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CombiSimilarity, an innovative method to compare environmental and health data sets with different attribute sizes example: Eighteen Organochlorine Pesticides in soil and human breast milk samples

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ABSTRACT

Human health and the health of the environment have entwined. In this paper we underpin this position by presenting a modeling approach named CombiSimilarity, which has been developed by the first author in the software tool PyHasse comprising a wide variety of partial ordering tools. A case study of 18 Organochlorine Pesticides (OCPs) detected in soil as well as in human breast milk samples in the Taurus Mountains in Turkey is carried out. Seven soil samples and 44 breast milk samples were measured. We seek to answer the question whether the contamination pattern in breast milk is associated with the contamination pattern in soil by studying the mutual quantitative relationships of the chemicals involved. We could demonstrate that there is a similarity with respect to the concentration profiles between the soil and breast milk pollution. Therefore the hypothesis may be formulated that the concentrations of chemicals in the milk samples are strongly related to the soil contamination. This supports the concept that soil could be a surrogate for human exposure at background locations.

1. Introduction

We find ourselves in an uneasy position due to the impact of the great industrial and technologic expansions. The mushrooming chemical industry, the wide application of nuclear energy, the revolutionary changes in food processing, and many other technological developments are affecting the environment and consequently the health of man, in multitudinous ways. The numerous benefits associated with these developments have been detracted from the recognition that the health factor may well be the limiting factor in the continuing development. It is amazing that these statements have already be recognized and published around 60 years ago (Ludwig, 1955). An approach to the identification of organic compounds hazardous to the environment and human health has already been initiated by the US National Science Foundation in the seventies (Stephenson, 1977). However, in the following decades environmental topics and health topics have not been regarded sufficiently in parallel. Only recently, these two interacting areas are acknowledged to be considered in closer conjunction. This implies that monitoring data are available not only on the environmental contamination side but also on the human tissue side.

The modeling aspects have been acknowledged by several approaches, e.g. an environmental health impact assessment approach (Knol et al., 2010), a hazard ranking model for environmental and human health hazard classifications for 55 plastic polymers (Lithner et al., 2011), human health risk assessment of chemicals at electronic waste sites in China (Chan and Wong, 2013).

The global pesticide use comes at the cost of its widespread occurrence in the environment and eventually in many cases in the human body. A special emphasis should be laid on the pesticides with endocrine effects. Endocrine disruptors are exogenous agents that interfere with the production, release, transport, metabolism, binding, action or elimination of the natural hormones from the body and are responsible for the maintenance of homeostasis and the regulation of developmental processes. Hence they can act like uncontrolled medicine (Birnbaum, 2013). In a recently performed

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Table 1
Eighteen OCPs detected in human and environmental samples in the Taurus Mountains, Turkey.

Nr.	Acronym	Standard abbreviation	Name	CAS-number
01	**AHCH**	alpha-HCH	alpha-Hexachlorcyclohexane	319-84-6
02	**BHCH**	beta-HCH	beta-Hexachlorcyclohexane	319-85-7
03	**GHCH**	gamma-HCH	gamma-Hexachlorcyclohexane	58-89-9
04	**PECB**	PCB	Pentachlorobenzene	608-93-5
05	**HCBE**	HCB	Hexachlorobenzene	118-74-1
06	**PPDT**	p, p′-DDT	p, p′-Dichlordiphenyltrichlorethane	50-29-3
07	**OPDT**	o, p′-DDT	o, p′-Dichlordiphenyltrichlorethane	789-02-6
08	**PPDD**	p, p′-DDD	p, p′-Dichlordiphenyldichlorethane	72-54-8
09	**OPDD**	o, p′-DDE	o, p′-Dichlordiphenyldichlorethane	53-19-0
10	**PPDE**	p, p′-DDD	p, p′-Dichlordiphenyldichlorethene	72-55-9
11	**OPDE**	o, p′-DDD	o, p′-Dichlordiphenyldichlorethene	3424-82-6
12	**OXYC**	Oxychlordane	Oxychlordane	27304-13-8
13	**CHCE**	cis-Heptachloroepoxide	cis-Heptachloroepoxide	1024-57-3
14	**DIEL**	Dieldrin	Dieldrin	60-57-1
15	**END1**	Endosulfan	Endosulfan-1	959-98-8
16	**END2**	Endosulfan	Endosulfan-2	33213-65-9
17	**MECH**	Methoxychlor	Methoxychlor	72-43-5
18	**MIRE**	Mirex	Mirex	2385-85-5

study the current knowledge of the potential endocrine impacts of 105 pesticides on human health is given (Mnif et al., 2011). Out of our test set of eighteen pesticides (see Table 1) seventeen have endocrine effects according to Mnif's study.

The occurrence of environmental chemicals in the Taurus Mountains in Turkey motivated an international study on POPs (Persistent Organic Pollutants) in environmental and human media. Eighteen OCPs (Organochlorine Pesticides) in samples of soils as well as in human breast milk were analyzed in different regions in the Taurus Mountains in Turkey (Turgut et al., 2012). The soil samples were taken in seven different geographical heights and composited according to the methods of the German Environment Specimen Bank (http://www.umweltprobenbank.de/en/documents/publications/15883). At each height only one soil sample was retained. Concerning the breast milk samples, women at five different heights were considered. At each height a different number (from three to fourteen) of human breast milk samples was analyzed.

The contamination of soils has already been evaluated and published in this journal by Turgut et al. (2012). The determination of the occurrence of OCPs in breast milk samples was the aim of a recently published study (Voigt et al., 2013a). Voigt et al. (2013b) demonstrated that in Finland, Demark and Turkey the concentration profiles (values of the concentrations in an ordered tuple of samples) of OCPs in breast milk samples are similar to that of the soil samples.

In our current study we evaluate the same number of chemicals, namely eighteen pesticides, in breast milk samples as well as in soil samples and aiming to find out as to how far, concentration profiles between the environmental soil samples (seven samples) can be considered as similar (see Section 2) to those of the human breast milk samples (44 samples). An appropriate data analysis method to answer such is the discrete mathematical method called the Hasse diagram technique (HDT) (Bruggemann et al., 2001). The software package used is the PyHasse software (Bruggemann et al., 2014). This software is written in Python by the first author and it is under constant development. It comprises more than 100 modules which are of great support especially in the data evaluation of environmental health data.

2. Material and methods

2.1. Data matrix

In this approach we want to examine the occurrence of eighteen OCPs presented in Table 1 in a human medium, namely breast milk, as well as in an environmental medium, namely mountain soil. In Table 1 we can see the eighteen chemicals with their used acronym, standard abbreviation, name, and CAS-number. The list comprises persistent organic pollutants and their degradation products. Most of these chemicals have already been banned worldwide in the Stockholm Convention (United Nations, 2013). This convention is a global treaty to protect human health and the environment from persistent organic pollutants (POPs). The Stockholm Convention focuses on eliminating or reducing releases of twelve POPs, the so-called Dirty Dozen. The twelve key POPs that are targeted by the Convention include Aldrin, Chlordane, DDT, Dieldrin, Dioxins, Endrin, Furans, Hexachlorobenzene, Heptachlor, Mirex, PCBs and Toxaphene. Alfa-hexachlorocyclohexane, beta-hexachlorocyclohexane, gamma-hexachlorocyclohexane (lindane) and pentachlorocyclohexane are now included as POPs in Annexes A and C of the Stockholm Convention (2009). Mirex is a good example for POPs traveling long distances in the air and be deposited in areas far from where they were released because Mirex has never been produced and used in Turkey.

These listed organochlorine chemicals are known to pose a serious threat to the environment and consequently to human health. Especially the endocrine disruption potential of some of these chemicals should initiate action worldwide. In a review concerning the history of the discovery of the widespread toxicity of chlorinated hydrocarbons by Rosner and Markowitz (2013), the authors conclude the enormous lag between identification of danger and ultimate regulation of these products which is still a major public challenge.

2.2. Ranking

2.2.1. Partial order relation

Often a ranking aim is not directly measurable. As a proxy for the ranking aim suitable indicators are introduced, which can be measured or calculated by mathematical models. Taken many objects to be ranked and a set of indicators a data matrix results. The data matrix can be considered as a multi-indicator system (abbr.: mis) (Bruggemann and Patil, 2011). The columns of this data matrix represent indicator values expressing a non-measurable ranking aim. That means, the indicators are oriented in a manner that increases in values express increase with respect to the ranking aim.

To rank objects, whose ranking aim is expressed by several indicators as proxies is by far not trivial. The inherent difficulties will be evident when the manifold of different ranking aggregation methods is inspected. Munda and Nardo (2008) write that there is indeed an inherent ambiguity, which can be traced back to the works of Borda and Condorcet in the eighteenth century (Borda, 1784; Condorcet, 1785). Here we apply simple elements of partial order theory, which do not aggregate the indicators and which are therefore not affected by the above-mentioned built-in ambiguity.

Partial orders in multi-indicator systems can be introduced in many different ways. Most obvious is to set:

Let X be an object set and $x, y \in X$, and let q_i $(i=1,...,m)$ be the m indicators which we conveniently consider as elements of a set too, namely of the "information base", IB and $m=|IB|$ (Bruggemann et al., 1995). Note we use objects and elements of a set interchangeably. Elements of a set will not always be objects; hence both notions are needed. We define then:

$$x \le y : \Leftrightarrow q_i(x) \le q_i(y) \text{ for all } q_i \in IB. \tag{1}$$

In application of Eq. (1) we assume that objects equivalent to each other with respect to their profiles $(q_1(),q_2(),...,q_m())$ are identified and only representatives of the equivalence classes are retained. If needed, the equivalent elements are taken into consideration appropriately.