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The concept of stability fields and hot spots in ranking of environmental chemicals

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Abstract

In contrast to conventional multi-criteria decision aids, such as the well known PROMETHEE approach, AHP or the different versions of ELECTRE, we support the basic assumption of environmetrics: let first the data speak, and then let us include subjective preferences in order to get a unique decision. In the present paper we introduce and discuss the decision support system METEOR (Method of Evaluation by Order Theory). The basis of the method is a data matrix. The rows are defined by the objects which are to be evaluated; the columns are defined by the attributes, which characterize the objects with respect to the evaluation problem. By means of the attributes a partial order is derived. In subsequent steps attributes are aggregated by a weighting procedure, allowing a high degree of participation of stakeholders and other participants of the planning process. The aim is to enrich the partial order stepwise, until the objects of interest can be compared. The software WHASSE written in Delphi is available for scientific purposes from the first author.

As an example we evaluate 12 high production volume chemicals (HPVC) which have been detected in the environment by four attributes and discuss the enriched partial order after introducing some weights. It turns out that in some cases the weights have almost no influence concerning the evaluation result, whereas in some other cases slight variations of weights drastically change the evaluation result. Therefore, the metric space spanned by weights can be partitioned in so-called ‘‘stability fields’’ where the evaluation result is invariant and in so-called ‘‘hot spots’’, where the evaluation is strongly changing. This characterisation of the space of weights is helpful for stakeholders to express their preferences.

Keywords: HPV chemicals; Environmental chemicals; Ranking; Posets; Hasse diagram technique (HDT); Decision support systems; Cluster analysis; Method of Evaluation by Order Theory (METEOR); Stability fields; Environmetrics; Environmental software

1. Introduction

Multi-criteria decision making becomes more and more important in environmental sciences and hence quite a few research projects focus on this topic. For example the MULINO Decision Support System (mDSS) has been developed for implementing the European Water Framework Directive, namely integrating environmental, social and economic concerns (Giupponi, 2007). Another example concerning the Integrated Water Resources Management (IWRM), is a multi Objective Decision Support System (MODSS) which has been developed and applied to the planning of the Lake Maggiore (Castelletti and Soncini-Sessa, 2006). The Elbe-Decision Support System is a computer based system for integrated river basin management of the German river Elbe basin and is therefore another example for an environmental decision

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support system (Berlekamp et al., 2007). A methodology based on a hybrid approach that combines fuzzy inference systems and artificial neural networks has been used to classify the ecological status in surface waters. This methodology is applied to sampling sites in the Ebro river basin and can support decision makers in evaluation and classification of ecological status, as required by the EU Water Framework Directive (Ocampo-Duque et al., 2007). The chemical speciation model BIOCHEM comprises ecotoxicological transfer functions for uptake of metals (As, Cd, Cu, Ni, Pb, and Zn) by plants and soil invertebrates and is another example for a flexible and dynamic decision support system (DSS) to analyse natural or anthropogenic changes that occur in river systems (Vink and Meeussen, 2007). A further interesting work including the spatial factor is a multi-criteria decision making approach applied to urban water management (Makropoulos and Butler, 2006). Concepts for the use of techniques of decision analysis to structure scientist and stakeholder involvement in river rehabilitation decisions are published by Reichert et al. (2007). The software, named proDEX is also applied as a multi-criteria decision support model in environmental sciences (Znidarsic et al., 2006).

Decisions concerning risk assessment of chemicals are to be supported by information about exposure and effects of chemicals. Both, exposure and effects are used as attributes/indicators to evaluate the chemicals under investigation. For the subsequent evaluation of chemicals, many methodological approaches are available, requiring in principle the same working steps, which are discussed in more detail in Simon et al. (2005) and Klauer et al. (2001). One step, namely the evaluation algorithm is often almost disregarded in real evaluations. The chosen evaluation approach however influences the evaluation result and the participation of stakeholders. The efficiency of participation of stakeholders and the acceptance of the decision result in turn depends on the transparency of the evaluation procedure. For example: decisions about complex problems such as chemical risk assessment will include conflicting attributes. To solve such conflicts, the most commonly used approaches include the methodological step of attributes' aggregation. The benefit of the aggregation step is that finally a linear ranking of the objects (here: chemicals) can be obtained, identifying *one* best solution, e.g. the chemical with the lowest risk. Aggregation often implies a trade off among attributes: a bad evaluation in one or more attribute(s) can be compensated for by a good evaluation in other attributes. However, attributes can represent fundamentally different aspects such as accumulation, mobility and toxicity. Therefore the methodological idea followed in this paper is to take first a purely statistical explorative point of view (i.e. "let first the data speak") and to include additional knowledge, e.g. the preferences of the stakeholder, in separate steps in order to keep a maximal control over the effect of including additional knowledge.

The paper is organized as follows: in Section 2 the example of 12 high-production volume chemicals (HPVC) is introduced, the methods Hasse diagram technique (HDT) and Method of Evaluation by Order Theory (METEOR) and the concept of crucial weights together with their analysis toward the introduction of "*g*-spectra, stability fields and hot spots" are explained. Whereas for the sake of demonstration a simpler example is used, Section 3 shows the application of METEOR on the HPVC data matrix. A detailed discussion about possible extensions of the method concludes the paper. Additionally, there are appendices 1–4, where abbreviations, symbols and concepts are listed (Appendix 1) and where some counting formulas are explained (Appendices 2–4).

2. Materials and methods

2.1. Data preprocessing

With publication of the White Book of the EU (EEC, 2001) and of the REACH-procedure (European Commission, 2006) the interest in ranking of chemicals as a preparatory step is renewed: here the data matrix (12 high production volume chemicals) define the rows, and 4 attributes define the columns), first published by Lerche (2002a) is taken as a ranking example and is more extensively described in the Section 3. We are calling the set of objects (i.e. of chemicals) C.

"Results". Note, that we refer to 'objects' instead of chemicals as long we are not discussing the real life example.

Often it is necessary to transform a data matrix into the appropriate form i.e. into the closed interval [0,1] for an evaluation:

(i) a normalization by

$$\bar{q}_i(j) := \frac{q_i(j) - q_i(\min)}{q_i(\max) - q_i(\min)}, \quad i = 1, \ldots, 4, \quad j \in \mathrm{C}$$

(ii) check for a common orientation (high numerical value indicates a high risk) by multiplying attributes – if necessary – with −1 or another appropriate transformation
(iii) shifting negative values to positive entries by adding a positive number to the attribute values.

The subjective preferences of stakeholders are expressed by weights, which are taken from the closed interval [0,1]. We consider the weights as 'external knowledge', whereas the data matrix expresses the basic information taken from measurements or modelling.

2.2. Hasse diagram technique

Several well-known evaluation algorithms are available such as PROMETHEE (Brans and Vincke, 1985), AHP (Saaty, 1994), MAUT (Schneeweiss, 1991), ELECTRE (Roy, 1990) or NAIADE (Matarazzo and Munda, 2001). All these methods include an aggregation of attributes by including subjective preferences and therefore cannot be considered as purely data explorative methods. Beyond this it is difficult to trace back how the evaluation result was influenced by parameters to run those algorithms. Hence we consider these high sophisticated methods on the one side as efficient, as they deliver a unique decision, but on the other side as not transparent and difficult to handle as all preferences must be at hand simultaneously.

An alternative approach is provided by simple elements of partial order theory, such as Hasse diagram technique (HDT) (Brüggemann and Voigt, 1995; Brüggemann and Welzl, 2002; Brüggemann and Carlsen, 2006; Brüggemann et al., 1994, 2001, 2006a; Voigt et al., 2004a,b, 2006). For the sake of clarity we define some important concepts used in this paper.

Definition 1. We call x an object and C the ground set that is the set of objects.

Definition 2. $q_i(x)$ is the ith attribute of the object x and $\mathrm{IB} = \{q_i | i = 1, 2, \ldots, m\}$ the set of m attributes (information base).

Definition 3. Let $x, y \in \mathrm{C}$ and $q_i \in \mathrm{IB}$, then $x \le y$ if $q_i(x) \le q_i(y)$ for all $i = 1, 2, \ldots, m$. We say that x and y are comparable. If the orientation does not play a role, we write $x \perp y$ to express that x and y are comparable.