MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **54** (2005) 551-560

ISSN 0340 - 6253

Posets and Lattices, Contexts and Concepts

Adalbert Kerber,
Lehrstuhl II für Mathematik,
Universität Bayreuth,
D-95440 Bayreuth

Abstract

The present paper contains a brief description of the order theoretic foundations of the application of partial orders, in particular in environmental sciences. Posets and lattices are introduced as well as the corresponding Hasse diagrams which are an important tool for their visualization. Then we define the notion of concept. It is very helpful (and relatively new), since one of the main achievements of human society is *conceptual thinking*. We consider one- and many-valued contexts as well as generalizations, the L-fuzzy contexts which show up in many daily situations. They serve very well in the organization of interviews, tests and evaluations and so they play a role as a tool to support decisions in environmental risk management, for example.

1 Posets and Lattices

A *partially ordered set,* for short: a **poset**, is a set X together with a binary relation $\preceq$, say, which means that we are given, together with X, a set of certain pairs (x, x') of elements $x, x' \in X$, for short:

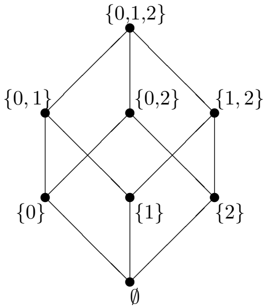
$$x \preceq x',$$

such that the following conditions are satisfied:

- $\preceq$ is *reflexive*: $x \preceq x$, for each $x \in X$.
- $\preceq$ is *antisymmetric*: $x \preceq x', x' \preceq x$ imply $x = x'$, for each $x, x' \in X$.
- $\preceq$ is *transitive*: $x \preceq x', x' \preceq x''$ imply $x \preceq x''$ for each $x, x', x'' \in X$.

The point is that there may exist elements $x, x' \in X$, for which neither $x \preceq x'$ nor $x' \preceq x$ holds, in which case we say that x and x' are *incomparable.* Hence partial orders are helpful in cases when some of the elements are comparable while others are not. Such situations occur quite often in daily life.

Partial orders can nicely be visualized by their **Hasse diagram**, the *nodes* (also called *vertices*) of which represent the elements of the set, and where two nodes are connected by an edge if and only if they are (immediate) *neighbors* with respect to the partial order. The Hasse diagram is usually *read from bottom to top*, the smaller elements are lower down. Here is, as an example, the Hasse diagram of the partial order $\subseteq$ on the set X, consisting of all the eight subsets of the set $\{0, 1, 2\}$:



The use of posets in chemistry is the topic of a special issue of MATCH ([12]), edited by D. Klein and J. Brickmann. The Prolegomenon of this issue, written by D. Klein, is strongly recommended, as are the other contributions.

Many examples of partial orders that occur in environmental sciences can be found in the publications of R. Brüggemann, for example in [4], where 13 pesticides are considered with respect to environmental hazards, based on their persistence T (half-life in soils), aqueous solubility W (in mg/L), vapor pressure of the pure substance V (in mPa) and the yearly usage U in Italy (in tons per year). Hence, for each of these pesticides there is a quadruple of values. For example, to propanil there corresponds the quadruple

$$(T, W, -V, U) = (1, 200, -5.3, 694),$$

while for alachlor we find

$$(T, W, -V, U) = (15, 240, -1.87, 1537),$$

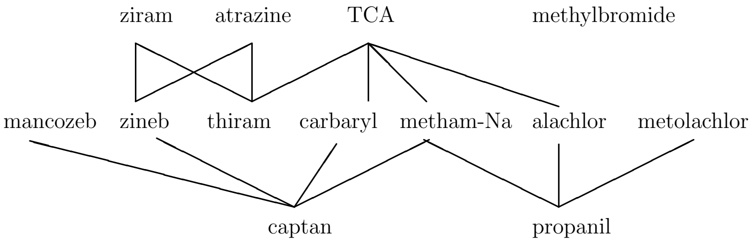
and for carbaryl

$$(T, W, -V, U) = (10, 120, -0.16, 590).$$

The bigger the entries are, the worse is the influence of the pesticide on the environment, and so there is *a natural partial order according to the given measurements.* It models the ranking according to "worse in every respect":

$$(T, W, -V, U) \preceq (T', W', -V', U') \iff T \leq T', W \leq W', -V \leq -V', U \leq U'.$$

Using this partial order, alachlor is worse than propanil, while carbaryl can neither be compared with alachlor nor with propanil. The Hasse diagram obtained is



Among other things we note that methylbromide is incomparable with the other pesticides. In other words: Compared with any one of the other pesticides *it has advantages as well as disadvantages.*

Partial orders are **lattices** if for any two elements there exists an *infimum* $x \wedge x'$ and a *supremum* $x \vee x'$. In our example of subsets of $\{0, 1, 2\}$, the infimum of two subsets is their intersection: $x \wedge x' = x \cap x'$, and their supremum is their union: $x \vee x' = x \cup x'$. In the case of divisibility, the infimum is the greatest common divisor: $x \wedge x' = gcd\{x, x'\}$, while the supremum is the least common multiple: $x \vee x' = lcm\{x, x'\}$. A lattice is said to be *complete*, if there is an infimum and a supremum not just for two elements, but also for any subset.
In the partial order on the set of pesticides mentioned above we have, for example,

$$\text{ziram} \wedge \text{TCA} = \text{thiram},$$

but it is *not* a lattice because, for example, there does not exist an infimum of methylbromide and TCA, the infimum of ziram and atrazine is not defined, and many other violations of the definition of lattice can be found.

2 Contexts and their concepts

We are now going to apply the notions of partial order and of lattice to situations of the following sort of kind: Suppose that we are given *information on properties of certain objects,* say on chemical substances and some of their environmental properties. We call this knowledge a **context,** and we should like to explore the information contained in it. For example, we should like to

- *visualize* its content,
- to *draw conclusions,*
- or to form *hypotheses,*

based on the context and on nothing else.

For this purpose, we can use *concept analysis,* introduced by R. Wille about twentyfive years ago. Its main tool is the notion of **lattice of concepts,** which is a particular *partial order* that beautifully reflects the information contained in the given context.

The notion of concept, mathematically modelled by concept analysis, is in fact due to the 17-th century philosophy of *Port-royal,* (Pascal et al., see e.g. [1], also Leibniz had some influence) where it was called *idée universelle* (in German: Begriff).

The definition of idée universelle, given there, reads as follows:

- ... dans ces idées universelles il y a deux choses qu'il est très important de bien distinguer, la comprehension et l'étendue...
- ...J'appelle *comprehension* de l'idée, les attributs qu'elle enferre en soi, & qu'on ne lui peut ôter sans détruire, comme la comprehension de l'idée du triangle conferme extension, figure, trois lignes, trois angles, & l'égalité de ces trois angles á deux droits, & c...
- ...J'appelle *étendue* de l'idée, les sujets á qui cette idée convient...

The standard reference for its *mathematical model* is the book [7] by Ganter and Wille.

Corresponding to the philosophical definition, a concept consists of two sets, the *extent* (étendue, Umfang) the set of objects (sujets, Gegenstände) implied in the concept, and the *intent* (comprehension, Inhalt), a set of attributes (attributs, Merkmale).

Hence, this notion of concepts applies in particular to situations, where the information given is of the form

The object ω has (has not) the attribute α

for a given set of objects $\omega \in \Omega$, and a given set of attributes $\alpha \in A$. Such a set of informations can be gathered e.g. in the form of a table, a **context.**
Here is the oldest context of environmental chemistry ([2]). It describes the classical "four elements":

$\omega\backslash\alpha$	w	c	d	h
F	1	0	1	0
E	0	1	1	0
W	0	1	0	1
A	1	0	0	1

Its objects are: <u>F</u>ire, <u>E</u>arth, <u>W</u>ater, <u>A</u>ir, and the attributes: <u>w</u>arm, <u>c</u>old, <u>d</u>ry, <u>h</u>umid. The entry at the intersection of the row corresponding to an object ω and the column of the attribute α is put to 1 (or $\times$) if the object *has* this property, otherwise it is put to 0 (or left empty).

The **concepts** reflect its information content. They are pairs (B, C), $B \subseteq \Omega, C \subseteq A$, such that the corresponding entries form a rectangle of 1s, *not* contained in a bigger rectangle full of 1s: For example, if $B = \{b_1, \ldots, b_m\}$ is the extent of a concept and $C = \{c_1, \ldots, c_n\}$ its intent, the situation looks as follows (after a suitable rearrangement of rows and columns):

$$
\begin{array}{c|ccccc}
\omega\backslash\alpha & \dots & c_1 & \dots & c_n & \dots \\
\hline
\vdots & & & & & \\
b_1 & & 1 & \cdots & 1 & \\
\vdots & & \vdots & \cdots & \vdots & \\
b_m & & 1 & \cdots & 1 & \\
\vdots & & & & &
\end{array}
$$

In formal terms: If we define the *derivation of* B by

$$B' := \{\alpha \in A \mid \text{ each } \omega \in B \text{ has the attribute } \alpha\},$$

and, analogously, the *derivation of* C:

$$C' := \{\omega \in \Omega \mid \text{ each } \alpha \in C \text{ is an attribute of } \omega\},$$

then (B, C) is a concept, if and only if

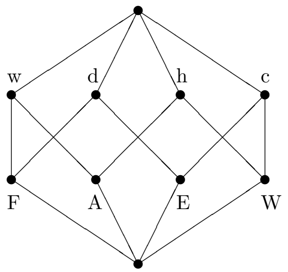
$$B = C' \text{ and } C = B'.$$

We note in passing that this implies $C'' = C$ as well as $B'' = B$.

The concepts obtained from a given context form a partial order $\preceq$, defined by

$$(B, C) \preceq (D, E) \iff B \subseteq D \iff C \supseteq E,$$

(B, C) is said to be a *subconcept* of (D, E), (D, E) a *superconcept* of (B, C). This partially ordered set of concepts is even a lattice, i.e. for two concepts there exists both an infimum (= the biggest subconcept of both of them) and a supremum (= the smallest superconcept of them). Hence we may call this partial order **the lattice of concepts** corresponding to the context in question. It is in fact a complete lattice.
Here is, for example, the Hasse diagram of the lattice of concepts corresponding to the context on the "four elements":



The letters F, A, E, W label the smallest concepts containing the objects F, A, E, W in their content, i.e. F, for example, labels the concept $(B, C) = (\{F\}'', \{F\}')$. Correspondingly, the attribute w, say, labels the concept $(B, C) = (\{w\}', \{w\}'')$. It is important to notice that the lattice of concepts given obviously allows to reconstruct the context

$\omega\backslash\alpha$	w	c	d	h
F	1	0	1	0
E	0	1	1	0
W	0	1	0	1
A	1	0	0	1

and in fact, also in the general case, the lattice of concepts, better say **the Hasse diagram of the lattice of concepts perfectly reflects and visualizes the information contained in the context** in question! For example, we can easily read off from the above diagram, that fire is supposed to be warm and dry (and neither humid nor cold). This is why Hasse diagram techniques (HDT) are so helpful and important.

This context on the four elements contains, besides zeros, entries of just one further value. We call such contexts **one-valued contexts.** There is an obvious generalization, for example the following context that may express our feeling that water is more humid than air, for example,

$\omega\backslash\alpha$	w	c	d	h
F	2	0	2	0
E	0	1	1	0
W	0	1	0	2
A	1	0	0	1

Such contexts are called **many-valued contexts.** They can easily be transformed into a one-valued context. This transformation is called **scaling**, and the scale can be chosen in a problem oriented way. For example, a self-explaining scaling of the above two-valued context is

$\omega\backslash\alpha$	w≥ 2	w≥ 1	c≥ 2	c≥ 1	d≥ 2	d≥ 1	h≥ 2	h≥ 1
F	1	1	0	0	1	1	0	0
E	0	0	0	1	0	1	0	0
W	0	0	0	1	0	0	1	1
A	0	1	0	0	0	0	0	1

A different scaling uses the attributes

$$w \leq 2, w \leq 1, c \leq 2, c \leq 1, d \leq 2, d \leq 1, h \leq 2, h \leq 1,$$

for example.

Sometimes there are too many different entries, and the entries are not integral. In this case we can use a method that Brüggemann et al. applied to environmental contexts: Take the mean-value m in a column and replace an entry in that column by 0 if it is $< m$, by 1 otherwise (see [5]). Clearly, they also consider a more refined view, using more than two intervals.

Generalizing the situation of one-valued contexts we obtain the following definition:

Definition: *A* ***generalized context*** *or* ***order context*** *is a triple* $\mathbb{K} = (X, Y, \varphi)$, *where both* X *and* Y *are partially ordered sets and* $\varphi: X \to Y$ *is a* Galois mapping *(i.e. there exists another mapping* $\psi: Y \to X$ *such that* (φ, ψ) *is a* Galois connection *between the posets, which means that both mappings are antitone and their compositions* $\varphi\psi$ *and* $\psi\varphi$ *are extensive). A special case is a* ***power set context***, *where*

$$X = P(\Omega) = \{M \mid M \subseteq \Omega\},\ Y = P(A) = \{N \mid N \subseteq A\},$$

the power sets of Ω *and* A, *respectively, ordered by inclusion, and* φ, ψ *the derivations*

$$\varphi: P(\Omega) \to P(A), B \mapsto B',\ \psi: P(A) \to P(\Omega), C \mapsto C'.$$

Hence the one-valued contexts are power set contexts. More important is that this definition allows an easy generalization to the fuzzy case as well.

Consider L**-contexts,** where the entries are elements of a partial order, or even a lattice L. An example of an $L-$context about environment can be obtained from Brüggemann's table on pollution (by Pb, Cd, Zn and S) of the regions of Baden-Württemberg ([5]), measured in herb layers (HL), tree leaves (TL) etc.:

region\pollution	$(HLPb, HLCd, HLZn, HLS)$	$(TLPb, TLCd, TLZn, TLS)$	$\ldots$
06	$(1, 0.07, 29, 1750)$	$(0.6, 0.04, 22, 1620)$	$\ldots$
08	$(1.5, 0.07, 27, 1750)$	$(0.9, 0.1, 33, 1890)$	$\ldots$
$\vdots$			

For example, the two entries in the first column are incomparable, while the entries in the second column can be compared:

$$(0.6, 0.04, 22, 1620) < (0.9, 0.1, 33, 1890).$$

Simple examples taken from environmental chemistry are not available, hence for demonstration a fictitious example is given. Let Ω be the set of objects $\{N, P, S, T\}$. Let furthermore the set A of attributes be $\{a, b, c, d, e, f\}$. Then an L-context may be given as follows (it is in fact a context containing test results published in the computer journal c't some time ago, and the reason that the entries are pairs of evaluation results is due to the fact that the objects were read/write machines for compact discs and for DVD's and that there are two different standards for reading and writing such discs):

	a	b	c	d	e	f
N	$++, ++$	$-, -$	$--, \circ$	$+, -$	$-, --$	$+, \circ$
P		$+, -$	$-, -$	$\circ, -$	$--, +$	$-, \circ$
S		$++, ++$	$\circ, +$	$+, \circ$	$++, --$	$-, -$
T		$\circ, -$	$\circ, \circ$	$-, -$	$+, +$	$+, \circ$

The partial order used is the cartesian product of the linear order $-- < - < \circ < + < ++$ with itself:

$$L = \{-- < - < \circ < + < ++\} \times \{-- < - < \circ < + < ++\}.$$

The elements of L are pairs (x, y), the components x, y of which belong to the totally ordered set $\{-- < - < \circ < + < ++\}$, and the partial order L of pairs is defined by

$$(v, w) \leq (x, y) \iff v \leq x \text{ and } w \leq y.$$

It is clear how such a context containing pairs can be replaced by a one-valued context via separating the components of the pairs of the entries, obtaining a many valued context and then scaling (cf. [8],[9],[10],[14],[3]).

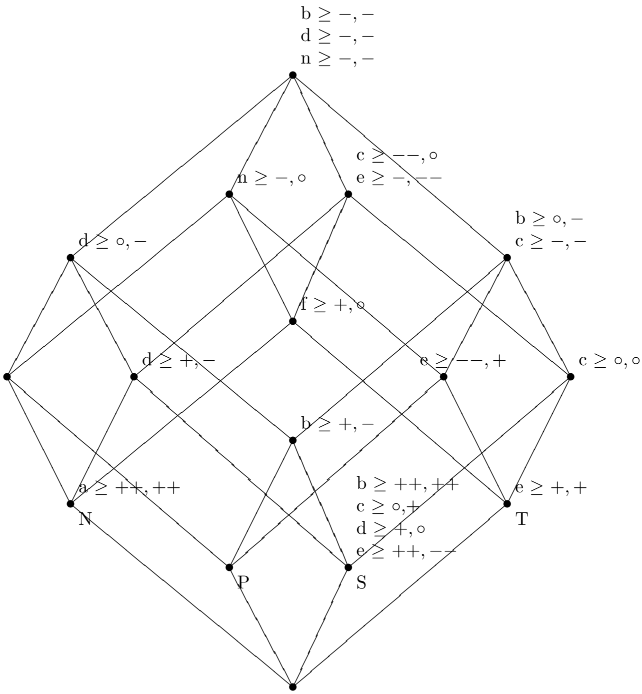
Thus, most generally, we consider a set Ω of objects ω, a set A of attributes α, together with a *lattice* $(L, \wedge, \vee)$ i.e. a partial order such that for each pair of elements $\lambda, \mu \in L$ there exists the infimum $\lambda \wedge \mu$ and the supremum $\lambda \vee \mu$. For sake of simplicity we assume that Ω, A and L are finite, as in most applications, and we define the L-power set of M (for more details on fuzzy sets and concepts see [13],[11],[14]) to be the set $P_L(\Omega)$ of mappings $B_L: M \rightarrow L$ (ordered by $B_L \subseteq B_L^*$ iff $B_L(m) \leq B_L^*(m)$, for each $m \in M$). Using this notation we define:

Definition: *An L-**Fuzzy power set context** is a triple $\mathbb{K} = (P_L(\Omega), P_L(A), \varphi)$, where*

$$\varphi: P_L(\Omega) \rightarrow P_L(A)$$

*is a Galois mapping. An L-**Fuzzy concept** is a pair (B_L, C_L) of L-Fuzzy subsets B_L in $P_L(\Omega)$ and C_L in $P_L(A)$ such that $\varphi(B_L) = C_L$ and $\psi(C_L) = B_L$, if (φ, ψ) is the Galois connection.*

Here is the lattice of L-Fuzzy concepts corresponding to the example of an L-Fuzzy context given above ([3]). It shows, among many other things, that with respect to both attributes c and d, the object S has the best test results, while T is best with respect to e. N and T are the best – and of equal quality – with respect to the attribute f. Moreover, if we are looking for an object with $c \geq \circ, \circ$, then we can choose between S and T, and if we insist that also $d \geq \circ, \circ$, the only product that remains is S.



For more details, see [10] and [14].

References

[1] Arnauld, A. Nicole, P.: *La Logique ou L'Art de penser, contenant, outre les Règles communes, plusieurs observations nouvelles, propres à former le jugement.* Sixième Édition revue et de nouveau augmentée. A Amsterdam, Chez Abraham Wolfgang (1685). German translation by Axelos, C., 2. edition, Wiss. Buchges., Darmstadt (1994)

[2] Bartel, H.-G.: *Formale Begriffsanalyse und Materialkunde.* MATCH Commun. Math. Comput. Chem. **32**, 27-46 (1995)

[3] Bögelein, A.: *Computerunterstützte Berechnung der Begriffsverbände von Fuzzy-Kontexten und deren Anwendung.* Diploma thesis, Bayreuth 2005.

[4] Brüggemann, R., Bartel, H.-G.: *A Theoretical Concept To Rank Environmentally Significant Chemicals.* J. Chem. Inf. Comput. Sci. **1999,** 39, 211-217

[5] Brüggemann, R., Welzl, G., Voigt, K.: *Order Theoretical Tools for the Evaluation of Complex Regional Pollution Patterns.* J. Chem. Inf. Comput. Sci. **43**, 1771-1779 (2003)

[6] Ganter, B.: *Begriffe und Implikationen.*

[7] Ganter, B., Wille, R.: *Formal Concept Analysis* – Mathematical Foundations. Springer Verlag, Berlin (1999)

[8] Gugisch, R. *Verallgemeinerung der formalen Begriffsanalyse und Anwendung auf mehrwertige Kontexte.* Diplomarbeit, Uni Bayreuth (1997)
http://www.mathe2.uni-bayreuth.de/ralfg/papers/diplom.ps.gz

[9] Gugisch, R. *Lattice Contexts – a Generatization in Formal Concept Analysis.* handout to ICCS 2000, Darmstadt (2000)
http://www.mathe2.uni-bayreuth.de/ralfg/papers/iccs2000.ps.gz

[10] Gugisch, R. *Many-Valued Context Analysis Using Descriptions.* In: Delugach, H., Stumme, G., editors, Conceptual Structures: Broadening the Base. Lecture Notes in Artificial Intelligence 2120. Springer, Berlin-Heidelberg-New York (2001) 157-168

[11] Kerber, A., Lex, W.: *Kontexte und ihre Begriffe.* (1997)
http://www.mathe2.uni-bayreuth.de/kerber/begriffe.ps

[12] Klein, D.J., Brickmann, J. (eds.): Partial Orderings in Chemistry. MATCH Commun. Math. Comput. Chem. **42** (2000), 290 pp.

[13] Klir, G. J., Bo Yuan: *Fuzzy Sets and Fuzzy Logic (Theory and Applications).* Prentice Hall 1995.

[14] Pollandt, S.: *Fuzzy-Begriffe, Formale Begriffsanalyse unscharfer Daten.* Springer-Verlag 1997.