Inter*net* Electronic Journal of Molecular Design

February 2005, Volume 4, Number 2, Pages 151–172

Editor: Ovidiu Ivanciuc

Proceedings of the Internet Electronic Conference of Molecular Design, IECMD 2003
November 23 – December 6, 2003
Part 8

A Lattice–Theoretical Shape Concept

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Received: October 24, 2003; Revised: July 22, 2004; Accepted: September 7, 2004; Published: February 28, 2005

Citation of the article:
I. Bálint and A. Kocsor, A Lattice–Theoretical Shape Concept, *Internet Electron. J. Mol. Des.* **2005**, *4*, 151–172, http://www.biochempress.com.

Inter*net* Electronic Journal of Molecular Design

BioChem Press
http://www.biochempress.com

A Lattice–Theoretical Shape Concept [#]

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Internet Electron. J. Mol. Des. **2005**, *4* (2), 151–172

Abstract

This report is on the lattice–theoretical characterization of the 'shape' of topological sets. The reported procedure is abstract enough to have a wide area of applications in those fields, where the classification relies on 'similarity' or 'neighborhood-ness'. A possible huge field is the searching for molecules with predetermined pharmacological properties. The targets of comparison can be the various type electron densities of the interacting molecular systems, when the procedure is able to give a hierarchically ordered set of more and more detailed shape characterizations, a distance concept and topology. Actually the shapes of continuous *n*–variable functions are investigated and the electron densities are chosen for representatives of this class, but instead of real–life computations an easy to grasp artificial example is given.

Keywords. Lattice theory; shape theory; similarity measures.

Abbreviations and notations

EDSs, electron density surfaces	PESs, potential energy surfaces

1 INTRODUCTION

Although the 'common sense' meaning of the 'shape' of a 3–dimensional object is quite familiar to everyone, this meaning is not unique and not even well–defined in a mathematical sense. Our practice in comparing and classifying objects as 'identical', 'similar', or 'different' is based on learning, taste, actual conditions and so on. The mathematical definition is not a trivial problem either, because the 'shape' of the object can be described in a number of ways. These descriptions are not equivalent and emphasize different characteristics of the object. This is the reason that

[#] Presented in part at the Internet Electronic Conference of Molecular Design 2003, IECMD 2003.
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various branches of universal algebra, topology [1], or algebraic topology [2–5] can serve for suitable (but not equivalent!) tools of the 'shape–description' problem. To characterize the shape is a widespread intention [7–8]. Classification problems relying on the 'similarity' of the elements of a set are important, but require a mathematically sound and in the practical sense suitable definitions of the shape. Practical applicability prefers such a schemes, which can provide gradually more and more detailed characterization of the objects, a distance concept and a neighborhood–topology, which is a mathematically well–established close analogue of our perception. A shape characterization of this kind gives a result which corresponds to our common, every–day practice, when approaching a set of objects and coming closer more and more details appear. Since a possible application of this scheme is in quantum–chemistry instead of 'topological sets' we talk about the shape of continuous *n*–variable functions and as representative about electron densities. Our intention is the theoretical foundation of the scheme and no real–life but only an easy artificial example will be given.

In quantum chemistry the notion of shape occurs mostly in relation with atomic or molecular orbitals, electron density surfaces (EDSs), potential energy surfaces (PESs), exchange–correlation hole, nuclear wave and density functions [1–2,4–6], etc. The shapes of these mathematical objects are in relationships with the physical behaviors of the associated systems.

Our primary interest is focused on EDSs. From the simple model of Thomas and Fermi [9] grew a whole new branch of computational quantum mechanics based on local density approximation [10–11]. By the theorems of Hohenberg and Kohn [8], the one–electron density function plays the central role in all these methods. Besides the one–electron densities, also the two–electron and transition densities are of great importance concerning the correlation effects and dynamic molecular interactions. This is the reason, why the 'shapes' of electron density functions attract considerable attentions, when explaining molecular properties. But, beyond the theoretical interest, there is also a great practical significance in the shape–description problem, because it helps to select molecules with prespecified chemical or pharmacological behaviors. In this way the hunting for pharmacologically active compounds can be shortened significantly.

Our aim is to give a general lattice–algebraic scheme, where a distributive lattice is associated with each electron density function and the 'structures' of the shapes of electron densities are characterized by the structures of the associated lattices. We want to give measures, which assign 'distances' to couples of lattices/functions and induce topologies. The measures are intended to quantify the fine details in the similarity of the compared functions making the similarity 'structured'. The subjects of our shape characterization scheme are the electron density functions, but only implicitly. The method will be discussed in abstract terms referring to the class of continuous functions. Since also electron densities belong to this class, the generality of our discussion will not mean lose speaking. To focus our attention to the method itself, the illustrations

will refer to unspecified functions. The report is structured as follows: the next section is devoted to technicalities, then the shape lattices are defined with measure, then come the main results and finally the conclusions close the discussion. To make the reading easier, the proofs of assertions are collected into a separate section (Appendix 1) and some background material on lattice theory is given in Appendix 2.

2 THE LATTICE OF CONGRUENCIES

The presented scheme is intended to compare objects in relation of 'geometrical identity' and those, which arise from each other by 'continuous deformations'. In this report we adhere to objects that can be represented in a single coordinate frame, as (*n*+1)–dimensional point sets of the form:

$$O = \{(\vec{x}, f(\vec{x})) \ : \ \vec{x} \in \mathbf{R}^n\}, \ f(\vec{x}) \textit{ is absolutely continuous}, \ f(\vec{x}) : \mathbf{R}^n \to \mathbf{R}, \tag{1}$$

where $f(\vec{x})$ can be a density function.

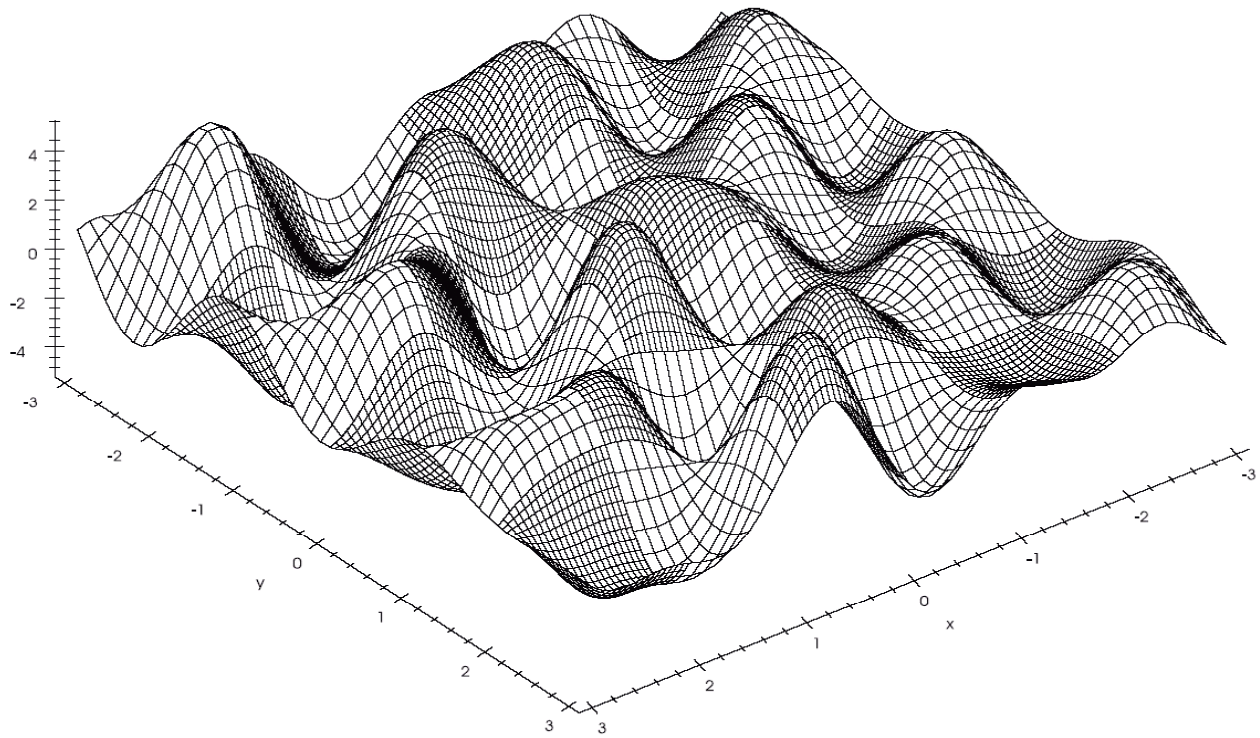

Figure 1. The graph of $f(\vec{x})$ partitioned into building blocks.

To keep the forthcoming discussion formally simple and concrete, let the co–ordinate space be two–dimensional ($n = 2$), the function be restricted to the closed domain $D \subset \mathbf{R}^n$, which is partitioned (by a regular grid) into disjoint cells:

$$D = \{\cup\, d_{kl} \ : \ k = 1,...,M_K, \ l = 1,...,M_L, \ kl \neq k'l' \Rightarrow d_{kl} \cap d_{k'l'} = \varnothing\}. \tag{2}$$

(To avoid an abuse of indexes, the double–indexes will not be separated, $(kl) \equiv (k,l)$). Each cell

supports a restriction of $f(\vec{x})$, which is illustrated on Figure 1 by a (6×6)–element set of "sample building blocks".

The building blocks will be represented by abstract 'brackets':

$$(kl,\theta(kl)) \leftrightarrow \{(\vec{x}, f(\vec{x})) \ : \ \vec{x} \in d_{kl}\}, \tag{3}$$

where the first element of the ordered pair is the double–index of the cell, the second element is a set function (denoted shortly) $\theta(kl) \equiv \theta(d_{kl}) \in \mathbf{R}$, and we call it 'property' function. A set function θ is an admissible property function, if refining the partitioning infinitely, it converges to f. This means for every contracting sequence of measurable sets $\delta_i \subset \mathbf{R}^n$:

$$(\lim_{i\to\infty} diam(\delta_i) = 0, \ \cap_i \delta_i = \{\vec{x}\}\ ) \Rightarrow \ \theta(\delta_i) \to f(\vec{x}). \tag{4}$$

Some of the possible choices are the integral mean $\theta(d_{kl}) = \frac{1}{|d_{kl}|}\int_{d_{kl}} f(\vec{x})\, d\vec{x}$ (where $|\, d_{kl}\,|$ indicates area), the $\inf f(\vec{x}),$ *or* $\sup f(\vec{x}),$ $(\vec{x} \in d_{kl})$, respectively. Choosing a set function to characterize the building blocks is equivalent with the substitution of the continuous surface patches by a step function, as displayed on Figure 2.

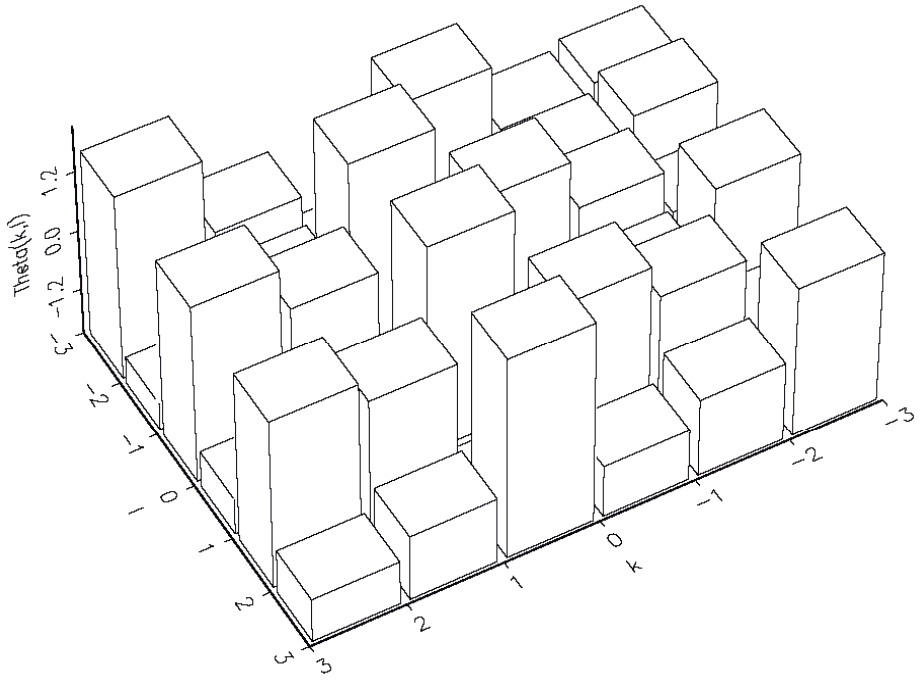

Figure 2. The graph of $\theta(kl)$.

Although in finitely dense grids a more detailed picture is obtained, if a whole parameter vector (for instance set functions of partial derivatives) is assigned to each cell, for practical simplicity only one parameter will be considered here. To construct a lattice over the brackets, the brackets are embedded into a Cartesian product set. The double–indexes are separated into $K = \{k \ : \ k = 1,...,M_K\}$ and $L = \{l \ : \ l = 1,...,M_L\}$ sets providing the Cartesian product:

$$K \times L \equiv KL = \{(k,l):\ k \in K,\ l \in L)\}, \tag{5}$$

where KL is shorthand for $K \times L$.

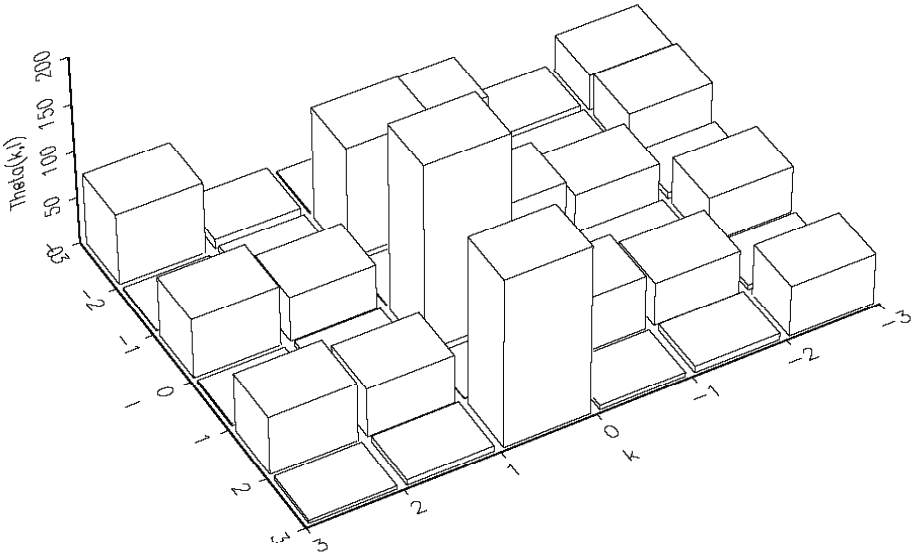

Figure 3. The graph of $\theta'(kl)$ isomorphic to $\theta(kl)$ on Figure 2.

The property function $\theta(kl)$ is concentrated to discrete points of a closed interval range of the real line. The function values are indexed by kl and ordered by the usual ordering $(\leq)$. The set of points includes the distinct function values $\Theta = \{\theta(kl):\ kl \in KL\}$. Concerning the cardinalities, $|K| = M_K$, $|L| = M_L$, but $|\Theta| \leq M_K M_L$, where we assume $M_K \geq 2,\ M_L \geq 2,\ |\Theta| \geq 2$. The Cartesian product of these sets is the set of 'generalized' brackets,

$$KL \times \Theta \equiv KL\Theta = \{(kl,\ \theta(k'l'))\ \ :\ \ kl,\ k'l' \in KL\}, \tag{6}$$

(where $KL\Theta$ is again a shorthand notation). The 'diagonal' elements (for which $kl = k'l'$) are the 'true' brackets, which belong to the primordial building blocks. The 'non–diagonal' elements (for which $kl \neq k'l'$) arise 'by transposing the surface patch $(k'l')$ into the cell (kl)', if a pictorial explanation is given. The lattices over K, L and Θ are simple chains. The operations are defined identically (in K for example), the meet and join will be:

Definition 1.

$$k \wedge k' = \min\{k,k'\},\quad k \vee k' = \max\{k,k'\} \tag{7}$$

and the lattices are $\mathbf{L}(K)$, $\mathbf{L}(L)$ and $\mathbf{L}(\Theta)$. If investigating the congruence relations of a lattice, a deeper insight is gained into the algebra. A congruence relation will be symbolized by λ (or λ_i), that particular congruence class, which includes elements congruent with a given k one is $[k]/\lambda$. All congruence relations of a lattice algebra can be partially ordered by inclusion into a 'congruence lattice', as $\mathbf{Con}(\mathbf{L}(K))$, $\mathbf{Con}(\mathbf{L}(L))$, $\mathbf{Con}(\mathbf{L}(\Theta))$. In the congruence lattice, the meet is the set–theoretical intersection, the join is the transitive closure [14]. For example,

$\mathbf{Con}(\mathbf{L}(K)) = \langle Con(\mathbf{L}(K)), \wedge, \vee \rangle$ is the algebra with base set $Con(\mathbf{L}(K))$ including all congruence relations and operations $\wedge, \vee$ (the base set is not boldface!, see Appendix 2.). The number of congruences is very large, therefore we shall only use an appropriately selected subset of all congruencies in $Con(\mathbf{L}(K))$, $Con(\mathbf{L}(L))$ and $Con(\mathbf{L}(\Theta))$. Allowed congruence relations (except the $\hat{0}$–congruence relation) will be those, which have only one congruence class with $m > 1$ element (this is called 'main class'), while all other classes have a single element. The main class will sometimes be denoted $[\lambda]$. To make a clear distinction from the general set of congruence relations, our specially chosen subset will be symbolized by lowercase letters, as $con(\mathbf{L}(K))$, $con(\mathbf{L}(L))$, $con(\mathbf{L}(\Theta))$.

Definition 2. *In any chain lattice those elements* $(k, k' \in K)$, *which satisfy*

$$k \vee k_i = k' \vee k_i, \; k_i \in (k_r] \tag{8}$$

are equivalent with respect to the congruence relation generated by the 'principal ideal' $(k_r] := \{k_i \in K \; : \; k_i \leq k_r\}$. *Those elements*, *which satisfy*

$$k \wedge k_i = k' \wedge k_i, \; k_i \in [k_s) \tag{9}$$

are equivalent with respect to the congruence relation generated by the 'principal dual ideal' $[k_s) := \{k_i \in K \; : \; k_i \geq k_s\}$ (*'principal filter'*).

We shall call these two types of congruence relations 'basis' congruence relations. Congruent elements will be denoted $k \equiv k' \pmod{\lambda}$. The universal bounds $\hat{0}^K$ and $\hat{1}^K$ determine the smallest and largest congruence relations:

$$k \equiv k' \pmod{\hat{0}^K}, \; if \; k = k' \; and \; \forall k, k' \, (k \equiv k' \pmod{\hat{1}^K}). \tag{10}$$

Lemma 1. *The congruence classes form convex sublattices* (*intervals*) *in the chain lattices* $\mathbf{L}(K)$, $\mathbf{L}(L)$ *and* $\mathbf{L}(\Theta)$.

In the set of chosen congruence relations, the operations are defined as follows:

Definition 3.

$$\lambda_i \wedge \lambda_j = \lambda_k, \; p \equiv p' \pmod{\lambda_k}, \; if \; (p \equiv p' \pmod{\lambda_i}) \bigwedge (p \equiv p' \pmod{\lambda_j}), \tag{11}$$

where the meet collapses those elements, *which are congruent with respect to both relations*. *The join of two allowed congruence relations is specially constructed to ensure*, *that the resulting relation be in the allowed subset*:

$$\lambda_i \vee \lambda_j = \lambda_k, \; p \equiv p' \pmod{\lambda_k}, \; if \; p \equiv p' \pmod{(\lambda_{i1} \; or \; \lambda_{j1}) \bigwedge (\lambda_{i2} \; or \; \lambda_{j2})}) \tag{12}$$

where $\lambda_i = \lambda_{i1} \wedge \lambda_{i2}$, $\lambda_j = \lambda_{j1} \wedge \lambda_{j2}$ *and* $\lambda_{i1}, \lambda_{j1}$ *are of type* (*8*), $\lambda_{i2}, \lambda_{j2}$ *of type* (*9*).

The join is the smallest (allowed) congruence relation, which collapses the classes of the operands. The whole set of allowed congruence relations $con(\mathbf{L}(K))$ arises through a single

application of the above operations onto the set of basis congruence relations. Our specially chosen congruence lattices will be the (lowercase!) algebras $\mathbf{con}(\mathbf{L}(K)) = \langle con(\mathbf{L}(K)), \wedge, \vee \rangle$, $\mathbf{con}(\mathbf{L}(L)) = \langle con(\mathbf{L}(L)), \wedge, \vee \rangle$ and $\mathbf{con}(\mathbf{L}(\Theta)) = \langle con(\mathbf{L}(\Theta)), \wedge, \vee \rangle$. Since the congruence relations are generated by (11) and (12) from the basis congruence relations, the main classes are intervals of chain lattices. The elementary congruence relations of a 3–element and a 5–element chain are displayed on figure 4. (4.1, 4.2 and 4.3, 4.4). Abandoning chain lattices, $\mathbf{L}(KL\Theta) = \mathbf{L}(K) \times \mathbf{L}(L) \times \mathbf{L}(\Theta)$ is defined on the Cartesian product set. The operations are imposed on the ordered pairs 'component–wise'.

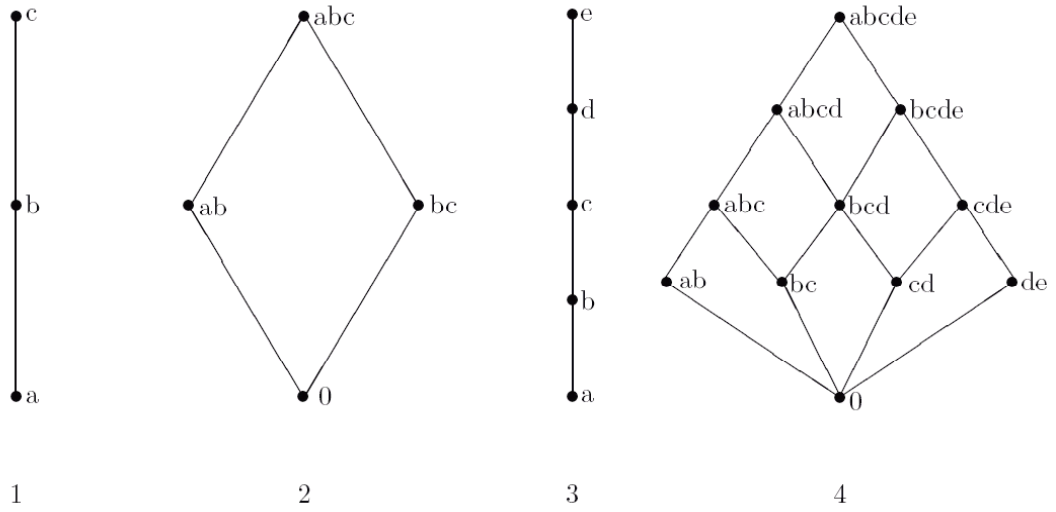

Figure 4. A 3–element and a 5–element chain with lattices of allowed congruence relations (Congruence relations are identified with collapsed elements).

Definition 4.

$$(kl, \theta(k'l')) \wedge (k''l'', \theta(k'''l''')) = (kl \wedge k''l'', \theta(k'l') \wedge \theta(k'''l''')), \tag{13}$$

$$(kl, \theta(k'l')) \vee (k''l'', \theta(k'''l''')) = (kl \vee k''l'', \theta(k'l') \vee \theta(k'''l''')), \tag{14}$$

which means that for elements of the ordered pairs, the meet and join come from $\mathbf{L}(KL)$ and $\mathbf{L}(\Theta)$. It is stressed, that also the double–index is understood component–wise, *i.e.* $(kl \wedge k''l'') \equiv \{(k,l) \wedge (k'', l'')\}$.

Lemma 2. *Lattice* $\mathbf{L}(KL\Theta)$ *is distributive.*

To have also a visual impression about $\mathbf{L}(KL\Theta)$, the Hasse–diagram of a (2×2)–partitioned (density) function is displayed on Figure 5. The marked dots denote true brackets associated with the following three distinct property function values $\theta(11) < \theta(12) = \theta(22) < \theta(21)$.

Since congruence relations of different chain lattices are independent, as well as the lattice operations in the Cartesian lattice are component–by–component defined, also the congruence relations of $\mathbf{L}(KL\Theta)$ are of product structure.

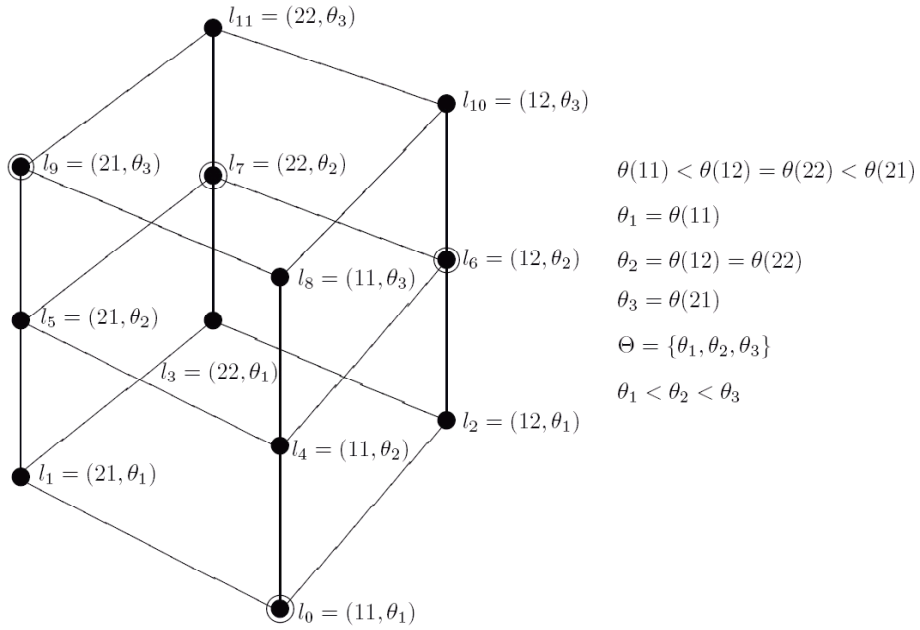

Figure 5. The Hasse–diagram of a (2×2)–partitioned density function with three different $\theta(kl)$ values.

Definition 5. *Any congruence relation* $\lambda_i \in con(\mathbf{L}(KL\Theta))$ *of a Cartesian lattice is the Cartesian product of the congruence relations of the component lattices* $\lambda_i^{KL} \in con(\mathbf{L}(KL))$ *and* $\lambda_i^{\Theta} \in con(\mathbf{L}(\Theta))$

$$\lambda_i^{KL\Theta} = \lambda_i^{KL} \times \lambda_i^{\Theta}, \tag{15}$$

where any of the components may be $\hat{0}^{KL}$, $\hat{0}^{\Theta}$ *or* $\hat{1}^{KL}$, $\hat{1}^{\Theta}$.

Henceforth, the component congruence relations will always be distinguished by superscripts $\lambda_i^{KL} \equiv \lambda_i^{K} \times \lambda_i^{L}$ and λ_i^{Θ}, while an unlabelled symbol is understood as $\lambda_i \equiv \lambda_i^{KL\Theta}$.

Definition 6. *Two brackets in* $KL\Theta$ *are congruent*, *if the first and second elements of the ordered pairs are congruent separately*,

$$\begin{aligned} &(kl, \theta(k'l')) \equiv (k''l'', \theta(k'''l''')) \pmod{\lambda_i^{KL} \times \lambda_i^{\Theta}}, \\ &\text{if } kl \equiv k''l'' \pmod{\lambda_i^{KL}} \text{ and } \theta(k'l') \equiv \theta(k'''l''') \pmod{\lambda_i^{\Theta}}. \end{aligned} \tag{16}$$

The universal bounds $\hat{0}^{KL\Theta}$ and $\hat{1}^{KL\Theta}$ of $\mathbf{con}(\mathbf{L}(KL\Theta))$ determine the smallest and largest congruence relations,

$$(kl, \theta(k'l')) \equiv (k''l'', \theta(k'''l''')) \,(\mathrm{mod}\, \hat{0}^{KL\Theta}),\ \textit{if}\ (kl, \theta(k'l')) = (k''l'', \theta(k'''l''')), \tag{17}$$

$$(kl, \theta(k'l')) \equiv (k''l'', \theta(k'''l''')) \,(\mathrm{mod}\, \hat{1}^{KL\Theta}),\ \forall (kl, \theta(k'l')), (k''l'', \theta(k'''l''')). \tag{18}$$

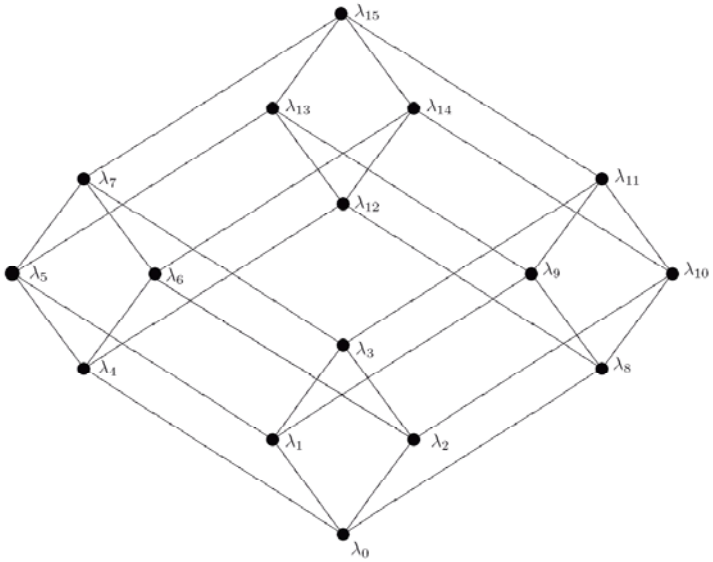

Figure 6. The congruence lattice $\mathbf{con}(\mathbf{L}(KL\Theta))$ of the lattice on figure 5.

The congruence classes $[(kl,\theta(k'l'))]/\lambda_i$ of allowed congruence relations $(\lambda_i \in con(\mathbf{L}(KL\Theta)))$ determine convex one–, two–, or three–dimensional intervals (points respectively). Although each elementary congruence relation has only one main class (with more than one element), this property is lost in the product formation and the product congruences have several multi–element classes. A congruence class $[(kl,\theta(kl))]/\lambda_i$ generated by a true bracket contains all those brackets, which belong to the rectangle $[(kl)]/\lambda_i^{KL}$ with property function values in the interval $[\theta(kl)]/\lambda_i^{\Theta}$. The congruence lattice $\mathbf{con}(\mathbf{L}(KL\Theta))$ associated with the (2×2)–partitioned (density) function with three distinct $\theta(kl)$ values (Figure 5.) has 16 allowed congruence relations listed in table 1. The two non–trivial congruence relations of $\mathbf{con}(\mathbf{L}(\Theta))$ have the main classes $[\gamma_1^{\Theta}]=\{\theta_1,\theta_2\}$ and $[\gamma_2^{\Theta}]=\{\theta_2,\theta_3\}$, as seen on Figures 4 and 5. The corresponding Hasse–diagram is displayed on Figure 6.

Table 1. The list of allowed congruence relations of the lattice on Figure 5

	λ^K	$\times$	λ^L	$\times$	λ^{Θ}			λ^K	$\times$	λ^L	$\times$	λ^{Θ}
λ_0	$\hat{0}^K$	$\times$	$\hat{0}^L$	$\times$	$\hat{0}^{\Theta}$		λ_4	$\hat{0}^K$	$\times$	$\hat{1}^L$	$\times$	$\hat{0}^{\Theta}$
λ_1	$\hat{0}^K$	$\times$	$\hat{0}^L$	$\times$	γ_1^{Θ}		λ_5	$\hat{0}^K$	$\times$	$\hat{1}^L$	$\times$	γ_1^{Θ}
λ_2	$\hat{0}^K$	$\times$	$\hat{0}^L$	$\times$	γ_2^{Θ}		λ_6	$\hat{0}^K$	$\times$	$\hat{1}^L$	$\times$	γ_2^{Θ}
λ_3	$\hat{0}^K$	$\times$	$\hat{0}^L$	$\times$	$\hat{1}^{\Theta}$		λ_7	$\hat{0}^K$	$\times$	$\hat{1}^L$	$\times$	$\hat{1}^{\Theta}$
λ_8	$\hat{1}^K$	$\times$	$\hat{0}^L$	$\times$	$\hat{0}^{\Theta}$		λ_{12}	$\hat{1}^K$	$\times$	$\hat{1}^L$	$\times$	$\hat{0}^{\Theta}$
λ_9	$\hat{1}^K$	$\times$	$\hat{0}^L$	$\times$	γ_1^{Θ}		λ_{13}	$\hat{1}^K$	$\times$	$\hat{1}^L$	$\times$	γ_1^{Θ}
λ_{10}	$\hat{1}^K$	$\times$	$\hat{0}^L$	$\times$	γ_2^{Θ}		λ_{14}	$\hat{1}^K$	$\times$	$\hat{1}^L$	$\times$	γ_2^{Θ}
λ_{11}	$\hat{1}^K$	$\times$	$\hat{0}^L$	$\times$	$\hat{1}^{\Theta}$		λ_{15}	$\hat{1}^K$	$\times$	$\hat{1}^L$	$\times$	$\hat{1}^{\Theta}$

Lemma 3. *The elementary congruence lattices* $\mathbf{con}(\mathbf{L}(K))$, $\mathbf{con}(\mathbf{L}(L))$, $\mathbf{con}(\mathbf{L}(\Theta))$ *are lower* (*dually*) *semi–modular*.

Since it is known [12] that the Cartesian product of semi–modular lattices is itself semi–modular,

con(**L**(*KL*Θ)) is a lower (dually) semi–modular lattice. For the congruence lattice of a lattice algebra is distributive [12–14], **con**(**L**(*KL*Θ)) is differing from the general **Con**(**L**(*KL*Θ)). This is because the actual algebra is defined only on a subset of all congruence relations, according to the special choice of the join operation.

Let us make a short summary on the ideas and results obtained up to this point. The density function under study has been decomposed into a set of building blocks. The building blocks have been mapped bijectively onto a set of abstract brackets defined as ordered pairs of a 'location index' and a 'property function'. The set of brackets has been embedded into the Cartesian product set of the indexes and the property function points and a Cartesian lattice was constructed over these generalized brackets. Congruence relations were defined on the component lattices, as well as on their product and a specially chosen subset of all congruence relations was selected. These allowed congruence relations formed the base set of the algebra resulting in the congruence lattice **con**(**L**(*KL*Θ)).

3 SHAPE LATTICE AND MEASURE

To have a deeply structured picture on the shape, **con**(**L**(*KL*Θ)) alone is not enough. The aim is to give a measure for the similarity of two density functions, but **con**(**L**(*KL*Θ)) is not distributive, therefore not admitting a measure. We shall construct a new lattice carrying the full information on the shape and admitting a measure, too.

Table 2. The congruence classes generated by the bracket $l_0 \equiv (11, \theta(11))$

$[l_0]/\lambda_0$	l_0											
$[l_0]/\lambda_1$	l_0	l_4										
$[l_0]/\lambda_2$	l_0											
$[l_0]/\lambda_3$	l_0	l_4	l_8									
$[l_0]/\lambda_4$	l_0	l_2										
$[l_0]/\lambda_5$	l_0	l_2	l_4	l_6								
$[l_0]/\lambda_6$	l_0											
$[l_0]/\lambda_7$	l_0	l_2	l_4	l_6	l_8	l_{10}						
$[l_0]/\lambda_8$	l_0	l_1										
$[l_0]/\lambda_9$	l_0	l_1	l_4	l_5								
$[l_0]/\lambda_{10}$	l_0											
$[l_0]/\lambda_{11}$	l_0	l_1	l_4	l_5	l_8	l_9						
$[l_0]/\lambda_{12}$	l_0	l_1	l_2	l_3								
$[l_0]/\lambda_{13}$	l_0	l_1	l_2	l_3	l_4	l_5	l_6	l_7				
$[l_0]/\lambda_{14}$	l_0											
$[l_0]/\lambda_{15}$	l_0	l_1	l_2	l_3	l_4	l_5	l_6	l_7	l_8	l_9	l_{10}	l_{11}

Each congruence relation ($\lambda_i \in con(\mathbf{L}(KL\Theta))$) structures the base set $KL\Theta$ into congruence classes. Each class is an ensemble of true and generalized brackets mixed. In case of several

(density) functions, the identical partitionings of the co–ordinate domains result in identical $\mathbf{L}_j(KL)$, $(j=1,...,m)$ lattices. If the cardinalities $|\Theta_j|$, $(j=1,...,m)$ are also identical, then $\mathbf{con}(\mathbf{L}_j(KL\Theta_j))$, $(j=1,...,m)$ coincide and do not characterize the individual shapes. However, the congruence classes generated by the true brackets are fully specific in each lattice and carry all informations on the shape. To be definite, the congruence classes generated by the true brackets $(l_0 \equiv (11,\theta(11))$, $l_6 \equiv (12,\theta(12))$, $l_7 \equiv (22,\theta(22))$ and $l_9 \equiv (21,\theta(21)))$ (identified on figure 5.) are listed in Tables 2–5.

Table 3. The congruence classes generated by the bracket $l_6 \equiv (12,\theta(12))$

$[l_6]/\lambda_0$	l_6											
$[l_6]/\lambda_1$	l_6	l_2										
$[l_6]/\lambda_2$	l_6	l_{10}										
$[l_6]/\lambda_3$	l_6	l_2	l_{10}									
$[l_6]/\lambda_4$	l_6	l_4										
$[l_6]/\lambda_5$	l_6	l_4	l_2	l_0								
$[l_6]/\lambda_6$	l_6	l_4	l_{10}	l_8								
$[l_6]/\lambda_7$	l_6	l_4	l_2	l_0	l_{10}	l_8						
$[l_6]/\lambda_8$	l_6	l_7										
$[l_6]/\lambda_9$	l_6	l_7	l_2	l_3								
$[l_6]/\lambda_{10}$	l_6	l_7	l_{10}	l_{11}								
$[l_6]/\lambda_{11}$	l_6	l_7	l_2	l_3	l_{10}	l_{11}						
$[l_6]/\lambda_{12}$	l_6	l_7	l_4	l_5								
$[l_6]/\lambda_{13}$	l_6	l_7	l_4	l_5	l_2	l_3	l_0	l_1				
$[l_6]/\lambda_{14}$	l_6	l_7	l_4	l_5	l_{10}	l_{11}	l_8	l_9				
$[l_6]/\lambda_{15}$	l_6	l_7	l_4	l_5	l_2	l_3	l_0	l_1	l_{10}	l_{11}	l_8	l_9

Table 4. The congruence classes generated by the bracket $l_7 \equiv (22,\theta(12))$

$[l_7]/\lambda_0$	l_7											
$[l_7]/\lambda_1$	l_7	l_3										
$[l_7]/\lambda_2$	l_7	l_{11}										
$[l_7]/\lambda_3$	l_7	l_3	l_{11}									
$[l_7]/\lambda_4$	l_7	l_5										
$[l_7]/\lambda_5$	l_7	l_5	l_3	l_1								
$[l_7]/\lambda_6$	l_7	l_{11}	l_5	l_9								
$[l_7]/\lambda_7$	l_7	l_5	l_3	l_1	l_{11}	l_9						
$[l_7]/\lambda_8$	l_7	l_6										
$[l_7]/\lambda_9$	l_7	l_6	l_3	l_2								
$[l_7]/\lambda_{10}$	l_7	l_6	l_{11}	l_{10}								
$[l_7]/\lambda_{11}$	l_7	l_6	l_3	l_2	l_{11}	l_{10}						
$[l_7]/\lambda_{12}$	l_7	l_6	l_5	l_4								
$[l_7]/\lambda_{13}$	l_7	l_6	l_5	l_4	l_3	l_2	l_1	l_0				
$[l_7]/\lambda_{14}$	l_7	l_6	l_5	l_4	l_{11}	l_{10}	l_9	l_8				
$[l_7]/\lambda_{15}$	l_7	l_6	l_5	l_4	l_3	l_2	l_1	l_0	l_{11}	l_{10}	l_9	l_8

Although the elements of congruence classes form convex sublattices of $\mathbf{L}(KL\Theta)$, the set of elements of those congruence classes, which are generated by the true brackets do not form generally a distributive lattice. Therefore a set of n–vectors is constructed by mapping only the true elements of congruence classes. The ensemble of these vectors characterizes the shape and proves to be suitable for constructing a distributive lattice admitting a measure, too.

Table 5. The congruence classes generated by the bracket $l_9 \equiv (21, \theta(21))$

$[l_9]/\lambda_0$	l_9											
$[l_9]/\lambda_1$	l_9											
$[l_9]/\lambda_2$	l_9	l_5										
$[l_9]/\lambda_3$	l_9	l_5	l_1									
$[l_9]/\lambda_4$	l_9	l_{11}										
$[l_9]/\lambda_5$	l_9											
$[l_9]/\lambda_6$	l_9	l_{11}	l_5	l_7								
$[l_9]/\lambda_7$	l_9	l_{11}	l_5	l_7	l_1	l_3						
$[l_9]/\lambda_8$	l_9	l_8										
$[l_9]/\lambda_9$	l_9											
$[l_9]/\lambda_{10}$	l_9	l_8	l_5	l_4								
$[l_9]/\lambda_{11}$	l_9	l_8	l_5	l_4	l_1	l_0						
$[l_9]/\lambda_{12}$	l_9	l_8	l_{11}	l_{10}								
$[l_9]/\lambda_{13}$	l_9											
$[l_9]/\lambda_{14}$	l_9	l_8	l_{11}	l_{10}	l_5	l_4	l_7	l_6				
$[l_9]/\lambda_{15}$	l_9	l_8	l_{11}	l_{10}	l_5	l_4	l_7	l_6	l_1	l_0	l_3	l_2

Definition 7. *For every congruence class* $o_{ji} \equiv [l_j]/\lambda_i$, *where* $\lambda_i \in con(\mathbf{L}(KL\Theta))$ *and* l_j *is an arbitrarily chosen true bracket*

$$\beta_{o_{ji}}(kl) = \begin{cases} \theta(kl)\tau_{kl}, & if \quad (kl, \theta(kl)) \in o_{ji} \\ 0, & otherwise. \end{cases} \tag{19}$$

where vector $\vec{\beta}_{o_{ji}} \equiv (\beta_{o_{ji}}(11), ..., \beta_{o_{ji}}(M_k M_l))^T$ *is called* (*shape*) *'property–vector'. The non–zero elements are the property function values* $\theta(kl)$ *multiplied by the* τ_{kl} *measure of the cell* d_{kl}. The image of all congruence classes is the vector set $V = \{\vec{\beta}_{o_{ji}}\}$.

Lemma 4. *The mapping* $\{o_{ji} \ : \ o_{ji} \equiv [l_j]/\lambda_i, \ \lambda_i \in con(\mathbf{L}(KL\Theta)), \ l_j$ *is a true bracket*$\} \to V$ *is surjective and order–preserving*,

$$o_{ji} \subseteq o_{j'i'} \Rightarrow \vec{\beta}_{o_{ji}} \le \vec{\beta}_{o_{j'i'}}. \tag{20}$$

The vectors are ordered according to the vector lattice operations specified in the sequel. To proceed in a formal generality, the operands will be denoted by capital letters $X, Y, Z, ...$

Definition 8. *The meet and join are constructed component–by–component*, *as the minimum and the maximum of the operands*,

$$X \wedge Y = Z, \quad Z_{kl} := \min\{X_{kl}, Y_{kl}\}, kl \in KL. \tag{21}$$

$$X \vee Y = Z, \quad Z_{kl} := \max\{X_{kl}, Y_{kl}\}, kl \in KL. \tag{22}$$

The order relations and lattice operations are connected in the usual way. The closure set $\overline{V}$ is obtained by finite applications of the specified operations. The constructed lattice $\mathbf{L}(\overline{V}) = \langle \overline{V}, \wedge, \vee \rangle$ is characteristic to the shape and will be called 'shape (property) lattice'. The universal bounds are $\hat{0}^{\overline{V}} = \wedge_{ji} \vec{\beta}_{o_{ji}}$ and $\hat{1}^{\overline{V}} = \vee_{ji} \vec{\beta}_{o_{ji}}$.

Lemma 5. *The shape* (*property*) *lattice* $\mathbf{L}(\overline{V})$ *is distributive*.

Unfortunately our example the (2×2)–partitioned density function has 10 distinct congruence classes, therefore the closure set $\overline{V}$ has too many elements to draw its Hasse–diagram. The lattice $\mathbf{L}(\overline{V})$ is characteristic to the shape and distributive, too. In any distributive lattice one can define a non–negative function μ with the following properties. If X, Y are elements of the lattice, then:

$$X = Y \Rightarrow \mu(X) = \mu(Y), \tag{23}$$

$$X \wedge Y = \hat{0} \Rightarrow \mu(X \vee Y) = \mu(X) + \mu(Y). \tag{24}$$

Under these circumstances μ is a (finitely additive) measure and it is strictly positive, if:

$$\mu(X) = 0 \Rightarrow X = \hat{0}. \tag{25}$$

Lemma 6. *The function*

$$\mu_\tau(X) := X \circ X, \quad X \in \overline{V} \tag{26}$$

(*where* $\circ$ *denotes scalar product*) *is a strictly positive measure on the distributive lattice* $\mathbf{L}(\overline{V})$.

If $O = \vee_{ji} o_{ji}$, then $\vec{\beta}_O \equiv \hat{1}^{\overline{V}}$ and measure $\mu_\tau(X / \| \vec{\beta}_O \|)$ is a density function. It provides information about the distribution of the considered property among the congruence classes generated by the true brackets. We shall call it 'property density function'.

4 THE MAIN RESULTS

This section is devoted to the implications of the former results. The aim is to obtain appropriate algebraic tools for finding those (density) functions in a set, which are 'similar' in some lattice–theoretical sense. The lattice–theory based similarity concept does not rely on the direct comparison of two functions, but the compared functions are decomposed into appropriate building blocks and the internal relationships of these building blocks are compared by means of lattice–theory. This way allows considering also the abstract internal structures of the functions, beyond the point–wise or integral differences.

Definition 9. *The function set under further study is a family of continuous* (*density*) *functions* $f_w : D_w \to \mathbf{R}$, $(w \in W)$. *The supports are isometrically partitioned* $(D_w \equiv_\phi D_u,\ w,u \in W)$ (*Definition* 11.), *the indexes are running identically*, *the resulting index–lattices are identical*

$(\mathbf{L}_w(KL) \equiv \mathbf{L}_u(KL),\ w,u \in W)$. *Each function* f_w *is associated with the lattice* $\mathbf{L}_w(KL\Theta_w)$, *relating to an admissible property function* $\theta_w(kl)$.

Definition 10. *Two domains* $D_w,\ D_u \subset \mathbf{R}^n,\ w,u \in W$ *are isometrically isomorph with respect to bijection* $\phi\ :\ D_w \leftrightarrow D_u$ $(D_w \equiv_\phi D_u$ *'domain congruent'*$)$, *if* $\vec{x},\vec{y} \in D_w,\ \Rightarrow \| \vec{x}-\vec{y} \|_2 = \| \phi(\vec{x}) - \phi(\vec{y}) \|_2$.

Definition 11. *Two isometrically isomorph domains are 'isometrically partitioned', if bijection* ϕ *induces a one–to–one mapping of the partitions*.

Property function $\theta_w(kl) \equiv \theta_w(d_{kl})$ is a set function with argument labeled by the index of the supporting cell. It is a piecewise constant approximation function to the shape–generating f_w. The lattice–ordering $\mathbf{L}_w(\Theta_w)$ orders the points of set $Range(\theta_w(kl)) \equiv \theta_w(KL) \equiv \Theta_w$, therefore neither $\mathbf{L}_w(\Theta_w)$, nor $\mathbf{L}_w(KL\Theta_w)$ reflects the connections between function values $\theta(kl)$ and arguments. As a consequence, the concept of isomorphism can be strengthened for 'strong isomorphism'.

Definition 12. *Two continuous* (*density*) *functions* $f_w,\ f_u$ (*Definition* 9.) *are 'strongly isomorphic', if their associated lattices are strongly isomorphic*, $\mathbf{L}_w(KL\Theta_w) \cong_{st} \mathbf{L}_u(KL\Theta_u),\ (w,u \in W)$.

Definition 13. *Two lattices are 'strongly isomorphic'* $\mathbf{L}_w(KL\theta_w(KL)) \cong_{st} \mathbf{L}_u(KL\theta_u(KL))$, *if their elements satisfy*,

$$\forall kl,k'l' \left(\theta_w(kl) \le \theta_w(k'l') \Leftrightarrow \theta_u(kl) \le \theta_u(k'l') \right),\ kl,k'l' \in KL. \tag{27}$$

From the two–way implication of strong isomorphism condition follows that the property function lattices are isomorphic $\mathbf{L}_w(\Theta_w) \cong \mathbf{L}_u(\Theta_u)$, *i.e.* the number of distinct function values are equal in Θ_w and Θ_u. In consequence $\mathbf{L}_w(KL\Theta_w) \cong \mathbf{L}_u(KL\Theta_u),\ (w,u \in W)$ supporting the 'strong isomorphism' terminology. Strong isomorphism asserts that under the conditions of *Definition 9*, the lattice–ordering of property function values induces the identical permutations of their arguments. It is an important concept, because the strongest condition for the 'similarity' of two functions and easy to detect. It is enough to check, whether the pairing by arguments $\theta_w(kl) \leftrightarrow \theta_u(kl)$ is order–preserving. Although strong isomorphism ensures 'similarity', a further condition is needed to ensure the equality of two functions.

Definition 14. *Two strongly isomorphic continuous* (*density*) *functions* $f_w,\ f_u$ (*Definition* 9.) *are 'exchange isomorphic'* $(\mathbf{L}_w(KL\Theta_w) \cong_{ex} \mathbf{L}_u(KL\Theta_u),\ w,u \in W)$, *if their associated lattices are exchange isomorphic*.

Definition 15. *Two strongly isomorphic lattices* $\mathbf{L}_w(KL\Theta_w),\ \mathbf{L}_u(KL\Theta_u),\ (w,u \in W)$ *are exchange isomorphic* $\mathbf{L}_w(KL\Theta_w) \cong_{ex} \mathbf{L}_u(KL\Theta_u)$, *if and only if* $\forall k_0 l_0$,

$$\left(\mathbf{L}_w\left(KL\left(\theta_w(KL\setminus k_0l_0)\cup\theta_u(k_0l_0)\right)\right)\cong_{st}\mathbf{L}_u\left(KL\left(\theta_u(KL\setminus k_0l_0)\cup\theta_w(k_0l_0)\right)\right)\right),\ k_0l_0\in KL. \qquad (28)$$

Exchange isomorphism requires that interchanging systematically every element $(k_0l_0=\{11,...,M_kM_l\})$ of the approximation function $\theta_w(kl)$, the generated lattices remain strongly isomorphic.

Definition 16. *Two continuous* (*density*) *functions* f_w, f_u (*Definition* 9.) *are identical* ($f_w\equiv_\phi f_u$ *'shape–congruent'*), *if* $\forall\vec{x}(f_w(\vec{x})=f_u(\phi(\vec{x})),\ \vec{x}\in D_w$.

Theorem 1. *Two continuous* (*density*) *functions* f_w, f_u (*Definition* 9.) *are identical* ($f_w\equiv_\phi f_u$), *if and only if the coupled elements of lattice sequences* ($\mathbf{L}_w^n(K_nL_n)\equiv\mathbf{L}_u^n(K_nL_n),\forall n$) (*belonging to monotone and infinitely refining isometric partitionings of* D_w *and* D_u ($refin(D_w)=refin(D_u)\to 0$)) *are exchange isomorphic for all* n, $\mathbf{L}_w^n(K_nL_n\Theta_w^n)\cong_{ex}\mathbf{L}_u^n(K_nL_n\Theta_u^n)$.

Exchange isomorphism ensures that isomorphism coupled elements of two strongly isomorphic lattices do not differ more, than they differ from their immediate lattice neighbors (covering and preceding elements). If this property is invariant in the infinite refinement limit, the two functions are identical. Although Theorem 1 asserts a known result (that two different sequences with infinitely approximating elements have a common limit), this global statement (on the identity of two functions) is established by the lattice structure of their discretized parts. While the identity of two (density) functions is (more or less) easily recognizable, the strong isomorphism does not define easily perceptible similarity. This is illustrated on Figure 3, where the displayed $\theta'(kl)$ – function is strongly isomorphic with $\theta(kl)$ on Figure 2, although they look different. Strong isomorphism represents a deeply rooted relationship. If two density functions are strongly isomorphic, their inherent similarities are indisputable. However, the 'basically similar' molecular interactions are affected by individual effects characterizing the system. In this report we only deal with strongly isomorphic (density) functions and the weaker types of similarity will be discussed elsewhere.

The strong and exchange isomorphism concepts are important in qualitative sense, but do not say anything about the 'degree of correspondence' of two functions, or the territorial distribution of the considered property. The assembling of elements in **con**($\mathbf{L}(KL\Theta)$) provides only qualitative information on the internal dependencies of the elements, but the measure on the distributive shape property lattice $\mathbf{L}(\overline{V})$ provides quantitative information.

Definition 17. *If given two continuous* (*density*) *functions* f_w, f_u (*Definition* 9.) *associated with strongly isomorphic lattices*,

$$GlobDist(\mathbf{L}_w, \mathbf{L}_u) := \mu_\tau(\vec{\beta}_{O_w} - \vec{\beta}_{O_u}) \tag{29}$$

is the 'lobal shape distance' and

$$PartDist(o^w_{ji}, o^u_{pq}) := \mu_\tau(\vec{\beta}_{o^w_{ji}} - \vec{\beta}_{o^u_{pq}}) \tag{30}$$

is the 'partial shape distance', where $\mathbf{L}_w \equiv \mathbf{L}_w(KL\Theta_w)$, $\mathbf{L}_u \equiv \mathbf{L}_u(KL\Theta_u)$ *and* $o^w_{ji} \in \mathbf{L}_w / \lambda_i$ *is generated by the true bracket* l_j, *while* $o^u_{pq} \in \mathbf{L}_u / \lambda_q$ *is generated by the true bracket* l_p (*or both belong to the same factor lattice*).

Lemma 7. $GlobDist(\mathbf{L}_w, \mathbf{L}_u)$ *and* $PartDist(o^w_{ji}, o^u_{pq})$ $(w,u \in W)$ *satisfy the conditions to be a metric*.

Theorem 2. *If given two continuous* (*density*) *functions* f_w, f_u (*Definition* 9.) *and exchange isomorphic*, *infinitely refining lattice sequences* (*Theorem* 1.), *the global shape distance approaches 0 in the infinite refinement limit*,

$$GlobDist(\mathbf{L}^n_w, \mathbf{L}^n_u) \to 0, \ if \ n \to \infty. \tag{31}$$

In case of partial shape distance, *the assertion is implied for every strong isomorphism coupled congruence class*. *This means that*:

$$PartDist(o^{n,w}_{ji}, o^{n,u}_{ji}) \to 0, \ if \ n \to \infty \tag{32}$$

where $o^{n,w}_{ji} \in \mathbf{L}^n_w(K_n L_n \Theta^n_w) / \lambda_i$ *and* $o^{n,u}_{ji} \in \mathbf{L}^n_u(K_n L_n \Theta^n_u) / \lambda_i$.

Measure μ_τ separates strongly isomorphic, but not exchange isomorphic density functions assigning a single scalar to couples of lattices. Function *PartDist* does the same with a couple of congruence classes. The meaning of the former is the 'degree of similarity' in the whole co–ordinate domain and full range of $\theta(kl)$. The meaning of the latter is the 'degree of similarity' in a sub–domain of the coordinates space and a subinterval of the property function range. If systematically applying *PartDist* to every pair of congruence classes in $\mathbf{L}_w$ and $\mathbf{L}_u$, $(w,u \in W)$ (can be also identical), the matrix:

$$PD_{L_w, L_u} = [PartDist(o^w_{ji}, o^u_{pq})]_{ji,pq} \tag{33}$$

of partial shape distances is obtained. Unlike the single parameter *GlobDist*, this matrix carries a well structured characterization of similarity.

If given a set of density functions with associated strongly isomorphic lattices $\{\mathbf{L}_w(KL\Theta_w) \ : \ w \in W\}$, two ε–neighbor (metric) topologies can be established. The open sets of these topologies include those lattices, which are 'similar enough' to a chosen lattice. This lattice is in the center of a ball with radius of length ε and all its ε–neighbors are in the open interior of the

ball. In the one topology, the distance is measured by $GlobDist$, in the other, by $PartDist$.

Definition 18. *Given a set of continuous strongly isomorphic* (*density*) *functions* (*Definition* 9.) *with associated lattices* $L_w(KL\Theta_w),(w\in W)$, *a global* ε*–neighbor* $GlobNb_\varepsilon(\mathbf{L}_u(KL\Theta_u))$ *is a set of lattices in the* ε*–ball around the central lattice*,

$$GlobNb_\varepsilon(\mathbf{L}_u(KL\Theta_u))=\{\mathbf{L}_w(KL\Theta_w):\ GlobDist(\mathbf{L}_u,\mathbf{L}_w)<\varepsilon,\ w\in W\},\ u\in W. \tag{34}$$

The partial ε*–neighbor is defined analogously*, *by the distances between elements of a set of congruence classes* $o_{pq}^W:=\{o_{pq}^w\ :\ o_{pq}^w\in\mathbf{L}_w(KL\Theta_w)/\lambda_q,\ w\in W\}$ *and the fixed element* $o_{ji}^u\in\mathbf{L}_u(KL\Theta_u)/\lambda_i,\ (u\in W)$,

$$PartNb_\varepsilon(o_{ji}^u,o_{pq}^W)=\{\mathbf{L}_w(KL\Theta_w):\ PartDist(o_{ji}^u,o_{pq}^w)<\varepsilon,\ w\in W\},\ u\in W. \tag{35}$$

Lemma 8. *The closure sets* $\overline{GlobNb}$ *and* $\overline{PartNb}$ *constructed by the set–theoretical unions and intersections of* $GlobNb_\varepsilon(\mathbf{L}_u(KL\Theta_u))$ *and* $PartNb_\varepsilon(o_{ji}^u,o_{pq}^W)$ *are topologies*.

The ε–neighbor of a given lattice includes exactly those lattices we are looking for. In general, if a set of density functions is given, our aim is to select those functions, which are similar to each other. The global distances can be arranged into the matrix $[GlobDist(\mathbf{L}_u,\mathbf{L}_w)]_{u,w}$, while the partial distances into the hyper–matrix $[PD_{L_u,L_w}]_{u,w}$, $(u,w\in W)$. These measures satisfy the triangle inequality and serve for generalized (similarity) distance functions. The intersections and unions of the open sets of established topologies include lattices satisfying entangled metric conditions concerning distances from several fixed lattices. The open sets of $\overline{PartNb}$ allow to find those lattices, which are 'similarly shaped' only partially, in some (important) domains. The partial similarity distances allow defining any combination of similarity requirements and provide versatile tools for structuring a set by the similarity properties of their elements. Since the lattices and discretized density functions are in one–to–one relationship, a set of density functions can be structured in any required accuracy by studying the lattices of their building blocks.

5 CONCLUSIONS

In the general case, there is a set of continuous (shape determining) functions or more specifically a set of (electron) density functions and the aim is to select those functions, which are similar in some sense. The practical significance of this task might be quite challenging. The shape of the appropriately chosen kinds of the electron density functions of the molecular systems are closely related to their chemical and pharmacological behaviors. This is the reason, why studying their shapes is of long-term interest. We have chosen a lattice algebraic approach to this question, because the nature of lattice theory especially fits the problem. Although in this report only a tiny

portion of the whole problem is attacked, some useful results could be obtained.

For analyzing the shape of a function, the function was discredited in a way, which ensured that in the infinite refinement limit the original function was recaptured. The set of discrete ‘brackets’ became the carrier of the properties of the original function and the immediate subject of our investigation. A distributive lattice was constructed on the brackets and two functions were compared by their associated lattices. If they exhibited the so called strong isomorphism property, the functions were said to be ‘similar’, in spite of the fact that the everyday experience might have judged such functions quite different looking. The established exchange isomorphism concept provided a necessary and sufficient condition for being two functions shape–congruent in the infinite refinement limit. But, such a deep–lying similarity as embodied in the strong isomorphism concept is not satisfactory for the demands of application. Therefore, the brackets were collected into congruence classes using a special subset of all congruence relations. The congruence classes express the connections of the brackets. The connections are characterized by the locations of elements, as well as by the associated properties. Because of the nature of congruence relations these connections are relative. Since the applications required a tool to define also the degree of similarity, the congruence classes were projected onto a set of vectors and a distributive vector lattice was constructed with a measure. The measure served for a property density function yielding detailed information about the distribution of the studied property, as well as for a distance function. The measure allowed to define a 'global' and a 'partial' shape distance of two functions. The main goal of applications was to find all those functions in a set, which were 'similar' in some specified degree. The distance functions provided appropriate tools to establish a 'global' and a 'partial' ε–neighbor topology. The open sets of these topologies included those functions, which were similar in a specified degree in the whole coordinate domain and property function range, or only partially in a sub–domain and subinterval. The partial similarity distance made the similarity structured allowing very fine statements on the shapes of the functions. In accordance, the topologies decomposed a set of functions on the basis of the fine details of this structured similarity.

In a set of electron density functions (or any other continuous functions), the global and partial shape distances and the associated neighborhood topologies accomplished our goal exactly. We are able to pick out those functions, which correspond to each other in some sense. But, this correspondence can be much more intricate, than mere ‘close overlapping’. Although in this report we restricted ourselves to strongly isomorphic systems, strong isomorphism allows a very wide class of shapes far beyond of the similarity judgment of our everyday experience. In spite of the analytically based similarity concepts, the lattice theoretical footing of the procedure provides a

firm basis to make separate statements on the similarity of (density) functions in the qualitative sense of strong isomorphism and on the degree of similarity in the quantitative sense of similarity distances.

Acknowledgment

The useful comments on the topic of Prof. Cs. Szepesvári are gratefully acknowledged.

Appendix 1 (Proofs of the assertions)

Lemma 1.

Proof. Let us choose $\mathbf{L}(K)$ for example and let $\lambda \in \mathbf{con}(\mathbf{L}(K))$. It is assumed, that exists $a,b,c \in K$ with $a < b < c$ and $[a]/\lambda = [c]/\lambda \neq [b]/\lambda$. Since $a\lambda c$ and $b\lambda b$, the substitution property implies $(a \wedge b)\lambda(c \wedge b) = a\lambda b$ and $(a \vee b)\lambda(c \vee b) = b\lambda c$ proving the convexity by contradiction.

Lemma 2.

Proof. The proof will be restricted to $\mathbf{L}(K)$, since the operations in $\mathbf{L}(KL\Theta)$ are defined component–by–component, therefore distributivity is preserved. The distributive identity is $a,b,c \in K$

$$a \wedge (b \vee c) = (a \wedge b) \vee (a \wedge c), \quad a \vee (b \wedge c) = (a \vee b) \wedge (a \vee c).$$

Taking into account Definition 1., this means, for the first identity

$$\min\{a, \max\{b,c\}\} = \max\{\min\{a,b\}, \min\{a,c\}\}$$

and similarly for the second

$$\max\{a, \min\{b,c\}\} = \min\{\max\{a,b\}, \max\{a,c\}\}.$$

But in a chain lattice, these equalities are always obeyed.

Lemma 3.

Proof. Lower (dual) semi–modularity requires $(\lambda_i \vee \lambda_j) \succ \lambda_i \Rightarrow (\lambda_i \wedge \lambda_j) \prec \lambda_j$. Since the elementary lattices are chains and their congruence relations are restricted to have one mainclasses, the covering relation means, that the larger mainclass collapses one more element of the chain. Taking into account the definitions of the meet and the join, the following sequence of implications proves the statement,

$$\lambda_i \prec (\lambda_i \vee \lambda_j) \Rightarrow |[\lambda_i]| = |[(\lambda_i \vee \lambda_j)]| - 1 \Rightarrow |[\lambda_i]| = |[\lambda_j]|$$

$$|[\lambda_i]| = |[\lambda_j]| \Rightarrow |[(\lambda_i \wedge \lambda_j)]| = |[\lambda_j]| - 1 \Rightarrow (\lambda_i \wedge \lambda_j) \prec \lambda_j.$$

Lemma 4.

Proof. The surjectivity is trivial, the isotonicity follows from the definitions of the operations and the subsequent implications,

$$o_{ji} \subseteq o_{j'i'} \Rightarrow (\beta_{o_{ji}}(kl) \leq \beta_{o_{j'i'}}(kl)), \; kl \in KL.$$

Lemma 5.

Proof. The vector lattice $\mathbf{L}(\overline{V})$ can be considered for products of chain lattices defined over the components. But, for chain lattices the statement has been proved in Lemma 2.

Lemma 6.

Proof. Condition (23) and (25) are satisfied trivially. If the vectors have empty intersection, then for $kl \in KL$ either $\beta_{o_{ji}}(kl)$ or $\beta_{o_{j'i'}}(kl)$ is 0 . Since (24) is satisfied component–by–component, it is satisfied also for the sum of the components, i.e. by the properties of the scalar product.

Theorem 1.

Proof. The two lattices $\mathbf{L}_w(KL\Theta_w)$ and $\mathbf{L}_u(KL\Theta_u)$, $(w,u \in W)$ are strongly isomorphic. The conditions of exchange isomorphism ensure that for every lattice interval $\theta_w^n(k'l') \prec \theta_w^n(kl) \prec \theta_w^n(k''l'')$ (^{n} refers to the n –th refinement!) also $\theta_w^n(k'l') \prec \theta_u^n(kl) \prec \theta_w^n(k''l'')$ is satisfied. If $refin(D_w) = refin(D_u) \to 0$, then

$$(|\theta_w^n(k'l') - \theta_w^n(k''l'')| \to 0) \Rightarrow (|\theta_w^n(kl) - \theta_u^n(kl)| \to 0) \Rightarrow |f_w(\vec{x}) - f_u(\phi(\vec{x}))| \to 0,$$

$$\vec{x} \in D_w,\ \phi(\vec{x}) \in D_u.$$

The sequence of opposite implications is trivial.

Lemma 7.

Proof. The following conditions are satisfied for all $\mathbf{L}_w, \mathbf{L}_u, \mathbf{L}_v$ lattices,

$$GlobDist(\mathbf{L}_w, \mathbf{L}_u) = GlobDist(\mathbf{L}_u, \mathbf{L}_w) \geq 0 = GlobDist(\mathbf{L}_w, \mathbf{L}_w)$$

$$GlobDist(\mathbf{L}_w, \mathbf{L}_u) + GlobDist(\mathbf{L}_u, \mathbf{L}_v) \geq GlobDist(\mathbf{L}_w, \mathbf{L}_v),$$

since the above functions are defined for the usual Euclidean distance. The assertion is implied for the $PartDist(o_{ji}^w, o_{pq}^u)$ function.

Theorem 2.

Proof. If τ_{kl}^n (^{n} refers to the n –th refinement!) is the measure of the cell d_{kl}^n in the n –th refinement, then $GlobDist(\mathbf{L}_w^n, \mathbf{L}_u^n)$ is the square integral of $(\theta_w^n - \theta_u^n)$, which are the n th approximations to the function $(f_w - f_u)$. From Theorem 1. follows that, $n \to \infty \Rightarrow \theta_w^n \to f_w,\ \theta_u^n \to f_u \Rightarrow (\theta_w^n - \theta_u^n) \to (f_w - f_u)$ and $\int(\theta_w^n - \theta_u^n)^2 \tau^n \to 0 \Rightarrow \int(f_w(\vec{x}) - f_u(\phi(\vec{x})))^2 d\vec{x} = 0$, what is exactly the statement.

Lemma 8.

Proof. The $GlobDist(\mathbf{L}_w, \mathbf{L}_u)$, $PartDist(o_{ji}^w, o_{pq}^u)$ functions satisfy the conditions to be a metrics. Therefore, the $GlobNb_\varepsilon(\mathbf{L}_u(KL\Theta_u))$ and $PartNb_\varepsilon(o_{ji}^u, o_{pq}^W)$ are open neighbourhoods including the empty set, as well as the total base set, too. Their closures contain also all unions and intersections forming the referred ε –neighbourhood topologies.

Appendix 1. (Basics of lattice theory)

The content of this section is to be found in many textbooks of algebra or lattice theory [12–16]. It is included here only for convenience, therefore the statements are given without formal proofs. The forthcoming discussion refers to finite lattices. It is more general than our actual topic and the notation will distinctly differ from the previous symbolism.

Lattice theory, as a branch of algebra refers to a set endowed with some operations. The ordered pair $\langle L, \Gamma \rangle$ specifies a lattice, if L is a non–empty set and $\Gamma = \{\gamma_i : i \in I\}$ is an ensemble of operations obeying some conditions. Set L is the 'universe' of the (lattice) algebra and $\gamma_i \in \Gamma,\ (i \in I)$ are the basic operations in it. The operations can be of rank $0,1,2$ and they are functions from the product sets L^0, L^1, L^2 into L . Set L^0 is identified with $\{\varnothing\}$, therefore the rank 0 operation selects only a special element of L , but in the actual report only operations of rank two appear explicitly. By a convention we shall use boldface letters ($\mathbf{L}$) to denote algebras and simple uppercase letters (L) for their universes. Lattices can be seen equivalently as special (partially) ordered sets or binary (rank 2) algebras. To be a (partially) ordered set, (order) relation ρ must be,

- i.) reflexive, i.e. $\forall b(b \rho b)$
- ii.) anti–symmetric, i.e. $b \rho b',\ b' \rho b \ \Rightarrow\ b = b'$
- iii.) transitive, i.e. $b \rho b',\ b' \rho b'' \ \Rightarrow\ b \rho b''$.

If L is a (partially) ordered set with order relation $\leq$, properties i.)–iii.) are obeyed and if every non–void subset $X \subseteq L$ has a least upper bound (l.u.b.) [$a \in L$ is an upper bound of X , if $x \leq a$ for all $x \in X$ and $a \in L$ is a least upper bound of X , if b is also an upper bound of X and $a \leq b$], as well as a greatest lower bound (g.l.b.) [$a \in L$ is a lower bound of X , if $a \leq x$ for all $x \in X$ and $a \in L$ is a greatest lower bound of X , if b is also a lower bound of X and $b \leq a$], then $\mathbf{L}$ is a lattice. If considering lattices as binary algebras with operations denoted by $\vee$ and $\wedge$, the following identities must be satisfied for every $x, y, z \in L$:

- $\lambda 1.)$ $x \wedge x = x;\ x \vee x = x$ (idempotency).
- $\lambda 2.)$ $x \wedge y = y \wedge x;\ y \vee x = x \vee y$ (commutativity).
- $\lambda 3.)$ $x \wedge (y \wedge z) = (x \wedge y) \wedge z;\ x \vee (y \vee z) = (x \vee y) \vee z$ (associativity).

- $\lambda 4.)\ \ x \wedge (x \vee y) = x \vee (x \wedge y) = x$ (absorption law).

The lattice operations and order relations are consistent in the following way,
$a \le b,\ if\ a = a \wedge b\ and\ b = a \vee b.$
The lattice operations assign to each couple of elements their l.u.b. ($\vee$) and g.l.b. ($\wedge$). The lattice is complete if every subset has a g.l.b and a l.u.b.. The least element is $\hat{0}$, the greatest is $\hat{1}$. An element b covers a , if $a < b$ and $a \le c \le b \Rightarrow a = c$ or $c = b$. The upper covers of $\hat{0}$ are the 'atoms' of the lattice, while elements exactly below $\hat{1}$ are the 'dual atoms'. Elements a, b are comparable, whenever $a \le b$ or b $\le a$ and incomparable ($a \| b$), otherwise. Those elements, which are comparable pairwise form a chain, while those which are incomparable form an anti–chain. Using the covering relation, finite lattices can be displayed by drawing a Hasse diagram. Here the elements of L are represented by points on a plane, where each point is connected to the (point–)representatives of upper and lower cover elements. Some subsets of L are closed with respect to one or both of the lattice operations. If U is non–empty, $U \subseteq L$ and for all $b \in L$, if $b \le a \Rightarrow b \in U$, furthermore $a, b \in U \Rightarrow (a \vee b) \in U$, then U is an 'ideal' of the lattice denoted by $(U]$. By dualization we arrive at the concept of the 'filter' of the lattice. If U is non–empty, $U \subseteq L$ and for all $b \in L$, if $b \ge a \Rightarrow b \in U$, furthermore $a, b \in U \Rightarrow (a \wedge b) \in U$, then U is a filter (dual ideal) of the lattice denoted by $[U)$. If $a = U$, the 'principal ideal' and 'principal filter' is obtained. A sublattice is closed with respect to both of the operations, i.e. if U is non–empty, $U \subseteq L$ and $(a,b) \in U \Rightarrow (a \vee b) \in U$, $(a \wedge b) \in U$, then U is a sublattice. The sets of ideals (filters, sublattices) can be ordered by the set–theoretic inclusion giving the ideal lattice $\mathbf{I}(L)$.
The morphism concept covers mappings from a lattice into a lattice (possible the same one). Let $\phi : L1 \to L2$ be a function from $L1$ to $L2$. The mapping is isotone, if $x \le y \Leftrightarrow \phi(x) \le \phi(y)$. It is a meet morphism, if $\phi(x \wedge y) = \phi(x) \wedge \phi(y)$, a join morphism, if $\phi(x \vee y) = \phi(x) \vee \phi(y)$ and a lattice (homo)morphism, if both properties are fulfilled. The mapping is an isomorphism, if it is a bijection, an epimorhism, if it is onto, an endomorphism, if it is a homomorphism and $L1 = L2$ and an automorphism, if it is isomorphism with $L1 = L2$.
A congruence relation is a special kind of equivalence relation. An equivalence relation exhibits similar properties as $i.) - iii.)$, except $ii.)$, which is replaced by

- ii'.) symmetric, i.e. $b \rho b' \Rightarrow b' \rho b.$

An equivalence relation ρ is a congruence relation, if the so called 'substitution property' is fulfilled, $x_0 \equiv y_0\ (\rho),\ x_1 \equiv y_1\ (\rho) \Rightarrow x_0 \wedge x_1 \equiv y_0 \wedge y_1\ (\rho),\ x_0 \vee x_1 \equiv y_0 \vee y_1\ (\rho)$, where $x \rho y$ was substituted with the notation $x \equiv y(\rho)$. All congruences of a lattice $\mathbf{L}$ can be ordered by inclusion to form the congruence lattice $\mathbf{Con}(\mathbf{L}(L)) =< Con(\mathbf{L}(L)), \wedge, \vee >$, where the meet is the set–theoretic intersection and the join is the transitive closure [14].
The lattices can be classified by those identities, which their elements satisfy. The 'modular' lattices are characterized by the modular identity,
$x \wedge (y \vee z) = (x \wedge y) \vee z,\ if\ x, y, z \in L,\ z \le x.$
In the class of 'distributive' lattices, the modular law appears in unrestricted form,
$x \wedge (y \vee z) = (x \wedge y) \vee (x \wedge z),\ if\ x, y, z \in L.$
The Boolean lattices are distributive, contain the universal bounds $\hat{0}$ and $\hat{1}$ and every element has a unique complement x' , with the following properties $x \wedge x' = \hat{0},\ x \vee x' = \hat{1}$.
We do not intend to pick out further elements of lattice theory, this short overview hopefully covers the topic we are interested in.

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