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Fuzzy lattice reasoning (FLR) type neural computation for weighted graph partitioning

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ABSTRACT

The fuzzy lattice reasoning (FLR) neural network was introduced lately based on an inclusion measure function. This work presents a novel FLR extension, namely agglomerative similarity measure FLR, or asmFLR for short, for clustering based on a similarity measure function, the latter (function) may also be based on a metric. We demonstrate application in a metric space emerging from a weighted graph towards partitioning it. The asmFLR compares favorably with four alternative graph-clustering algorithms from the literature in a series of computational experiments on artificial data. In addition, our work introduces a novel index for the quality of clustering, which (index) compares favorably with two popular indices from the literature.

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1. Introduction

Neural computation is typically pursued on numeric data in the Euclidean space R^N, where there is an abundance of mathematical tools available. Nonnumeric data were also considered including linguistic (fuzzy) data [32,46]. Alternative (nonnumeric) data of practical interest include *structured* (*graph*) data.

Our long-term interest, in the context of this work, is in partitioning a weighted graph, which represents a WWW-site as explained below. Advantages of meeting the aforementioned task by neural computing techniques include a capacity for massively parallel data processing as well as a capacity for both learning and generalization. A number of authors have pursued neural computing involving graphs as described next.

A structure (graph) was used as a vehicle for a unified data representation including arrays, sequences, and trees; in conclusion, a neural paradigm was proposed for learning, probabilistically, IO-isomorph transductions from an input- to an output- structured space, where transductions admit a recursive hidden state–space representation [18]. The latter work has spurred a lasting research activity including various enhancements and applications [1,2,8,20,47,48]. In addition, a number of technical issues were studied including ambiguity [19], nodecomplexity, etc. [21]. Extensions to Kohonen's self-organizing map (SOM) were also reported [27,29]. However, the aforementioned neural paradigm pursues learning by optimizing an "energy type"

objective (error) function in R^N using "number crunching" techniques. Hence, even though semantics may exist in (structured) input/ output data, nevertheless semantics is absent during data processing. Also, the aforementioned neural paradigm does not induce descriptive, decision-making knowledge for the general user.

On a different context, especially popular is an employment of the Hopfield neural network in graph-theoretic problems including: maximum cut [9], search [58], minimum vertex cover [66], etc. Note that, typically, a Hopfield network ignores semantics and it pursues optimization of an "energy type" *objective* function. Nevertheless, a different (Hopfield) network, which does not neglect graph-theoretical properties, preserved under isomorphism, was also presented for deciding whether two graphs are structurally equivalent [31].

Several works have dealt with the problem of *graph matching* using neural networks [62]. For instance, a general framework was proposed for *approximate graph matching* problems in image retrieval tasks [22]. Moreover, a (neural) graph matching technique was presented for object recognition [57], where a graph representation of the neuron positions/inter-connections reflects the structure of model objects. Furthermore, a pattern recognition problem was formulated as *labelled graph matching* towards finding the best match between an input graph and a stored graph [59].

The abovementioned graph matching techniques typically assume overlapping graphs, moreover an objective (cost) function is assumed. A recent work has introduced a (metric) graph edit distance (GED), derived from a metric cost function, in a set of graphs embedded in a labelled complete graph G_{Ω} , namely edit grid; moreover it demonstrated, comparatively, a successful pattern recognition application regarding a chemical information



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system [33]. Furthermore, three novel graph kernels were introduced for measuring similarity between feature vectors of chemical molecules towards classification of chemical compounds represented by graphs of covalent bonds [54].

The specifications of our task here, namely *weighted graph partitioning*, require different tools since we need to partition a graph into non-overlapping (sub)graphs by clustering, as explained below. There exists an abundance of graph (clustering) algorithms in various application domains including circuit partitioning [6], pattern recognition [15,25,65], structure comparison [26,33], etc. Note that the literature is dominated by *divisive* type clustering algorithms [4,16,61], where clusters are computed "top-down" by successively batch-splitting a graph. A different type of clustering, namely *agglomerative* (clustering), may proceed "bottom-up" by incrementally augmenting graphs. However, agglomerative clustering is not usually pursued mainly due to a shortage of enabling mathematical tools.

A fundamentally novel approach to neural computing was introduced lately applicable on partially(lattice)-ordered data including logic values, numbers, sets, symbols, and graphs [36,38,40,41]. In conclusion, the fuzzy lattice reasoning (FLR) emerged as an enhanced version of the learning algorithm employed by the neural-fuzzy classifier σ -FLN(MAP) [42]. The latter (classifier), in turn, has emerged as a lattice data domain extension of the well-known neural classifier fuzzy-ARTMAP, or FAM for short [40].

The operation of FLR was originally based on an *inclusion measure* function [39,42] towards inducing descriptive, decisionmaking knowledge (rules). A cluster, computed by FLR, is interpreted as an information granule [37]. A successful employment of a FLR version on graphs was already demonstrated using fuzzy lattice neurocomputing (FLN) [52], where clusters (namely, *hyperwords*) were computed in a master-graph, the latter encoded a thesaurus of English language synonyms; in conclusion, hyperwords were used for dimensionality reduction in a classification problem regarding large text documents. Nevertheless, the work in [52] ignores graph connectivity and treats, quite restrictively, a graph as an unstructured set of both *vertices* (or, *nodes*) and *edges* (or, *links*).

A substantial novelty of this work is consideration of graph connectivity by a different FLR version based on a novel *similarity measure* function. In conclusion, a master-graph is treated here as a (structured) data domain where, in contrast with the conventional data domain R, which includes a single shortest path between two different real numbers $a, b \in \mathbb{R}$ [40,42], there might be multiple shortest paths between two different nodes *a* and *b* in a master-graph.

Previous versions of FLR dealt either with hyperboxes in \mathbb{R}^{N} [42] or with FINs [39]; whereas, this work extends the applicability of FLR to graphs based on a metric distance. Note that a number of distances between graphs have been proposed by different authors [5,55].

There are similarities as well as substantial differences between FLR and previous graph processing algorithms. For instance, the latter algorithms have proposed a unification of graph/set/series data at a "representation" (encoding) level in the Euclidean space \mathbb{R}^N , whereas FLR proposes a disparate data fusion in a mathematical product-lattice $\mathbb{L} = \mathbb{L}_1 \times \cdots \times \mathbb{L}_N$ data domain [36,40]. In conclusion, previous algorithms carry out data processing by "number crunching" techniques, whereas FLR may retain semantics throughout data processing [34]. In addition, the FLR may induce descriptive decision-making knowledge (rules) from the training data. An additional advantage for FLR includes the capacity to introduce tunable nonlinearities [34,36,37,39,40,42].

This paper builds on previous work [43] including the following substantial novelties. First, we introduce a number of useful mathematical results including theoretical substantiation (i.e. proofs) and, second, we demonstrate comparatively a large number of new experimental results on artificial data. In addition, the work in [43] employs solely the *inner-transactions ratio* (ITR) index for evaluating the quality of graph clustering in a real-world application, where a weighted master-graph represents traffic. However, the ITR index "by definition" ascribes larger values to fewer clusters; hence, it encourages the computation of a single cluster. Whereas, the work here employs three different indices, including a novel one, for evaluating advantageously the quality of graph clustering. Future work will demonstrate a real-world application using the novel (mathematical) tools detailed here.

The layout is as follows. Section 2 defines metrics in measure (path) spaces. Section 3 summarizes the theory of fuzzy lattices including useful extensions; the practical relevance is also explained. Section 4 presents a novel neural computing algorithm for graph clustering. Comparative experimental results are presented in Section 5 including also a discussion. Section 6 concludes by summarizing the contribution of this work. Finally, Appendix A summarizes useful mathematical definitions and proofs.

2. Measurable paths and metrics

This section introduces useful metric distances between sets in a metric space; the latter emerges from measurable paths in a graph. Appendix A lists useful definitions.

2.1. Measurable paths

Inspired from measure theoretic analysis for path-planning in robotics [44], this section introduces useful terminology. Consider the following definition regarding a *path*.

Definition 2.1. Let *X* be a set and D be a totally-ordered "indexing set" with least- and greatest-elements *O* and *I*, respectively. A *path* from $a \in X$ to $b \in X$, symbolically $a \rightarrow b$, is a function $p_{ab}(.)$: $D \rightarrow X$ such that $p_{ab}(O) = a$ and $p_{ab}(I) = b$.

We point out that the indexing set D implies a totally-ordered complete lattice (D, \leq) , whose cardinality may be either *finite*, e.g. $D = \{0, 1, 2, ..., M\}$, or *infinite*; in turn, the latter could be either *countable*, e.g. $D = \{0, 1, 2, ...\}$, or *uncountable*, e.g. $D = \{0, 1, 2, ...\}$ or *uncountable*, e.g. $D = \{0, 1, 2, ...\}$ and $R^{\geq 0}$ have greatest element $I = +\infty$.

Our interest is in "measurable" paths $p_{ab}(.)$: $D \rightarrow X$ such that a measure space $(D, \Sigma_D, m_{\Sigma_D})$ can be defined with $0 < m_{\Sigma_D}(D) < +\infty$. The σ -algebra Σ_D includes intervals $[t_1, t_2]$, where $t_1, t_2 \in D$ with $t_1 \leq t_2$. In particular, $m_{\Sigma_D}(D) = m_{\Sigma_D}([O, I])$ is called *length* (of the path $a \rightarrow b$ from $a \in X$ to $b \in X$).

A measure function $m_{\Sigma_{D}} : \Sigma_{D} \to \mathbb{R}^{\geq 0}$ is induced from a measure space $(X, \Sigma_{X}, m_{\Sigma_{X}})$ as follows. Number $m_{\Sigma_{D}}(D)$ is calculated from a partition $\{D_{1},...,D_{N}\}$ of D such that there are no $x \neq y$ with $p_{ab}(x) = p_{ab}(y)$, i.e. there are no "cycles" on the path $a \to b$. In conclusion, $m_{\Sigma_{D}}(D) = m_{\Sigma_{X}}(p_{ab}(D_{1})) + \cdots + m_{\Sigma_{X}}(p_{ab}(D_{N}))$, where $p_{ab}(D_{i})$ denotes the image (set) of D_{i} , i = 1,...,N. We point out that any partition of D results in the same number $m_{\Sigma_{D}}(D)$.

Measure space $(D, \Sigma_D, m_{\Sigma_D})$ implies complete lattice (Σ_D, \subseteq) with least and greatest elements \emptyset and D, respectively; moreover, function $m_{\Sigma_D} : \Sigma_D \to \mathbb{R}^{\geq 0}$ is a positive valuation in lattice (Σ_D, \subseteq) [40]. Our interest, next, focuses on the (complete) indexing lattice (D, \leq) .

Function $v_{D}(x) = m_{\Sigma_{D}}([0,x]), x \in D$ is a positive valuation in the indexing lattice (D, \leq) because (1) $v_{D}(x) + v_{D}(y) = m_{\Sigma_{D}}([0,x]) + m_{\Sigma_{D}}([0,y]) = m_{\Sigma_{D}}([0,x \lor y]) + m_{\Sigma_{D}}([0,x \lor y]) = v_{D}(x \lor y) + v_{D}(x \land y)$

and (2) $x < y \Rightarrow m_{\Sigma_{D}}([0, x]) < m_{\Sigma_{D}}([0, y]) \Rightarrow v_{D}(x) < v_{D}(y)$. Hence, a metric d_{D} : $D \times D \to \mathbb{R}^{\geq 0}$ is given by $d_{D}(x, y) = v_{D}(x \lor y) - v_{D}(x \land y) = m_{\Sigma_{D}}([0, x \lor y]) - m_{\Sigma_{D}}([0, x \land y])$.

The greatest lower bound of all path $p_{ab}(.)$ lengths we call distance between a and b, symbolically $d_X(a,b)$. That is, distance $d_X(a,b)$ is the length of a shortest path from $a \in X$ to $b \in X$. Note that uniqueness of number $d_X(a,b)$ does not imply uniqueness of the shortest path between a and b since more than one path can have the same (shortest) length. In conclusion, a metric space (X,d_X) emerges from measurable paths between set X elements.

Definition 2.2. A subset $V \subseteq X$ in a metric space (X, d_X) is called *convex* if and only if it includes all shortest paths between set *V* elements.

In the context of this work, a convex set is interpreted as an *information granule* [50].

We define distance(s) between sets in a metric space (X,d_X) , next.

2.2. Metrics in a σ -algebra

The previous section has detailed how a measure space (X, Σ_X , m_{Σ_X}) gives rise to a metric space (X, d_X). This section presents three metrics in a σ -algebra Σ_X .

Proposition 2.3. Function $d_a: \Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ such that $d_a(A,B) = 0 \Leftrightarrow A = B$, moreover $d_a(A,B) = (1/(|A||B|))\sum_{i} d_X(a_i, b_i)$ is a metric.

The proof of Proposition 2.3 is shown in Appendix A.

We remark that Proposition 2.3 regards only sets of finite cardinality. More specifically, |A| in Proposition 2.3 denotes the *cardinality* of finite set *A*. In other words, |A| denotes the (integer) number of elements contained in set *A*, e.g. $|A = \{a,b,c\}| = 3$. Moreover, expression $\sum_{i,j} d_X(a_i, b_j)$ in Proposition 2.3 is a simplification for $\sum_{a_i \in A} [\sum_{b_i \in B} d_X(a_i, b_j)]$.

The following two metrics employ *unary* operations $\lor S$ and $\land S$, which equal, respectively, the supremum and the infimum of a set *S* of real numbers. Note that expressions $\lor S$ and $\land S$ are simplifications for expressions $\lor_{x\in S}S$ and $\land_{x\in S}S$, respectively. For a finite set *S*, numbers $\lor S$ and $\land S$ equal, respectively, the maximum and minimum number in *S*.

Proposition 2.4. Function $d_M: \Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ such that $d_M(A,B) = 0 \Leftrightarrow A = B$, moreover $d_M(A,B) = \bigvee_i \bigvee_j d_X(a_i,b_j)$ is a metric.

The proof of Proposition 2.4 is shown in Appendix A.

We remark that expression $\lor_i \lor_j d_X(a_i, b_j)$ in Proposition 2.4 is a simplification for expression $\lor_{a_i \in A} \{ \lor_{b_j \in B} \{ d_X(a_i, b_j) \} \}$. Consider the following condition.

Condition 2.5. Let *A*, *B*, *C* be sets in a metric space (X,d_X) , and let $a_i \in A$, $b_j \in B$, $c_k \in C$. For an index *k* suppose both $\exists I_k : I_k = \arg_i \{ \land_i d_X(c_k, a_i) \}$ and $\exists J_k : J_k = \arg_j \{ \land_j d_X(c_k, b_j) \}$. Then we define "Condition 2.5" as follows $d_X(a_{I_k}, b_{J_k}) \leq \max\{ \lor_i \land_j d_X(a_i, b_j), \lor_j \land_i d_X(b_j, a_i) \}$.

Proposition 2.6. Condition 2.5 is sufficient for a metric function $d_H: \Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ given by $d_H(A, B) = \max\{ \bigvee_i \wedge_j d_X(a_i, b_j), \bigvee_j \wedge_i d_X(b_i, a_i) \}.$

The proof of Proposition 2.6 is shown in Appendix A.

The metrics above are different from other ones between graphs [26,33] in that the latter quantify structural dissimilarity between graphs, whereas the metrics here quantify distance between graphs. More specifically, metric $d_H(.,.)$ is a generalization of the *Hausdorf* metric, the latter is typically defined in $\mathbb{R}^{\mathbb{N}}$ [13,35]. Moreover, metric d_a is applicable solely to sets of finite cardinality, whereas the other two metrics d_M and d_H are applicable between any sets.

2.3. Examples

In this section we demonstrate computation of metrics $d_M(.,.)$ and $d_H(.,.)$ including also geometric interpretations.

Example 2.7. Consider intervals [a,b] and [c,d] on the real line (Fig. 1). Sufficient Condition 2.5 holds, therefore it follows

 $d_{M}([a,b],[c,d]) = \max\{|a-d|,|b-c|\} \text{ for } [a,b] \neq [c,d] \text{ and }$

 $d_H([a, b], [c, d]) = \max\{|a - c|, |b - d|\}.$

Example 2.8. We represent a circle in the normed linear space $\mathbb{R}^{\mathbb{N}}$ by a pair (**c**,*r*), where $\mathbf{c} \in \mathbb{R}^{\mathbb{N}}$ and $r \ge 0$ is the (circle) radius. For instance, Fig. 2 shows circles (\mathbf{c}_{A} , r_{A}) and (\mathbf{c}_{B} , r_{B}) on the plane. A vector **r**, on the line defined by the centers of circles (\mathbf{c}_{A} , r_{A}) and (\mathbf{c}_{B} , r_{B}), is given by $\mathbf{r}(\lambda) = \mathbf{c}_{A} + \lambda (\mathbf{c}_{B} - \mathbf{c}_{A}), \lambda \in \mathbb{R}$. For intervals on the line $\mathbf{r}(\lambda)$ sufficient Condition 2.5 holds. Therefore, it follows

$$d_M((\mathbf{c}_A, \mathbf{r}_A), (\mathbf{c}_B, \mathbf{r}_B)) = \mathbf{r}_A + \|\mathbf{c}_A - \mathbf{c}_B\| + \mathbf{r}_B$$

for $(\mathbf{c}_A, r_A) \neq (\mathbf{c}_B, r_B)$ and

$$d_{H}((\mathbf{c}_{A}, r_{A}), (\mathbf{c}_{B}, r_{B}))$$

$$= \max\left\{ \left\| \left(\mathbf{c}_{A} - \frac{\mathbf{c}_{B} - \mathbf{c}_{A}}{\|\mathbf{c}_{B} - \mathbf{c}_{A}\|} r_{A} \right) - \left(\mathbf{c}_{B} - \frac{\mathbf{c}_{B} - \mathbf{c}_{A}}{\|\mathbf{c}_{B} - \mathbf{c}_{A}\|} r_{B} \right) \right\|,$$

$$\left\| \left(\mathbf{c}_{A} + \frac{\mathbf{c}_{B} - \mathbf{c}_{A}}{\|\mathbf{c}_{B} - \mathbf{c}_{A}\|} r_{A} \right) - \left(\mathbf{c}_{B} + \frac{\mathbf{c}_{B} - \mathbf{c}_{A}}{\|\mathbf{c}_{B} - \mathbf{c}_{A}\|} r_{B} \right) \right\| \right\}$$

$$= \max\{|r_{A} + \|\mathbf{c}_{A} - \mathbf{c}_{B}\| - r_{B}|, |r_{B} + \|\mathbf{c}_{A} - \mathbf{c}_{B}\| - r_{A}|\},$$

where $\|\cdot\|$ denotes the norm of its vector operand, and $|\cdot|$ denotes the absolute value of its real number operand.

3. Fuzzy lattices and useful extensions

This section introduces useful functions based on the theory of fuzzy lattices [36,37,40,42] summarized below including novel extensions.

3.1. Power-lattices

Lattice theory was compiled creatively by Garrett Birkhoff [3]. This section considers the power-set 2^{L} of a lattice (L, \leq). Next, we introduce a *binary* relation $\leq \subseteq 2^{L} \times 2^{L}$ such that for $U = \{u_1, ..., u_l\}$

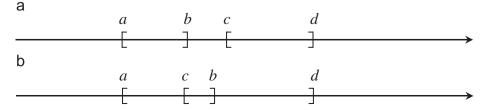


Fig. 1. (a) Non-overlapping intervals [a,b] and [c,d] on the real line and (b) overlapping intervals [a,b] and [c,d] on the real line.

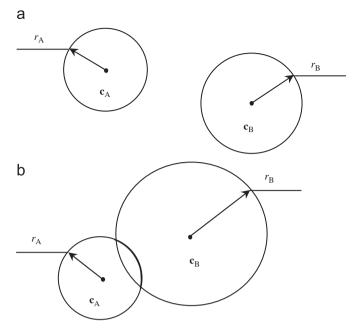


Fig. 2. (a) Non-overlapping circles (\mathbf{c}_{A}, r_{A}) and (\mathbf{c}_{B}, r_{B}) on the plane and (b) overlapping circles (\mathbf{c}_{A}, r_{A}) and (\mathbf{c}_{B}, r_{B}) on the plane.

and $W = \{w_1, ..., w_j\}$ in 2^{\perp} it is $U \leq W$ if and only if $\forall i \in \{1, ..., l\}$, $\exists j \in \{1, ..., j\}$: $u_i \leq w_j$. It can be shown immediately that the aforementioned binary relation, first, is a partial order and, second, it is a lattice order. In conclusion, the *power-lattice* $(2^{\perp}, \leq)$ emerges with $U \wedge W = \bigcup_{i,i} \{u_i \wedge w_i\}$ and $U \vee W = \bigcup_{i,i} \{u_i \vee w_i\}$.

3.2. Fuzzy lattices

A fuzzy set is a pair (U,m), where U is a universe of discourse and m is a membership function $m:U \rightarrow [0,1]$. In particular, the core (of fuzzy set m) is the set $C \subseteq U$ for which $\sup_{x \in U} m(x)$ is attained. Fuzzy lattices emerged in mathematics as well as in computational intelligence [36] by fuzzifying the binary relation " \leq " in a (crisp) lattice as follows.

Definition 3.1. A *fuzzy lattice* is a triple (L, \leq, m) , where (L, \leq) is a crisp lattice and $(L \times L, m)$ is a fuzzy set such that m(x,y) = 1 if and only if $x \leq y$.

We remark that function $m:U \rightarrow [0,1]$ in Definition 3.1 is interpreted as a *weak* (*fuzzy*) partial order relation in the sense that both m(x,y) = 1 and m(y,z) = 1 imply m(x,z) = 1, whereas if either $m(x,y) \neq 1$ or $m(y,z) \neq 1$ then m(x,z) could be any number in the interval [0,1]. A (complete) lattice can be fuzzified by an *inclusion measure* function defined next.

Definition 3.2. Let (L, \leq) be a complete lattice with least element *O*. An *inclusion measure* is a function $\sigma: L \times L \rightarrow [0,1]$, which satisfies conditions: (I0) $\sigma(u,O) = 0$, $u \neq O$; (I1) $\sigma(u,u) = 1$, $\forall u \in L$; (I2) $u \wedge w < u \Rightarrow \sigma(u,w) < 1$; (I3) $u \leq w \Rightarrow \sigma(x,u) \leq \sigma(x,w)$ (The Consistency Property).

We remark that $\sigma(x,y)$ is interpreted as a (fuzzy) degree of inclusion of *x* in *y*. Therefore, notations $\sigma(x,y)$ and $\sigma(x \le y)$ are used interchangably. If $\sigma: L \times L \rightarrow [0,1]$ is an inclusion measure in lattice (L, \le) then (L, \le, σ) is a fuzzy lattice [36,42]. A couple inclusion measures can be defined based on a *positive valuation* function as follows [36,42,52].

Theorem 3.3. If $v: \perp \rightarrow \mathbb{R}^{\geq 0}$ is a positive valuation in a complete lattice (\perp, \leq) , with v(0) = 0, then both functions $s(x,u) = v(x \land u)/v(x)$ and $k(x,u) = v(u)/v(x \lor u)$ are inclusion measures.

We point out that Theorem 3.3 calls for a *nonnegative* positive valuation function v.

A novel inclusion measure can be introduced in a power-lattice as follows.

Proposition 3.4. Let function $\sigma_V: \mathbb{L} \times \mathbb{L} \to [0,1]$ be an inclusion measure in a lattice (\mathbb{L}, \leq) . Then function $\sigma: 2^{\mathbb{L}} \times 2^{\mathbb{L}} \to [0,1]$ given by the convex combination $\sigma(\{u_1, \dots, u_l\} = U \leq W = \{w_1, \dots, w_J\}) = \lambda_1 \max_i \sigma_V(u_1 \leq w_i) + \dots + \lambda_l \max_i \sigma_V(u_l \leq w_i)$ is an inclusion measure.

The proof of Proposition 3.4 is shown in Appendix A.

We remark that by "convex combination" we mean a set $\lambda_1, \ldots, \lambda_I$ of positive numbers such that $\lambda_1 + \cdots + \lambda_I = 1$.

3.3. Similarity measure functions

Various similarity measures are employed/defined in applications [11,53,55]. A novel definition is proposed next.

Definition 3.5. A *similarity measure* is a function $\mu: U \times U \rightarrow [0,1]$, which satisfies conditions: (S1) $\mu(x,y) = 1 \Leftrightarrow x = y$; (S2) $\mu(x,y) = \mu(y,x)$.

We remark that the advantage of our proposed Definition 3.5 is that it retains rigorously the essentials of a "common sense" notion of similarity while avoiding redundancies.

We define a *similarity space* as a pair (U,μ) including a nonempty set U and a similarity measure function $\mu: U \times U \rightarrow [0,1]$. The following proposition introduces a similarity measure in a (complete) lattice based on an inclusion measure function σ .

Proposition 3.6. Let (L, \leq) be a lattice with an inclusion measure $\sigma: L \times L \rightarrow [0,1]$. Then, function $\mu_{\sigma}: L \times L \rightarrow [0,1]$ given by $\mu_{\sigma}(x,y) = (\sigma(x \leq y) + \sigma(y \leq x))/2$ is a similarity measure.

The proof of Proposition 3.6 is shown in Appendix A.

The following proposition introduces a similarity measure, in a metric space.

Proposition 3.7. Let function $d: U \times U \to \mathbb{R}^{\geq 0}$ be a metric. Then, function $\mu_d: U \times U \to [0,1]$ given by $\mu_d(x,y) = 1/(1 + d(x,y))$ is a similarity measure.

The proof of Proposition 3.7 is shown in Appendix A.

3.4. Practical relevance

A metric space emerges below by adding up the weights of links and nodes along shortest paths in a weighted master-graph M = (V,E), where $V = \{v_1,...,v_N\}$ is the (non-empty) finite set of *vertices* (or, equivalently *nodes*) and $E \subseteq V \times V$ is the set of *edges* (or, equivalently, *links*).

A partition, also called *equivalence* relation, P of the set V of vertices in a master-graph is a (finite) collection of subsets $P_1,...,P_N$, namely *parts*, of V such that both $P_i \cap P_j = \{\}$ for $i \neq j$ and $P_1 \cup ... \cup P_N = V$ for an integer number N. Apparently, based on shortest path lengths, we can define different metric distances $d_a(...)$, $d_M(...)$, and $d_H(...)$ between *parts* of partitions, where a *part* represents a subgraph. Note that different authors have already proposed distances beyond space \mathbb{R}^N , e.g. in metric spaces for queries [64], in spaces of convex/concave bodies for optimization [7], etc. An additional, useful function is presented next.

Consider the family Π_V of all partitions of a set *V*. It is known that $(\Pi_{V_1} \leq)$ is a lattice-ordered by (partitions') refinement [56].

Step-0: Consider a partition $P = \{P_1, \dots, P_n\}$ of the vertices $V = \{v_1, \dots, v_N\}$ of a weighted

master-graph M = (V, E), where clusters $P_i \subseteq V$, i=1,...,n are such that both $\bigcup_{i=1}^n P_i =$

V and $P_i \cap P_j = \{\}$ for $i \neq j$.

- Step-1: While (a user-defined Assimilation Condition is satisfied) do
- Step-2: Compute, in parallel, the similarity measure values $\mu_d(P_i, P_j) = 1/(1+d(P_i, P_j))$,
 - $i,j \in \{1,...,n\}.$
- Step-3: Competition among pairs of clusters.

Winner in pair (I,J) $\in \mathsf{P} \times \mathsf{P}$ such that (I,J) $\doteq \arg \max_{i,j} \mu_d(P_i,P_j)$, where I \neq J.

Step-4: Merge P_1 and P_1 by replacing them with the (single) cluster $P_1 \cup P_1$; $n \leftarrow n-1$.

Fig. 3. The agglomerative similarity measure FLR (asmFLR) neural computing algorithm for partitioning the nodes of a master-graph by clustering.

More specifically, lattice $(\Pi_{V,\leq})$ is a sublattice of power-lattice $(2^{L},\leq)$, where $(L = 2^{V},\leq)$ is the power-set (lattice) of V.

In this work we have considered (in a master-graph) inclusion measure "type" functions defined as in Proposition 3.4 with $\lambda_1 = \cdots = \lambda_I$ for the following choices of σ_V :

(1)
$$\sigma_{V1}(P_i \leq Q_j) = \frac{|P_i \wedge Q_j|}{|P_i|}$$
, (2) $\sigma_{V2}(P_i \leq Q_j) = \frac{|Q_j|}{|P_i \wedge Q_j|}$, and
(3) $\sigma_{V3}(P_i \leq Q_j) \frac{|P_i \wedge Q_j|}{|P_i \vee Q_j|}$,

where the unary operator $|\cdot|$ returns the cardinality of its (set) operand; e.g. $|P_1 = \{a,b,c\}| = 3$.

It turns out that only functions $\sigma_{V1}(...)$ and $\sigma_{V2}(...)$ above are inclusion measures, according to Theorem 3.3; whereas, function $\sigma_{V3}(...)$ is not an inclusion measure as demonstrated by the following counter-example.

Consider the (totally-ordered) lattice (\mathbb{R}, \leq) of real numbers. For $1 = u \leq w = 2$ it is straightforward to confirm that the Consistency Property $u \leq w \Rightarrow \sigma(x,u) \leq \sigma(x,w)$ of Definition 3.2 does not hold for x = 0.5, because $0.5 \land 1/0.5 \lor 1 = 0.5 > 0.25 = 0.5 \land 2/0.5 \lor 2$. Hence, function $\sigma_{V3}(...)$ is not an inclusion measure. Nevertheless, function $\sigma_{V3}(...)$ has produced the best experimental results as demonstrated below.

4. A FLR-type neural network

FLR has emerged as an enhanced version of the learning algorithm employed by fuzzy neural network σ -FLN(MAP) [42]. The latter, in turn, has emerged as a lattice data domain enhancement of neural network fuzzy-ART(MAP) [40].

The operation of FLR was originally based on an *inclusion measure* function [37,39,42] towards inducing descriptive, decision-making knowledge (rules). Lately, there was an effort to extend FLR in space \mathbb{R}^N based on a "non-rigorously defined" similarity measure function [12]. Inspired from the latter we introduce, in the following, a FLR version for clustering in a graph, based on a rigorously defined similarity measure function.

4.1. The agglomerative similarity measure FLR (asmFLR) algorithm

The agglomerative similarity measure FLR (asmFLR) algorithm for master-graph partitioning by clustering is presented in Fig. 3 for neural computing subgraphs, namely granules or, equivalently, clusters. Data processing by asmFLR repeats, conditioned on a user-defined Assimilation Condition (Fig. 3, Step-1), a number of cycles. Each aforementioned cycle carries out, in parallel, "batch processing" computations. Overall, it can be claimed that the *asmFLR* algorithm carries out *lattice computing* (LC), the latter is defined as lattice-theory-based computational intelligence [23].

4.2. Algorithm asmFLR details

The *asmFLR* may set out learning without *a priori* knowledge; however, a priori knowledge can be supplied in the form of an initial set of subgraphs/clusters (Fig. 3, Step-0). In particular, for n = N it follows that each master-graph node constitutes a (trivial) cluster.

There can be different user-defined Assimilation Conditions (Fig. 3, Step-1). For instance, a naive Assimilation Condition could be "n > 1" meaning that clustering proceeds until all master-graph nodes are put in one cluster. Another Assimilation Condition may define a maximum threshold size for a computed cluster, etc.

Generalization can be effected as follows. A cluster $Q \subseteq V$ in a weighted master-graph $\mathbb{M} = (V,E)$ defines a fuzzy set $(\Sigma_X, \mu_d(P;Q))$ such that cluster Q corresponds to the *core* of fuzzy set $(\Sigma_X, \mu_d(P;Q))$. Note that in notation " $\mu_d(P;Q)$ " symbol "P" denotes a variable, whereas symbol "Q" denotes a parameter. Hence, generalization becomes feasible beyond core Q.

We remark that the original *FLR* classifier, which employs an inclusion measure function, supports two different modes of reasoning, namely *Generalized Modus Ponens* and *Reasoning by Analogy* [42]. None of the aforementioned modes of reasoning is supported by *asmFLR* since the latter is a scheme for clustering based on a similarity measure function. Next, we compute the complexity of *asmFLR*.

Algorithm *asmFLR* (Fig. 3) includes a number of O(N) cycles. Each cycle computes $O(N^2)$ similarity measure function values. Moreover, each of the latter (values) requires the length (i.e. the metric distance) of the shortest path between two master-graph nodes; nevertheless, there is no additional computational overhead since all aforementioned metric distances are computed once, in a data preprocessing step. It follows that the learning (clustering) complexity of *asmFLR* is cubic $O(N^3)$ in the number "*N*" of master-graph nodes.

4.3. Comparative discussion

There are inherent similarities as well as substantial differences between *asmFLR* and *FLR*. More specifically, a cluster computed by either algorithm corresponds to the core of a fuzzy set. Nevertheless, a cluster for *FLR* is a *N*-tuple FIN in space \mathbb{R}^N , the latter is the Cartesian product of N totally-ordered lattices \mathbb{R} [42]; whereas, the *asmFLR* here is applied in the partially-ordered lattice ($\Pi_{V,\leq}$) of partitions of the set $V = \{v_1,...,v_N\}$ of vertices in a weighted master-graph $\mathbb{M} = (V,E)$. Moreover, *asmFLR* is a data-orderindependent extension of the data-order-dependent *FLR* such that *asmFLR* is based on a *similarity measure* function, whereas *FLR* is based on an *inclusion measure* function. In addition, the *FLR* learns rapidly with complexity O(n) in the number *n* of data, whereas the learning complexity of *asmFLR* is $O(N^3)$ in the number *N* of mastergraph nodes as shown above.

5. Comparative experimental results

We applied (neural) algorithm *asmFLR*, comparatively, on metric spaces emerged from master-graphs as described above. Master-graphs were generated as described next.

5.1. Artificial data generation and preprocessing

A user defined a number of parameters for generating, randomly, a *dataset*. The aforementioned parameters included: the number *M* of master-graphs in a dataset, the number *C* of *graph-clusters* in a master-graph, both the minimum number v_{min} and the maximum number v_{max} of vertices per graph-cluster and, finally, both an *intra-connection ratio* $r_{in} \in [0,1]$ and an *inter-connection ratio* $r_{out} > 0$. A single master-graph was generated as detailed next.

For a graph-cluster $c \in \{1,...,C\}$, a number $v_c \in [v_{\min}, v_{\max}]$ of vertices was drawn randomly. Then, we computed the number n_{in} of *intra-cluster* links between a vertex and different ones in graph-cluster c such that n_{in} equals the integer nearest to real number $r_{in}(v_c-1)$. Next, we randomly selected (eligible) intra-cluster links from the list of all links in graph-cluster c. Hence, a total number C of graph-clusters were computed.

The graph-clusters computed above were connected by randomly generated *inter-cluster* links as follows. We computed the (constant) number n_{out} of links between a vertex in graph-cluster $c \in \{1,...,C\}$ with vertices in different graph-clusters such that n_{out} equals the smallest integer above real number $r_{in}(v_c - 1)r_{out}$. In addition, we required vertex intra-connectivity (within a cluster) to be larger than the corresponding vertex inter-connectivity (with different clusters) in order to produce clearly separated graph-clusters (in a master-graph). Note that different authors often generate inter-cluster links "probabilistically" [49] resulting in, unfortunately, "not clearly separated" graph-clusters. Finally, we randomly drew (eligible) inter-cluster links from the list of all links in the master-graph. Hence, a master-graph was generated.

We repeated the above procedure M times. In conclusion, one *dataset* was generated including M (different) master-graphs. The next example demonstrates dataset generation.

Example 5.1. Fig. 4 (as well as Fig. 5) displays a *dataset* with M = 2 different master-graphs; each of the aforementioned master-graphs includes C = 5 identical graph-clusters with $v_{\min} = 3$, $v_{\max} = 5$. Note that it is $r_{in} = 1.0$ in both Figs. 4 and 5, i.e. each graph-cluster is completely intra-connected. A user defined $r_{out} = 0.3$ for the dataset in Fig. 4, and $r_{out} = 0.6$ for the dataset in Fig. 5.

Due to the master-graph generation procedure detailed above, it turns out that the (actual) r_{out} of a specific vertex is, typically, different than the user-defined r_{out} . Therefore, for each vertex, we computed the (actual) r_{out} as the ratio of (number of) inter-cluster

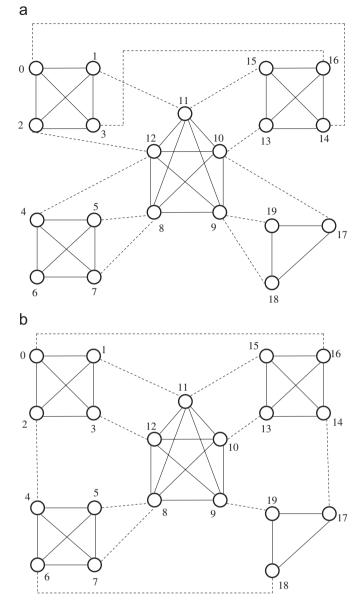


Fig. 4. A *dataset* including two master-graphs, i.e. M = 2, each of whom has C = 5 identical graph-clusters with 3, 4, or 5 vertices. A master-graph has both a user-defined *intra-connection ratio* $r_{in} = 1.0$ and a user-defined *inter-connection ratio* $r_{out} = 0.3$: (a) a master-graph with average r_{out} equal to 0.38 and standard deviation 0.23 and (b) a master-graph with average r_{out} equal to 0.36 and standard deviation 0.24.

links over (number of) intra-cluster links. Finally, we computed both the average r_{out} and the corresponding standard deviation in a master-graph in Fig. 4 as well as in Fig. 5. It turns out that the average r_{out} is different than the user-defined r_{out} , as expected.

As soon as a master-graph was generated, we used (in a datapreprocessing step) Floyd's algorithm [17] in order to compute the distances between any two nodes in the master-graph. We point out that Floyd's algorithm receives as input the corresponding master-graph's "adjacency matrix" and outputs the required "distance matrix" with cubic complexity $O(N^3)$ in the number *N* of master-graph nodes. Note that in our experiments we considered master-graph links of "unit" length, moreover the vertices in a master-graph did not have a weight.

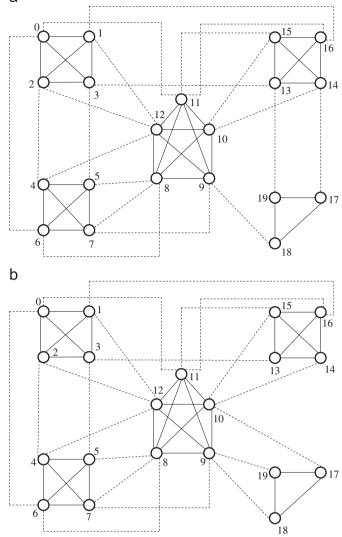


Fig. 5. A *dataset* including two master-graphs, i.e. M = 2, each of whom has C = 5 identical graph-clusters with 3, 4, or 5 vertices. A master-graph has both a user-defined *intra-connection ratio* $r_{in} = 1.0$ and a user-defined *inter-connection ratio* $r_{out} = 0.6$: (a) a master-graph with average r_{out} equal to 0.63 and standard deviation 0.10 and (b) a master-graph with average r_{out} equal to 0.62 and standard deviation 0.13.

Table 1
Statistics regarding five datasets ds1, ds2, ds3, ds4, and ds5.

	Dataset	No. of clusters C	Cluster size					User- defined	r _{out}	
		clusters e	v_{\min}	$v_{\rm max}$	Average	Std.		r _{out}	Average	Std.
	ds1	10	5	15	11.6	3.565	1	0.5	0.532	0.031
1	ds2	10	5	15	11.6	3.565	1	0.7	0.755	0.051
1	ds3	10	5	15	11.6	3.565	1	0.9	0.937	0.043
1	ds4	10	5	15	11.6	3.565	1	1.0	0.996	0.031
1	ds5	10	5	15	11.6	3.565	1	1.2	1.255	0.046

5.2. Comparative experiments

We generated five (different) datasets **ds1**, **ds2**, **ds3**, **ds4**, **ds5**, respectively, for $r_{out} \in \{0.5, 0.7, 0.9, 1.0, 1.2\}$. A master-graph in a dataset included C = 10 (identical) graph-clusters with $v_{min} = 5$ and $v_{max} = 15$. Table 1 summarizes various dataset statistics including average cluster size as well as the corresponding

standard deviation 11.6 and 3.565, respectively. Table 1 also shows the user-defined intra-connection ratio $r_{\rm in} = 1$, that is each vertex in a graph-cluster was connected to all other vertices. The next column in Table 1 indicates the user-defined inter-connection ratio $r_{\rm out}$. The last two columns in Table 1 display the actual (average) $r_{\rm out}$ as well as the corresponding standard deviation in a dataset.

In a data-preprocessing step we calculated (and stored) the metric distances between all pairs of nodes in a master-graph, for fast access.

We employed algorithm *asmFLR* using a similarity measure $\mu_d(...)$ based on three different metrics, namely $d_a(...)$, $d_M(...)$, and $d_H(...)$. Notation *asmFLR*(d_X) below means algorithm *asmFLR* based on metric d_X , $X \in \{a, M, H\}$. For comparison, we implemented and applied four alternative graph clustering algorithms, namely *MajorClust* [61], *MinCutTrees* [10,16], *Modularity* [49], and *SingleLink* [30]. Where applicable, the aforementioned algorithms were executed until 10 graph-clusters were computed.

Tables 2–6 summarize our experimental results regarding datasets ds1, ds2, ds3, ds4, and ds5, respectively. Algorithms MajorClust and MinCutTrees terminated by computing a small number $C \leq 3$ of graph-clusters. The other algorithms terminated when a total number of C = 10 graph-clusters were computed as shown in the second column of Tables 2-6. The next four columns in Tables 2-6 display size statistics regarding graph-clusters computed by an algorithm. Symbol "NaN", i.e. Not-a-Number, appears in the std (standard deviation) column in a Table when a single cluster was computed, hence computation of std is meaningless. Column "No. of trivials" in a Table indicates the (average) number of trivial graph-clusters in a total number of C = 10 graphclusters computed by an algorithm. The last three columns in a table show the corresponding values of (graph-clustering) indices *Purity* [67], *Entropy* [68], and *similarity measure* $\mu_{\sigma}(...)$. Note that we used a different *similarity measure* function $\mu_{\sigma}(...)$ as an index than the similarity measure function $\mu_d(...)$ used by algorithm asmFLR towards producing unbiased results.

Fig. 6, as well as Fig. 7, demonstrates comparatively the performance of algorithms $asmFLR(d_a)$ and Modularity using three indices, namely Purity (curve in light gray color), Entropy (curve in dark gray color), and index $\mu_{\sigma}(...)$ (curve in black color), versus a (decreasing) number of computed graph-clusters for dataset ds1. First, Figs. 6a and b correspond to algorithms $asmFLR(d_a)$ and Modularity, respectively, where both aforementioned figures use index $\mu_{\sigma}(...)$ based on inclusion measure $\sigma_{V2}(P_i \leq Q_i) = |Q_i|/|P_i \vee Q_i|$. Note that similar curves were obtained by the aforementioned alternative graph clustering algorithms, also for $\sigma_{V1}(P_i \leq Q_i) =$ $|P_i \wedge Q_i|/|P_i|$, for other datasets as well. Second, Figs. 7a and b correspond to algorithms $asmFLR(d_a)$ and Modularity, respectively, where both aforementioned figures use index $\mu_{\sigma}(...)$ based on $\sigma_{V3}(P_i \leq Q_i) = |P_i \wedge Q_i|/|P_i \vee Q_i|$. Note that similar curves were obtained also by the aforementioned alternative graph clustering algorithms, for other datasets as well.

5.3. Discussion of the results

Our computational experiments have clearly demonstrated a favorable comparison for our proposed *asmFLR* algorithms. In addition, our experimental work has confirmed the value of our proposed index function $\mu_{\sigma}(...)$ as detailed next.

First, an index value (in Figs. 6 and 7) was calculated by comparing a partition, computed by a graph clustering algorithm, to an "optimum" partition. The latter was the one, which included the C = 10 graph-clusters used for generating a master-graph as described above. Note that index *Purity*, by definition, indicates the average largest percentage of a computed cluster inside an "optimum" cluster; hence, larger values of *Purity* are preferable.

Table 2

Statistics of experimental	results regarding dataset	ds1 by various	s graph clustering algorithms.

Algorithm name	No. of clusters C	Cluster siz	e			No. of trivials	Purity	Entropy	Similarity measure $\mu_{\sigma}()$
		Min	Max	Average	Std.				
asmFLR (d _a)	10	4.8	16	11.6	3.818	0	0.957	0.062	0.921
$asmFLR(d_M)$	10	3.7	33.7	11.6	9.049	0	0.731	0.252	0.665
Modularity	10	1	22.5	11.6	7.529	2.5	0.816	0.156	0.659
MajorClust	3	9	92	38.6	46.285	0	0.336	0.698	0.510
$asmFLR(d_H)$	10	1	90.2	11.6	27.704	3.2	0.309	0.729	0.269
MinCutTrees	1	116	116	116	NaN	0	0.129	0.979	0.114
SingleLink	10	1	107	11.6	33.520	9	0.206	0.899	0.111

The results are arranged in the order of decreasing *similarity measure* $\mu_{\sigma}(...)$ values.

Table 3

Statistics of experimental results regarding dataset ds2 by various graph clustering algorithms.

Algorithm	No. of clusters C	Cluster siz	:e			No. of trivials	Purity	Entropy	Similarity
name	clusters c	Min	Max	Average	Std.				measure $\mu_{\sigma}(.,.)$
asmFLR (d _a)	10	5	17.9	11.6	3.818	0	0.888	0.148	0.817
Modularity	10	1	23.7	11.6	7.529	2.1	0.824	0.147	0.705
$asmFLR(d_M)$	10	2.1	38.4	11.6	9.049	0.3	0.606	0.375	0.512
MajorClust	2	32	84	58	46.285	0	0.258	0.723	0.261
$asmFLR(d_H)$	10	1	94.3	11.6	27.704	3.8	0.282	0.780	0.220
MinCutTrees	1	116	116	116	NaN	0	0.129	0.979	0.114
SingleLink	10	1	107	11.6	33.520	9	0.206	0.899	0.111

The results are arranged in the order of decreasing *similarity measure* $\mu_{\sigma}(.,.)$ values.

Table 4

Statistics of experimental results regarding dataset ds3 by various graph clustering algorithms.

Algorithm name	No. of clusters C	Cluster siz	ze			No. of trivials	Purity	Entropy	Similarity measure $\mu_{\sigma}()$
	clusters e	Min	Max	Average	Std.	tiviais			measure $\mu_{\sigma}()$
asmFLR (d _a)	10	5.6	18.4	11.6	4.109	0	0.869	0.176	0.788
Modularity	10	1	24.4	11.6	8.269	2.7	0.787	0.190	0.623
$asmFLR(d_M)$	10	1.5	49.2	11.6	14.720	0.6	0.517	0.470	0.429
$asmFLR(d_H)$	10	1	98.5	11.6	30.562	4.4	0.256	0.819	0.185
MajorClust	1	116	116	116	NaN	0	0.129	0.979	0.114
MinCutTrees	1	116	116	116	NaN	0	0.129	0.979	0.114
SingleLink	10	1	107	11.6	33.520	9	0.206	0.899	0.111

The results are arranged in the order of decreasing *similarity measure* $\mu_{\sigma}(.,.)$ values.

 Table 5

 Statistics of experimental results regarding dataset ds4 by various graph clustering algorithms.

Algorithm name	No. of clusters C	Cluster siz	ze			No. of trivials	Purity	Entropy	Similarity measure $\mu_{\sigma}(.,.)$
	clusters e	Min	Max	Average	Std.	tiviais			measure $\mu_{\sigma}(.,.)$
asmFLR (d _a)	10	4.2	21	11.6	5.296	0.3	0.804	0.246	0.697
Modularity	10	1	22.4	11.6	7.281	2.4	0.799	0.185	0.629
$asmFLR (d_M)$	10	1.2	54.3	11.6	16.323	1.1	0.466	0.532	0.370
$asmFLR(d_H)$	10	1	96.4	11.6	29.841	4	0.274	0.794	0.207
MajorClust	1	116	116	116	NaN	0	0.129	0.979	0.114
MinCutTrees	1	116	116	116	NaN	0	0.129	0.979	0.114
SingleLink	10	1	107	11.6	33.520	9	0.206	0.899	0.111

The results are arranged in the order of decreasing *similarity measure* $\mu_{\sigma}(.,.)$ values.

Whereas, index *Entropy*, by definition, is (roughly) the complement of index *Purity*; hence, smaller values of *Entropy* are preferable.

A disadvantage of both indices *Purity* and *Entropy* is that "more" graph-clusters may be characterized by better (index) values than the optimum number of C = 10 graph-clusters as demonstrated in

both Figs. 6 and 7. Whereas, index $\mu_{\sigma}(...)$ has a global optimum value at C = 10 graph-clusters as demonstrated in both Figs. 6 and 7. Note in both Figs. 6 and 7 that the *Purity* index drops sharply for fewer than C = 10 graph-clusters, as expected, since "10" is the optimum number of clusters. Moreover, the *Purity* index in both Figs. 6 and 7 is less than 1 at C = 10 due to the fact that the

Table 6
Statistics of experimental results regarding dataset ds5 by various graph clustering algorithms.

Algorithm name	No. of clusters C	Cluster siz	e			No. of trivials	Purity	Entropy	Similarity measure $\mu_{\sigma}(.,.)$
nume	clusters c	Min	Max	Average	Std.	triviais			measure $\mu_{\sigma}()$
$asmFLR(d_a)$	10	3.4	21.6	11.6	5.566	0.3	0.800	0.258	0.687
Modularity	10	1	23.5	11.6	7.175	2.1	0.806	0.197	0.649
$asmFLR(d_M)$	10	1.2	62.8	11.6	19.133	1.1	0.402	0.602	0.317
$asmFLR(d_H)$	10	1	94.1	11.6	29.032	3.7	0.287	0.786	0.214
MajorClust	1	116	116	116	NaN	0	0.129	0.979	0.114
MinCutTrees	1	116	116	116	NaN	0	0.129	0.979	0.114
SingleLink	10	1	107	11.6	33.520	9	0.206	0.899	0.111

The results are arranged in the order of decreasing similarity measure $\mu_{\sigma}(.,.)$ values.

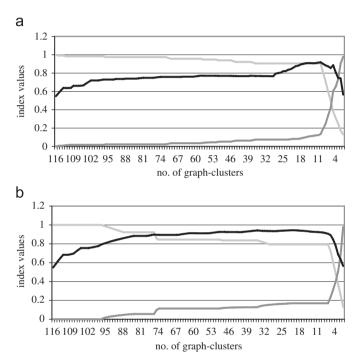


Fig. 6. Values of (graph clustering) indices *Purity* (curve in light gray color), *Entropy* (curve in dark gray color), and index $\mu_{\sigma}(...)$ (curve in black color), the latter is based on inclusion measure $\sigma_{V2}(P_i \leq Q_j) = |Q_j|/|P_i \lor Q_j|$, versus a (decreasing) number of graph-clusters for dataset **ds1** by: (a) neural algorithm *asmFLR*(d_a) and (b) algorithm *Modularity*.

computed 10 clusters are not identical to the original ("optimal") ones in a dataset. An inherent drawback of index *Purity* is its trustworthy capacity mainly for comparing partitions of the same cardinality. Whereas, by definition, index $\mu_{\sigma}(...)$ is also reliable for comparing partitions of different cardinalities.

Index $\mu_{\sigma}(...)$ based on $\sigma_{V3}(P_i \leq Q_i) = |P_i \land Q_j|/|P_i \lor Q_j|$ (Fig. 7) is preferable to index $\mu_{\sigma}(...)$ based on $\sigma_{V2}(P_i \leq Q_i) = |Q_i|/|P_i \lor Q_j|$ (Fig. 6) because the index $\mu_{\sigma}(...)$ curves in Fig. 7 have a "sharper" global maximum than the corresponding curves in Fig. 6. Hence, the graph-clustering algorithms in Tables 2–6 were arranged in the order of "decreasing" values of index $\mu_{\sigma}(...)$ based on $\sigma_{V3}(P_i \leq Q_j) =$ $|P_i \land Q_j|/|P_i \lor Q_j|$. Note also that, in our computational experiments, only index $\mu_{\sigma}(...)$ based on σ_{V3} has retained nearly the same ordering in the performance of the alternative four algorithms *Modularity*, *MajorClust*, *MinCutTrees*, and *SingleLink* as the popular *Purity* index; whereas, index $\mu_{\sigma}(...)$ based on either σ_{V1} or σ_{V2} has produced different orderings. The latter is one more reason for preferring σ_{V3} . Furthermore, note that function σ_{V3} , also known

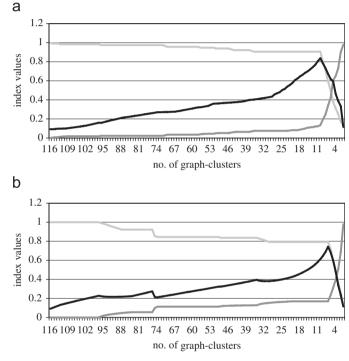


Fig. 7. Values of (graph clustering) indices *Purity* (curve in light gray color), *Entropy* (curve in dark gray color), and index $\mu_{\sigma}(...)$ (curve in black color), the latter is based on function $\sigma_{V3}(P_i \leq Q_j) = |P_i \land Q_j| / |P_i \lor Q_j|$, versus a (decreasing) number of graph-clusters for dataset **ds1** by: (a) neural algorithm *asmFLR*(*d*_{*a*}) and (b) algorithm *Modularity*.

in the literature as *Jaccard* (similarity measure) *coefficient*, has demonstrated a superior performance as compared to seven well-known similarity measure functions in a series of computational experiments elsewhere [45]. The extensive experimental evidence presented in this work has confirmed the superiority of the *Jaccard coefficient* σ_{V3} .

Second, algorithm $asmFLR(d_a)$ invariably tops all the other algorithms in Tables 2–6. In the second and third places appear algorithms *Modularity* and $asmFLR(d_M)$. In the fourth and fifth places appear algorithms *MajorClust* and $asmFLR(d_H)$. Finally, algorithm *MinCutTrees* is always in the sixth place, whereas algorithm *SingleLink* is always in the last (seventh) place in all Tables 2–6. It is remarkable that the aforementioned arrangement of algorithms essentially remains the same (with minor differences) in Tables 2–6, for either index *Purity* or *Entropy*. Therefore, based on experimental evidence, it can be claimed that algorithm $asmFLR(d_a)$ approaches the "optimum" graph clustering better than any other graph clustering algorithm in this work. Furthermore, it is a remarkable advantage that algorithm $asmFLR(d_a)$ typically avoids computing trivial graph-clusters.

We, further, pursued computation of *convex* subgraphs in a master-graph. In a large number of experiments, using various indices of performance, we recorded a "non-statistically significant" deterioration of performance for the same number of computed subgraphs. In addition, the time required for computing convex subgraphs grew significantly (i.e. exponentially) in the number of nodes. Therefore, we conclude that convex subgraphs do not improve performance here. The explanation is that the artificial master-graphs, generated in the context of this work, as described above, were not convex in the first place.

6. Conclusion

This work has introduced novel mathematical perspectives and tools for clustering in a general metric space. In conclusion, the *agglomerative similarity measure FLR* (*asmFLR*) neural computing algorithm was introduced for partitioning-by-clustering. In addition, our work introduced a novel index for evaluating the quality of clustering.

A metric space emerged here from a weighted graph. Experimental results have confirmed, comparatively, the viability of our proposed techniques/tools on artificial data (graphs) generated randomly. A real-world application of practical interest is to partition a master-graph, whose link-weights represent Webtraffic, towards Web-navigation support [14,51,60,63]. The preliminary experimental work in [43] will be extended in the future using the tools here. Future work may also consider alternative weighted graph partitioning problems including an approximate solution to the "minimum cut" problem [16].

Appendix A

This Appendix A lists useful definitions. It also includes the proofs of six novel propositions.

A.1. Lattice theory

For elementary definitions regarding lattice theory the reader may refer to [3,24,39]. The following definition is important in the sequel.

Definition A.1. A *positive valuation* in a lattice (L, \leq) is a real function $v:L \rightarrow R$, which satisfies both $v(x)+v(y) = v(x \land y)+v(x \lor y)$ and $x \lt y \Rightarrow v(x) \lt v(y)$.

A positive valuation $v: \bot \rightarrow R$ in a lattice (\bot, \leqslant) implies a *metric* function $d: \bot \times \bot \rightarrow R^{\ge 0}$ given by

$$d(a,b) = v(a \lor b) - v(a \land b) \tag{E1}$$

For definition of a metric function see below.

It is remarkable that the latter metric (distance) is used implicitly in the "graph literature" without reference to lattice theory. More specifically, (metric) distance $d_{mcs1}(G_0,G_1) = |V_0| + |V_1| - 2|V_{01}|$ is used in [33], which (distance d_{mcs1}), in the context of lattice theory, can be produced as follows. Function v(G(V,E,l)) = v(V) = |V| is a positive valuation in the power-set (lattice) of vertices. Hence, $d_{mcs1}(G_0,G_1) = v(G_0 \vee G_1) - v(G_0 \wedge G_1) = v(V_0 \vee V_1) - v(V_0 \wedge V_1)$, where both $V_0 \wedge V_1 = V_{01}$ and $v(V_0 \vee V_1) + v(V_0 \wedge V_1) = v(V_0) + v(V_1)$ hold. It follows, $d_{mcs1}(G_0,G_1) = v(V_0) + v(V_1) - 2v(V_0 \wedge V_1) = |V_0| + |V_1| - 2|V_{01}|$.

A.2. Measure spaces

Consider the following definition [28].

Definition A.2. A σ -algebra Σ_X over a set X is a collection of subsets of X that satisfies:

 $(\Sigma 1) \varnothing \in \Sigma_X$, $(\Sigma 1) A \in \Sigma_X$ implies $(X-A) \in \Sigma_X$, and $(\Sigma 3)$ for a collection of sets $A_i \in \Sigma_X$ indexed by a countable indexing set D it follows $(\bigcup_{i \in D} A_i) \in \Sigma_X$.

In words, a σ -algebra includes the empty set and it is closed under both complementation and countable (including finite) unions.

A measure is a set function $m_S: S \to \mathbb{R}^{\geq 0}$, which assigns a size to every "measurable set" element in *S*. Note that a measure m_S is required, by definition, to satisfy: (1) $m_S(\emptyset) = 0$, and (2) for any countable (including finite) indexing set *D*, and any collection of pairwise disjoint sets $A_i \in S$ indexed by $i \in D$ it holds $m_S(\bigcup_{i \in D} A_i) = \sum_{i \in D} m_S(A_i)$. In this work *S* is a σ -algebra, i.e. $S = \Sigma_X$.

A measure space $(X, \Sigma_X, m_{\Sigma_X})$ includes a set X, a σ -algebra Σ_X over X, and a measure m_{Σ_X} over Σ_X . We remark that a probability space is a measure space such that $m_{\Sigma_X}(X) = 1$.

A.3. Metric spaces

Consider the following definition.

Definition A.3. A *metric* in a set *U* is a nonnegative real function $d: U \times U \rightarrow \mathbb{R}^{\geq 0}$, which satisfies the following laws.

- (M0) $d(x,y) = 0 \Rightarrow x = y;$ (M1) d(x,x) = 0;
- (M2) d(x,y) = d(y,x);
- (M3) $d(x,y) \leq d(x,z) + d(z,y)$ (Triangle Inequality).

If only conditions (M1)–(M3) are satisfied in Definition A.3 then *d* is called *pseudo-metric*. A *metric space* is a pair (*U*,*d*) including both a set *U* and a metric $d: U \times U \rightarrow \mathbb{R}^{\geq 0}$.

A.4. Proofs of novel propositions

This section presents the proofs of six novel propositions.

Proposition 2.3. Function $d_a: \Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ such that $d_a(A,B) = 0 \Leftrightarrow A = B$, moreover $d_a(A,B) = (1/(|A||B|))\sum_{i,i}d_X(a_i,b_j)$ is a metric.

Proof. Let $A,B,C \in \Sigma_X$. Real function $d_a(A,B)$ is nonnegative. We show next that function $d_a(A,B)$ satisfies the four laws of a metric (in Definition A.3).

(M0) and (M1) hold by definition.

(M2) $d_a(A, B) = (1/(|A||B|))\sum_{i,j} d_X(a_i, b_j) = (1/(|B||A|))\sum_{j,i} d_X(b_j, a_i) = d_a(B, A).$

(M3) Given $(a_i,b_j) \in A \times B$ it follows $d_X(a_i,b_j) \leq d_X(a_i,c_k)+d_X(c_k,b_j)$, for $c_k \in C$. Summing up for all $c_k \in C$ it follows $\sum_k d_X(a_i,b_j) \leq \sum_k [d_X(a_i,c_k) + d_X(c_k,b_j)] \Rightarrow d_X(a_i,b_j) \leq (1/|C|) \sum_k [d_X(a_i,c_k) + d_X(c_k,b_j)]$. Furthermore, summing up for all pairs $(a_i,b_j) \in A \times B$ it follows $\sum_{i,j} d_X(a_i,b_j) \leq \sum_{i,j} (1/|C|) \sum_k [d_X(a_i,c_k) + d_X(c_k,b_j)]$. Hence,

$$\frac{1}{|A||B|} \sum_{ij} d_X(a_i, b_j)$$

= $d_a(A, B) \leq \frac{1}{|A||B||C|} \sum_{ij,k} [d_X(a_i, c_k) + d_X(c_k, b_j)]$

$$= \frac{1}{|A||C|} \sum_{i,k} d_X(a_i, c_k) + \frac{1}{|C||B|} \sum_{k,j} d_X(c_k, b_j)$$

= $d_a(A, C) + d_a(C, B).$

Proposition 2.4. Function $d_M: \Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ such that $d_M(A,B) = 0 \Leftrightarrow A = B$, moreover $d_M(A,B) = \bigvee_i \bigvee_j d_X(a_i,b_j)$ is a metric.

Proof. Let $A,B,C \in \Sigma_X$. Real function $d_M(A,B)$ is nonnegative. We show next that function $d_M(A,B)$ satisfies the four laws of a metric (in Definition A.3).

(M0) and (M1) hold by definition.

(M2) $d_M(A, B) = \bigvee_i \bigvee_i d_X(a_i, b_i) = \bigvee_i \bigvee_i d_X(b_i, a_i) = d_M(B, A).$

(M3) Let $a_i \in A$, $b_j \in B$, and $c_k \in C$. Apparently, $d_X(a_i,b_j) \leq d_X$ $(a_i,c_k)+d_X(c_k,b_j)$. Since both inequalities $d_X(a_i,c_k) < \lor_i \lor_k d_X(a_i,c_k)$ and $d_X(c_k,b_j) < \lor_k \lor_j d_X(c_k,b_j)$ hold, it follows $d_X(a_i,b_j) \leq \lor_i \lor_k d_X$ $(a_i,c_k) + \lor_k \lor_j d_X(c_k,b_j)$. Furthermore, since the latter inequality holds for any $(a_i,b_j) \in A \times B$ it follows $\lor_i \lor_j d_X(a_i,b_j) \leq \lor_i \lor_k d_X(a_i,c_k) + \lor_k \lor_j d_X(c_k,b_j)$. Hence, $d_M(A,B) \leq d_M(A,C) + d_M(C,B)$. \Box

Proposition 2.6. Condition 2.5 is sufficient for a metric function d_H : $\Sigma_X \times \Sigma_X \to \mathbb{R}^{\geq 0}$ given by $d_H(A, B) = \max\{\forall_i \land_j d_X(a_i, b_j), \forall_j \land_i d_X(b_j, a_i)\}.$

Proof. Let $A,B,C \in \Sigma_X$. Real function $d_H(A,B)$ is nonnegative. We show next that function $d_H(A,B)$ satisfies the four laws of a metric (in Definition A.3).

- (M0) $d_H(A, B) = 0 \Rightarrow \max\{\forall_i \land_j d_X(a_i, b_j), \forall_j \land_i d_X(b_j, a_i)\} = 0$. Therefore, $\forall a_i \in A, \exists b_j \in B: d_X(a_i, b_j) = 0$, and $\forall b_j \in B, \exists a_i \in A: d_X(b_j, a_i) = 0$. Hence, $\forall a_i \in A, \exists b_j \in B$ such that $a_i = b_j$, and $\forall b_j \in B, \exists a_i \in A$ such that $b_j = a_i$. In conclusion, A = B.
- (M1) $d_H(A,A) = \max\{ \bigvee_{a_i \in A} \wedge_{b_i \in A} d_X(a_i, b_j), \bigvee_{b_i \in A} \wedge_{a_i \in A} d_X(b_j, a_i) \} = 0.$
- (M2) $d_H(A, B) = \max\{\forall_i \land_j d_X(a_i, b_j) \lor_j \land_i d_X(b_j, a_i)\} = \max\{\forall_j \land_i d_X(b_j, a_i), \forall_i \land_i d_X(a_i, b_j)\} = d_H(B, A).$
- (M3) Let $a_i \in A$, $b_j \in B$, and $c_k \in C$. Consider, first, Condition 2.5 $d_X(c_{K_i}, b_{J_i}) \leq \max\{\forall_k \land_j d_X(c_k, b_j), \forall_j \land_k d_X(b_j, c_k)\}$, and, second, triangle inequality $d_X(a_i, b_j) \leq d_X(a_i, c_k) + d_X(c_k, b_j) \Rightarrow \land_j d_X$ $(a_i, b_j) \leq \land_k d_X(a_i, c_k) + d_X(c_{K_i}, b_{J_i})$. Hence, $\forall_i \land_j d_X(a_i, b_j) \leq \forall_i \land_k d_X(a_i, c_k) + \forall_i d_X(c_{K_i}, b_{J_i}) \leq \forall_i \land_k d_X(a_i, c_k) + \max\{\forall_k \land_j d_X(c_k, b_j), \forall_j \land_k d_X(b_j, c_k)\}$.

By rotating sets *A* and *B* we obtain $\lor_j \land_i d_X(b_j, a_i) \leqslant \lor_j \land_k d_X(b_j, c_k) + \max\{\lor_k \land_i d_X(c_k, a_i), \lor_i \land_k d_X(a_i, c_k)\}$. Hence, $\max\{\lor_i \land_j d_X(a_i, b_j), \lor_j \land_i d_X(b_j, a_i)\} \leqslant \max\{\lor_i \land_k d_X(a_i, c_k) + \max\{\lor_k \land_j d_X(c_k, b_j), \lor_j \land_k d_X(b_j, c_k)\}, \lor_i \land_k d_X(b_j, c_k) + \max\{\lor_k \land_i d_X(c_k, a_i), \lor_i \land_k d_X(b_j, c_k)\}$

 $d_X(a_i, c_k)$

We consider four cases, next.

(1) Both $\lor_k \land_j d_X(c_k, b_j) \ge \lor_j \land_k d_X(b_j, c_k)$ and $\lor_k \land_i d_X(c_k, a_i) \ge \lor_i \land_k d_X(a_i, c_k)$. Hence, max{ $\lor_i \land_k d_X(a_i, c_k) + \lor_k \land_j d_X(c_k, b_j), \lor_i \land_k d_X(b_j, c_k)$

Hence, $\max\{\forall_i \land_k a_X(a_i, k_k) + \forall_k \land_j a_X(c_k, b_j), \forall_j \land_k a_X(b_j, c_k) + \forall_k \land_i d_X(c_k, a_i)\} \leq \forall_k \land_j d_X(c_k, b_j) + \forall_k \land_i d_X(c_k, a_i).$

(2) Both $\forall_k \land_j d_X(c_k, b_j) \ge \forall_j \land_k d_X(b_j, c_k)$ and $\forall_k \land_i d_X(c_k, a_i) < \forall_i \land_k d_X(a_i, c_k)$. Hence, max $\{\forall_i \land_k d_X(a_i, c_k) + \forall_k \land_j d_X(c_k, b_j), \forall_j \land_k d_X(b_j, c_k)\}$

 $+ \bigvee_{i} \wedge_{k} d_{X}(a_{i}, c_{k}) \} = \bigvee_{i} \wedge_{k} d_{X}(a_{i}, c_{k}) + \bigvee_{k} \wedge_{j} d_{X}(c_{k}, b_{j}), \forall_{j} \wedge_{k} d_{X}(a_{j}, c_{k}) + \bigvee_{k} \wedge_{j} d_{X}(c_{k}, b_{j}).$

- (3) Both $\vee_k \wedge_j d_X(c_k, b_j) < \vee_j \wedge_k d_X(b_j, c_k)$ and $\vee_k \wedge_i d_X(c_k, a_i) \ge \vee_i \wedge_k d_X(a_i, c_k)$. Hence, $\max\{\vee_i \wedge_k d_X(a_i, c_k) + \vee_j \wedge_k d_X(b_j, c_k), \vee_j \wedge_k d_X(b_j, c_k) + \vee_k \wedge_i d_X(c_k, a_i)\} = \vee_i \wedge_k d_X(b_j, c_k) + \vee_k \wedge_i d_X(c_k, a_i)$.
- (4) Both $\vee_k \wedge_j d_X(c_k, b_j) < \vee_j \wedge_k d_X(b_j, c_k)$ and $\vee_k \wedge_i d_X(c_k, a_i) < \vee_i \wedge_k d_X(a_i, c_k)$.

Hence, $\max\{\forall_i \land_k d_X(a_i, c_k) + \forall_j \land_k d_X(b_j, c_k), \forall_j \land_k d_X(b_j, c_k) + \forall_i \land_k d_X(a_i, c_k)\} = \forall_i \land_k d_X(a_i, c_k) + \forall_j \land_k d_X(b_j, c_k).$

In conclusion, $d_H(A,B) = \max\{\forall_i \land_j d_X(a_i, b_j), \forall_j \land_i d_X(b_j, a_i)\} \leqslant \max\{\forall_i \land_k d_X(a_i, c_k) + \max\{\forall_k \land_j d_X(c_k, b_j), \forall_j \land_k d_X(b_j, c_k)\}, \forall_j \land_k d_X(b_j, c_k) + \max\{\forall_k \land_i d_X(c_k, a_i), \forall_i \land_k d_X (a_i, c_k)\}\}$ = $\max\{\forall_i \land_k d_X(a_i, c_k), \forall_k \land_i d_X(c_k, a_i)\} + \max\{\forall_k \land_j d_X(c_k, b_j), \forall_j \land_k d_X(b_j, c_k)\} = d_H(A, C) + d_H(C, B). \square$ **Proposition 3.4.** Let function $\sigma_V: \mathbb{L} \times \mathbb{L} \to [0,1]$ be an inclusion measure in a lattice (\mathbb{L}, \leq) . Then function $\sigma: 2^{\mathbb{L}} \times 2^{\mathbb{L}} \to [0,1]$ given by the convex combination $\sigma(\{u_1, \dots, u_l\} = U \leq W = \{w_1, \dots, w_j\}) = \lambda_1 \max_j \sigma_V(u_1 \leq w_j) + \dots + \lambda_l \max_j \sigma_V(u_l \leq w_j)$ is an inclusion measure.

Proof. First, we prove (by contraposition) the following Lemma.

Lemma: $U \land W < U \Rightarrow \exists i \in \{1, ..., I\}$ such that $\forall j \in \{1, ..., J\}$ it is $u_i \land w_j < u_i$.

Proof of the Lemma: NOT[$\exists i \in \{1,...,I\}$ such that $\forall j \in \{1,...,J\}$ it is $u_i \land w_j < u_i$] $\Rightarrow \forall i \in \{1,...,I\}$, $\exists j \in \{1,...,J\}$ such that $u_i \land w_j = u_i \Rightarrow \forall i \in \{1,...,I\}$, $\exists j \in \{1,...,J\}$ such that $u_i \leqslant w_j \Rightarrow \text{NOT}[U \land W < U]$. It follows, $U \land W < U \Rightarrow \exists i \in \{1,...,I\}$ such that $\forall j \in \{1,...,J\}$ it is $u_i \land w_j < u_i$.

Next, we resume the proof of Proposition 3.4. More specifically, we show that function $\sigma(U \leq W)$ satisfies the four laws of an inclusion measure (in Definition 3.2).

- (10) $\sigma(U \leq 0) = \lambda_1 \max_j \sigma_V(u_1 \leq 0) + \dots + \lambda_I \max_j \sigma_V(u_I \leq 0) = \lambda_1 0 + \dots + \lambda_I 0 = 0.$
- (I1) $\sigma(U \leq U) = \lambda_1 \max_i \sigma_V(u_1 \leq u_i) + \dots + \lambda_I \max_i \sigma_V(u_l \leq u_i) = \lambda_1 + \dots + \lambda_I = 1.$
- (12) From the above Lemma we have $U \wedge W < U \Rightarrow \exists i \in \{1, ..., l\}$ such that $\forall j \in \{1, ..., l\}$ it is $u_i \wedge w_j < u_i$. Hence, $U \wedge W < U \Rightarrow \exists i \in \{1, ..., l\}$ such that $\forall j \in \{1, ..., l\}$ it is $\sigma(u_i, w_j) < 1$. In conclusion, $\sigma(U \leq W) = \lambda_1 \max_j \sigma_V(u_1 \leq w_j) + \dots + \lambda_l \max_j \sigma_V(u_l \leq w_j) < \lambda_1 + \dots + \lambda_l = 1$.
- (13) $U \leqslant W \Rightarrow \forall i \in \{1, \dots, I\}, \exists j \in \{1, \dots, J\}: u_i \leqslant w_j \Rightarrow \sigma_V(x_k \leqslant u_i) \leqslant \sigma_V(x_k \leqslant w_j), \\ \forall k \in \{1, \dots, K\} \Rightarrow \forall k \in \{1, \dots, K\}, \max_i \sigma_V(x_k \leqslant u_i) \leqslant \max_j \sigma_V(x_k \leqslant w_j) \Rightarrow \lambda_1 \max_i \sigma_V(x_1 \leqslant u_i) + \dots + \lambda_K \max_i \sigma_V(x_K \leqslant u_i) \leqslant \lambda_1 \max_j \sigma_V \\ (x_1 \leqslant w_j) + \dots + \lambda_K \max_j \sigma_V(x_K \leqslant w_j) \Rightarrow \sigma(X, U) \leqslant \sigma(X, W). \quad \Box$

Proposition 3.6. Let (L, \leq) be a lattice with an inclusion measure $\sigma: L \times L \rightarrow [0,1]$. Then, function $\mu_{\sigma}: L \times L \rightarrow [0,1]$ given by $\mu_{\sigma}(x,y) = (\sigma(x \leq y) + \sigma(y \leq x))/2$ is a similarity measure.

Proof. We show next that function $\mu_{\sigma}(x,y)$ satisfies the two laws of a similarity measure (in Definition 3.5).

- (S1) $\mu_{\sigma}(x,y) = (\sigma(x \leqslant y) + \sigma(y \leqslant x))/2 = 1 \Leftrightarrow \sigma(x \leqslant y) = 1 = \sigma(y \leqslant x) \Leftrightarrow x \leqslant y \text{ and } y \leqslant x \Leftrightarrow x = y.$
- (S2) $\mu_{\sigma}(x,y) = (\sigma(x \leq y) + \sigma(y \leq x))/2 = (\sigma(y \leq x) + \sigma(x \leq y))/2 = \mu_{\sigma}(y,x).$

Proposition 3.7. Let function $d: U \times U \rightarrow R^{\geq 0}$ be a metric. Then, function $\mu_d: U \times U \rightarrow [0,1]$ given by $\mu_d(x,y) = 1/(1 + d(x,y))$ is a similarity measure.

Proof. We show next that function $\mu_d(x,y)$ satisfies the two laws of a similarity measure (in Definition 3.5).

(S1) $\mu_{d}(x,y) = 1/(1+d(x,y)) = 1 \Leftrightarrow d(x,y) = 0 \Leftrightarrow x = y.$ (S2) $\mu_{d}(x,y) = 1/(1+d(x,y)) = 1/(1+d(y,x)) = \mu_{d}(y,x).$

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