## Data analysis by partial order methodology

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The present paper reviews data analysis applying partial order methodology. Hence, in addition to a short introduction to the basics of partial ordering a series of central tools of partial order methodology is presented and discussed based on exemplary studies applying a dataset comprising 12 obsolete pesticides characterized by their environmental persistence, bioaccumulation and toxicity.

Partial orders are often visualized by the so-called Hasse diagrams where the characteristics of partial ordering immediately become evident through the structure of the diagrams by levels, chains and antichains. Especially the presence of incomparabilities due to conflicting indicator values calls for attention.

The paper presents tools to a) estimate the relative importance of the single indicators applied, b) disclose the presence of so-called 'peculiar' objects that have one or more unexpected high or low indicator values, c) calculate the average order of the single element as partial ordering a priori does not lead to an absolute ordering that often is wanted, d) apply various weighting regimes in order to qualify the ordering, and e) disclose and visualize the actual nature of the incomparabilities that are in inherent part of partial ordering.

**Keywords**: data analysis; partial ordering; Hasse diagram; indicator importance; peculiar objects; average order; weight regimes; incomparabilities.

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## Деректерді талдаудың ішінара жүйелеу әдісі

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Бұл мақалада ішінара реттік жүйелеу әдісін пайдалана отырып деректерді талдау тәсілі сипатталған. Ішінара жүйелеу негіздерінің кіріспесіне қоса ескірген 12 пестицидтер туралы деректер жинағы негізінде, яғни олардың қоршаған ортадағы тұрақтылығы мен биожинақтағыштығы, улылығы туралы мәліметтер негізінде осы әдіснаманың негізгі құралдары сипатталып талқыланды.

Ішінара жүйелер көбінесе Хассе диаграммалары түрінде көрсетіледі. Бұл диаграммалардың деңгейлерге, тізбектерге және антитізбектерге бөлінген құрылымы есебінен ішінара жүйелеудің сипаттамалары анық көрінеді. Атап айтқанда индикаторлардың қайшылықты мәндерінен кейін шашырандылықтардың болуы ерекше маңызды.

Мақалада а) әрбір қолданылған индикатордың салыстырмалы маңыздылықтарын бағалау, б) бір немесе бірнеше күтпеген жоғары немесе төмен индикатор мәніне ие «ерекше» нысандарды анықтау, в) ішінара жүйелеу әрдайым қажетті абсолютті жүйелеуге алып келмейтін болғандықтан, әрбір элементтің орташа жүйесін есептеу, г) жүйелеуді сапалық бағалау үшін әртүрлі жүктеме режимдерін қолдану, және д) ішінара жүйелеудің ажырамас бөлігі болып табылатын шашырандылықтың шынайы табығатын анықтау және көзге көрсету құралдары сипатталған.

**Түйін сөздер:** деректерді талдау; ішінара жүйелеу; Хассе диаграммасы; индикаторлардың маңыздылығы; ерекше нысандар; орташа жүйе; жүктемелер режимі; шашырандылық.

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## Анализ данных методом частичного порядка

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В данной статье описан анализ данных с использованием метода частичного порядкового ранжирования. В дополнение к введению в основы частичного ранжирования, представлены и обсуждены основные инструменты данной методологии на примере набора данных о 12 устаревших пестицидов, включающего их устойчивость и биоаккумуляцию в окружающей среде, а также токсичность.

Частичные ранги часто представляют в виде так называемых диаграмм Хассе, на которых четко видны характеристики частичного ранжирования за счет структуры диаграмм по уровням, цепочкам и антицепочкам. В особенности важно присутствие несопоставимостей вследствие конфликтующих значений индикаторов.

В статье описаны средства для а) оценки относительных важностей каждого использованного индикатора, б) выявления так называемых «особенных» объектов, которые имеют одно или более неожиданно высокое или низкое значение индикаторов, в) расчета среднего порядка каждого элемента, так как частичное ранжирование не ведет к часто желаемому абсолютному ранжированию, г) применения различных режимов нагрузки для качественной оценки ранжирования, и д) выявления и визуализации истинной природы несопоставимостей, которые являются неотъемлемой частью частичного ранжирования.

**Ключевые слова:** анализ данных; частичное ранжирование; диаграмма Хассе; важность индикаторов; особенные объекты; средний порядок; режимы нагрузок; несопоставимости.

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## 1. Introduction

Data analysis is an omnipresent challenge is a wide variety of areas in science, social studies etc. as well as in daily life. The desire to disclose what is better and what is worse are dilemmas we constantly are facing. Just imagine buying a new car. How many different aspects should be included in the decision? And they are definitely all changing in the same direction. The performance increases (good) but at the same time the fuel consumption may increase (bad), price increases (bad) and the comfort increases (good). And just to complicate the picture, a series of subjective indicators may play a role as well such as color tradition. How can we possibly process the information?

Typically, as just demonstrated, the choice cannot be based on a single indicator expressing what the obvious and thus best decision is. Thus, in order to rank the different possible options requires that several indicators are taken into account simultaneously. Hence, we are dealing with a so-called multi-indicator system (MIS) [7].

One often seen way to handle a MIS is a mathematical mapping of the single indicator values to get a one-dimensional scalar, eventually to be used as the ranking indicator [1]. However, such a mapping process, e.g., by aggregating the single indicators through a weighted sum, not only hides all background information but may also cause unwanted compensation effects [32].

It is recognized and acknowledged that there are many well-known methods to obtain a linear (or with respect to technical aspects also a weak, i.e., including ties) order from a multivariate data matrix. Methods like PROMETHEE [3], or the ELECTRE family [35, 36, 22, 26, 2] serve as good examples. It should be stressed that all these methods require additional parameters beyond the data matrix in order to do the job and has in some cases even be criticized from a theoretical point of view [32].

The concepts of partial order methodology constitutes an attractive alternative to these methods and the present paper will review a series of tools that allow, based on such a set of indicators to obtain information concerning mutually to rank the single option/object under investigation and in addition to obtain some ideas to what extent a given option/object is better than another.

Partial ordering is, from a mathematical point of view, simple, applying only the relation "≤" and appears as an advantageous way to look at MIS [8].

## 2. Methodology

As mentioned below (sect. 2.7) the software applied for studying partially ordered data sets (PyHasse), often denoted posets, today includes more than 100 specialized modules. The objective with the present review is obviously not to deliver a complete presentation of all aspects of the partial order methodology. Hence, in the following the basics of partial ordering are described together with a small selection of appropriate modules.

### *2.1 Basics of partial order methodology*

The basis for partial ordering is the relation among the objects to be ordered. The only mathematical term in this context is "≤" [5, 15, 6]. Thus, the "≤"-relation is the basis for a comparison of objects and constitutes a graph, the so-called Hasse diagram (see below). Two objects are connected with each other if and only if the relation $x \leq y$ holds. However, since each object is characterized by a series of indicators $r_j$ the obvious questions is how $x \leq y$ should understood. As a given object, x, is characterized by the a set of indicators $r_j(x)$, $j = 1,...,m$, it can be com-

pared to another object y, characterized by an identical set of indicators $r_j(y)$, if

$$r_i(x) \leq r_i(y) \text{ for all } i = 1,\ldots,m \quad (1)$$

It is obvious that eqn. 1 is a rather strict requirement for having a comparison as all indicator values of object x must be lower (or at least equal) to those of object y. In more technical terms: Let X be the group of objects studied, i.e., X = {O1, O2, O3, ……, On}, then object Oy will be ranked higher than object Ox, i.e., Ox < Oy if at least one of the indicator values for Oy is higher than the corresponding indicator value for Ox and no indicator for Oy is lower than the corresponding indicator value for Ox. On the other hand, if $r_j(Oy) > r_j(Ox)$ for some indicator j and $r_i(Oy) < r_i(Ox)$ for some other indicator i, Oy and Ox will be called incomparable (notation: Oy ‖ Ox) due to the mathematical contradiction expressed by the conflicting indicator values. A set of comparable objects are called a chain, whereas a set of mutually incomparable objects is called an antichain (see below; 2.1.1). In cases where all indicator values for two objects, Oy and Ox, are equal, i.e., $r_j(Oy) = r_j(Ox)$ for all j, the two objects will be considered as equivalent, i.e., labx ~ laby, which in ranking terms means that they will have the same rank.

Eqn. 1 is the basis for the so-called Hasse diagram technique (HDT) [5, 15, 6]. HDT is a special (statistically oriented part of partial order theory). Hasse diagrams are visual, graphical representation of the partial order.

*2.1.1 The Hasse diagram*

In a Hasse diagram, comparable objects are connected by a sequence of lines [6, 14, 18]. Consequently incomparable object appear non-connected in the Hasse diagram. For construction of a sensible Hasse diagram, it is mandatory that all indicators have a uniform orientation, i.e., high indicator values correspond, e.g., to "good" objects and low values to "bad" objects (or vice versa). As an illustrative example, we may use the following data set (Table 1; [20]).

The corresponding Hasse diagram is depicted in Fig. 1.

A Hasse diagram (cf. Fig 1) is characterized with it structure that comprises levels, chains and antichains.

Levels are the horizontal arrangement of objects within a Hasse diagram. The level structure gives a first approximation to a weak order of the objects from "bad" (bottom) to "good" (top). Unfortunately, this will often give rise to many tied ranks as all objects in a level automatically will be assigned identical ranks [21]. Thus, in the above case we will see (Fig. 1) O7 < O3 < O2 = O5 < O4 = O6 < O1.

**Table 1** – Set of 7 objects characterized by 3 indicators

| Object | Indicator 1 | Indicator 2 | Indicator 3 |
|---|---|---|---|
| O1 | 1 | 1 | 1 |
| O2 | 0.739 | 0.581 | 0.520 |
| O3 | 0.417 | 0.240 | 0.141 |
| O4 | 0.852 | 0.623 | 0.909 |
| O5 | 0.035 | 0.011 | 0.603 |
| O6 | 0.065 | 0.689 | 0.413 |
| O7 | 0 | 0 | 0 |

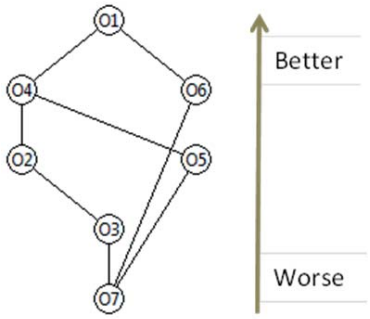


**Figure 1** – Hasse diagram constructed based on the data set given in Table 1

Typically, the degree of tied ranks is wanted to be as low as possible, i.e., there is a need for a linear ranking of the single objects. This is to some extent obtained by looking at chains only. However, it is not immediately obtainable when incomparable objects are included (Further discussion: see Sect. 2.4).

Chains are subsets of X, i.e., $X' \subseteq X$, where all objects in X' fulfill eqn. 1. Chains are characterized by their height that equals the number of objects in X'. Chains are specifically interesting as they constitute complete orders, or ranking of the objects of X'. Hence, for objects within a given chain, all indicators are monotonously varying, i.e., simultaneously decreasing from top (start vertex) to bottom (end vertex).

Antichains are subsets $X' \subseteq X$, where no object fulfills eqn. 1, i.e., all objects in X' are mutually incomparable. Thus, for any two objects within an antichain, there is at least one conflict in indicator values. Levels per definition constitute an antichain, whereas the reverse not necessarily is true.

*2.2 Indicator Importance*

The relative importance of the single indicators in play can be determined through a sensitivity analysis [13]. The basic idea is to construct partial ordered sets excluding the single indicators one at the time. Subsequently, the distances from these posets to the original poset are determined. The indicator, whose elimination from the original poset leads to the maximal distance to the original one, in other words causing the highest degree of changes in the Hasse diagram is most important for the structure of the original partial order. As the effect of elimination single indicators is studied, this kind of sensitivity analysis can be called 'indicator-related sensitivity'.

Within the PyHasse software package, the module sensitivity20_5 is available for disclosing indicator importance.

*2.3 Peculiar objects*

The Hasse diagram in Fig. 1 shows that eqn. 1 is sufficiently often fulfilled. Thus, it expresses qualitatively that most often an increase in one of the indicators is implying an increase in another indicator. Thus, for the [0,1] normalized poset, the "mainstream" objects are found distributed in a more or less slim ellipsoid around the line connecting the two extremes (0,0,…..,0) and (1,1,……,1) [9]. On other words, the single objects can be represented by a pattern, generally described by the set.

$$h(m) = \{0,1\}^m - \{(0,0,\ldots,0), (1,1,\ldots,1)\} \quad (2)$$

In the simple example, as illustrated in Fig. 1, m = 3 it can accordingly be expected that the majority of points representing the single objects are located around a straight line starting in (0,0,0), corresponding to non-remedied situation and ending in (1,1,1) that corresponds to the fully remedied site (Fig. 2). Objects deviating from the "mainstream" will be located closer to one of the other 6 corners of h(3) as for example to (1,0,0) or (0,1,0). Such objects are defined as peculiar as they, verbally expressed deviate from the "mainstream" [9].

Bruggemann and Carlsen [9] introduced a "near-enough-factor", f, calculated as the squared Euclidian distance between two points. The maximum value in the m-dimensional case is the distance between (0,0,….0) and (1,1,…,1). Thus, in h(m) $D_{max}$ = m. Consequently the distance between two given points will be on a scale from 0 to m. Introducing f objects where the distance, d, to one of the corners in h(m) is lower that f times the maximum distance, i.e., $d < f \bullet D_{max}$, will be regarded as peculiar as these objects appears to have what can be denoted as an unbalanced indicator profile and thus away from the mainstream.

Turning to the simple 3-dimensional case, an f equal to 0.05 only objects with highly unbalanced indicator profiles would be recognized, i.e., being found very close to one of the 6 corners of interest, the term 'very close' referring to the relative distance to the maximal distance. Thus, an f = 0.05 can be interpreted 5% of the maximal distance, i.e., 3. In other words, when d ≤ 0.15 for a given point to one of the 6 peculiar corners, this object will be denoted peculiar or extreme, i.e., displaying a significant unbalance in the indicator profile, meaning that on a 95 % level, such objects will not be found located around the (0,0,0)-(1,1,1) straight line (cf. fig. 2). For a somewhat less strict requirement as, e.g., 90 % level (f = 0.1) the limit would be d ≤ 0.30.

Peculiar objects are disclosed using the module incompposet4_1 of the PyHasse software package.

*2.4 Average orders*

Looking at the Hasse diagram, the level structure

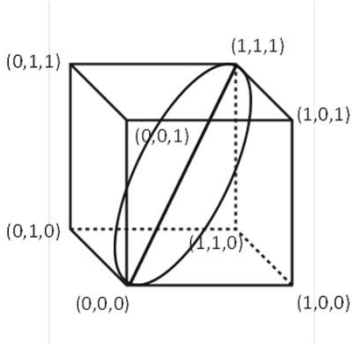


**Figure 2** – The extreme points of the cube h(3)

constitutes a first approximation to ordering (cf. Section 2.1.1). However, as all objects in a level automatically will be assigned identical orders such an ordering will obviously cause many tied orders. Obviously, it is desirable with a degree of tiedness as low as possible. Hence, ultimately a linear ordering of the single objects is desirable. However, when incomparable objects are included in the study, this is obviously not immediately obtainable. Looking at Fig. 1 as an illustrative example, the O5 may be located between O4 and O2, O2 and O3 or O3 and O7, respectively; each possible location will obviously correspond to a different absolute order.

Partial order methodology provides a weak order, where tied orders are not excluded. This is obtained by calculating the average order of the single objects as, e.g., described by Bruggemann and Annoni [4]. If the number of objects included in the study is relatively low (typically < 25) the average orders may be calculated by an exact method based on lattice theory [31, 41, 23]. For larger systems, approximations are available [7]. The calculations [39, 29, 17, 41, 23, 31, 7] deducting a weak ordering will assign an average order to the individual objects.

Within the PyHasse software package, the module avrank5_2 calculate exact average orders based on the lattice theory. The module LPOMext6_1 is available for larger posets applying an approximate method.

*2.5 Introducing weight regimes*

In many cases a numerical aggregation of the single indicators are made in order to obtain a single composite indicator CI, which subsequently will allow an absolute ordering of the studied objects.

$$CI = \Sigma\, g_i * rn_i \quad g_i\text{: weights,} \qquad i = 1,..3 \quad (3)$$

Such an introduction of weights is from various perspectives problematic. From a scientific point, the aggregation will cause a loss of potential important information and, possibly even worse, such aggregation may unequivocally lead to compensation effects where high values in one indicator may compensate low values in another [32]. Hence, assume a poset with three indicators

that for one object adopt the values 0.001, 1 and 1, respectively and for another object the values 0.667, 0.667 and 0.667, respectively. A simple aggregation would in both cases lead to the same CI = 0.667, despite the two objects obviously are quite different.

A further obvious problem is the assignment of weights to the single indicators. This may often lead to extended discussions and possible compromises with little or even no scientific basis in order to get to consensus. However, it appears that a significantly easier process would be to reach consensus about weight intervals for the indicators [16, 11]. It is still clear that introducing weight intervals will not lead to an absolute (linear) order but it will typically lead to an enriched Hasse diagram, i.e., to a reduction of incomparisons and therefore strengthen a subsequent ordering based on averaged orders (cf. 2.4).

Within the PyHasse software a specialized module, HDweightMC6_2, is available for studying various weight regimes.

*2.6 Dealing with incomparabilities*

Incomparabilities are often seen as a major obstacle in using partial ordering. Looking at the eqn. 1, it is obvious that even very small differences in indicator values may lead to incomparisons. In many cases such minor differences may be regarded as noise and should be neglected, i.e., below a certain limit such values should be regarded as identical. In other cases, it may be of significant interest to elucidate which indicators lead to incomparisons. Within the partial order methodology tools are available for such studies.

*2.6.1 Neglecting small differences in indicator values*

Due to the very nature of the partial order methodology (cf. eqn. 1), even small differences in indicator values may lead to incomparabilities, if all incomparabilities are looked upon without regard to the possible importance of the single incomparabilities. This is obviously not always the truth and a somewhat more nuanced view is necessary. Thus, a Δ-value can be introduced so only if the differences in indicator values are larger than this value, the incomparability between two objects, Objx and Objy, is considered as relevant. Thus, only remarkable data differences are to be contextually interpreted as exerting a real conflict. In mathematical terms this can be expressed as eqn. 4.

The module scanincomp4_4 in the PyHasse software package is designed to study the effect of neglecting small differences in indicator values applying the values of the scanning parameter Δ (min, max, steps from min to max) as input [9]. The lower the Δ values the smaller differences between the indicators values will be regarded as real.

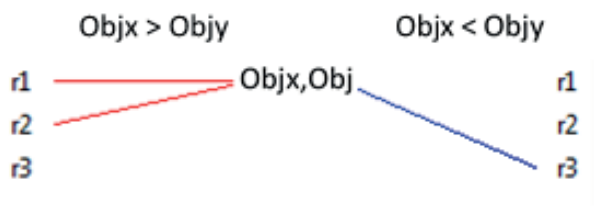


**Figure 3** – Example of a tripartite graph

The tool may be used directly on the original data set or on the [0,1] normalized set. An option to normalize is included in the module. If the normalized data set is used, the Δ-value reflects the percentage variation in the indicator values allowed before the values are regarded as different.

*2.6.2 The tripartite graphs*

In order visually to display and thus better understand the role of individual indicators for incomparisons, the concept of tripartite graph was introduced by [19]. Here an intuitive approach is presented again assuming a case with three indicators. Imagine that Objx has worse values (i.e. higher values) in comparison to Objy in the first and second indicator, but better value (i.e. lower value) in the third indicators. This fact can be graphically represented as follows (Fig. 3).

Tripartite graphs may be obtained using the module antichain20_4 from the PyHasse software package. For studies where small differences are to be disregarded, the module sepanalcoloured16_2 is offered with an optional input of the Δ-values, i.e., the limit under which a given indicator is assumed to be negligible. Thus working with the [0,1] normalized poset the Δ-values can be seen as a percentage of the maximum value, i.e., 1.0, under which the given indicator for the given object is regarded as negligible.

*2.7 Software*

All partial order analyses were carried out using the PyHasse software [12]. PyHasse is programmed using the interpreter language Python (version 2.6) [25, 28, 40, 33]. The term 'Hasse' refers to the German mathematician Helmut Hasse [27], who made the Hasse diagram popular. It should be noted that in the US and other nations,

$$|r_i(Objx)-r_i(Objy)| > \Delta \text{ and } |r_j(Objx)-r_j(Objy)| > \Delta, \text{ and} \quad (4)$$

$$\text{sgn}(r_i(Objx)-r_i(Objy)) \neq \text{sgn}(r_j(Objx)-r_j(Objy)) \text{ with } \text{sgn}(...) \neq 0 \quad (5)$$

with sgn(x) = -1,0,+1 according to x < 0, =0, >0, respectively.

where $r_i(Objx)$ is the value of Object x with respect to the $i^{th}$ indicator.

also the concept 'line diagram' is commonly used for the visualization of a partial order Today, the software package contains more than 100 specialized modules designed to solve specific tasks in the context of partial ordering. This 'pro' version is available upon request from the developer, Dr. R.Bruggemann (brg_home@web.de).

A simplified version of PyHasse operating on a web-based browser is available. Currently only few tools are included. However, this web-based tool is under continuous development to include the most often used modules of the PyHasse family (see *www.pyhasse.org*).

Statistical analyses in connection with the data generation were carried out applying the freely available software R [34].

### 3. Exemplary studies

In the following sections, applications of the above described tools will be presented applying an exemplary data set of 12 obsolete pesticides [38] characterized by three indicators, i.e., their persistence (Pers), bioaccumulation (BioA) and toxicity (Tox), respectively, in general noted as the PBT characteristics [37]. The ordering of the pesticides simultaneously including of the three indicators is believed to constitute an ordering according to the environmental hazard [37, 10]. The [0,1] normalized poset is given in Table 2. It should be noted that the values for the single indicators are ordered with an equal orientation. Thus, for all three indicators, a high value means "bad" whereas a low value means "good" (cf. 2.1.1).

In Fig. 4, the resulting Hasse diagram based on the data in Table 2 is visualized. The diagram is by five levels that gives a first indication of the mutual hazard ranking of the pesticides. The Hasse diagram has in total 35 comparisons and 31 incomparisons.

From the diagram (Fig. 4), it is immediately clear that from an environmental point of view, the compounds DDT, ALD and CHL are the most hazardous whereas LIN apparently is the least problematic of this series. However, it must be emphasized that all 12 pesticides are banned according to the Stockholm Convention [38].

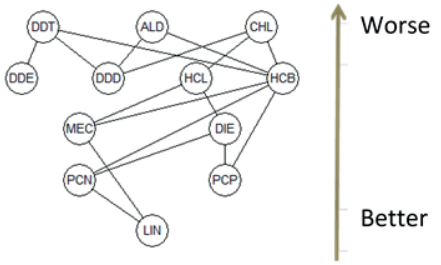


**Figure 4** – Hasse diagram based on the pesticide data given in Table 2

*3.1 Indicator Importance*

An obvious question to ask is: which of the indicators are the more important? The sensitivity analysis (cf. sect. 2.2) is a tool specifically designed to answer this question. The result of the sensitivity analysis is shown graphically in Fig. 5.

By normalizing the data depicted in Table 2, the relative importances of the three indicators are calculated to be 0.742, 0.194 and 0.065, respectively, for the indicators Pers, BioA and Tox, respectively. Some readers may find it surprising that the importance of the toxicity indicator is so low; however, the results fit nicely with the EU chemical legislation REACH on PBT substances [24] stating that if the persistence and bioaccumulation values are very high, i.e., we are talking about the so-cally vPvB substances, the toxicity does not play a role in the legislation, as an illustration of the high importance of persistence (Pers) and bioaccumulation (BioA).

In a future section (sect. 3.4), we will return to a possible use of the relative importances of the single indicators.

**Table 2** – Normalized (column-wise) data matrix (rounded to three decimals) of 12 pesticides (PBT-substances) included in the [37] study where also details on the data generation can be found

| Pesticide | Trivial name | Pers | BioA | Tox |
|---|---|---|---|---|
| DDT | p,p-DDT | 0.084 | 1.000 | 1.000 |
| DDE | p,p-DDE | 0.009 | 0.856 | 0.160 |
| DDD | p,p-DDD | 0.000 | 0.679 | 0.171 |
| MEC | Methoxychlor | 0.027 | 0.339 | 0.101 |
| ALD | Aldrin | 0.263 | 0.852 | 0.627 |
| DIE | Dieldrin | 0.293 | 0.383 | 0.041 |
| HCL | heptachlor | 0.428 | 0.480 | 0.104 |
| CHL | chlordane | 1.000 | 0.751 | 0.212 |
| LIN | lindane (γ-HCH) | 0.027 | 0.000 | 0.000 |
| HCB | hexachlorbenzene | 0.057 | 0.574 | 0.187 |
| PCN | pentachlor nitrobenzene | 0.054 | 0.180 | 0.028 |
| PCP | pentachlor phenol | 0.012 | 0.354 | 0.010 |

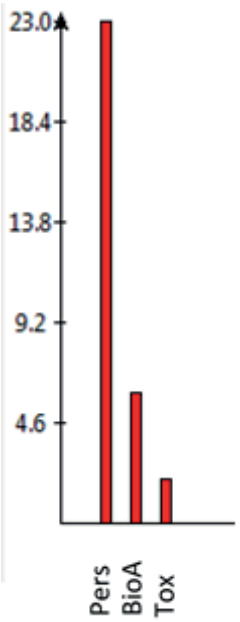


**Figure 5** – Relative indicator importance

*3.2 Peculiar objects (cf. sect. 2.3)*

When looking at the graphical representation of the poset given in Table 2 (Fig. 4) it is clear that an overall trend is that the 12 pesticides are mutually arranged on a scale from 'better' to 'worse'. As already also discussed, the partial order as displayed in the Hasse diagram (Fig. 4) is characterized by levels, chains and antichain, i.e. comparabilities and incomparabilities. So it is expected that in general the variation in the indicator values goes from (0,0,0) to (1,1,1).

If each of the three indicator values monotonously varied from 0 to 1, the resulting order would be a total ordering of the compounds, i.e., all compounds would be located on the line from (0,0,0) to (1,1,1). This is obviously not the case as the ordering results in the partial ordering as visualized by the Hasse diagram, the various incomparabilities being results of conflicting indicator values (cf. sect. 2.1). Thus, it is expected that the majority of the compounds would be located in an ellipsoid around the (0,0,0) – (1,1,1) line (Fig. 2). However, for certain compounds, the so-called peculiar compounds, one or two of the three indicators may display values that are either peculiarly high or low compared to the 'mainstream' (cf. sect. 2.3).

In Table 3, the results of an analysis of the dataset (Table 2) revealed that 4 compounds appear as peculiar applying a 95% level, i.e., we are 95% certain that these compounds in one way or another are peculiar (cf. Section 2.3).

The reasons for the peculiarities of these four compounds are thus easily disclosed. In the cases of DDE and DDD, the Pers and the Tox values are very low whereas the BioA value is rather high. For DDT and CHL, it is seen that the values for Pers and Tox, respectively, are rather low whereas the other two indicator values are rather high. As a consequence, these four compounds are located far away from the (0,0,0) - (1,1,1) line, i.e., close to one of the other six corners of the h(3) cube (cf. sect. 2.3) as thus appear as peculiar. Hence, this analysis is a further qualification of the general analysis of the partial order by disclosing compounds (objects) with odd indicator tuples that possibly may call for further attention or investigations.

**Table 3** – Peculiar objects on the 95% level (f = 0.05)

***object: DDT*** data :0.084, 1.0, 1.0,
pattern: [0, 1, 1] with minimal distance 0.007
---
***object: DDE*** data :0.009, 0.856, 0.16,
pattern: [0, 1, 0] with minimal distance 0.046
---
***object: DDD*** data :0.0, 0.679, 0.171,
pattern: [0, 1, 0] with minimal distance 0.132
---
***object: CHL*** data :1.0, 0.751, 0.212,
pattern: [1, 1, 0] with minimal distance 0.107
---

**Table 4** – Average orders based on the exact method (cf. 2.4)

| Pesticide | Average order |
|---|---|
| DDT | 10.602 |
| DDE | 5.301 |
| DDD | 4.672 |
| MEC | 4.304 |
| ALD | 10.32 |
| DIE | 6.757 |
| HCL | 9.087 |
| CHL | 11.216 |
| LIN | 1.587 |
| HCB | 7.285 |
| PCN | 3.832 |
| PCP | 3.039 |

*3.3 Average orders*

As it is clear from the above, the partial ordering, as the name indicates, does not lead to an absolute ordering of the objects studied. Due to the actual nature of the partial ordering, not least the incomparabilities of the single objects may take a variety of ranks still maintaining the order preserving nature of the poset. However, this is often a requirement or demand from decision makers. To accommodate such wishes, partial order methodology offers the possibility to calculate the average orders of the objects (cf. sect. 2.4).

For relatively small systems, typically including up to 20-25 objects an exact method is available [31, 41, 23,]. For the present exemplary study, the results of such calculations are shown in Table 4.

For larger systems, approximate methods are available as the so-called LPOMext. In the LPOMext method, a further feature is available as the actual span of possible orders for the single objects are given, i.e., the range from the lowest to the highest possible rank. This may be regarded as some kind of uncertainty of the average orders estimated. In Table 5, the results for the dataset in Table 2 based on the approximate method is given. It is noted that for some of the pesticides, relatively wide ranges of possible ranks are found. To get further insight in the probability of the possible ranks for the single objects

**Table 5** – Average orders based on the approximate method LPOMext (cf. 2.4)

| Pesticide | Average order | Uncertainty |
|---|---|---|
| DDT | 10.967 | 8...12 |
| DDE | 5.333 | 1...11 |
| DDD | 4.25 | 1...9 |
| MEC | 4.052 | 2...7 |
| ALD | 10.425 | 7...12 |
| DIE | 6.821 | 4...10 |
| HCL | 9.274 | 6...11 |
| CHL | 11.4 | 9...12 |
| LIN | 1.504 | 1...4 |
| HCB | 7.108 | 5...9 |
| PCN | 3.583 | 2...6 |
| PCP | 2.676 | 1...6 |

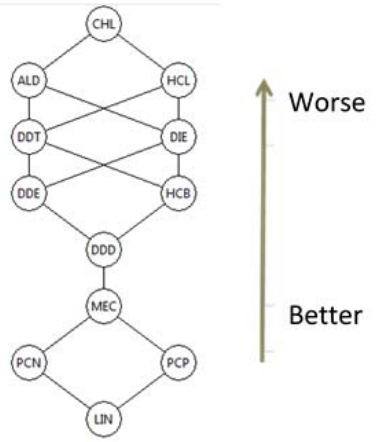


**Figure 6** – Hasse diagram based on the weight intervals

studied a method based on random linear extensions have been reported by [30] leading to probability distributions for the single objects. This is not further studied in the present review; thus, the reader is recommended to the original studies [30] and references therein).

*3.4 Introducing weight regimes*

The introduction of weight appears in the best case controversial. Agreeing on the relative weight of the single indicators is often a troublesome process and the resulting aggregated indicator hides potentially important information and is, as described above, subject to compensation effects (cf. 2.5). As an alternative that typically will be easier to agree upon is to introduce weight intervals.

In section 3.1 the relative importance of the indicators were retrieved, and it appears that these values constitute an appropriate starting point for developing weight intervals. Thus, as an illustrative example ranges of $\pm$ 25% around the relative importances of the single indicators are used (cf. Table 6). In the present case, 1000 Monte Carlo simulations were used and for each of the simulations the set of indicator values were collected and eventually used to construct a Hasse diagram that is now significantly enriched, i.e. displaying a lower number of incomparabilities that the original (Fig. 6). Thus, the diagram displayed in Fig. 6 only contains four incomparabilities in contrast to the original diagram (Fig. 4) displaying 35 incomparabilities.

It is noted (Table 6) that the calculated minimum, mean and maximum values of the weights as a result of the Monte Carlo simulations are rather close to the input values. This is not surprising as this corresponds to the original intervals. It is in this connection important to stress that other weight intervals will lead to different results just as possible aggregated indicators will depend on the actual weights used.

The resulting data, as visualized in the Hasse diagram (Fig. 6), leads to calculation of the average orders based on the enriched poset (Table 7) that should be compared to the average orders obtained from the original poset (Table 5).

Overall the two orderings are found to be rather close as it can be seen from Fig. 7, the correlation coefficient being 0.947.

Despite the good correlation (Fig. 7) some variations are that in the average orders. Thus, following the use of weight intervals is it noted that DDT is now ordered below ALD and HCL, and HCB is now found below DIE and DDE. Apart from the new relative locations of DDT and HCB,

**Table 6** – Input to - and output (Results) from weight interval calculations

| | Indicator | | | |
|---|---|---|---|---|
| Input | | Lower limit | Importance | Upper limit |
| | Pers | 0.557 | 0.742 | 0.928 |
| | BioA | 0.146 | 0.194 | 0.243 |
| | Tox | 0.049 | 0.065 | 0.081 |
| | | | | |
| Output | | | | |
| | | Min. value | Mean | Max value |
| | Pers | 0.647 | 0.739 | 0.815 |
| | BioA | 0.133 | 0.195 | 0.279 |
| | Tox | 0.042 | 0.066 | 0.098 |

**Table 7** – Average orders based on the LPOMext method (cf. 2.4) applying weight intervals (cf. Table 6)

| Pesticide | Average order | Uncertainty |
|---|---|---|
| DDT: | 8.5 | 8...9 |
| DDE: | 6.5 | 6...7 |
| DDD: | 5.0 | 5...5 |
| MEC: | 4.0 | 4...4 |
| ALD: | 10.5 | 10...11 |
| DIE: | 8.5 | 8...9 |
| HCL: | 10.5 | 10...11 |
| CHL: | 12.0 | 12...12 |
| LIN: | 1.0 | 1...1 |
| HCB: | 6.5 | 6...7 |
| PCN: | 2.5 | 2...3 |
| PCP: | 2.5 | 2...3 |

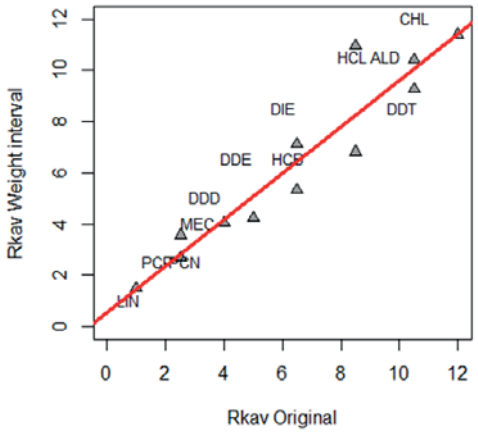


**Figure 7** – Correlation between the average orders obtained based on the original dataset (Table 2) and following application of weight intervals (Table 6)

the remaining mutual orders are reproduced. However, the average orders generated this way are, due to the enrichment of the Hasse diagram significantly more reliable provided the weight intervals have been selected carefully and appropriately and as such this procedure is qualifying the determination of the average orders, which is immediately seen when comparing the 'uncertainty' columns in the Tables 5 and 7.

*3.5 Dealing with incomparabilities*

By nature, partial ordering includes incomparabilities, a fact that is often seen as a significant disadvantage of the methodology and thus apparently appears prohibitive for a broader application of partial order technology. However, the incomparabilities may be looked upon as a valuable source of information [1, 9, 10, 11, 21].

*3.5.1 Neglecting small differences in indicator values*

One potential obvious problem in relation to partial ordering is that even minute differences in indicator values may lead to incomparabilities (cf. sect. 2.6.1). Unambiguously, small variations/differences in indicator values may be regarded as negligible and without scientific significance.

In Table 8, it is shown that if we assume a Δ-value = 0.3, i.e., only if the differences in indicator values are larger than 0.3, the incomparability between two pesticides is considered as relevant, only five pesticides couple apparently are still in play. The remaining pesticides are in this example consequently regarded as being equivalent.

*3.5.2 The tripartite graphs*

To visualize the reasons for incomparabilities, tripartite graphs (cf. sect. 2.6.2) appear as an advantageous tool. As an illustrative example, the tripartite graph displays the conflicts between the pesticides DDD, DDE, HCL and HCB, i.e., the pesticides in level 4 (Fig. 4). It should be noted that these four pesticides constitute an antichain, and as such per definition are incomparable. Hence, the tripartite graph gives further insight into the actual nature of these incomparabilities. Here it is seen that, e.g., HCB and DDE are incomparable as the values for Pers and Tox are higher for HCB than for DDE, whereas the value for BioA is higher for DDE than for HCB.

Again all differences in the indicator values counts, i.e., we a priori use a Δ = 0.0. However, it is possible to filter out incomparabilities due to minute differences in indicator values. In Fig. 9, the resulting tripartite graphs for Δ = 0.0, 0.05 and 0.1 are displayed. It should here be noted that rather small Δ values are applied as a consequence of using a [0,1] normalized poset (Table 2).

**4. Conclusions and Outlook**

The present paper provides a short review on how

**Table 8** – The 5 pesticide couples and corresponding indicator pair still in play assuming a Δ = 0.3

| Pesticide couple | Indicator pair | Difference Indicator 1 | Difference indicator 2 |
|---|---|---|---|
| DDT : HCL | Pers : BioA | -0.344 | 0.52 |
| DDT : HCL | Pers : Tox | -0.344 | 0.896 |
| DDT : CHL | Pers : Tox | -0.916 | 0.788 |
| DDE : HCL | Pers : BioA | -0.419 | 0.376 |
| ALD : CHL | Per : Tox | -0.736 | 0.415 |

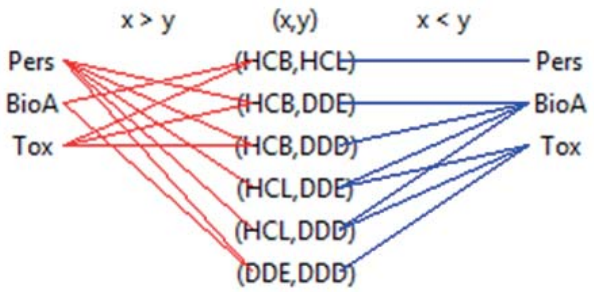


**Figure 8** – Tripartite graph displaying the indicator conflicts for DDD, DDE, HCL, HCB (cf. Fig. 4)

data analyses advantageously can be carried out applying partial order methodology. Hence, the basic equation for partial ordering is presented and discussed based on a simple example. Further a series of central partial order tools is presented and the background being explained. The possible applications of these tools are elucidated through exemplary studies using a dataset comprising 12 obsolete organochlorine pesticides characterized by three indicators, i.e., their environmental persistence, bioaccumulation and toxicity, respectively.

The tools presented in the paper comprise methods to a) estimate the relative importance of the single indicators applied, b) disclose the presence of so-called 'peculiar' objects, i.e., objects that possess odd, or peculiar, indicator tuples by displaying one or more unexpectedly high or low indicator values, c) calculate the average order of the single element as partial ordering *a priori* does not lead to an absolute ordering that often is wanted, d) apply various weighting regimes in order to qualify the ordering, including a discussion of introduction of weight intervals instead of attempting an assignment of exact weight to the indicators eventually leading to an absolute order, and e) disclose and visualize the actual nature of the incomparabilities that are in inherent part of partial ordering as, e.g., done through the application of so-called tripartite graphs.

Apart from presenting the various tools, the review further is an illustration of the use of the PyHasse software.

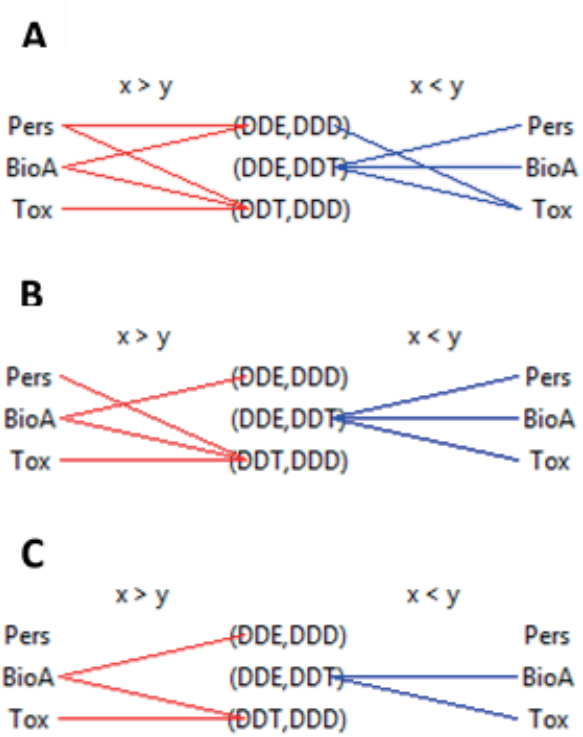


**Figure 9** – Tripartite graphs displaying the relationships between DDT, DDD and DDE, respectively as function of Δ: A: Δ = 0, B: Δ = 0.05 and C: Δ = 0.1.

Today the software package contains 100+ more or less specialized modules to cope with the various challenges in data analyses and thus decision support.

The development of specialized tools for data analysis is an ongoing process both in relation to the development of tools focusing at specific problems as well as tools of more general nature. The actual development of the PyHasse software is made by Dr. Rainer Bruggeman, Berlin, Germany.

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