MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 413-432

ISSN 0340 - 6253

Weighting Intervals and Ranking, Exemplified by Leaching Potential of Pesticides

R. Bruggemann[1], G. Restrepo[2, 3], K. Voigt[4], P. Annoni[5]

[1] *Leibniz-Institute of Freshwater Ecology and Inland Fishery, Berlin, Germany*
brg_home@web.de

[2] *Interdisciplinary Research Institute, Universidad de Pamplona, Bogotá, Colombia*

[3] *Laboratorio de Química Teórica, Universidad de Pamplona, Pamplona, Colombia*
grestrepo@unipamplona.edu.co

[4] *Helmholtz Zentrum Muenchen, German Research Center for Environmental Health, Institute of Biomathematics and Biometry, Germany*
kvoigt@helmholtz-muenchen.de

[5] *JRC-European Commission, Unit of Econometrics and Applied Statistics, Ispra, Varese, Italy*
paola.annoni@jrc.ec.europa.eu

(Received November 7, 2011)

Abstract

Often a ranking based on a multi-indicator system is performed by construction of a composite indicator, which is generally computed as a weighted average of the indicators. The set of weight-tuples is introduced: the g-space. Each point of this space represents a tuple of weight values, which lead together with the indicators of an object to a certain value of the composite indicator.
The composite indicator induces a weak or linear order, when the associated space of an object set together with a data matrix is available. Each hypercube in the g-space, corresponding to intervals of the weights, can be represented by a partial order which is not necessarily a weak or even a linear order. Changing from one point of the hypercube to another will often not change the partial order. We have a freedom of changing weights according to the dimensionality of the g-space -1 (because of normalization). When other hypercubes are selected, then other partial orders can be found. The boundary between two hypercubes with different partial orders is a lower dimensional sphere, with fewer degrees of freedom. In the current paper we treat these two points: (i) how to use weight intervals to determine the resulting partial orders and (ii) if the number of indicators is not too large and if the focus is on a pair of objects instead on the whole set, then equations are given which can be helpful.
As example pesticides are taken, for which three attributes are available. These pesticides are a subset of a set of 50 Italian pesticides, whose leaching potential to groundwater is investigated in Galassi et al.,1996.

1. Introduction

In environmental sciences, and even more often in social economic sciences a ranking is needed, see for instance Bruggemann, Patil, 2010, Bruggemann, Patil, 2011, Annoni, Bruggemann, 2008, Annoni et al., 2011. The usual scientific method is to search for indicators which measure the properties of the objects to be ranked, and then to aggregate them (mostly by weighted sums) eventually to super-indicators, often called pillar scores. Composite indices ("composites") are then computed by further aggregating the pillar scores to get a single, final score for each object. Composites are attractive because they always allow for a unique ranking of the objects. But they are also more and more criticized as linear aggregation always implies compensability between dimensions (see for example the vast literature on measuring well-being (Stiglitz et al., 2010). A good idea to overcome the drawback is to stop the aggregation at least at the level of pillars and see what conclusions can be drawn from the partial order resulting from the ordinal analysis of the pillar scores.

The main issue when performing linear aggregations is the weighting scheme which is often the result of subjective choices and, as a consequence, can be easily criticized thus weakening the trust in the ranking from the composite. In the last years many efforts were directed towards the problem of how to determine the weights, see for example Nardo, 2008.

In this context partial order theory can be of help. One of the recent extensions of the so-called Hasse Diagram Technique (HDT) is the introduction of the concept of step-wise aggregation of indicators, to have a control about the role of the weight values. This concept, which has several realizations, is called METEOR (method of evaluation by order theory), see Simon et al., 2005, 2006, Voigt, Bruggemann, 2005. In the new software package PyHasse (Bruggemann, Voigt, 2009) there are actually six modules tackling the concept of step-wise aggregation. Unfortunately this kind of analysis is too complex to be realized in all practical cases, although many studies show the usefulness of the concept (Simon et al., 2005, 2006).

Are there alternatives? Let us go back to the indicators, denoted by q_j, j=1, …, m and compute the composite indicator I as the weighted sum:

$$I(x) = \Sigma\, g_j * q_j(x) \quad j=1,..,m,\ x \in X, \text{ with X the object set and } g_j \in [0,1] \text{ and } \Sigma\, g_j = 1, \qquad (1)$$

In the general case the weights g_j are not known exactly but a range of variability can be assigned to each of them. We assume that the values of the indicators are observable and known, for a partial order analysis, if these property values are unknown, see Sørensen, et al, 2000, Denouex et al., 2005.

This paper shows how weight-intervals can be applied in terms of simple elements of partial order theory and is organized as follows:

After a brief introduction to the basic material concerning partially ordered sets, we moot a convenient notation, then we show by a simple example how the analysis can be performed. The reader may see that there is some analogy between thermodynamics of phase equilibria and the concepts studied here.

2. Material and Methods

2.1 Basics of the theory of partially ordered sets

Although there are many papers, from where basics of partially ordered sets are described (Bruggemann, Patil, 2010, Bruggemann, Patil, 2011, Bruggemann, Voigt, 2008, Bruggemann et al., 2001), we give a brief overview for the convenience of the reader.

Definition of component-wise order

Let us assume that a finite "object set" X (in technical terms also called a "ground set") is of interest. We wish to compare n objects x, y,... $\in$ X on the basis of m indicators, measured at least on an ordinal scale, characterizing them with respect to the ranking aim, i.e. an n $\times$ m data matrix is at hand. Therefore the comparison is performed by applying the special order relation called component - wise order: Let x, y be two different objects of the object set X. Let Q be the space of measurements that may be of different scaling levels. Let q(x) be the data row for x and q(y) that for y, i.e q(x), q(y) $\in$ Q:

$x < y$ if and only if $q(x) < q(y)$, $q(x) < q(y)$ if and only if for the components of q it is valid

$q_j(x) \leq q_j(y)$ for all j, j = 1, 2, …,m

and there is at least one attribute q_{i*}, for which a strict inequality

$q_{i*}(x) < q_{i*}(y)$ is found. (2)

Sets X equipped with a partial order, such as the specific one, defined in (2) are called partially ordered sets (posets).

Aim of ranking

An analysis of the data matrix by partial order is meaningless without the information about the aim of ranking. When the aim of ranking is known, the indicators are to be checked for their common orientation with respect to the aim. If necessary, the columns of the data matrix must be appropriately transformed (for example by multiplication by -1). Thus, for example, if one is ranking chemicals according to two indicators, say bioconcentration (BC) and biodegradation (BD), then high BC values indicate a problematic chemical, while high BD values indicate a desirable chemical. In this case one need to orientate indicators in such a way that high scores of both indicate either problematic or desirable chemicals.

Equivalence

If x, y are different objects but $q(x) = q(y)$, i.e. $q_j(x) = q_j(y)$ for all j, then the objects x and y are called equivalent under the equivalence relation 'equality'. Equivalence is denoted as: $x \cong y$. In empirical data matrices equivalence relations may appear, then we consider representatives of each equivalence class and add the information about the other equivalent elements, whenever needed.

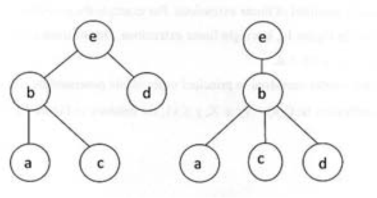
Further notations:

(i) Posets based on a data matrix are indicated by (X, IB), whereby $IB=\{q_1,..,q_m\}$ is the set of indicators, also called the information base (Bruggemann et al., 1995). (ii) We speak of 'elements' if their membership to a set is considered and of objects in a more general sense. (iii) If a partial order is to be denoted without reference to a set of indicators, we use the notation
$(X, \leq)$. (iv) When a set A is a finite set, we denote by $|A|$ the number of its elements.

2.2 Hasse diagrams

We first introduce the 'cover-relation': x is covered by y if there is no element $z \in X$ for which $x < z$ and $z < y$. We write this as $x \leq: y$. With the cover-relation at hand, we can get a diagrammatic representation of the partially ordered set: Let us consider x and y, and assume that $x \leq: y$. Then we draw x in a vertical plane below y and connect both with a straight line.

This is repeated for every ordered pair of the cover relation, i.e. for all pairs of two objects for which ≤: - relation holds. The resulting diagram is known as Hasse diagram. Example: X= {a, b, c, d, e} (Figure 1):



(a) (b)

Figure 1. (a): Hasse diagram representing a poset (X, ≤) (b)Hasse diagram after selecting an interval for the weights (see text below).

2.3 Some additional concepts:

1. Because of transitivity, couples such as $a \le e$ can easily be deduced from the Hasse diagram by finding strictly downward or upward paths of lines connecting a and e.
2. Objects x,y which are incomparable are denoted as $x \parallel y$.
3. If there is no incomparability, then we speak of a complete, total or linear order. In the case of a complete order, the objects $x \in X$ can be arranged in a sequence $x_1 < x_2 <\ldots < x_n$, i.e. a ranking is found.
4. Chain: If a subset $X' \subset X$ can be found such that for all $x \in X'$, a complete order is obtained, then this subset, together with the partial order relation, is called a chain.
5. Weak order: Representative elements of equivalence classes are in a chain, but there are equivalence classes. The equivalence classes can also be singletons, hence the weak order includes the linear or complete order as a specific case.
6. Antichain: If a subset $X' \subset X$ can be found such that, for no $(x, y) \in X' \times X'$, $x \perp y$, i.e. $x \le y$ or $y \le x$ holds, then this subset, equipped with the partial order relation, is called an antichain.
7. Maximal, minimal and isolated elements: An element x, for which no element y can be found with $y \ge x$ is called a maximal element. An element x, for which no element y can be found with $y \le x$ is called a minimal element. An element, which is at the same

time a maximal and a minimal element is called an isolated element. In Figure 1a: the maximal element is e, and the minimal ones are a, c, d; there is no isolated element.

8. Linear extension: A linear order derived from a partially ordered set, preserving all order relations, is called a linear extension. When a partially ordered set is not a linear order, then there exist a manifold of linear extensions. For example the partially ordered set, visualized in Figure 1a, has eight linear extensions. One of them is a < c < b < e < d, another: e < c < a < b < d.
9. Order ideal: (Here we restrict ourselves to principal order ideals generated by just one element O(x). The definition is: $O(x) := \{y \in X, y \leq x\}$, for instance in Figure 1a: $O(b) = (\{a,b,c\},\leq)$..

2.4 Weak or linear orders

There is a high interest to directly derive weak or linear orders from a partially ordered set. The basic idea is derived from the concept, published by Winkler, 1982: Identify all linear extensions and compute for each element $x \in X$ the average rank. By the average rank a weak order can be derived. This is an important concept, not because the theory of composite indicators is to be replaced, but because we have now the possibility of a cross-checking to find out, for example, great discrepancies between the position of an object in a ranking from a composite indicator and from average ranks indicate that the selection of weights may be crucial.

There are, however, two pitfalls in the method of average ranks:

1. As the number of linear extensions can increase with $|X|!$, we are faced with a computational problem. Consequently in the last years many research activities were focused on this point (De Loof et al., 2006, 2012, Bruggemann et al., 2004 and 2005, Bruggemann, Carlsen, 2011).

2. Because of order theoretical symmetries very often a high degree of ties among the average ranks is observed. This causes different objects to be ranked in the same position with a resulting degeneracy, which is unwanted in decision making.

Our proposal is to use weight intervals in order to improve the theory of composite indicators with respect to the choice of the weighting scheme.

2.5 Intervals of weights and their posetic consequences

Let us assume that we have m [0,1]-normalized indicators, and n objects (n= |X|, m=|IB|.)

Def. 1: G-space: $G:=\{(g_1,...,g_m)=: 0 \leq g_i \leq 1\}$. We speak of an m-tuple $g \in G$,

Def. 2: Normalized G-space: $G_n:=\{(g_1,..,g_m): \Sigma g_i=1, 0 \leq g_i \leq 1\}$

Def. 3: Composite indicator: $I(g,x):= \Sigma\, g_j*q_j(x)$, $(g_1,..,g_m) \in G_n$

I(g,.) indicates the set of values of the composite indicator, without specifying the

object x.

Def. 4: Hypercube: $H(g):=\{(g_1,...,g_m) \in G_n: g_j \in [g_j(\text{below}), g_j(\text{above})]\}$

The quantities g_j(below) and g_j(above) are the limiting values of the weight g_j and may come from experts' knowledge or previous studies such as for example the Regional Competitiveness Index where weights are based upon the World Economic Forum weights.

The edges of the hypercube H(g) are defined by the weight intervals.

Def. 5: g-point: An m-tuple $g \in G_n$.

Def. 6: g-poset: Let $H_i(g)$ be a hypercube, identified by the subscript i, then each single g-point in $H_i(g)$ identifies a weak order. The determination of all the common pairwise order relations leads to a g-poset. A g-poset is denoted by (X, IB, $H_i(g)$).

Obviously to each g-point belongs exactly one and only one composite indicator. And each composite indicator obtained from the points in $H_i(g)$ induces a weak order.

In Bruggemann et al. 2008, Restrepo et al., 2008a, Bruggemann, Patil, 2010 we discussed two- or three-dimensional G-spaces and we introduced the concepts of hot spots and stability fields. In simple words: "hot spots" are the points in the G_n-space where a slight variation of g crossing the hot spot implies many changes in the order, due to I(g,.). "Stability field" (hypercube in one dimension) is the dual concept: here a slight variation of the weights in all dimensions of G_n has no consequence in the order of the objects. The concepts developed in the context with stability fields can be extended too, indeed Restrepo et al. , 2008b, showed how this extension into a three dimensional space G_n can be done. However, the mathematical procedures can be tedious and visualization will be difficult in higher dimensions of G_n. In this paper the more pragmatical point of view of a stakeholder is the focus:

1) What is the consequence of knowing only intervals for each weight in posetic terms?

and

2) What can be done if the order relation between two objects is of interest?

Def. 7: g-phase: The union of hypercubes for which a given order relation between two objects, say x > y holds: $gph(x > y) := \bigcup_{x>y} H(g)$

Figure 2 shows, how hypercubes and g-phases are related.

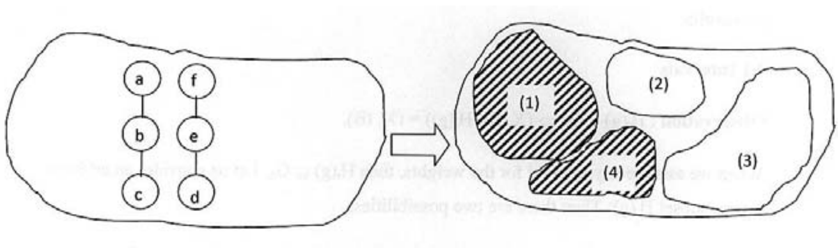


Figure 2. (a) Schematic presentation of G_n , the weights vary in the interval [0,1]. The effect of some more knowledge about weights is shown in (b) (see text).

From a normalized G-space G_n a poset can be built which represents the common order relations deduced from all composite indicators computed from all g-points, i.e.: In Figure 2 a poset is obtained, whose Hasse diagram shows two 3-element chains. The order relations a > b, a > c, b > c, f > e, f > d and e > d are the only common order relations, when all possible composites are examined for their orders. Assuming some knowledge concerning the weights (b) four different scenarios for the weights (weight models) are supposed. Correspondingly four sets of g-intervals are selected. Each of the hypercube defined by its set of intervals has now only a restricted set of composites, therefore the partial order will be enriched. We assume now that the hatched areas (1) and (4) contain g-posets for which b>d is in common. The union of these two areas would be a g-phase. Area 3 may contain g-posets with b<d, whereas in (2) b || d may appear.

The g-posets of certain g-phases can be seen as molecules in different physico-chemically defined phases. When we manipulate g by starting in a subset of G_n, where x<y and stop in a subset of G_n, where x>y, we have performed a “phase transition”. Coexistence of phases implies a phase rule, quantifying the number of freedoms, coexistence of g-phases reduces the number of freedoms too.

3. Results

3.1 Intervals

Observation : $H_i(g) = G_n \Rightarrow (X, IB, H_i(g)) = (X, IB)$.

When we assume any interval for the weights, then $H_i(g) \subseteq G_n$. Let us consider an arbitrary proper subset $H_i(g)$: Then there are two possibilities:

(1): We can find a hypercube $H_1(g)$, where a variation of g does not change the linear (or weak) order among the objects, due to the composite indicator I. Any refinement (reducing the intervals for the weights) cannot have a consequence for the orders in $H_1(g)$.

(2): There may be a hypercube $H_2(g)$ where not a weak order is found but a partial order. Depending on the kind of refinement, by which $H_3(g) \subseteq H_2(g)$ is found, different enriched partial orders up to linear or weak orders (if the intervals are small enough) result.

In the first case we have, what we called a stability field, in the second case, we know that the hypercube $H_3(g)$ includes hot spots.

In $H_1(g)$ there is freedom to vary the g-tuples in all m-1 dimensions (we have one degree of freedom less because of the constraint $\Sigma\ g_i = 1$).

In $H_3(g)$ there are variations which change the order of objects.

3.2 Coexistence of two g-phases

Let us assume that in one g-point we find $x<y$ and in another one we find $x>y$ .Between these two g-points there may be a g-point where the two objects x and y are equivalent with respect to the value of the composite indicator. That is:

$I(g,x)-I(g,y) = 0$ or $\Sigma\ g_i(q_i(x)-q_i(y)) = 0$

Together with $\Sigma g_i=1$ a matrix equation can be formulated as follows:

After introducing the abbreviations:

$\Delta_j := q_j(x)\text{-}q_j(y) \qquad q_j(\cdot) \in [0,1]$

$$\delta_{i,j} := \Delta_i - \Delta_j \tag{4}$$

we obtain:

$$\begin{pmatrix} \Delta_1 & \dots & \Delta_m \\ 1 & \dots & 1 \end{pmatrix} \times \begin{pmatrix} g_1 \\ \dots \\ g_m \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{5}$$

If equation (5) can be solved, then we find g-points of coexistence. If m=2 (only two indicators), than (5) can be easily solved and the solution is unique. If m>2 infinite solutions in a space of dimension m-2, corresponding to the normalization and to the coexistence condition, can be found. Now let us assume, that m=3 and that

$$\Delta_1 \neq 0,\ \delta_{1,2} \neq 0 \tag{6}$$

In this simple case of three indicators, it is easy to show that the coexistence condition (3) and the constraint on the sum of weights imply

$$\begin{cases} g_1 = -\dfrac{\Delta_3}{\delta_{13}} - g_2 \dfrac{\delta_{23}}{\delta_{13}} \\ g_2 = -\dfrac{\Delta_3}{\delta_{23}} - g_1 \dfrac{\delta_{13}}{\delta_{23}} \\ g_3 = 1 - g_1 - g_2 \end{cases}$$

The coexistence condition is granted if

$$\begin{cases} g_1 = -\dfrac{\Delta_2}{\delta_{12}} + \dfrac{\delta_{23}}{\delta_{12}} t \\ g_2 = \dfrac{\Delta_1}{\delta_{12}} - \dfrac{\delta_{13}}{\delta_{12}} t \\ g_3 = t \end{cases} \tag{7}$$

for each $t \in [0,1]$. Equation (7) describes a line as a coexistence condition for two g-phases in the three-dimensional space of weights G, and in the twodimensional space of weights in G_n. Analogously it is possible to extend (7) to the case m>3.

For the general the following equation is valid:

$$g = K + A^*t \tag{8}$$

Therein is

- g a vector of dimension m,
- K is a vector of dimension m with the components ($-\Delta_2/\delta_{1,2}$, $\Delta_1/\delta_{1,2}$, 0....,0),
- t is a vector of dimension m-2 and freely variable,and
- A is an m*(m-2)-matrix. The A-matrix with is conveniently written as follows:

$$A=\begin{pmatrix} A2 \\ I_{m-2} \end{pmatrix}.$$

A2 is the matrix where the first two rows are:

$$a_{1k}=-\frac{1}{\delta_{1,2}}\times\frac{\Delta_k\times\delta_{1,2}-\Delta_2\times\delta_{1,k}}{\Delta_1}=\frac{\delta_{2,k}}{\delta_{1,2}}=:Q_{1,k} \quad (9)$$

$$a_{2,k}=-\frac{\delta_{1,k}}{\delta_{1,2:}}=:Q_{2,k} \quad (10)$$

I_{m-2} is the unit matrix with m-2 rows and columns, respectively.

Varying the free parameters t influences the variations of the weight –values g_j. The space spanned by equation (8) is called CoG, as it is the space of coexistence of two g-phases in G.

Hypercubes which contains such a boundary sphere CoG are crucial ones, at least for those object pairs which are defining the boundary.

Any variation following equation (8) keeps I(x,g)= I(y,g). Instead of varying m-1 weights freely (taking into account that Σ g_i = 1) condition (3) further reduces the degrees of freedom. We see this as (pretty trivial) analogy between thermodynamical phases where the equilibrium conditions are expressed by equality of chemical potentials.

3.3 Crossing the phase boundary

Crossing the phase boundary means to find that subspace orthG in G, which is orthogonal to that defined by equation (7). The dimensionality is 2 as both, the space of CoG and the space orthogonal to CoG must give the space G. If we denote with A2 the two first rows of the matrix A, then the orthogonality condition leads to the equation for orthG.

$$\begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \cdots \\ g_m \end{pmatrix} = b + \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ -Q_{1,1} & -Q_{2,1} \\ -Q_{1,2} & -Q_{2,2} \\ \cdots & \cdots \end{pmatrix} \times \begin{pmatrix} t_1 \\ t_2 \end{pmatrix} \tag{12}$$

There the vector b consists of values to assure the constraint that $\Sigma\ g_i = 1$. The third to mth rows of the matrix in eq. (12) is just the matrix A2, transposed ($A2^t$) and multiplied by (-1). Hence we can write equation (12) in a more elegant way as:

$$\begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \cdots \\ \cdots \\ g_m \end{pmatrix} = b + \begin{pmatrix} I_2 \\ -A2^t \end{pmatrix} \times \begin{pmatrix} t_1 \\ t_2 \end{pmatrix}$$

I_2 is the 2*2 unit matrix.

4. A real life example

4.1 Data matrix

In De Loof et al., 2012 a data set about pesticides is used in order to show some new tools in partial order theory. Here the starting point is the same data set (Galassi et al., 1996) but restrict ourselves to those pesticides whose annual usage is over 1500 tons. Six out of 50 pesticides are then considered. For these pesticides the span of values of the vapour pressure is more than 10^8 which would need extra consideration as to how the vapour pressure values should be normalized in a meaningful manner, but this is not the main line of this paper. In Table 1 the data matrix of the six pesticides and the normalized indicator values for persistence (Tn), for the leaching tendency (Ln) and the usage (Usagen) are shown.

Table 1. Subset of the data matrix of Galassi et al, [0,1]-normalized indicators (rounded after the third digit)

name	id	Tn	Ln	Usagen
alachlor	a0	0.127	0.308	0
mancozeb	h2	1	0	0.545
metham-Na	i0	0	1	1
methylbromide	i5	0.762	0.643	0.692
ziram	n0	0.365	0.199	0.456
zineb	n1	0.365	0.043	0.232

4.2 Partial Order Analysis

The Hasse diagram of the six pesticides shows a pattern which is typical in evaluation problems: There is not a long chain with only some few incomparabilities: In contrast, the partial order consists of three components where two components are isolated elements, see Figure 3.

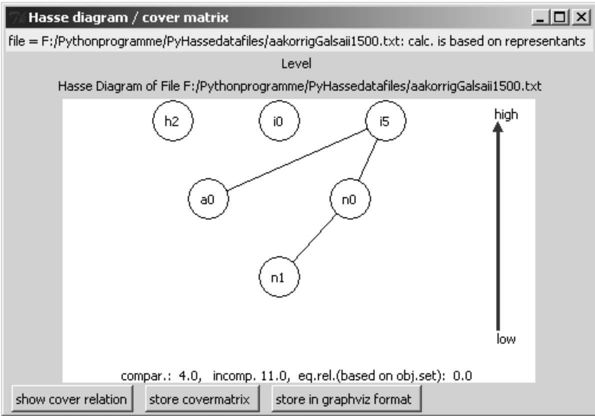


Figure 3. Hasse diagram derived from the data matrix in Table 1.(drawn with PyHasse software)

The leaching potential may be proportional to Usagen, Tn and Ln (in Halfon et al. , 1996 the vapour pressure is additionally taken into regard). Hence, the leaching potential should follow the sequence n1<n0<i5, or a0<i5. The fact that two isolated elements appear indicates that the leaching potential may be pretty high, when at least one of the three attributes is high. This suggests that also special mechanisms may be possible for the transfer from the soil to groundwater.

In former papers many techniques were developed to obtain more information out of this poor Hasse diagram (we called ‘poor’ for it does not show so many comparabilities). Beside the derivation of weak orders (see Bruggemann, Carlsen, 2011), one could apply the concept of tripartite graphs (Bruggemann, Voigt, 2011) to show which are the factors leading to separated subsets, or an antichain analysis could render more information about for instance the three maximal elements (Bruggemann, Voigt, 2012). Here, however we want to study the weight intervals and their influence on the enrichment of the original partial order shown in Figure 3.

4.3 Examples of enrichments

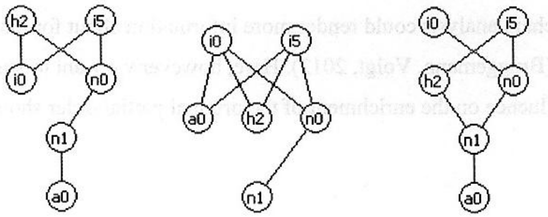
The module HDCI6.py of the software package PyHasse allows for calculating the composite indicator. By choosing equal weights (g_1=g_2=g_3= 0.3333), the composite indicator induces the following ranking: a0 < n1 < n0 < h2 < i0 < i5. However, the problem is: Is the selection of equal weights for all three indicators really appropriate? Should have usage or persistence more influence on the composite indicator? In Table 2 we discuss three weight models . In each of them one indicator is given a weight interval at the larger end of the weight scale, whereas the remaining two indicators get intervals at the lower end. The simulations are performed with 10000 Monte Carlo runs.

Table 2. Three weight models

Model	input	min	max	Volume of the hypercube	number of incomparabilities
a	[0.5, 1.0] [0.0, 0.3] [0,0.3]	0.471 0 0	0.994 0.358 0.355	0.066	4
b	[0,0.3] [0.5,1] [0,0.3]	0 0.466 0	0.368 0.995 0.349	0.068	6
c	[0,0.3] [0,0.3] [0.5,1]	0 0 0.466	0.358 0.356 1.0	0.068	3

Note that due to the weight constraint (Σg_i=1) the actual interval limits are different from the assigned limits (compare the values in columns 2, 3 and 4 of Table 2).

The Hasse diagrams of the corresponding partial orders are shown in Figure 4.



(a) (b) (c)

Figure 4. Hasse diagrams following three weight-interval models.

It can be observed that

- there is an enrichment of the partial order, all comparabilities found in the original poset are reproduced, however, new order relations are added: The original poset includes 11, the g-posets (Figure 4) have at maximum 6 incomparabilities
- Pesticide i5 is in all cases (including the original poset) a maximal element
- There is a change in the order relation for the pesticides h2 and i0: In Figure 6a: h2>i0, in Figure 4b, however: i0>h2, in Figure 4c: i0 || h2.
- Contextually the introduction of weight intervals leads to more chains, expressing the increase of the leaching potential and in two out of three models the chains are becoming longer.

When we measure the uncertainty in giving weights by the volume of the space G_n, which is 0.7, then the reduction in uncertainty, measured by the volumes of the hypercubes by almost factor 10 , reduces the incomparabilities by a factor of around 2.

4.4 Boundary of the g-phases

Let us discuss the g-phases where h2 > i0 and i0 > h2, respectively, as well as the g-phase boundary. According to equation (7) (or in many cases simply by directly manipulating the corresponding equations) the following results are obtained.

$g_1 = 0.5 - 0.2725 * g_3$

$g_2 = 0.5 - 0.7275 * g_3$

These two equations describe the CoG of those coexisting phases, where h2 > i0 and h2 < i0.

In fact this 1- dimensional space is the set of all three dimensional g-points, where the composite indicator score for pesticide h2 equals that for i0.

Knowing this pair of equation one can easily check points in G_n, so that h2 < i0 or h2 > i0.

In Table 3 four g-points are selected, following the equations for CoG and the corresponding configuration of i0 versus h2 is shown.

Table 3. Points in the G_n-space which are not on CoG.

g-model	g_1	g_2	g_3	configuration*)
1	0	0.3	0.7	h2 < i0
2	0	0.7	0.3	h2 > i0
3	0.466	0.2	0.334	h2 > i0
4	0	0.4	0.6	h2 < i0

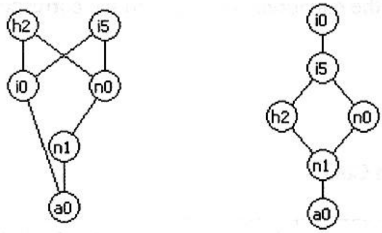
*): The order relation is related to an enriched partial order, where the selected weights are taken from an interval which does not include the g-point, corresponding to the coexistence condition.

When g-intervals are according to g-models 3 and 4 (see Table 4), then the partial orders are obtained, where h2 and i0 are in the order relation, as shown in Table 3.

Table 4. g-intervals according to g-models 3 and 4, respectively.

g-model	input gbelow	input gabove	realized g-values: min	realized g-values: max	order relation h2⊥i0
3	0.5 0.2 0.0	1 0.3 0.4	0.429 0.128 0.0	0.829 0.363 0.354	h2>i0
4	0 0.2 0.6	0.1 0.4 1.0	0.0 0.157 0.55	0.107 0.39 0.829	h2<i0

Then a partial order is obtained (Figure 5):



(a) (b)

Figure 5. (a) Partial order with intervals selected according to g-model 3.(b), according to g-model 4.

5. Discussion

Composite indicators play an enormous role, especially in political sciences, where for example nations of the European Union are to be measured with respect to educational level or innovation potential or as an actual example, economical power of nations (rating). After the absolutely not trivial selection of suitable properties the not trivial task begins to give weight values for the properties, so that from them the composite indicator can be calculated as a weighted sum. In decision support systems other procedures to obtain a ranking of objects are well known such as for example PROMETHEE (Brans, Vincke, 1985) or other systems, as described in Munda, 2008. Although the construction of composite indicators by a weighted sum is transparent and does not need additional steering parameters as it is the case for example in PROMETHEE, where the preference functions need to be fixed. The weights are not always known precisely and in general intervals are to be defined for each of them. A hypercube in the G_n-space may be small enough so that the partial order is in reality a linear or weak order. Often however the hypercubes contain a partial order where incomparabilities appear. Then there are either possible refinements such that hypercubes included in the original one now contain the desired linear order, or the enrichment is powerful enough to find decisions.

There are still open questions: The more direct approach would be to determine those hyperspaces of G_n which have all the same linear order. When n objects are to be analyzed, then n-1 equations can be found of the type I(g,x) = I(g,y). Then, however, we leave the supposition of independent incomparabilities, i.e. have to take care for transitivity. This is not sufficiently investigated and remains for future work.

Furthermore the approach shown here has some similarity with the reasoning in Paelinck 1977, 1978 and it seems to be an interesting task to deepen the comparison between the approach shown here and the approach discussed back in the seventies of the last century.

References

Annoni, P. 2007, Different ranking methods: Potentialities and pitfalls for the case of European opinion poll, *Environ. Ecol. Stat.* **14**:453-471.

Annoni, P., R. Bruggemann. 2008, The dualistic approach of FCA: A further insight into Ontario Lake sediments, *Chemosphere* **70**:2025-2031.

Annoni, P., R. Bruggemann. 2009, Exploring partial order of European countries, *Soc. Indicators Res.* **92**:471-487.

Annoni, P., M. Fattore, R. Bruggemann. 2008, Analyzing the structure of poverty by fuzzy partial order, in: J. Owsinski, R. Bruggemann (Eds.), *Multicriteria Ordering and Ranking: Partial Orders, Ambiguities and Applied Issues*, Sys. Res. Inst. Polish Acad. Sci., Warsaw, pp 107-124.

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

Annoni, P., K. Kozovska. 2010, EU Regional Competitiveness Index 2010. EUR 24346 EN, European Commission.

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

Bruggemann, R., G. P. Patil. 2010, Multicriteria prioritization and partial order in environmental sciences, *Environ. Ecol. Stats.* **17**:383-410.

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

Bruggemann, R., K. Voigt. 1995, An evaluation of online databases by methods of lattice theory, *Chemosphere* **31**:3585-3594.

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

Bruggemann, R., K. Voigt. 2009, Analysis of partial orders in environmental systems applying the new software PyHasse, in: J. Wittmann, M. Flechsig (Eds.), *Simulation in Umwelt- und Geowissenschaften- Workshop Potsdam 2009*, Shaker-Verlag, Aachen, pp. 43-55.

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

Bruggemann, R., K. Voigt. 2012, 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**:731-744.

Bruggemann, R., L. Carlsen. 2011, An improved estimation of averaged ranks of partially orders, *MATCH Commun. Math. Comput. Chem.* **65**:383-414.

Bruggemann, R., K. Voigt, G. Restrepo, U. Simon. 2008, The concept of stability fields and hot spots in ranking of environmental chemicals, *Environ. Modell. Softw.* **23**:1000-1012.

Bruggemann, R., P. B. Sørensen, D. Lerche, L. Carlsen. 2004, Estimation of averaged ranks by a local partial order model, *J. Chem. Inf. Comp. Sci.* **44**:618-625.

De Loof, K., B., De Baets, H. De Meyer. 2008, Properties of mutual rank probabilities in partially ordered sets, in: J. Owsinski, R. Bruggemann (Eds.), *Multicriteria Ordering and Ranking: Partial Orders, Ambiguities and Applied Issues*, Sys. Res. Inst. Polish Acad. Sci., Warsaw, pp. 146-165.

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

De Loof, K., B. De Baets, H. De Meyer, R. Bruggemann. 2008, A Hitchhiker's guide to poset ranking, *Combin. Chem. High Throughput Screen.* **11**:734-744.

De Loof, K., H. De Meyer, B. De Baets. 2006, Exploiting the lattice of ideals representation of a poset, *Fund. Informat.* **71**:309-321.

Denoeux, T., M. H. Masson, P. A. Hébert. 2005, Nonparametric rank-based statistics and significance tests for fuzzy data, *Fuzzy Sets Sys.* **153**:1-28.

Fattore, M., R. Bruggemann, J. Owsinski. 2011, Using poset theory to compare fuzzy multidimensional material deprivation across regions, in: S. Ingrassia, R. Rocci, M. Vichi (Eds.), *New Perspectives in Statistical Modeling and Data Analysis*, Springer-Verlag, Heidelberg, pp. 49-56.

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

Munda, G. 2008, *Social Multi-Criteria Evaluation for a Sustainable Economy*, Springer-Verlag, Berlin.

Nardo, M. 2008, *Handbook on Constructing Composite Indicators -Methodology and User Guide*, OECD, Ispra.

Paelinck, J. 1977, Qualitative multicriteria analysis: An application to airport location, *Environ. Planning A* **9**:883-895.

Paelinck, J. H. P. 1978, Qualiflex: A flexible multiple-criteria method, *Econ. Lett.* **1**:193-197.

Restrepo, G., R. Bruggemann. 2008, Dominance and separability in posets, their application to isoelectronic species with equal total charge, *J. Math. Chem.* **44**:577-602.

Restrepo, G., M. Weckert, R. Bruggemann, S. Gerstmann, H. Frank. 2008a. Ranking of refrigerants, *Environ. Sci. Technol.* **42**:2925-2930.

Restrepo, G., R. Bruggemann, M. Weckert, S. Gerstmann, H. Frank. 2008b. Ranking patterns, an application to refrigerants, *MATCH Commun. Math. Comput. Chem.* **59**:555-584.

Simon, U., R. Bruggemann, H. Behrendt, E. Shulenberger, S. Pudenz. 2006, METEOR: A step-by-step procedure to explore effects of indicator aggregation in multi criteria decision aiding - Application to water management in Berlin, Germany, *Acta Hydrochim. Hydrobiol.* **34**:126-136.

Simon, U., R. Bruggemann, S. Mey, S. Pudenz. 2005, METEOR - Application of a decision support tool based on discrete mathematics, *MATCH Commun. Math. Comput. Chem.* **54**:623-642.

Sørensen, P. B., M. Thomsen, P. Fauser, B. Münier. 2007, The usefulness of a stochastic approach for multi-criteria selection, in: O. Hryniewicz, J. Studzinski, A. Szediw (Eds.), *Environmental Informatics and Systems Research*, Shaker Verlag, Aachen, pp. 187-194.

Sørensen, P. B., B. B. Mogensen, L. Carlsen, M. Thomsen. 2000, The influence on partial order ranking from input parameter uncertainty - Definition of a robustness parameter, *Chemosphere* **41**:595-600.

Stiglitz, J. E., Sen A., Fitoussi J. P. 2010, *Mismeasuring Our Lives: Why GDP Doesn't Add Up*, The New Press.

Voigt, K., R. Bruggemann. 2005, water contamination with pharmaceuticals: Data availability and evaluation approach with hasse diagram technique and meteor, *MATCH Commun. Math. Comput. Chem.* **54**:671-689.

Winkler, P. 1982, Average height in a partially ordered set, *Discr. Math.* **39**:337-341.