	noise-equiv
$ATR \rightarrow NP$	$>$	$>$	$>$	noise-equiv
$ATR \rightarrow NA$	$>$	$=$	$>$	noise-equiv
$CNB \rightarrow NA$	$>$	$>$	$>$	noise-equiv

Table 4. noise-equiv: new equality due to simulation with respect to a single indicator

Only the small differences between the $Persist$ cause noise equiv. A larger p can also change the other differences significantly. The user can control the noise equiv by changing p. In the example, larger noise will influence the result as the next Tox. The cut-off parameter ϵ either includes or excludes the noise equiv nodes and controls the structure directly (see section 4).

4 Discussion

To address the main problem again, a small change of some values in a given data set can significantly change the structure of an HD. Although Kosko's approach could mitigate the problem, the numerical combination of indicator values and the selection of the best defuzzification are still problematic. The presented simulation technique offers a basis for interactive structure refinement together with the stakeholder. The introduction of noise in terms of a probability distribution (the uniform distribution was used here) together

with the "cut-off" parameter ϵ allows the simulation to be controlled. The fictitious example demonstrates the "fuzzy" change according to the *delta*. The much richer HPVC data set was used to demonstrate the influence of ϵ and p changed by the user. A larger p introduces more connections when ϵ is moderate: $\epsilon \in (0.1, 0.3]$ (using 2,000 simulation runs), which means that ϵ is somewhere in the "fuzzy" range. With higher ϵ, outside of the "fuzzy" range, the structure will become more simple again when p increases. This can be explained by the fact that large noise can break small dominance and a large ϵ will cut it.

The noise level that should be used depends on the uncertainty of the data and is often a priori unknown. For practical application it should be somewhere between $p \in [0.01, 0.5]$ and has to be estimated by trial and error. The cut-off parameter ϵ, on the other hand, can be used as an additional control parameter. If $\epsilon > 0.5$, then the resulting structure will be increasingly poor even if p increases. $\epsilon < 0.5$ can approach the "fuzzy" range and the structure becomes richer. Below the "fuzzy" range, the structure becomes meaningless.

The appearance of equivalence classes is relatively rare because, at the same time, x_i must dominate x_j, and vice versa, for all four indicators. Hence the effect of the Monte Carlo simulation is that similar indicator values are cancelled out so that only large numerical differences remain. Table 4 clearly shows this effect. The $<$ relation can only be broken to become noise equiv with a large amount of noise p. Even if all relations become noise equiv, the ϵ parameter will probably cut off these equivalence classes or noise equivalences. The crucial role of ϵ is demonstrated in Figure 7.

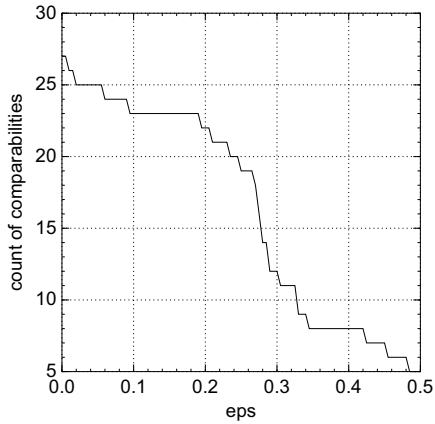

Figure 7. Count of comparabilities versus eps (ϵ), HPVC-data set

As can be seen in Figure 7 the number of comparabilities is changing were we selected our $\epsilon \approx 0.2$ (Figure 5, based on original data and Figure 6 based on $p = 0.05$ and $\epsilon = 0.2$).

Thus the crucial criss-cross of data profiles of objects, which often seriously hampers the analysis due to partial order, can be avoided. The downside is that, as in Kosko's method, new parameters such as p and ϵ are introduced.

5 Conclusion

One of the main problems of partial order analysis in the context of ranking and decision support is the appearance of incomparabilities. Whereas an incomparability itself merely indicates the existence of a conflict in the characterizing indicators, which is or should be considered a positive result, incomparabilities caused by small data differences must be considered disadvantageous. In the literature, therefore, several attempts concerning HDT are discussed. Examples include a discretization of the indicators only, see [4], and the fuzzy approach (Kosko's method).

Kosko's approach combines indicator values and, indeed, the normalization can lead to different partial orders! We therefore conclude that the approach by Monte Carlo simulation can be a good starting point for a refined application of HDT in rankings or decision support systems. An approach was discussed in [16] to directly combine a Monte Carlo simulation with an fuzzy approach, which leads in the same direction. The derivation of recipes for selecting "best" ϵ, p remains a task for the future.

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