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Problem Driven Evaluation of Chemical Compounds and Its Exploration

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Abstract

We continue [5] by generalizing the indicator–driven evaluation. The mathematical basis is now a general complete lattice L. We show that this allows a *problem–orientation* by choosing a suitable set theory and logic. It leads, for example, to a problem–oriented subsethood degree relation that generalizes Kosko's subsethood degree applied in [5]. In addition we shall discuss an *exploration* of the evaluation, using tools from data bank theory and formal concept analysis. We give a brief introduction to various mathematical tools and methods appropriate for dealing with this kind of problems. Having listed the mathematical basics we describe in particular the acquisition of knowledge obtainable from an evaluation. It is illustrated by an evaluation of chemical compounds using ecologically relevant parameters. We demonstrate the use of free software in order to get a basis of *all* the attribute implications that can be derived from an evaluation.

1 Orders

Evaluation is needed for *ranking objects* with respect to certain attributes, and ranking means to put an *order* on the set of objects. The order is obtained by first associating with each pair (o, a) consisting of an object o and an attribute a a value $\mathcal{E}(o, a)$, for example, a real number or a symbol like $\oplus \oplus /\ominus$, and we shall assume that this value belongs to a complete lattice,

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i.e., a *partial* order, because we need to allow incomparabilities. Having the sequence of values associated with a fixed object and the sequence of all the attributes at hand, we evaluate this particular object by this sequence of values. The set of sequences corresponding to the set of objects is also partially ordered in a canonical way, and it is this order on all these sequences that we call the canonical partial order or ranking of the objects.

Orders are particular relations on sets, and so we first recall the definition of relation: Let S denote a set. A *relation* R on S is a subset of

$$S \times S = \{(s, s') \mid s, s' \in S\},$$

which means that R is a set of pairs (s, s') of elements of S, for short: $R \subseteq S \times S$. If such a pair (s, s') is contained in R we write $(s, s') \in R$ or, for short, sRs'. If (s, s') or (s', s) are contained in R, the elements s and s' of S are *related* or *comparable*, otherwise they are *unrelated* or *incomparable*.

1.1 Definition (order, partial order, total order)

A relation R on L is called a partial order, if it is

- *reflexive, i.e., if all the pairs (s, s), $s \in S$, are contained in R, sRs, for all $s \in S$,*
- *antisymmetric, if sRs' and $s'Rs$ together imply that $s = s'$, and*
- *transitive as soon as sRs' together with $s'Rs''$ yields sRs''.*
- *A partial order R is a total order if any two elements $s, s' \in S$ are comparable.*

Hence, partial order is the general notion, total orders are particular cases. We may simply speak of an order, when we need not specifiy if it is total or not.

$\diamond$

Let us collect a few prominent partial orders that show up in the applications: Well known to the reader is the notation $r \leq s$, for two real numbers r and s, which indicates that $s - r$ is not negative, for short: $0 \leq s - r$. Moreover, the reader knows that $r < s$ indicates that $r \leq s$ and in addition $r \neq s$.

We first restrict attention to the 2–element set $S = \{0, 1\}$ consisting of the real numbers 0 and 1. It is totally ordered since $0 \leq 0$, $0 \leq 1$ and $1 \leq 1$. We can express this total order in terms of pairs as

$$R = \{(0, 0), (0, 1), (1, 1)\}$$

or (as a set) by the following abbreviation:

$$S = \{0 < 1\}.$$

The cartesian square

$$S^2 = S \times S = \{0,1\} \times \{0,1\} = \{(0,0),(0,1),(1,0),(1,1)\}$$

is partially but not totally ordered (since neither $(0,1) \leq (1,0)$ nor $(1,0) \leq (0,1)$) via

$$(s,s') \leq (s'',s''') \iff s \leq s'' \text{ and } s' \leq s'''.$$

Similarly, we have the total order on $\{0,1,2\}$ that gives a partial order on $\{0,1,2\}^2$. An arbitrarily selected small set of chemicals (cf. [18]) will demonstrate an idea to use it in an evaluation.

No.	Chemical name
1	Hexabromobenzene
2	Hexachlorobenzene
3	Perylo[3,4-cd:9,10-c'd']dipyran-1,3,8,10-tetrone
4	Bis(2,4-dichlorobenzoyl)peroxide
5	Tetradecafluorohexane
6	1,1,2,2,3,3,4,4,5,5,5-Undecafluoropentane-1-sulfonyl fluoride
7	1,1,2,2,3,3,4,4,5,5,6,6,6-Tridecafluorohexane-1-sulfonyl fluoride
8	3',6'-Bis(diethylamino)-spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one

We use the parameters

$nBCF$, the normalized bioconcentration factor, and

$nBDP$, the normalized and correctly oriented biodegradation potential.

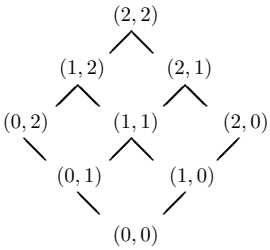
Note that large values of the parameters $nBCF$ and $nBDP$ indicate an environmental hazard. A discretization into three intervals with equal length was performed, just to obtain objects with indicator values taken from the set $\{0,1,2\}$. The data matrix, i.e., the evaluation obtained is

No.	$nBCF$	$nBDP$
1	0	1
2	0	0
3	0	0
4	0	0
5	0	2
6	2	1
7	0	2
8	2	0

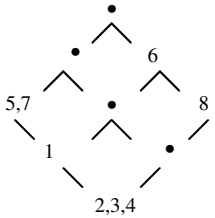
This means that, for example, the chemical compound of number 5 is evaluated by the element

$$(0,2) \in S^2 = \{(0,0),(0,1),(0,2),(1,0),(1,1),(1,2),(2,0),(2,1),(2,2)\}.$$

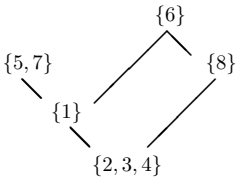
A *visualization* of this evaluation can be obtained from the *Hasse diagram* of the partially ordered set S^2. It shows the elements of S^2, connected by lines with their immediate neighbors. The smallest elements are usually shown at the bottom. E.g., the Hasse diagram of the partial order on $\{0,1,2\}^2$ looks as follows:



Replacing pairs of parameter values by the labels of the compounds with these parameter values and the other pairs by bullets we obtain



It demonstrates the relation between the compounds with respect to the chosen parameters. The compounds numbered 2, 3 and 4 cannot be distinguished by their parameter values, the same holds for 5 and 7. Hence, we obtain the sets of numbers of compounds that are 'equivalent': $\{2,3,4\}$, $\{5,7\}$, $\{1\}$, $\{6\}$ and $\{8\}$. The result is the following *ranking* of the compounds:



It shows that the compounds with numbers 5 and 7 are of the same quality, and they are worst with respect to these parameters. Another compound that is also worst (but incomparable with 5 and 7) is the compound number 6. Moreover, the compounds with numbers 2, 3 and 4 are best, and of the same quality.

Another well–known example of a partial order that is a cartesian power of a total order is obtained from the closed interval $S = [0, 1]$ of real numbers between 0 and 1, including 0 and 1. There is the total order $\leq$ on $[0, 1]$ as well, also defined by $s \leq s'$ if and only if the real number $s' - s$ is nonnegative. Thus, the third cartesian power $[0, 1]^3$ of $[0, 1]$ is partially ordered by $\leq$, if we define that order in the following way: $[0, 1]^3$ consists of triples (r, s, t) of elements in $[0, 1]$, and the definition of $\leq$ in this case is

$$(r, s, t) \leq (r', s', t') \iff r \leq r' \text{ and } s \leq s' \text{ and } t \leq t'.$$

We used this partial order for an evaluation of 18 refrigerants in [5]. More generally, we can obtain partial orders by forming cartesian powers like $[0, 1]^n$ of totally ordered sets, using $\leq$ 'coordinatewise'. Such partial orders of cartesian products of totally ordered sets are called *canonical* partial orders.

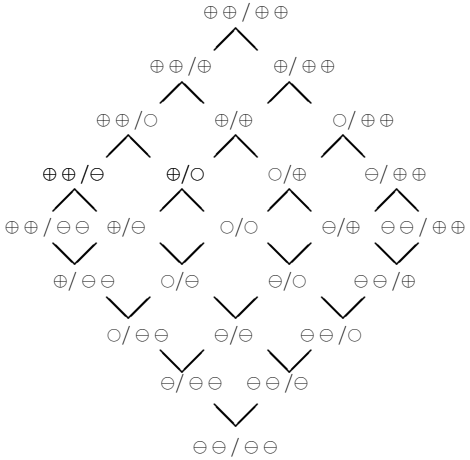
Here is a further canonical partial order that the interested reader may have met reading a test of electronic devices that can be found in the computer journal 'c't'. As reading and writing devices for CDs as well as for DVDs run under two different norms $\pm R$, tests of such machines may look as follows, and this table may be considered as an evaluation of such devices:

Label	$wDVD$	wCD	$rDVD$	rCD	$eDVD/CD$	$nDVD/CD$
a	$\oplus\oplus/\oplus$	$\ominus/\ominus$	$\ominus\ominus/\bigcirc$	$\oplus/\ominus$	$\ominus\ominus/\ominus$	$\oplus/\bigcirc$
b	$\oplus/\ominus$	$\oplus/\ominus$	$\ominus/\ominus$	$\bigcirc/\ominus$	$\ominus\ominus/\oplus$	$\ominus/\bigcirc$
c	$\bigcirc/\bigcirc$	$\oplus\oplus/\oplus\oplus$	$\bigcirc/\oplus$	$\oplus/\bigcirc$	$\oplus\oplus/\ominus\ominus$	$\ominus/\ominus$
d	$\oplus/\oplus$	$\bigcirc/\ominus$	$\bigcirc/\bigcirc$	$\ominus/\ominus$	$\oplus/\oplus$	$\oplus/\bigcirc$

The set of objects is $\{a, b, c, d\}$, a set of devices (but the table of the test is fictive). The set of attributes consists of $wDVD$ and wCD, the qualities in writing DVDs or CDs, of $rDVD$ and rCD, the qualities in reading, $eDVD/CD$ for electronic quality, while $nDVD/CD$ evaluates the noise. The values in the table are elements of the following partial order:

$$\begin{aligned} S^2 &= \{\ominus\ominus < \ominus < \bigcirc < \oplus < \oplus\oplus\}^2 \\ &= \{\ominus\ominus/\ominus\ominus, \ominus\ominus/\ominus, \ldots, \oplus\oplus/\oplus\oplus\}. \end{aligned}$$

Its Hasse diagram looks as follows, showing that there are many incomparabilities:



For example, $s = \ominus/\bigcirc$ and $s' = \bigcirc/\ominus$ are clearly incomparable. At first glance, this order may look strange, but it can be identified — up to the labels used — with the cartesian square of the total order $\{-2 < -1 < 0 < 1 < 2\}$.

In the following we shall use the symbol $\leq$ as a general symbol for an order, and we indicate an ordered set S, together with its order $\leq$, as a pair $(S, \leq)$. Particular elements in an ordered set S, related to a subset $M \subseteq S$, are of special interest:

1.2 Definition (lower, upper bounds, least, greatest element, minimal, maximal elements)

— *$s \in S$ is called a lower (upper) bound of $M \subseteq S$ if $s \leq s'$ ($s' \leq s$), for all $s' \in M$.*

— *$s' \in M$ is the least (the greatest) element of M if $s' \leq s''$ ($s'' \leq s'$) for each $s'' \in M$. It is easy to see that such elements are uniquely determined if they exist.*

— *$s' \in M$ is a minimal (a maximal) element of M if $s'' \in M$ together with $s'' \leq s'$ ($s' \leq s''$) implies that $s' = s''$. Such elements need not be uniquely defined. Least elements are minimal, greatest elements are maximal.*

— *If a least element exists in $M \subseteq S$, it will be denoted by $\min M$, and a greatest element will be indicated by $\max M$, if it exists.*

$\diamond$

Obviously, the interval $[0,1] \subset \mathbb{R}$, equipped with its total order $\leq$, contains a least and a greatest element: $\min[0,1] = 0$ and $\max[0,1] = 1$, while the open interval $(0,1) \subset \mathbb{R}$ contains neither a least nor a greatest element.

In particular, we shall consider situations where sets of lower (upper) bounds have a greatest (a least) element:

1.3 Definition (infimum and supremum)

Consider a set S, a subset $M \subseteq S$ and a partial order $\leq$ on S. In the case when the set of lower (upper) bounds of M in S contains a greatest (least) element, then we call this element the infimum (the supremum) of M and denote it by $\bigwedge M$ (by $\bigvee M$).

$\diamond$

We note that infima and suprema need not exist. For example, if $S = M = (0,1)$, the open interval, then the subset $M = S$ has the empty set as set of lower bounds as well as set of upper bounds, and the empty set contains, by definition, neither a greatest nor a least element.

2 Lattices

The values or 'degrees' that we associate in an evaluation with the pairs (o,a) consisting of an object o and an attribute a will usually be taken from a completely distributive lattice, an ordered set where suprema and infima exist, and which we denote by the letter L. In order to emphasize that we consider lattices we shall use small Greek letters for their elements.

2.1 Definition (complete and completely distributive lattices)

Consider an ordered set $(L,\leq)$.

— *$(L,\leq)$ is a lattice, if 2-element subsets $\{\alpha,\beta\} \subseteq L$ possess an infimum and a supremum, denoted by $\alpha \wedge \beta$ and $\alpha \vee \beta$, respectively.*

— *We note the close relationship between infimum, supremum and partial order, expressed by the equivalences*

$$\alpha \leq \beta \iff \alpha \wedge \beta = \alpha \iff \alpha \vee \beta = \beta.$$

It means that we may either speak of the lattice $(L,\leq)$, i.e. of the pair consisting of the set L and its partial order $\leq$, or of the triple $(L,\wedge,\vee)$, consisting of L and the mappings

$$\wedge\colon L \times L \to L\colon (\alpha,\beta) \mapsto \alpha \wedge \beta \text{ and } \vee\colon L \times L \to L\colon (\alpha,\beta) \mapsto \alpha \vee \beta.$$

For short, we may simply speak of the lattice L.

— *The lattice L is a complete lattice, if each subset $M \subseteq L$ possesses an infimum and a supremum, $\bigwedge M$ and $\bigvee M$, respectively. The infimum and the supremum of L itself will be denoted by 0 and by 1, or, more explicitly, by 0_L and 1_L,*

$$\bigwedge L = 0_L \text{ and } \bigvee L = 1_L.$$

— *If, in addition, the following equations hold for all subsets $M \subseteq L$ and every α in the lattice L,*

$$\bigvee\{\beta \wedge \alpha \mid \beta \in M\} = \Big(\bigvee M\Big) \wedge \alpha \text{ and } \bigwedge\{\beta \vee \alpha \mid \beta \in M\} = \Big(\bigwedge M\Big) \vee \alpha,$$

the lattice is called a completely distributive lattice.

$\diamond$

Complete distributivity is needed if the sets are not finite and suprema or infima have to be calculated. Complete lattices contain an element 0 and an element 1, and so all of them contain the complete lattice $\{0, 1\}$ if they contain more than one element. Therefore, *the use of a suitable completely distributive lattice L generalizes the classical binary (or Boolean) approach, and, in addition, it allows a problem–driven choice of methods in order to attack evaluation problems*, as we shall see in a minute. The choice of L is mostly obvious from the evaluation in question.

Examples of lattices are, of course, the totally ordered sets, since the infimum $\alpha \wedge \beta$ is the smallest of the elements α, β, correspondingly, the supremum ist the biggest one. So, for example, $[0, 1]$ is a lattice. Moreover, cartesian products of total orders are lattices, and so $[0, 1]^3$ is a lattice (with $0_L = (0, 0, 0)$ and $1_L = (1, 1, 1)$) as well as $\{\ominus\,\ominus \,/\, \ominus\,\ominus, \ldots\}$, where $0_L = \ominus\,\ominus \,/\, \ominus\,\ominus$, while $1_L = \oplus\,\oplus \,/\, \oplus\,\oplus$. We have seen how these lattices can be used for evaluation of chemical compounds as well as of electronic devices. Next, we show further examples where evaluation is of interest.

3 Two typical examples

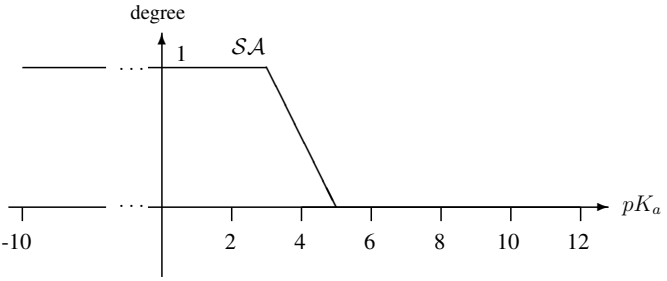
A model of a linguistic expression

In order to model the linguistic expression ‘strong acid’, we use a mapping

$$\mathcal{SA}\colon \mathbb{R} \to [0, 1]$$

that evaluates expressions of the form $pKa(p,T,x) = -\log_{10}(K_a)$. K_a means the thermodynamical equilibrium constant, describing the dissociation of an acid x in water at temperature $T = 273.15\ K$ and pressure $p = 1$ bar, see for instance [21], Table 9.2.

Such a mapping can serve as a mathematical model for the evaluation of 'x is a strong acid' by associating to x via its $pK_a(T,p,x)$–value the real number $\mathcal{SA}(pK_a(T,p,x))$ between 0 and 1, a *degree* that says in which sense the statement is true *according to that particular mapping or model*. For example, we may use the following mapping:



It takes, e.g., the values

$$\mathcal{SA}(2) = 1,\ \mathcal{SA}(4) = 0.5,\ \mathcal{SA}(8) = 0.$$

And this means, that a compound x with $pK_a(p,T,x) = 2$ is considered a strong acid, while in the case when $pK_a(p,T,x) = 4$ there is some doubt if x should be called a strong acid, and it is certainly not a strong acid if $pK_a(p,T,x) = 8$.

An evaluation of refrigerants

Another case is the evaluation of chemical compounds, for example of refrigerants, with respect to environmental properties. In [5, 17, 19, 20] refrigerants RE are evaluated using triples

$$(RE(ODP), RE(GWP), RE(ALT)) \in [0,1]^3$$

of parameter values, where ODP means *ozone depletion potential*, GWP means *global warming potential*, and ALT stands for the *atmospheric lifetime*. The parameter values are real numbers. We used a normalized and properly oriented version of the parameters, i.e., each value is contained in the interval $[0,1]$ and smaller values are the better ones: RE is at least as good as RE' if and only if the following is true:

$RE(ODP) \leq RE'(ODP)$ and $RE(GWP) \leq RE'(GWP))$ and $RE(ALT) \leq RE'(ALT)$.

This kind of evaluation using real–valued parameters allows an embedding into 'fuzzy mathematics' (a terrible name that should never be used since not the mathematics is fuzzy but the situations that are modeled), using ideas due to [15]. We shall give details below.

The evaluation of 18 refrigerants in [5] (motivated by [17]) used the following table of normalized and oriented values of the parameters, taken from [17]:

Label	Name	ODP	GWP	ALT
1	R11	0.19608	0.31622	0.01406
2	R12	0.16078	0.72432	0.03125
6	R141b	0.02353	0.04818	0.00290
7	R142b	0.01275	0.15338	0.00559
8	R23	0.00008	0.96689	0.08437
16	R290	0	0.00135	0.00001
21	R744	0	0.00007	0.03750
22	R1281	1	0.08784	0.00343
23	RC318	0	0.67568	1
29	HFE-125	0	1	0.05156
32	R40	0.00392	0.00108	0.00040
33	R113	0.17647	0.40541	0.02656
35	R114	0.16667	0.66216	0.09375
36	R13/1	0	0.00007	0.00003
37	–	0	0.00007	0
38	R717	0	0	0.00007
39	HFE-143	0	0.04432	0.00178
40	HFE-245	0	0.04709	0.00125

The first column contains the labels i of the 18 refrigerants RE_i, chosen from the 40 refrigerants that were evaluated in [17]. The second column contains the standard abbreviations, the technical names of these refrigerants, while the third, fourth, and fifth column contain the parameter values, the evaluation of the refrigerants that we use. More formally and more generally, we can introduce 'evaluation' as follows:

3.1 Definition (evaluation of a set of objects with respect to given attributes)

Consider a finite set O of objects $o \in O$ and a finite set A of attributes $a \in A$, together with a complete lattice L of values (e.g., of parameter values). Then an evaluation of the objects with respect to the attributes is a table of the following form:

$$\mathcal{E} = (\mathcal{E}(o, a)).$$

It can be considered as a mapping

$$\mathcal{E}\colon O \times A \to L\colon (o, a) \mapsto \mathcal{E}(o, a)$$

from $O \times A$ to L, or, as an L–subset (see below, Definition 4.1) of the cartesian product $O \times A$. The entry $\mathcal{E}(o, a)$ of this matrix, contained in the row corresponding to the object o and the column corresponding to the attribute a is the result of evaluating to which degree object o has attribute a.

$\diamond$

For example, the evaluation of the refrigerants is a matrix consisting of 18 rows, a column containing labels, and three columns containing parameter values. In the row of the third refrigerant (with its label 6) and in the column that corresponds to the parameter GWP it contains the value 0.04818, supposed we choose $L = [0, 1]$. If we choose $L = [0, 1]^3$, the matrix will consist of 18 rows and besides the column with the labels just a single column, its entries being triples of real numbers. For example, the third row contains the triple $(0.02353, 0.04818, 0.00290)$. So we have to choose if L is $[0, 1]$, which means that we want to separate the parameters, or if we put $L = [0, 1]^3$, i.e., to put the parameters together. *If we choose $L = [0, 1]^3$ then the evaluation (or ranking) is just the order of the triples of values being elements of the lattice.*

Having decided which lattice we use, the next question is if we want to use a problem–orientation that is different from the standard one, arising from the standard Boolean set theory and the corresponding logic. So let us discuss a few of the many possible choices that we have.

4 Set theory over L

Having chosen a lattice L as set of admissible values in an intended evaluation, the second step is the choice of a suitable set theory, a generalization of the standard 'binary' or 'Boolean' set theory allowing only an 'either or', i.e., it admits the values 0 and 1 only. Here is the corresponding notion:

4.1 Definition (*L*–subsets of crisp sets)

Assume that L was chosen, together with a crisp set X, i.e., a set in the classical sense where an object x either belongs to X or not.

— *Crisp subsets of X can be identified with mappings from X to $\{0, 1\}$, where the mapping $S\colon X \to \{0, 1\}$ corresponds to the subset of objects x in X mapped onto 1, $S(x) = 1$.*

— *More generally, an L–subset of X can be recognized as an element of*

$$L^X = \{\mathcal{S} \mid \mathcal{S} : X \to L\},$$

the set of mappings from X to L. The value $\mathcal{S}(x) \in L$ of $\mathcal{S}$ at $x \in X$ is an element in L that evaluates the statement 'x belongs to $\mathcal{S}$'.

— *We define the L–inclusion $\subseteq_L$ of L–subsets $\mathcal{S}, \mathcal{T} \in L^X$ by the equivalence*

$$\mathcal{S} \subseteq_L \mathcal{T} \iff \forall\, x \in X\colon\, \mathcal{S}(x) \leq \mathcal{T}(x).$$

$\diamond$

Our next step is the definition of various *intersections* of L–subsets using mappings that have the most important properties an intersection should have:

4.2 Definition (*t*–norms, intersections of *L*–subsets)

Consider a lattice L.

— *A t–norm on L is a mapping $\tau : L \times L \to L$ with the following properties:*

- *τ is symmetric, $\tau(\alpha, \beta) = \tau(\beta, \alpha)$,*
- *τ satisfies the boundary conditions: $\tau(\alpha, 1_L) = \alpha$ and $\tau(\alpha, 0_L) = 0_L$,*
- *τ is monotonous, $\beta \leq \gamma$ implies $\tau(\alpha, \beta) \leq \tau(\alpha, \gamma)$,*
- *τ is associative, $\tau(\alpha, \tau(\beta, \gamma)) = \tau(\tau(\alpha, \beta), \gamma)$.*

— *The τ–intersection $\mathcal{S} \cap_\tau \mathcal{T}$ of $\mathcal{S}, \mathcal{T} \in L^X$ is the L–subset $\mathcal{I} \in L^X$ with*

$$\mathcal{I}(x) = (\mathcal{S} \cap_\tau \mathcal{T})(x) = \tau(\mathcal{S}(x), \mathcal{T}(x)).$$

The most important t–norms are the following ones:

— *The standard norm is*

$$s(\alpha, \beta) = \alpha \wedge \beta, \text{ so that } (\mathcal{S} \cap_s \mathcal{T})(x) = \mathcal{S}(x) \wedge \mathcal{T}(x)\,.$$

— *The drastic norm is defined by*

$$d(\alpha, \beta) = \begin{cases} \alpha & \text{if } \beta = 1_L, \\ \beta & \text{if } \alpha = 1_L, \\ 0_L & \text{otherwise}. \end{cases}$$

Thus, the d–intersection reads as follows:

$$(\mathcal{S} \cap_d \mathcal{T})(x) = \begin{cases} \mathcal{T}(x) & \text{if } \mathcal{S}(x) = 1_L, \\ \mathcal{S}(x) & \text{if } \mathcal{T}(x) = 1_L, \\ 0_L & \text{otherwise}\,. \end{cases}$$

— *If* $L = [0,1]$*, there is the algebraic product*

$$a(\alpha,\beta) = \alpha \cdot \beta\,, \text{ in which case } (\mathcal{S} \cap_a \mathcal{T})(x) = \mathcal{S}(x) \cdot \mathcal{T}(x)\,,$$

and in addition the bounded difference

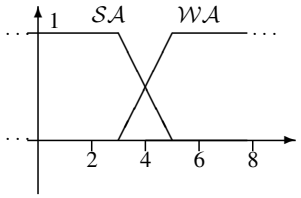
$$b(\alpha,\beta) = \max\{0, \alpha+\beta-1\}, \text{ hence } (\mathcal{S} \cap_b \mathcal{T})(x) = \max\{0, \mathcal{S}(x)+\mathcal{T}(x)-1\}.$$

◇

Let us rephrase one of the examples in terms of these notions.

The model of a linguistic expression

Besides the model $\mathcal{SA}$ of the linguistic expression *strong acid*, we may also want to model the linguistic expressions *weak acid* by another [0,1]–subset $\mathcal{WA}$, say in the following way:



Thus if we use the standard norm, we evaluate the statement 'an acid with pK_a–value 4 is both strong acid and weak acid' by 0.5, while the use of the drastic norm implies that we do not accept that there is any acid being both a strong acid and a weak acid, since, by definition of the drastic norm, we have, for every real number r that

$$(\mathcal{SA} \cap_d \mathcal{WA})(r) = 0$$

(although $\mathcal{SA}(4) = \mathcal{WA}(4) = 0.5$). We are in fact using kind of *semantic notion of truth*, based on the chosen t-norm, the truth value is obtained via a fixed mathematical formalism, the definition of d–intersection. In chemistry certainly the standard norm seems better to describe the transition zone between a strong acid and a weak one. Nevertheless, a problem–driven choice might sometimes be useful, in particular since for each t–norm $\tau\colon [0,1]\times[0,1] \to [0,1]$ we have

$$d(\alpha,\beta) \le \tau(\alpha,\beta) \le s(\alpha,\beta).$$

We may in fact say that the choice of the drastic intersection is advisible if a pessimistic or a precautious thinking might be better, while the choice of the standard intersection is the most optimistic one (all the others are in between these two). The introduction of unions of L–subsets is similar, it uses *conorms* σ, but we do not need that now. We just mention that usually particular pairs (τ, σ) are chosen that fit together (which means that, e.g., Morgan's laws of set theory hold).

So this is the *second* chance to do a problem–driven choice. The first one was the choice of L, the second one is the choice of a suitable t–norm τ. The third one is the choice of a logic. We shall see that the choice of a logic is more or less automatic after the choice of a t–norm.

5 A corresponding logic over L

It is crucial to note that to the t–norms s, d, a and b (and various other norms and conorms) a unique mapping of the following form exists:

5.1 Definition (residuum of a *t*–norm)

A mapping $\tilde{\tau} : L \times L \to L$ is called a residuum corresponding to a t–norm τ, if it satisfies the following condition: For all $\alpha, \beta, \gamma \in L$,

$$\tau(\alpha, \beta) \leq \gamma \iff \alpha \leq \tilde{\tau}(\beta, \gamma).$$

A t–norm with a residuum is called a residual t–norm.

$\diamond$

There may be several residua, but in many cases, depending on the chosen L, the residuum is uniquely defined. In particular, if L is completely distributive, the residuum of τ has the values

$$\tilde{\tau}(\alpha, \beta) = \bigvee\{\gamma \mid \tau(\gamma, \alpha) \leq \beta\}. \tag{1}$$

For example, if $L = [0, 1]$, the residua of the standard norm s, the drastic norm d, the algebraic product a and the bounded difference b are unique and they have the following values:

$$\begin{aligned}
\tilde{s}(\alpha, \beta) &= \begin{cases} 1 & \text{if } \alpha \leq \beta, \\ \beta & \text{otherwise,} \end{cases} \\
\tilde{d}(\alpha, \beta) &= \begin{cases} \beta & \text{if } \alpha = 1, \\ 1 & \text{otherwise,} \end{cases} \\
\tilde{a}(\alpha, \beta) &= \begin{cases} \beta/\alpha & \text{if } \alpha \neq 0, \\ 1 & \text{otherwise,} \end{cases} \\
\tilde{b}(\alpha, \beta) &= \min\{1, 1 - \alpha + \beta\}.
\end{aligned}$$

In order to generalize the Boolean logic over $L = \{0, 1\}$, we can argue as follows: The classical table of truth values of statements that are composed from statement A (with given truth value α) and statement B (with its truth value β) is

A	B	$\neg A$	$A \wedge B$	$A \vee B$	$A \Rightarrow B$
α	β	$1 - \alpha$	$\min\{\alpha, \beta\}$	$\max\{\alpha, \beta\}$	$\min\{1, 1 - \alpha + \beta\}$

.

In terms of the bounded difference this reads as follows:

A	B	$\neg A$	$A \wedge B$	$A \vee B$	$A \Rightarrow B$
α	β	$\widetilde{b}(\alpha, 0)$	$\min\{\alpha, \beta\}$	$\max\{\alpha, \beta\}$	$\widetilde{b}(\alpha, \beta)$

.

Hence, it can be generalized as follows: Assume a residual t-norm τ and use the following evaluation of compositions of statements in terms of the residuum $\tilde{\tau}$:

$$\tilde{\tau}(\neg \mathcal{A}) = \tilde{\tau}(\alpha, o) \text{ and } \tilde{\tau}(\mathcal{A} \Rightarrow \mathcal{B}) = \tilde{\tau}(\alpha, \beta), \tag{2}$$

supposed the value of $\mathcal{A}$ is α and that of $\mathcal{B}$ is β. This leads to the following table of values that we obtain once we have chosen a residual t–norm τ and a suitable t-conorm σ:

A	B	$\neg A$	$A \wedge B$	$A \vee B$	$A \Rightarrow B$
α	β	$\tilde{\tau}(\alpha, 0)$	$\tau(\alpha, \beta)$	$\sigma(\alpha, \beta)$	$\tilde{\tau}(\alpha, \beta)$

. (3)

And it is the choice of suitable logic described by this table that we call ‘problem–orientation’. In this way, we obtain, for example, a problem–oriented evaluation of subsethood of two L–subsets $\mathcal{A}, \mathcal{B} \in L^X$:

5.2 Definition (the subsethood degree)

Consider two L–subsets $\mathcal{A}$ and $\mathcal{B}$ of X and a residual t–norm τ. The evaluation of $\mathcal{A} \subseteq_L \mathcal{B}$, the truth value of $\mathcal{A}$ being contained in $\mathcal{B}$, with respect to $\tilde{\tau}$, is clearly

$$\bigwedge_{x \in X} \tilde{\tau}(\mathcal{A}(x), \mathcal{B}(x)) \in L.$$

It yields the mapping

$$\mathcal{SH}\colon L^X \times L^X \to L\colon (\mathcal{A}, \mathcal{B}) \mapsto \bigwedge_{x \in X} \tilde{\tau}(\mathcal{A}(x), \mathcal{B}(x)) \in L,$$

the τ–subsethood degree on L^X.

$\diamond$

The implication $\mathcal{A} \subseteq_L \mathcal{B}$ is true if and only if this value is 1, i.e., if and only if

$$\bigwedge_{x \in X} \tilde{\tau}(\mathcal{A}(x), \mathcal{B}(x)) = 1,$$

or, more explicitly, if and only if

$$\forall\, x \in X\colon\ \tilde{\tau}(\mathcal{A}(x), \mathcal{B}(x)) = 1.$$

For example, if $L = [0, 1]$ we have $\tilde{\tau} = \tilde{b}$, and so

$$\tilde{\tau}(\mathcal{A}(x), \mathcal{B}(x)) = \min\{1, 1 - \mathcal{A}(x) + \mathcal{B}(x)\} = 1 \iff \mathcal{A}(x) \leq \mathcal{B}(x),$$

in accordance with the definition of $[0, 1]$–subset.

In summary, we can say that evaluation generalizes the Boolean situation. It opens an approach to further applications, for example, modeling of linguistic expressions. In particular we can use a problem–driven (or at least problem–oriented) way of mathematical modeling in many cases. The method is to

— choose a suitable lattice L as set of values, truth values or degrees,

— take a suitable residual t-norm τ in order to establish a set theory over L,

— use the corresponding residuum $\tilde{\tau}$ in order to get a logic that can be applied in the evaluation of statements.

Thus, we mean by problem–orientation the suitable choice of a quintuple $(L, \wedge, \vee, \tau, \tilde{\tau})$, Pollandt calls it an L–fuzzy algebra, see [16] for more details. Let us go back to our main example.

The evaluation of the refrigerants

We used the parameters ODP, GWP, ALT, obtaining for a refrigerant RE the triple of parameter values

$$\mathcal{RE} = (RE(ODP), RE(GWP), RE(ALT)) \in [0, 1]^{\{ODP, GWP, ALT\}}.$$

Putting $L = [0, 1]$ we can easily formulate the following discussion in terms of the theory of $[0, 1]$–subsets. Of course, we can also formulate it in terms of $[0, 1]^3$–subsets.

The data base used in [5] for the evaluation of the refrigerants was

0.19608	0.31622	0.01406
0.16078	0.72432	0.03125
0.02353	0.04818	0.00290
0.01275	0.15338	0.00559
0.00008	0.96689	0.08437
0	0.00135	0.00001
0	0.00007	0.03750
1	0.08784	0.00343
0	0.67568	1
0	1	0.05156
0.00392	0.00108	0.00040
0.17647	0.40541	0.02656
0.16667	0.66216	0.09375
0	0.00007	0.00003
0	0.00007	0
0	0	0.00007
0	0.04432	0.00178
0	0.04709	0.00125

,

a table consisting of 18 $[0,1]$–subsets of the parameter set $\{ODP, GWP, ALT\}$, supposed we choose $L = [0,1]$. And we note the main result that *the ranking of the refrigerants can be modeled in terms of* $[0,1]$*–subsets and* $[0,1]$*–inclusion of the parameter sets by the following equivalence*:

$$RE \text{ is at least as good as } RE' \iff \mathcal{RE} \subseteq_{[0,1]} \mathcal{RE}'. \tag{4}$$

In words: *Refrigerant* RE *is at least as good as refrigerant* RE' *if and only if the corresponding evaluation* $\mathcal{RE}$ *is a* $[0,1]$*–subset of* $\mathcal{RE}'$.

If we choose $L = [0,1]^3$ we interpret the table as a set of 18 $[0,1]^3$–subsets $\mathcal{RE}_i$ of the set of refrigerants and obtain the following result: *Refrigerant* RE *is at least as good as refrigerant* RE' *if and only if the corresponding element of the lattice* $\mathcal{RE} \in [0,1]^3$ *is less than or equal to the element* $\mathcal{RE}' \in [0,1]^3$.

$$RE \text{ is at least as good as } RE' \iff \mathcal{RE} \leq \mathcal{RE}'. \tag{5}$$

This is, of course, trivial since we use the canonical partial order where smaller values are the better ones. Similarly, of course, for more than three real–valued, normalized and properly oriented parameters.

In the next section we consider certain chains of subsets of X that arise from a given $\mathcal{S} \in L^X$ and correspond to chains of elements in the lattice L. When applied to an evaluation they yield

chains of rankings that become successively coarser and successivley less dependent of the precision of measurement of the parameters.

6 Cutsets of *L*–subsets

We consider particular crisp subsets of X induced by an $\mathcal{S} \in L^X$ and the $\alpha \in L$:

6.1 Definition (cutsets and level sets)

The cutset of $\mathcal{S} \in L^X$ that corresponds to $\alpha \in L$ is defined as

$$\mathcal{S}_{\geq\alpha} = \{x \in X \mid \mathcal{S}(x) \geq \alpha\},$$

a crisp subset of X. (Correspondingly, there are open cutsets $\mathcal{S}_{>\alpha} := \{x \in X \mid \mathcal{S}(x) > \alpha\}$ and level sets $\mathcal{S}_\alpha := \{x \in X \mid \mathcal{S}(x) = \alpha\}$, but they will not be used here.)

$\diamond$

The crucial point is that *chains in L yield chains of cutsets*, as clearly

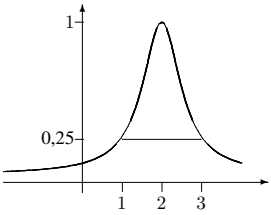
$$\alpha \leq \beta \Longrightarrow \mathcal{S}_{\geq\alpha} \supseteq \mathcal{S}_{\geq\beta}. \tag{6}$$

Here is a simple example: Choose $L = [0,1] \subset \mathbb{R}$, put $X = \mathbb{R}$ and consider the following 'fuzzy 2' that can be expressed in terms of the functions

$$l : (-\infty, 2] \to [0,1] : x \mapsto \frac{1}{1+3(x-2)^2}\,,$$

$$r : [2, \infty) \to [0,1] : x \mapsto \frac{1}{1+3(x-2)^2}\,.$$

The drawing shows the cutsets $\mathcal{S}_{\geq 0.25} = [1,3]$ and $\mathcal{S}_{>0.25} = (1,3)$, together with the level set $\mathcal{S}_{0.25} = \{1,3\}$.



It is most important for our purposes that in many cases chains of cutsets of structures yield chains of useful structures, as the example later in the text will clarify. In fact, *the partial orders that we shall finally obtain in an evaluation come from cutsets of equivalence relations*. Hence our next step is the introduction of relations and in particular of equivalence relations.

7 L-Relations

We introduced crisp relations on crisp sets, in particular orders. The corresponding notions over a given complete lattice L are obtained by replacing the lattice $\{0,1\}$ by a complete lattice L.

7.1 Definition (L–relations, L–equivalence relations, L–partial orders)

Consider a crisp set X and a complete lattice L.

— *We recall that a crisp relation on X is a mapping $R \in \{0,1\}^{X\times X}$ and that the elements $(x,x') \in X \times X$ with $R(x,x') = 1$ are usually called the elements of R.*

— *Correspondingly, an L-relation on X is an L–subset $\mathcal{R} \in L^{X\times X}$. We introduce its support as*

$$supp(\mathcal{R}) = \{(x,x') \mid \mathcal{R}(x,x') > 0\} \subseteq X \times X,$$

so that the support of $\mathcal{R}$ consists, in a sense, of the 'elements' of $\mathcal{R}$. It is

  — *reflexive, if and only if $\mathcal{R}(x,x) = 1_L$, for every $x \in X$,*

  — *it is symmetric, if and only if always $\mathcal{R}(x,y) = \mathcal{R}(y,x)$,*

  — *and it is transitive, if and only if $\mathcal{R}(x,y) \leq \tau(\mathcal{R}(x,z), \mathcal{R}(z,y))$, for all $x,y,z \in X$.*

— *L–equivalence relations are the L–relations that are reflexive, symmetric and transitive.*

◇

8 Cutsets yield partial orders

We assume an evaluation $\mathcal{E} = (\mathcal{E}(o,a))$ of a finite number of objects $o \in O$, with respect to a finite number of attributes $a \in A$, together with the lattice L containing the values $\mathcal{E}(o,a)$, the results of the evaluation. The rows $\mathcal{E}(o,-)$ of this matrix are the evaluations of the objects, where the entry $\mathcal{E}(o,a)$ evaluates the degree of a being an attribute of object o. Hence, we consider the mappings

$$\mathcal{E}(o,-)\colon A \to L\colon a \mapsto \mathcal{E}(o,a).$$

These L–subsets form a finite crisp subset S of L^A, the set of all the mappings from A to L,

$$S = \{\mathcal{E}(o,-) \mid o \in O\} \subseteq L^A.$$

We form the cartesian product $S \times S$ and consider the subsethood degree:

$$\mathcal{SH}\colon S \times S \to L\colon (\mathcal{E}(o,-),\mathcal{E}(o',-)) \mapsto \bigwedge_{a\in A} \tilde{\tau}(\mathcal{E}(o,a),\mathcal{E}(o',a)).$$

Thus, $\mathcal{SH}$ is an L–subset of $S \times S$, an L–relation on S. It is reflexive, $\tilde{\tau}(\mathcal{E}(o,a),\mathcal{E}(o,a)) = 1$. There exists a transitive closure of this relation, according to the following theorem, due to [8]:

8.1 Theorem (the transitive closure of an L–relation on a finite set)

A reflexive relation $\mathcal{R}\colon S^2 \to L$ on a finite set S of order $|S| = n$ has the following transitive closure $\mathcal{TR}$ with respect to a t–norm τ:

$$\mathcal{TR} = \bigcup_{k=1}^{n-1} \mathcal{R}_\tau^{(k)},$$

where the relation $\mathcal{R}_\tau^{(k)}$ is recursively defined by

$$\mathcal{R}_\tau^{(1)} = \mathcal{R} \text{ and, for } k \geq 2, \text{ by } \mathcal{R}_\tau^{(k)} = \mathcal{R}_\tau^{(k-1)} \circ_\tau \mathcal{R}_\tau^{(1)},$$

and where the τ–composition of such matrices is defined by

$$\mathcal{R}_\tau^{(k)}(s,s') = (\mathcal{R}_\tau^{(k-1)} \circ_\tau \mathcal{R}_\tau^{(1)})(s,s') = \bigvee_{s''\in S} \tau(\mathcal{R}_\tau^{(k-1)}(s,s''),\mathcal{R}_\tau^{(1)}(s'',s')).$$

$\diamond$

Having constructed the transitive closure $\mathcal{TR}$ we obtain on each of its cutsets $\mathcal{TR}_{\geq\alpha}$ an *equivalence relation* $\mathcal{ETR}_\alpha$ by collecting pairs in order to obtain a *symmetric* relation:

$$(x,y) \in \mathcal{ETR}_\alpha \iff (x,y) \in \mathcal{TR}_{\geq\alpha} \text{ and } (y,x) \in \mathcal{TR}_{\geq\alpha}.$$

These equivalence relations form a chain, since obviously

$$\alpha \leq \beta \Longrightarrow \mathcal{ETR}_\alpha \supseteq \mathcal{ETR}_\beta,$$

which implies that each equivalence class of $\mathcal{ETR}_\beta$ is a subset of an equivalence class in $\mathcal{ETR}_\alpha$. The cutsets are important since each one of them permits to assess the order relationships between the objects to rank at certain levels of data relaxation linked to α (cf. [13]). Thus, the bigger α, the lower the data relaxation. De Baets/De Meyer used in [8] the following helpful formulation for this interesting fact:

‘Incomparability disappears at the cost of increasing indifference’.

The final step is the introduction of a partial order $\leq_\alpha$ on the classes of the equivalence relation $\mathcal{ETR}_\alpha$ that corresponds to $\alpha \in L$. We denote the equivalence class of x in $\mathcal{ETR}_\alpha$ by

$$[x]_\alpha$$

and define the partial order as follows: For each $[x]_\alpha \neq [y]_\alpha$ we put

$$[x]_\alpha \ <_\alpha \ [y]_\alpha \iff (x,y) \in \mathcal{TR}_{\geq\alpha} \text{ and } (y,x) \notin \mathcal{TR}_{\geq\alpha}. \tag{7}$$

This completes our collection of notions and results that we need in order to do the first steps in the evaluation of a finite collection of objects $o \in O$ according to a given finite set of attributes $a \in A$, and a complete lattice L of 'truth values'. The application to the set of 18 refrigerants RE_i, the set of parameters $A = \{ODP, GWP, ALT\}$ and the lattice $L = [0,1]$ using the software package PyHasse [3] was described in [5]. The application to evaluation reads as follows:

— If we are given finite sets O of objects, A of attributes, we choose a suitable complete lattice L of values and a residual t-norm τ on the set $L^{O\times A}$. The evaluation yields a matrix

$$\mathcal{E} = (\mathcal{E}(o,a)),$$

i.e., an L–subset of $O \times A$, where the value $\mathcal{E}(o,a)$ is the degree of $a \in A$ as an attribute of the object $o \in O$.

— The ranking directly obtained from $\mathcal{E}$ is the canonical order of the rows of $\mathcal{E}$.

As this result of the evaluation, the canonical order, depends of the precision of the measurements that gave the parameter values, we may procede as follows, in order to obtain a chain of rankings that form a chain of rankings, order homomorphisms of the canonical order:

— We consider a suitable chain of values in L, say

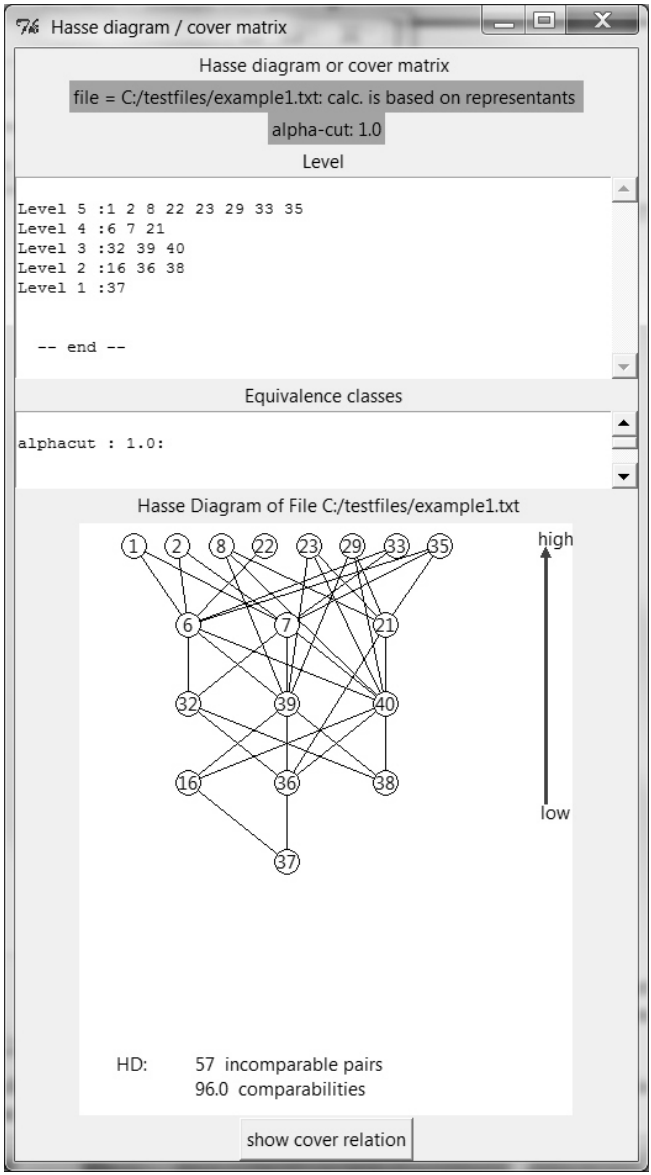
$$0_L = \alpha_1 < \alpha_2 < \ldots < \alpha_{n-1} < \alpha_n = 1_L.$$

and the corresponding equivalence relations

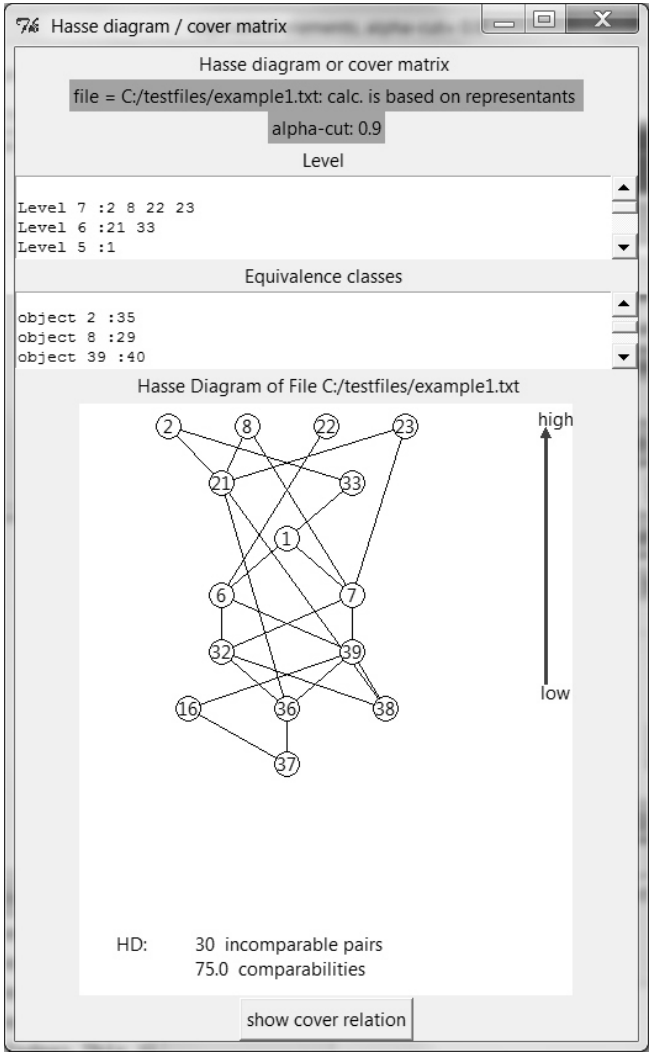
$$\mathcal{ETSH}_{\alpha_i},$$

obtained from the cutsets of the transitive closure of $\mathcal{SH}$, the relation subsethood degree.

The canonical partial order obtained by an application of PyHasse, cf. [5], to the 18 refrigerants looked as follows:



where the 18 nodes represent the refrigerants and the lines lead from a refrigerant to its neighbors in the partial order. The neighborhood relation can be checked via the button 'show cover relation'. The coarser ranking obtained for $\alpha = 0.9$ leads to 15 equivalence classes of refrigerants since RE_2 turned out to be equivalent to RE_{35}, RE_8 to RE_{29} and RE_{39} to RE_{40}:



9 Exploring an evaluation

In this section we discuss the application of an important result from *data bank theory*, cf. [9, 10, 11, 16]. It allows the exploration of the knowledge contained in an evaluation by providing a 'basis' of the set of attribute implications, a set of implications from which we can derive *every* attribute implication that can be obtained from the evaluation. *This is also of general interest since it formalizes a common model of learning and even of doing research.* The idea is the following:

— Assume a *possibly infinite* class Ω of interesting *objects*, e.g., the set of refrigerants, and a finite set A of their *attributes*, e.g. values of parameters. We want to derive conditions for the attributes $a \in A$ to hold in Ω, but Ω might be infinite or at least too big to evaluate. The plan is to evaluate a suitable *finite* subset of $O \subset \Omega$, obtaining

$$\mathcal{E} \in L^{O \times A},$$

for a suitably chosen L, to derive attribute implications from $\mathcal{E}$ and then to check if they hold in Ω or at least in a subset of Ω that is bigger than O.

— A typical example would be the class Ω of all refrigerants known or used today, and the set of attributes $A = \{ODP, GWP, ALT\}$. Having the evaluation $\mathcal{E}$ of the 18 refrigerants at hand, we may ask for its implications in order to find chemical properties of refrigerants that are not among the 18.

— This means, that we want to *explore* $\mathcal{E}$, i.e., to find a description of the knowledge that it contains. By 'knowledge' we usually mean *attribute implications* (implications between sets of attributes) that follow from $\mathcal{E}$. The description will be the Duquenne/Guigues basis, a set of attribute implications from which we can derive every attribute implication that can be obtained from $\mathcal{E}$. The elements of this basis can be considered as hypotheses on Ω. Thus, the exploration of $\mathcal{E}$ can be considered as a *generator of hypotheses* on Ω.

— Once we constructed this basis for the implications of $\mathcal{E}$, we check its elements on Ω. If we can find counterexamples, contradictions, we may extend O to $O' \subseteq \Omega$ by adding the counterexamples, evaluate O' obtaining $\mathcal{E}'$, calculate the implication basis of the new evaluation $\mathcal{E}'$, and so on until we end up with a subset $O^* \subseteq \Omega$, where we do not find any further counterexample or contradiction. If the remaining implications can be proven

for the whole class O^* we are ready as far as the objects in O^* and the attributes in A are concerned, 'we have understood the situation, and the evaluation $\mathcal{E}^*$ properly describes the relationship between O^* and A'. The Duquenne/Guigues basis of $\mathcal{E}'$ is a reasonable set of hypotheses on Ω, and we should try to prove them.

Moreover, it should be emphasized that we obtain this basis automatically, e.g., by computer, and it 'contains' the whole knowledge covered by the evaluation. Note what that means: We have an automatic generator of a full set of hypotheses! So let us introduce the notions and methods that we can use:

— Consider $\mathcal{E} \in L^{O\times A}$. We say that object o *has* attribute a if and only if $\mathcal{E}(o,a) > 0$.

— An L–subset $\mathcal{A}$ of the given set of attributes is evaluated at $o \in O$ and *with respect to the evaluation* $\mathcal{E}$ by the truth value of '$\mathcal{A}$ holds for $o \in O$ *in* $\mathcal{E}$', which is

$$\mathcal{A}'(o) = \tilde{\tau}(\mathcal{A} \Longrightarrow_{\mathcal{E}} \mathcal{E}) = \bigwedge_{a\in A} \tilde{\tau}(\mathcal{A}(a), \mathcal{E}(o,a)).$$

This defines an L–subset $\mathcal{A}'$ of O, since $\mathcal{A}' \in L^O$. Correspondingly, for each L–subset $\mathcal{O} \in L^O$, there is the set $\mathcal{O}' \in L^A$, where

$$\mathcal{O}'(a) = \tilde{\tau}(\mathcal{O} \Longrightarrow_{\mathcal{E}} \mathcal{E}) = \bigwedge_{o\in O} \tilde{\tau}(\mathcal{O}(o), \mathcal{E}(o,a)).$$

Iterating this we obtain the L–subsets $\mathcal{A}'', \mathcal{O}''$ that we shall use in a minute.

— If $\mathcal{A}, \mathcal{B} \in L^A$ then we evaluate '$\mathcal{A}$ implies $\mathcal{B}$ in the evaluation $\mathcal{E}$', in formal terms:

$$\mathcal{A} \Longrightarrow_{\mathcal{E}} \mathcal{B}.$$

This implication is evaluated by:

$$\begin{aligned} \tilde{\tau}(\mathcal{A} \Longrightarrow_{\mathcal{E}} \mathcal{B}) &= \bigwedge_{o\in O} \tilde{\tau}(\mathcal{A}'(o), \mathcal{B}'(o)) \\ &= \bigwedge_{o\in O} \tilde{\tau}\Big(\bigwedge_{a\in A} \tilde{\tau}(\mathcal{A}(a), \mathcal{E}(o,a)), \bigwedge_{a\in A} \tilde{\tau}(\mathcal{B}(a), \mathcal{E}(o,a))\Big). \end{aligned}$$

— Clearly, $\mathcal{A} \Longrightarrow_{\mathcal{E}} \mathcal{B}$ *holds* in $\mathcal{E}$ if and only if $\tilde{\tau}(\mathcal{A} \Longrightarrow_{\mathcal{E}} \mathcal{B}) = 1$, i.e., if and only if $\mathcal{A}' \subseteq_L \mathcal{B}'$. And the problem is to find a set of implications that gives the set of *all* the implications that hold in $\mathcal{E}$. Such a set will be described next.

— Consider an evaluation $\mathcal{E}$ with finite object and attribute sets, so that we can recursively define L–subsets $\mathcal{P} \in L^A$, called *pseudo–contents*, by

$$\mathcal{P} \neq \mathcal{P}'' \text{ and for each pseudo–content } \mathcal{Q} \subset_L \mathcal{P} \text{ we have that } \mathcal{Q}'' \subseteq_L \mathcal{P}\,.$$

— *The decisive result is the following set of implications which implies every attribute implication following from* $\mathcal{E}$. This set is the *Duquenne/Guigues–basis*, cf. [9]:

$$\mathbb{P} = \{\mathcal{P} \Longrightarrow_{\mathcal{E}} (\mathcal{P}'' \setminus \mathcal{P}) \mid \mathcal{P} \text{ pseudo–content}\}.$$

There is a way of successively constructing the pseudo–contents, and so it remains to explain what 'follows' means.

— We say that $\mathcal{D} \in L^A$ *respects* the implication $\mathcal{A} \Longrightarrow \mathcal{B}$, if and only if

$$\mathcal{SH}(\mathcal{A}, \mathcal{D}) \leq \mathcal{SH}(\mathcal{B}, \mathcal{D}).$$

— Assume a set $\mathbb{I}$ of L–attribute implications $\mathcal{I}$. $\mathcal{D} \in L^A$ *respects* $\mathbb{I}$ if $\mathcal{D}$ respects every $\mathcal{I} \in \mathbb{I}$. Moreover, we say that $\mathcal{A} \Longrightarrow \mathcal{B}$ *follows* from $\mathbb{I}$ if every $\mathcal{D} \in L^A$ that respects $\mathbb{I}$ also respects $\mathcal{A} \Longrightarrow \mathcal{B}$. The point is that such an $\mathbb{I}$ from which every attribute implication follows can be given, at least for finite sets of objects and attributes!

A binary evaluation of the refrigerants

We consider again the 18 refrigerants, a subset of the altogether 40 refrigerants evaluated in [17]. The intention is to establish an evaluation $\mathcal{E}$ over $L = \{0, 1\}$ of the refrigerants in order to demonstrate its exploration using available free software. Attributes will be parameters ODP^*, GWP^* and ALT^*, obtained from ODP, GWP and ALT as follows: Using that the third quartiles (as we want to find out the reasons for refrigerants being bad with respect to the ecological properties) of the refrigerants are 0.162 for ODP, 0.666 for GWP and 0.041 for ALT, we obtain the following definition of the new binary parameters:

$$RE(ODP^*) = \begin{cases} 1 & \text{if } RE(ODP) > 0.162 \text{ (=3.quartile)}, \\ 0 & \text{otherwise}, \end{cases}$$

$$RE(GWP^*) = \begin{cases} 1 & \text{if } RE(GWP) > 0.666 \text{ (=3.quartile)}, \\ 0 & \text{otherwise}, \end{cases}$$

$$RE(ALT^*) = \begin{cases} 1 & \text{if } RE(ALT) > 0.041 \text{ (=3.quartile)}, \\ 0 & \text{otherwise}. \end{cases}$$

In addition we consider as attributes the existence of Cl, F, Br, I in RE, the Ether–function, i.e., if RE is an ether, and whether or not RE is CO_2 or NH_3. Moreover we use a parameter nC which is defined as follows:

$$RE(nC) = \begin{cases} 1 & \text{if } RE \text{ contains at least two sp3-C-atoms,} \\ 0 & \text{otherwise.} \end{cases}$$

In order to derive the evaluation we consider the molecular formulas of the refrigerants. They are shown in the next table, together with the names of the corresponding substances, needed in order to specify the respective structural formula. It might be interesting for the reader to check the constitutional isomers corresponding to the molecular formulas via the online version of the molecular structure generator MOLGEN, available via

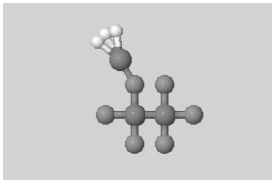
`http://www.molgen.de`

in order to identify the refrigerants. Click there at MOLGEN–ONLINE, press the button 2D, submit a molecular formula of one of the refrigerants, and all corresponding structures will be displayed immediately. Slightly more time is required to generate the structures in a 3D view. For details on the molecular structure generator, its various versions and their applications see [12, 14]. The following table provides the molecular formulas and names of the refrigerants considered.

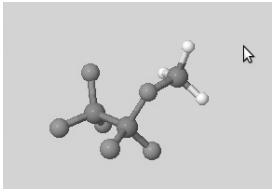
Label	Formula	Name
1	CCl_3F	Trichlorofluoromethane
2	CCl_2F_2	Dichlorodifluoromethane
6	$C_2H_3Cl_2F$	1,1-Dichloro-1-fluoroethane
7	$C_2H_3ClF_2$	1-Chloro-1,1-difluoroethane
8	CHF_3	Trifluoromethane
16	C_3H_8	Propane
21	CO_2	Carbon dioxide
22	$CBrClF_2$	Bromochlorodifluoromethane
23	C_4F_8	Octafluorocyclobutane
29	C_2HF_5O	Pentafluorodimethyl ether
32	CH_3Cl	Chloromethane
33	$C_2Cl_3F_3$	1,1,2-Trichloro-1,2,2-trifluoroethane
35	$C_2Cl_2F_4$	1,2-Dichloro-1,1,2,2-tetrafluoroethane
36	CF_3I	Trifluoroiodomethane
37	C_2H_6O	Dimethyl ether
38	NH_3	Ammonia
39	$C_2H_3F_3O$	Methyl trifluoromethyl ether
40	$C_3H_3F_5O$	Methyl pentafluoroethyl ether

Use MOLGEN–Online in order to check how many connectivity isomers of these compounds exist. For example, you will find that there are 30 isomers with the molecular formula $C_3H_3F_5O$.

Which of them is the technically applied refrigerant methyl pentafluoroethyl ether? Here is a picture of it:



A placement in 3D space, obtained by an application of a reduced version of the MM2 energy model (click 3D instead of 2D) looks as follows:



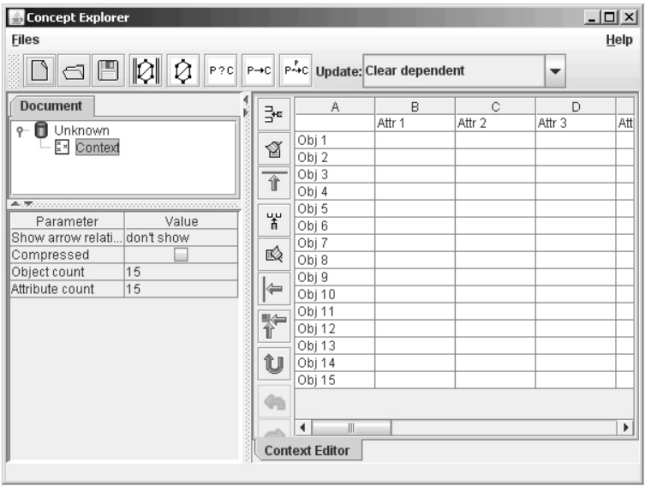
We obtain the following evaluation:

$\mathcal{E}$	ODP^*	GWP^*	ALT^*	nC	Cl	F	Br	I	Ether	CO_2	NH_3
1	1	0	0	0	1	1	0	0	0	0	0
2	0	1	0	0	1	1	0	0	0	0	0
6	0	0	0	1	1	1	0	0	0	0	0
7	0	0	0	1	1	1	0	0	0	0	0
8	0	1	1	0	0	1	0	0	0	0	0
16	0	0	0	1	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	1	0
22	1	0	0	0	1	1	1	0	0	0	0
23	0	1	1	1	0	1	0	0	0	0	0
29	0	1	1	1	0	1	0	0	1	0	0
32	0	0	0	0	1	0	0	0	0	0	0
33	1	0	0	1	1	1	0	0	0	0	0
35	1	0	1	1	1	1	0	0	0	0	0
36	0	0	0	0	0	1	0	1	0	0	0
37	0	0	0	1	0	0	0	0	1	0	0
38	0	0	0	0	0	0	0	0	0	0	1
39	0	0	0	1	0	1	0	0	1	0	0
40	0	0	0	1	0	1	0	0	1	0	0

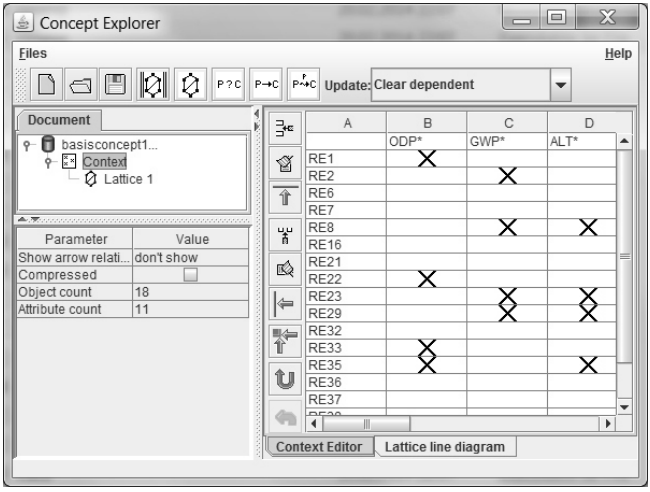
In order to explore this evaluation, the interested reader should download conexp-1.3, developed by S. A. Yevtushenko [23], from

`http://www.sourceforge.net`

and doubly click conexp.jar so that the following screen opens:



Enter, on the left hand side, the numbers of objects and attributes that you want to enter, 18 as number of objects, and 11 for the number of attributes. Enter also the notations of the refrigerants and the attributes, as well as $\times$ where in our table the entry is 1. You will obtain the table of the evaluation, the upper left hand corner of which is shown in the following screenshot:



You may want to save this evaluation under conexp1.cex somewhere. The final step is the evaluation of the Duquenne/Guigues–basis of implications and its reduction due to chemical arguing.

In the binary case, i.e., when $L = \{0, 1\}$, an L–subset $\mathcal{A}$ of the set of attributes is a crisp subset, and similarly for the L–subsets $\mathcal{O}$ of the set of objects. Moreover we easily obtain the corresponding subsets $\mathcal{A}'$ and $\mathcal{O}'$ as well as $\mathcal{A}''$ and $\mathcal{O}''$: The evaluation is binary, and so $\mathcal{A}'$ is the set of objects that have all the attributes contained in $\mathcal{A}$ while $\mathcal{O}'$ consists of all the attributes that all the objects $o \in \mathcal{O}$ have. For example, the following sets $\mathcal{A}$ consisting of a single attribute yield

$$\begin{aligned} \{ODP^*\}' &= \{1, 22, 33, 35\}, \\ \{GWP^*\}' &= \{2, 8, 23, 29\}, \\ \{ALT^*\}' &= \{8, 23, 29, 35\}. \end{aligned}$$

These equations are in fact abbreviations. For example, the first equation means that exactly the objects labeled 1, 22, 33 and 35 have the attribute ODP^*, i.e., the equation indicates that just

$$RE_1(ODP^*) = RE_{22}(ODP^*) = RE_{33}(ODP^*) = RE_{35}(ODP^*) = 1.$$

An application of the mapping $-'$ to $\{ODP^*\}'$ yields

$$\{ODP^*\}'' = \{ODP^*, Cl, F\},\ \{GWP^*\}'' = \{GWP^*, F\},\ \{ALT^*\}'' = \{ALT^*, F\}.$$

Now we note that

$$\mathcal{P} = \{ODP^*\} \neq \{ODP^*\}'' = \mathcal{P}''.$$

This inequality, together with $\emptyset = \emptyset''$ (which implies that the empty set is not a pseudo–content) shows that the set of attributes $\{ODP^*\}$ is a pseudo–content, and similarly for $\{GWP^*\}$ and $\{ALT^*\}$. Thus, we obtain the following attribute implications contained in the basis of the attribute implications, the Duquenne/Guigues–basis:

$$\begin{aligned} \{ODP^*\} &\Longrightarrow_{\mathcal{E}} \{Cl, F\}, \\ \{GWP^*\} &\Longrightarrow_{\mathcal{E}} \{F\}, \\ \{ALT^*\} &\Longrightarrow_{\mathcal{E}} \{F\}. \end{aligned}$$

They show that $RE_i(ODP^*) = 1$, i.e., a high ODP implies the existence of Cl and F, while a high GWP or a high ALT needs the presence of F but not of Cl. *But we should carefully note that this is true for just the 18 refrigerants evaluated by the binary evaluation shown above.* Of course, this is more or less trivial. Our focus here is not the set of implications per se but the fact that they were obtained *automatically and that they contain the whole knowledge about attribute implications contained in the evaluation of the 18 refrigerants that we consider.* The complete Duquenne/Guigues–basis is obtained as follows: Open conexp1.cex and look at its toolbar:

Click the button $P \to C$ and you will get the screen with 24 implications shown on the following page. These 24 implications form the Duquenne/Guigues–basis, and it remains to discuss which of them have to be taken into account since this basis contains, for example, trivial implications. Consider the implications number 10 and 11 on the table:

10 < 1 > ALT* nC F Ether ==> GWP*;
11 < 0 > nC NH3 ==> ODP* GWP* ALT* Cl F Br I Ether CO2;

Implication number 10, colored in *blue*, reads as follows:

$$10 < 1 > \quad ALT^* \; nC \; F \; Ether \implies GWP^*;$$

This means that there is exactly one of the 18 refrigerants fulfilling the condition that its parameter values of ALT^*, nC, F are 1 and that it is an ether. In fact, a glance at $\mathcal{E}$ shows that exactly 29 has this property,

$$RE_{29}(ALT^*) = RE_{29}(nC) = RE_{29}(F) = RE_{29}(Ether) = 1.$$

In contrast to this implication, the eleventh implication is colored in *red*, it reads as follows:

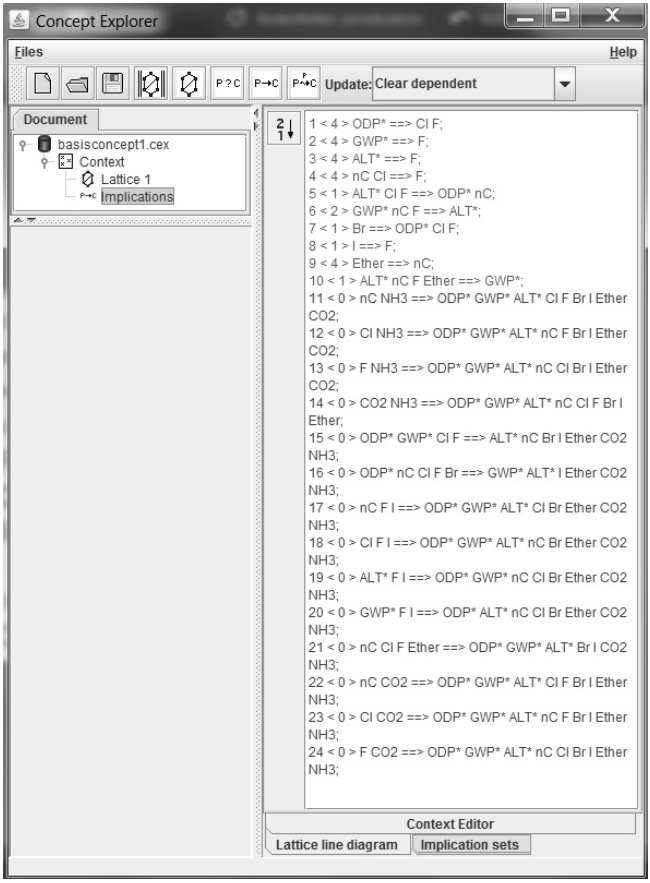
$$11 < 0 > \; nC \; NH3 \implies GWP^*;$$

The assumption is $\{nC, NH_3\}$ is valid only for such refrigerants i where

$$RE_i(nC) = RE_i(NH_3) = 1.$$

But there is clearly no chemical compound that has the molecular formula NH_3 and contains at least 2 carbon atoms. Thus, the assumption of implication 11 is contradictory *although the*

Table 1: The Duquenne/Guigues basis of attribute implications obtained for the binary evaluation of the 18 refrigerants and the 11 attributes



implication is true by the laws of formal logic. We can therefore skip this implication as it is trivial. The same holds for the implications 12, 13 and 14. Similarly for the implications 22, 23 and 24. They can be skipped without loosing information.

The implications 15, ..., 21 also have assumptions that do not hold for any of the 18 refrigerants considered, and so they are true 'in this evaluation'. *But these implications cannot be skipped because of their assumption since we do not know if there are refrigerants (besides the 18 refrigerants considered) that match these implications. Nevertheless they can be skipped because of their contradictory conclusions if we restrict attention to the 18 refrigerants.* It therefore remains to consider the following 10 implications contained in the Duquenne/Guigues–basis of our evaluation of the 18 refrigerants:

$$\begin{aligned}
\{ODP^*\} &\Longrightarrow_{\mathcal{E}} \{Cl, F\}\\
\{GWP^*\} &\Longrightarrow_{\mathcal{E}} \{F\}\\
\{ALT^*\} &\Longrightarrow_{\mathcal{E}} \{F\}\\
\{nC, Cl\} &\Longrightarrow_{\mathcal{E}} \{F\}\\
\{ALT^*, Cl, F\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, nC\}\\
\{GWP^*, nC, F\} &\Longrightarrow_{\mathcal{E}} \{ALT^*\}\\
\{Br\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, Cl, F\}\\
\{I\} &\Longrightarrow_{\mathcal{E}} \{F\}\\
\{Ether\} &\Longrightarrow_{\mathcal{E}} \{nC\}\\
\{ALT^*, nC, F, Ether\} &\Longrightarrow_{\mathcal{E}} \{GWP^*\}
\end{aligned}$$

This is what we gained from the binary evaluation of the 18 refrigerants using the 11 attributes. It is expressed in terms of implications that cover every attribute implication that we can deduce from the evaluation. One might therefore call the calculation of this basis *the exploration of the evaluation* expressed by the binary matrix given above. Of course, the binary context is just one of the contexts that we can obtain. It is quite special since it uses the third quartiles of the parameter values of ODP, GWP and ALT. We might, of course, also consider a context that uses 0.5 instead of the third quartiles, and so on. Nevertheless, it is a set of 10 implications that are true for the 18 refrigerants, and we may use them as conjectures on bigger sets of refrigerants that we might be interested to check. For example, the last implications means that

for every refrigerant i among the 18 we found that

$$RE_i(ALT^*) = RE_i(nC) = RE_i(F) = 1$$

implies that $RE_i(GWP) = 1$.

The next step is a check which of these implications might hold for a bigger set Ω of refrigerants. For example, if we extend to the 40 refrigerants that were evaluated, we remain with the following implications obtained by reduction of the Duquenne/Guigues–basis:

$$\begin{aligned}
\{ODP^*\} &\Longrightarrow_{\mathcal{E}} \{Cl, F\} \\
\{GWP^*\} &\Longrightarrow_{\mathcal{E}} \{F\} \\
\{ALT^*, nC\} &\Longrightarrow_{\mathcal{E}} \{GWP^*, F\} \\
\{ALT^*, Cl\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, GWP^*, F\} \\
\{nC, Cl\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, F\} \\
\{ALT^*, F\} &\Longrightarrow_{\mathcal{E}} \{GWP^*\} \\
\{GWP^*, Cl, F\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, ALT^*\} \\
\{Br\} &\Longrightarrow_{\mathcal{E}} \{ODP^*, Cl, F\} \\
\{I\} &\Longrightarrow_{\mathcal{E}} \{F\} \\
\{Ether\} &\Longrightarrow_{\mathcal{E}} \{nC\} \\
\{CO_2\} &\Longrightarrow_{\mathcal{E}} \{ALT^*\}
\end{aligned}$$

One reason for the difference between this set of 11 implications and the former set of 10 is the fact that the quartiles have changed. The third quartiles for the 40 refrigerants are in fact considerably smaller than those for the 18, here is the corresponding table:

3. quartiles of	ODP	GWP	ALT
40 refrigerants	0.0042	0.282	0.0131
18 refrigerants	0.162	0.666	0.041

The reduced bases show that five of the ten implications that hold for the 18 refrigerants are true for the 40 refrigerants as well.

The 11 implications may be considered as conjectures on the properties of further refrigerants RE. For example we are faced with *hypotheses* like

$RE(ODP) > 0.0042$ implies the presence of both Cl and F in RE,

$RE(GWP) > 0.282$ implies the presence of F in RE,

$\vdots$

If we doubt such an implication we have to look for refrigerants that do not meet this implication. If this is true, i.e., if we found counterexamples, we better increase the set O by adding the counterexamples obtaining $O' \supset O$, consider the corresponding evaluation $\mathcal{E}'$ and its Duquenne/Guigues–basis, reduce it and check the resulting set of implications, and so on until we cannot find any further contradiction. More generally, any new or controversely discussed refrigerant can be added to the data matrix, the table extended by the corresponding row and the new reduced Duquenne/Guigues–basis compared with the old basis consisting of the eleven implications. For example, the interested reader may add R1234yf — if the parameter values are available — and check what happens.

In contrast to such implications that hold for every object in the evaluation, in data mining there is also interest in implications that are not that strict, i.e., they need not be true for every object $o \in O$. They are called *association rules*. The base of association rules consists of the Duquenne-Guigues-Basis and additionally the following set of rules or implications:

9.1 Definition (the Luxenburger base)

This base is the set of implications of the following form, for sets of attributes which satisfy $\mathcal{A}_i = \mathcal{A}_i''$*,*

$$\mathcal{A}_1 \Longrightarrow_{\mathcal{E}} (\mathcal{A}_2 \setminus \mathcal{A}_1),$$

where no $\mathcal{A}_3$ *exists with* $\mathcal{A}_1 \subset \mathcal{A}_3 \subset \mathcal{A}_2$. $\diamond$

conexp allows to calculate this base of association rules. Here is the base for the association rules of our binary context:

```
1 < 0 > ODP* GWP* Cl F =[100%]=> < 0 > ALT* nC Br I Ether CO2 NH3;
2 < 0 > ODP* nC Cl F Br =[100%]=> < 0 > GWP* ALT* I Ether CO2 NH3;
3 < 4 > ODP* =[100%]=> < 4 > Cl F;
4 < 2 > GWP* nC F =[100%]=> < 2 > ALT*;
5 < 0 > GWP* F I =[100%]=> < 0 > ODP* ALT* nC Cl Br Ether CO2 NH3;
6 < 4 > GWP* =[100%]=> < 4 > F;
7 < 1 > ALT* nC F Ether =[100%]=> < 1 > GWP*;
8 < 1 > ALT* Cl F =[100%]=> < 1 > ODP* nC;
9 < 0 > ALT* F I =[100%]=> < 0 > ODP* GWP* nC Cl Br Ether CO2 NH3;
10 < 4 > ALT* =[100%]=> < 4 > F;
11 < 0 > nC Cl F Ether =[100%]=> < 0 > ODP* GWP* ALT* Br I CO2 NH3;
12 < 4 > nC Cl =[100%]=> < 4 > F;
13 < 0 > nC F I =[100%]=> < 0 > ODP* GWP* ALT* Cl Br Ether CO2 NH3;
14 < 0 > nC CO2 =[100%]=> < 0 > ODP* GWP* ALT* Cl F Br I Ether NH3;
15 < 0 > nC NH3 =[100%]=> < 0 > ODP* GWP* ALT* Cl F Br I Ether CO2;
16 < 0 > Cl F I =[100%]=> < 0 > ODP* GWP* ALT* nC Br Ether CO2 NH3;
17 < 0 > Cl CO2 =[100%]=> < 0 > ODP* GWP* ALT* nC F Br I Ether NH3;
18 < 0 > Cl NH3 =[100%]=> < 0 > ODP* GWP* ALT* nC F Br I Ether CO2;
19 < 0 > F CO2 =[100%]=> < 0 > ODP* GWP* ALT* nC Cl Br I Ether NH3;
20 < 0 > F NH3 =[100%]=> < 0 > ODP* GWP* ALT* nC Cl Br I Ether CO2;
21 < 1 > Br =[100%]=> < 1 > ODP* Cl F;
22 < 1 > I =[100%]=> < 1 > F;
23 < 4 > Ether =[100%]=> < 4 > nC;
24 < 0 > CO2 NH3 =[100%]=> < 0 > ODP* GWP* ALT* nC Cl F Br I Ether;
25 < 8 > Cl =[88%]=> < 7 > F;
26 < 10 > nC =[80%]=> < 8 > F;
```

Consider, for example, the 26th association rule:

$$26 \ < \ 10 \ > \ nC \ = [80\%] \Rightarrow < \ 8 \ > \ F;$$

An easy check shows that $\{nC\}'' = \{nC\}$, as well as $\{F\}'' = \{F\}$, for the sets of attributes that are involved and their second derivation (which is in fact the closure). Clearly there is no other set of attributes between these sets of attributes. The number 10 that is part of that rule says that the number of objects for which the assumption $\mathcal{A} = \{nC\}$ holds is 10, while the number 8 shows that there are exactly 8 objects for which both the assumption and the conclusion $\{F\}$ hold. The checks are easy.

10 The lattice of concepts

A disadvantage of the attribute implications is that on both sides of the implications just attributes occur but no objects. For this reason we should also consider the main notation of

Formal Concept Analysis, established by Rudolf Wille and his school at Darmstadt, see [10] around 1980. It describes a very important connection between particular sets of objects and particular sets of attributes and is helpful in evaluation, too, cf. [1, 2, 6, 22].

10.1 Definition (concepts and lattices of concepts)

Consider an evaluation $\mathcal{E} \in L^{O\times A}$ of a set O of objects with respect to a set A of attributes. We shall use the mappings $\mathcal{A} \mapsto \mathcal{A}'$ and $\mathcal{O} \mapsto \mathcal{O}'$ introduced above, as well as their iterations:

— *A concept in $\mathcal{E}$ is a pair of L–subsets $(\mathcal{O}, \mathcal{A})$, where $\mathcal{O} \in L^O$ and $\mathcal{A} \in L^A$, such that*

$$(\mathcal{O}, \mathcal{A}) = (\mathcal{O}'', \mathcal{O}') = (\mathcal{A}', \mathcal{A}'').$$

$\mathcal{O}$, an L–subset of the set O of objects, is called the extent of the concept, $\mathcal{A} \in L^A$ the intent of the concept.

— *The set of all the concepts in $\mathcal{E}$ is partially ordered by*

$$(\mathcal{O}, \mathcal{A}) \leq (\mathcal{O}^*, \mathcal{A}^*) \iff \mathcal{O} \subseteq_L \mathcal{O}^* \iff \mathcal{A}^* \subseteq_L \mathcal{A}.$$

In this case we call $(\mathcal{O}, \mathcal{A})$ a subconcept of $(\mathcal{O}^*, \mathcal{A}^*)$ and $(\mathcal{O}^*, \mathcal{A}^*)$ a superconcept of $(\mathcal{O}, \mathcal{A})$.

— *The concepts form a lattice with respect to that partial order, it is called the lattice of concepts.*

◇

Let us see what this means in the binary case:

10.2 Example (binary contexts, their concepts and lattices of concepts)

If $L = \{0, 1\}$ then $\mathcal{O} \in L^O = \{0, 1\}^O$ is a crisp subset of O, a crisp set of objects. The corresponding $\mathcal{O}' \in L^A = \{0, 1\}^A$ has the values

$$\mathcal{O}'(a) = \bigwedge_{o\in O} \tilde{\tau}(\mathcal{O}(o), \mathcal{E}(o, a)).$$

As the residuum is $\tilde{b}$, this means that

$$\mathcal{O}'(a) = \bigwedge_{o\in O} \tilde{b}(\mathcal{O}(o), \mathcal{E}(o, a)) = \bigwedge_{o\in O} \min\{1, 1 - \mathcal{O}(o) + \mathcal{E}(o, a)\}.$$

The minimum $\min\{1, 1 - \mathcal{O}(o) + \mathcal{E}(o, a)\}$ is 1 if and only if $\mathcal{O}(o) = \mathcal{E}(o, a)$, i.e.,

$$\mathcal{O}' = \{a \in A \mid \forall\, o \in \mathcal{O} : \mathcal{E}(o, a) = \mathcal{O}(o)\},$$

so that also

$$\mathcal{O}'' = \{o \in O \mid \forall\, a \in \mathcal{A} : \mathcal{E}(o, a) = \mathcal{O}'(a)\},$$

and so on. Correspondingly we get

$$\mathcal{A}' = \{o \in O \mid \forall\, a \in \mathcal{A} : \mathcal{E}(o, a) = \mathcal{A}(a)\},$$

so that also

$$\mathcal{A}'' = \{a \in A \mid \forall\, o \in \mathcal{O} : \mathcal{E}(o, a) = \mathcal{A}'(o)\},$$

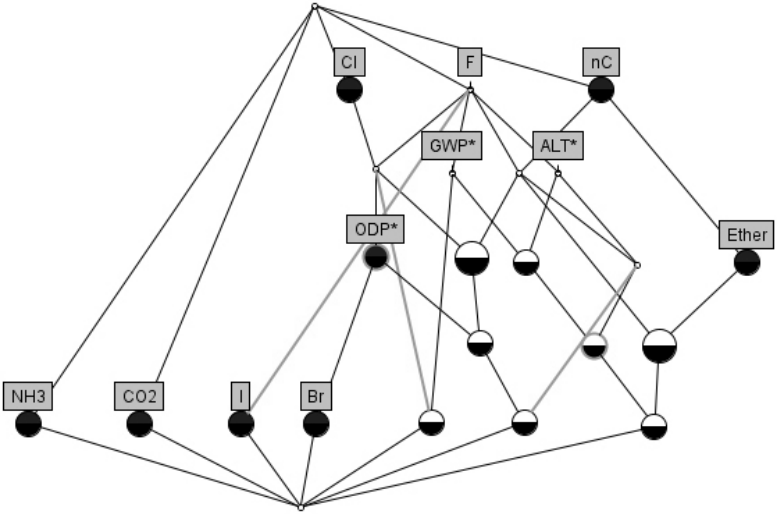
etc..

A concept is a pair $(\mathcal{O}, \mathcal{A})$ consisting of a crisp set $\mathcal{O}$ of objects, together with a crisp set $\mathcal{A}$ of attributes such that $(\mathcal{O}, \mathcal{A}) = (\mathcal{O}'', \mathcal{O}') = (\mathcal{A}', \mathcal{A}'')$. Hence, according to the above equations, $\mathcal{O} = \mathcal{A}'$ consists of just the objects that have the attributes contained in $\mathcal{A}$, while the set $\mathcal{A} = \mathcal{O}'$ consists of just the attributes that all the objects have which are elements of $\mathcal{O}$. Our binary context

Label	$nODP^*$	$nGWP^*$	$nALT^*$	nC	Cl	F	Br	I	$ether$	CO_2	NH_3
1	1	0	0	0	1	1	0	0	0	0	0
2	0	1	0	0	1	1	0	0	0	0	0
6	0	0	0	1	1	1	0	0	0	0	0
7	0	0	0	1	1	1	0	0	0	0	0
8	0	1	1	0	0	1	0	0	0	0	0
16	0	0	0	1	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	1	0
22	1	0	0	0	1	1	1	0	0	0	0
23	0	1	1	1	0	1	0	0	0	0	0
29	0	1	1	1	0	1	0	0	1	0	0
32	0	0	0	0	1	0	0	0	0	0	0
33	1	0	0	1	1	1	0	0	0	0	0
35	1	0	1	1	1	1	0	0	0	0	0
36	0	0	0	0	0	1	0	1	0	0	0
37	0	0	0	1	0	0	0	0	1	0	0
38	0	0	0	0	0	0	0	0	0	0	1
39	0	0	0	1	0	1	0	0	1	0	0
40	0	0	0	1	0	1	0	0	1	0	0

has the lattice of concepts, shown on the next page, it was obtained by an application of conexp. The 24 nodes represent the 24 concepts. From the 'User Guide' of that helpful software package we quote the following description:

Table 2: The lattice of concepts corresponding to the binary evaluation of the 18 refrigerants



So called reduced labeling is used in order to succinctly represent information about intents and extents of formal context. If label of attribute A is attached to some concept, that means, that this attribute occurs in intents of all concepts, reachable by descending paths from this concept to zero concept (bottom element) of lattice. If label of object O is attached to some concept, this means, that object O lays in extents of all concepts, reachable by ascending paths in lattice graph from this concept to unit concept (top element) of lattice. If drawing of node contains blue filled upper semicircle, that means, that there is an attribute, attached to this concept. If drawing of node contains black filled lower semicircle, that means, that there is a object, attached to this concept. Sometimes node or edge in line diagrams is displayed in red color. This means, that this edge or node are located very near or overlap with some other node. In order to improve layout, try manual adjustment of layout or some other layout.

On the lowest level we find one node, it corresponds to the trivial concept

$$(\emptyset, \{nODP^*, nGWP^*, nALT^*, nC, Cl, F, Br, I, ether, CO_2, NH_3\}).$$

On the last but one level we find two concepts with a 1-element extent and a 1-element intent, labeled by the attribute contained in the intent:

$$(\{RE_{38}\}, \{NH_3\}), (\{RE_{21}\}, \{CO_2\}),$$

and there is also a concept with a 1-element extent but a 2-element intent, and another one with a 1-element extent but a 4-element intent:

$$(\{RE_{36}\}, \{F, I\}), (\{RE_{22}\}, \{nODP^*, Cl, F, Br\}).$$

The other three (unlabeled) nodes correspond to three further concepts that have a 1-element extent as well:

$$(\{RE_1\}, \{nODP^*, Cl, F\}), (\{RE_2\}, \{nGWP^*, Cl, F\}),$$

$$(\{RE_8\}, \{nGWP^*, nALT^*, F\}), (\{RE_{36}\}, \{I\}), (\{RE_{22}\}, \{Br\}),$$

$$(\{RE_{16}\}, \{nC\}), (\{RE\}, \{ether\}),$$

and so on.

◇

For more examples and details see the cited literature [1, 2, 6, 22].

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See also `http://sourceforge.net/projects/conexp`