FCA2VEC: Embedding Techniques for Formal Concept Analysis

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Abstract Embedding large and high dimensional data into low dimensional vector spaces is a necessary task to computationally cope with contemporary data sets. Superseding ‘latent semantic analysis’ recent approaches like ‘word2vec’ or ‘node2vec’ are well established tools in this realm. In the present paper we add to this line of research by introducing ‘fca2vec’, a family of embedding techniques for formal concept analysis (FCA). Our investigation contributes to two distinct lines of research. First, we enable the application of FCA notions to large data sets. In particular, we demonstrate how the cover relation of a concept lattice can be retrieved from a computational feasible embedding. Secondly, we show an enhancement for the classical node2vec approach in low dimension. For both directions the overall constraint of FCA of explainable results is preserved. We evaluate our novel procedures by computing fca2vec on different data sets like, wiki44 (a dense part of the Wikidata knowledge graph), the Mushroom data set and a publication network derived from the FCA community.

Keywords: Vector Space Embedding · Covering Relation · Link Prediction · Word2Vec · Complex Data · Formal Concept Analysis · Closed Sets · Low Dimensional Embedding

1 Introduction

A common approach for the study of complex data sets is to embed them into appropriate sized real-valued vector spaces, e.g., \( \mathbb{R}^d \), where \( d \) is a small natural number with respect to the dimension of the original data. This enables the application of the well understood and extensive tool set from linear algebra. The practice is propelled by the presumption that relational and other features from the data will be translated to positions and distances in \( \mathbb{R}^d \), at least up to some extent. Especially relative distances of embedded entities are often meaningful, as shown in seminal works like [15]. For example, in [28] the authors employed

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the addressed embeddings for the complex data kind knowledge graphs (KG). Particularly the authors from [18, 22] demonstrated an embedding of the Wikidata KG [27] in a 100-dimensional model.

The embedding approaches were shown to be successful for many research fields like link prediction, clustering, and information retrieval. Hence, today they are widely applied. Despite that they also do exhibit multiple shortcomings. One of the most pressing is the fact that learned embeddings elude themselves from interpretation [9] and explanation, even though they are conducted in comparatively low dimension, e.g., 100. In our work we want to overcome this disadvantage. We step in with an exploration of the connection of formal concept analysis notions on the one side and proven embedding methods like word2vec or node2vec on the other. Our investigation is two fold and can be represented by two questions: First, how can vector space embeddings be exploited for coping more efficiently with problems from FCA? Secondly, to what extent can conceptual structures from FCA contribute to the embedding of formal context like data structures, e.g., bipartite graphs? In order to deal with the afore mentioned shortcomings, namely the non-interpretable/explainable, we limit our search for results to the posed questions using an additional constraint. We want to utilize only two and three dimensions for the to be calculated real-valued vector space embeddings. By doing so we ensure, at least to some extent, the possibility of some human comprehension, interpretation or even explanation of the results.

Equipped with this problem setting we perform different theoretical and practical considerations. We revisit previous work by Rudolph [24] and propose different models for learning closure operators using neural networks. Conversely to this we develop a natural procedure for improving low dimensional node embeddings using formal concepts. Here we may point out the peculiarity that our approach does not require the otherwise necessary parameter tuning. We evaluate the introduced techniques by experiments on covering relations and link prediction. Finally, we present some first ideas on how to treat, identify and extract functional dependencies (i.e., attribute implications and object implications) using partially learned closure operators.

The following is divided into five sections. First, we start with an overview over related work in Section 2. This will include in particular previous work from FCA. In Section 3 we recollect operations and notations from formal concept analysis and word2vec. The next section contains our modeling which connects the field of FCA with word2vec like approaches. Here we provide some theoretical insights into what aspects of closure operators can be learned through embeddings. This is followed by an experimental evaluation in Section 5 employing three medium sized data sets, i.e., the well known Mushroom context, a dense extract of the Wikidata KG, called wiki44k [12], and a bipartite publication graph consisting of authors in the FCA community.4 We conclude our work with Section 6 providing further research questions to be investigated.

4 The data was extracted from https://dblp.uni-trier.de/ and is part of the testing data set for the formal concept analysis software conexp-clj, which is hosted at GitHub, see https://github.com/tomhanika/conexp-clj/tree/dev/testing-data.
2 Related Work

We will employ in our work learning models based on neural networks, in particular but not limited to, word2vec [15] and derived works like node2vec [10]. To the best of our knowledge there are no previous works on embedding (FCA) closure systems into real-valued vector spaces using a neural network (NN) based learning setting. However, there is an plethora of principle investigations for embedding finite ordinal data in real vector spaces, first of all measurement structures [26] (which we found via [30]). In there the author investigated the basic feasibility of such an endeavor. Along this line of research in the realm of FCA is [29], which is also focused on ordinal structures, in particular ordinal formal contexts. The only FCA related learning model based approach we are aware of was investigated by authors in [5] and uses latent semantic analysis (LSA). Their analysis demonstrates that the LSA learning procedure does lead to useful structures. Nonetheless we refrain from considering LSA for our work. The by us investigated NN procedures posses a crucial advantage over LSA: they are able to cope with incremental updates of the relational data efficiently [20]. In the realm of modern complex data structures, such as Wikidata, this is a necessity. More research in the line of such data structures, namely Resource Description Framework Graphs, was explored by the works [18, 22, 28]. For this the authors use simple as well as sophisticated approaches. The overall goal in these compositions is to provide node similarity corresponding to the underlying relational structure. Since our goal is to excavate and employ a hidden conceptual relation we will develop an alternative NN method for formal context like data. For this we also foster from [24]. In there the author conducts a more fundamental approach for employing NN in the realm of closure systems. Notably, an encoding of closure operators through NN using FCA is presented.

3 Foundations

**Formal Concept Analysis** Before we start with our modeling, we want to recall necessary notions from formal concept analysis. For a detailed introduction we refer the reader to [8]. A formal context is a triple $K := (G, M, I)$, where $G$ represents the finite object set, $M$ the finite attribute set, and $I \subseteq G \times M$ a binary relation called incidence. We say for $(g, m) \in I$ that object $g \in G$ has attribute $m \in M$. In this structure we find a (natural) pair of derivation operators $\cdot' : \mathcal{P}(G) \rightarrow \mathcal{P}(M)$, $A \mapsto A' := \{m \in M \mid \forall g \in A : (g, m) \in I\}$ and $\cdot' : \mathcal{P}(M) \rightarrow \mathcal{P}(G)$, $B \mapsto B' := \{g \in G \mid \forall m \in B : (g, m) \in I\}$. Those give rise to the notion of a formal concept, i.e., a pair $(A, B)$ consisting of an object set $A \subseteq G$, called extent, and an attribute set $B \subseteq M$, called intent, such that $A' = B$ and $B' = A$ holds. The set of all formal concepts ($\mathfrak{B}(K)$) constitutes together with the order $(A_1, B_1) \leq (A_2, B_2) \iff A_1 \subseteq A_2$ a lattice [8], called formal concept lattice and denoted by $\mathfrak{B}(K) := (\mathfrak{B}(K), \leq)$. Throughout this work we consider formal contexts with $\forall g \in G : \{g\}' \neq \emptyset$ and $\forall m \in M : \{m\}' \neq \emptyset$. 
3.1 Word2Vec

We adapt the word2vec approach [15,16] that generates vector embeddings for words from large text corpora. The model gets as input a list of sentences. It is then trained using one of two different approaches: predicting for a target word the context words around it (the Skip-gram model, called SG); predicting from a set of context words a target word (the Continuous Bag of Words model, called CBoW). In detail, word2vec works as described in the following.

Let $\mathcal{V} = \{v_1, \ldots, v_n\}$ be the vocabulary. We identify $\mathcal{V}$ as a subset of the vectorspace $\mathbb{R}^n$ via $\phi : \mathcal{V} \rightarrow \mathbb{R}^n, v_i \mapsto e_i$, the $i$-th vector of the standard basis of $\mathbb{R}^n$. This identification is commonly known under the term one-hot encoding.

The learning task then is the following: Find for a given $d \in \mathbb{N}$ with $d \ll n$ a linear map $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}^d$, i.e., a matrix $W \in \mathbb{R}^{d \times n}$ which obeys the goal: words that appear in similar contexts shall be mapped closely by $\varphi$. The final embedding vectors of the words of the vocabulary are given by the map

$$\Upsilon : \mathcal{V} \rightarrow \mathbb{R}^d, v \mapsto \varphi(\phi(v)).$$  \hfill (1)

To obtain such an embedding, word2vec uses a neural network approach. This network consists of two linear maps and a softmax activation function, cf. Figure 1. The first linear function maps the input from $\mathbb{R}^n$ to $\mathbb{R}^d$, the second one from $\mathbb{R}^d$ back to $\mathbb{R}^n$. In detail, the neural net function has the structure

$$\text{NN} : \mathbb{R}^n \rightarrow \mathbb{R}^n, x \mapsto \text{softmax}(\psi(\varphi(x))),$$  \hfill (2)

where $\varphi : \mathbb{R}^n \rightarrow \mathbb{R}^d$ and $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^n$ are linear maps with corresponding matrices $W \in \mathbb{R}^{d \times n}$ and $U \in \mathbb{R}^{n \times d}$. The activation function softmax is given by

$$\text{softmax} : \mathbb{R}^n \rightarrow \mathbb{R}^n, \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mapsto \frac{1}{\sum_{i=1}^n \exp(x_i)} \begin{pmatrix} \exp(x_1) \\ \vdots \\ \exp(x_n) \end{pmatrix}.$$

The function $\varphi$ is then used in word2vec for creating embeddings of the words $v \in \mathcal{V}$ via Equation (1). If we use the notion of layers, as described in [4], the neural network function is a three-layer network, consisting of an input ($I_L$), hidden ($H_L$), and output layer ($O_L$). In this notation the hidden layer is used to determine the embeddings. We refer the reader again to Figure 1. In the realm of word2vec Mikolov et al. [15] proposed two different approaches to obtain the matrices $W$ and $U$ from input data. Those are called the Skip-gram and the Continuous Bag of Words architecture. We recollect them in the following.

**The Skip-Gram and the Continuous Bag of Words Architecture**

The SG architecture trains the network to predict for a given target word the context words around it. Training examples consist of a target word and a finite sequence of context words. We formalize these as tuples $(t, (c_i)_{i=0}^l) \in \mathcal{V} \times \mathcal{V}^{<\mathbb{N}}$, where $\mathcal{V}^{<\mathbb{N}}$ is the set of finite sequences of elements of $\mathcal{V}$. The SG architecture generates the input-output pairs $(\phi(t), \phi(c_0)), \ldots, (\phi(t), \phi(c_l))$ as training
Figure 1. Left: A generic neural network consisting of 3 layers. Right: The structure of the word2vec architecture. The neural network consists of an input and output layer of size $n$ and a hidden layer of size $d$, where $d \ll n$.

Examples, where $\phi$ is the one-hot encoding function, as introduced above. In the CBOW model, in contrast to SG, the training pairs are generated differently from $(t,(c_i))_{i=0}^l$. We take the middle point of the list of vectors $\phi(c_0), \ldots, \phi(c_l)$ and try to predict the target word $\phi(t)$, hence the generated input-output training pair is $(\frac{1}{l} \sum_{i=0}^{l} \phi(c_i), \phi(t))$. Both architectures employ the same kind of a loss function to learn the weights of $W$ and $U$. The error term is computed through cross-entropy loss. The backpropagation is done via stochastic gradient descent. A detailed explanation can be found in [23].

In word2vec, the pairs of target word and context words are generated from text data sequences, i.e., lists of sentences. The word2vec approach has a window size $m \in \mathbb{N}$ as parameter, i.e., for a given sentence $s = (w_i)_{i=0}^l \in \mathcal{V}^{<} \mathbb{N}$ pairs of target word and context word sequences are defined in the following manner. For every $i \in \{0, \ldots, l\}$ a reduced window size $m_i \in \{0, \ldots, m\}$ is chosen randomly and the pair $(w_i, (w_{i+k})_{k=-m_i, k \neq 0})$ is used as target word context word sequence pair. Of course, $m_i$ is to be chosen reasonable with respect to $l$.

Note, in the case of word embeddings, the size of the vocabulary often reaches a level where computing the softmax is computationally infeasible. Hence, the softmax layer is often approximated/replaced by one of the two following approaches. The hierarchical softmax [17] stores the elements of the vocabulary in a binary Huffman tree and then only uses the values to the path to an element to compute its probability. Another approach presented in [16] is negative sampling, which uses the sigmoid function. In the experimental part of this work we deal with formal contexts of a size where applying the softmax layer is possible.

4 Modeling

This section is split in two parts following the two mentioned research directions. In the first part we demonstrate how embeddings can be used in order to retrieve (classical) FCA relevant features from data. We will discover that different aspects of closure operators can be encoded into real-valued vector space embeddings through neural network techniques. In particular, we are looking at covering relations as well as canonical bases. In the second part we propose a straightforward approach for embedding objects and attributes with respect to their conceptual structure. While the first part deviates from the classical word2vec approach due to theoretical considerations, the second part translates
FCA notions to the word2vec model. Both investigations are governed by the overall goal from FCA to create explainable methods. To this end we apply for all our methods only low dimensional embeddings, i.e., two or three dimensions. Hence, these embeddings comprise the potential for human interpretability or even explainability, in contrast to high dimensional ones.

4.1 Retrieving FCA Features Through Closure2Vec

The goal of this section is to employ the ideas from word2vec to improve the computational feasibility of common tasks in the realm of Formal Concept Analysis. Doing so, we analyze different approaches and finally settle with a novel embedding technique that can provide more efficient computations. In particular, we consider the FCA problems of finding the covering relation of the concept lattice structure and the rediscovering of canonical bases. The linchpin of our investigation is the encapsulation of the closure operator of a formal context. analogue to the approach of word2vec we want to achieve a meaningful embedding of the closure operator into \( \mathbb{R}^d \) for \( d = 2 \) or \( d = 3 \). For the rest of this part we assume that for both, the attribute set and the object set are indexed, i.e., for some context \((G, M, I)\) we denote the object set by \( G = \{g_1, g_2, \ldots \} \) and the attribute set by \( M = \{m_1, m_2, \ldots \} \). This enables the possibility for defining the binary encoding of an object set \( A \) as the vector \( v \in \{0, 1\}^{|M|} \), with the \( v_i = 1 \) if and only if \( m_i \in A \). Dually this can be done for attribute sets.

Exact Representation of the Closure Operator Thanks to a previous work by S. Rudolph [24], we are aware that it is possible to represent any closure operator on a finite set into a neural network function using formal concept analysis. The network, as proposed in [24], consists of an input layer \( I_L := \{0, 1\}^{|G|} \), a hidden layer \( H_L := \{0, 1\}^{|M|} \) as well as an output layer called \( O_L := \{0, 1\}^{|M|} \). The mapping between \( I_L \) and \( H_L \) is defined as \( \phi = t \circ w \) consisting of a linear mapping \( w \) with transformation matrix \( W = (w_{jh}) \in \{-1, 0\}^{|M|\times|M|} \), such that

\[
    w_{jh} := \begin{cases} 0 & \text{if } (g_j, m_h) \in I, \\ -1 & \text{otherwise}, \end{cases}
\]

and a non-linear activation function \( t : \mathbb{R}^{|G|} \rightarrow \mathbb{R}^{|G|} \) with each component being mapped using the function \( \hat{t} : \mathbb{R} \rightarrow \{0, 1\} \) defined as

\[
    \hat{t}(x) = \begin{cases} 1 & x = 0, \\ 0 & x < 0. \end{cases}
\]

The mapping between \( H_L \) and \( O_L \) is defined analogously by \( \psi = \hat{t} \circ \hat{w} \), where once again \( \hat{w} \) is a linear mapping with transformation matrix \( W = W^T \). The function \( \hat{t} : \mathbb{R}^{|M|} \rightarrow \mathbb{R}^{|M|} \) is once again defined component wise with each component being \( \hat{t} \). Using this construction the function \( \phi \circ \psi \) encapsulates the closure operator. To find the closure of some attribute set \( B \subseteq M \), one has to
compute $\varphi \circ \psi$ of its binary encoding. Similar to the both derivation operators introduced in Section 3 does the mapping $\varphi$ compute the attribute derivation and the mapping $\psi$ the object derivation, both in their binary encoding.

Considering the Unconstraint Problem Considering the well established word2vec architecture the following idea seems intuitive. Take the neural network layers as defined in Rudolph’s architecture, but replace the hidden layer by a layer containing either two or three dimensions, i.e., we have $H_L = \mathbb{R}^d$. Instead of presetting $\varphi$ and $\psi$, as in the last section, we want to retrieve them through machine learning. However, it may be noted that it is not meaningful to allow arbitrary functions. To see this, consider the following example with $d = 1$. Let $s : \{0, 1\}^{|M|} \to \mathbb{N}$ be an injective mapping from the set of binary vectors of length $|M|$ to the natural numbers. Naturally there is an inverse map $s^{-1} : \{0, 1\}^{|M|} \to \{0, 1\}^{|M|}$, where $s[\{0, 1\}^{|M|}]$ denotes the image of $s$ of the domain. Since $\mathbb{N}$ is contained in $H_L$, we may find a natural continuation of $s^{-1}$ to $\mathbb{R}$ by $s^{-1} : \mathbb{R} \to \{0, 1\}^{|M|}$ such that $s^{-1}(x) := s^{-1}([x])$. Furthermore, let $cl$ be the double application of the derivation operator, i.e., $(\cdot)'$ in the binary encoding. Using this setup let $\varphi := s$ and $\psi := s^{-1} \circ cl$. Using these function one can easily see that even though the neural network is able to compute the closure operator, the layer $H_L$ contains no information about the formal context. This suggests that the set of possible functions has to be further constrained.

Representing Closure Operators Using Linear Functions Rudolph’s approach for representing a closure operator by a neural network function is sound and complete. It consists, as discussed of two linear functions and two non-linear activation functions. The later, however, is incompatible with the neural network proposed by word2vec. This procedure, as noted in Section 3.1, does consist of a linear map $\varphi$ from $I_L$ to $H_L$, which is also the final embedding we are looking for in our work. Note that it is not possible to represent a closure operator using a linear function, since the closure of the empty set is not necessary an empty set. The same fact is true for affine mappings, as showed in the following.

**Proposition 1.** Let $(G, M, I)$ be a formal context. The set of all affine linear mappings, which represent the closure operator on the attribute set in binary encoding, can be empty.

**Proof.** Consider the formal context from Figure 2. For the sake of simplicity we speak about attribute and object sets and their respective binary encodings
interchangeably. Assume that there is an affine mapping, which maps each attribute set to its closure. Then there is a linear mapping \( l \), such that for each attribute set \( v \in \{0, 1\}^{\mid M \mid} \) the vector \( v' = [1 \ v] \) is mapped to the closure of \( v \). Here \([1 \ v]\) denotes the vector which results from the concatenation of a single bit (valued 1) with \( v \). Using this one can infer that from

\[
\begin{align*}
\{\}\'' &= \{a, b, c\}' = \{
\{3\}'' &= \{a, b\}' = \{3
\{1, 2\}'' &= \{\}' = \{1, 2, 3
\{1, 2, 3\}'' &= \{\}' = \{1, 2, 3
\end{align*}
\]

follows that

\[
\begin{align*}
l(1, 0, 0, 0) &= (0, 0, 0)
l(1, 0, 0, 1) &= (0, 0, 1)
l(1, 1, 1, 0) &= (1, 1, 1)
l(1, 1, 1, 1) &= (1, 1, 1).
\end{align*}
\]

However, as \( l \) is a linear mapping, it is required that the following holds.

\[
l(1, 1, 1, 1) = l(1, 1, 1, 0) + l(1, 0, 0, 1) - l(1, 0, 0, 0)
\]

\[
= (1, 1, 1) + (0, 0, 1) - (0, 0, 0)
\]

\[
= (1, 1, 2),
\]

Hence, we obtain a contradiction. \( \square \)

**Corollary 1.** Let \((G, M, I)\) be a formal context. The set of all affine linear mappings, which represent the derivation operator on the attribute set in binary encoding, can be empty.

**Proof.** Assume there is such an affine linear map \( a \). By duality we know that there must be an affine linear map \( a^d \) on the object set. A suitable composition of those mapping, i.e., using augmentation, contradicts with Proposition 1. \( \square \)

**Linear Representable Part of Closure Operators** We know from the last section that it is neither possible to represent the closure operator nor the derivation operator using an affine linear function. Still, it might be possible to obtain a meaningful approximation of an embedding using a linear map. In order to obtain some empirical evidence if studying this approach is fruitful we conduct a short experiment. Consider the neural network architecture as depicted in Figure 1 (left). Furthermore, let the input layer \( I_L \) of size \( |M| + 1 \) be connected to a hidden layer \( H_L \) of low dimension, i.e., two or three, by a linear function \( \varphi \). The layer \( H_L \) is connected to the output layer \( O_L \) that is of dimension \( M \) using a function \( \psi \) that consists of a linear function together with a sigmoid activation function. The first bit of \( I_L \) is always set to 1 and therefore a so-called bias unit.
For our experiment we now train the neural network by showing it randomly sampled attribute sets as inputs and their attribute closures as output, both in their binary encoding. We employ for this mean squared error as the loss function and a learning rate of 0.001. Even though the neural network starts to memorize the samples it has seen after around 20 epochs, it does not generalize to attribute sets not previously seen in training. Furthermore, the resulting embedding into $\mathbb{R}^d$ does empirically not expose a meaningful structure. Additionally, this observation does not alter by changing the function $\psi$ to a linear function. Also, experiments in which we investigated learning only the derivative operator were not fruitful. This is the expected behavior from our considerations in the last section. We do not claim that there are no better performing, approaches for this task. However, for us this result motivate a progression to different task.

**Non-linear Embedding through Closure2Vec** As linear embeddings do not seem to work out for our learning task, we employ a different approach. Let the closure Hamming distance (chd) for two attribute sets $A \subseteq M$ and $B \subseteq M$ be the distance function $d(A, B) := d_H(A^b, B^b)$, where $A^b$ denotes the binary representation and $d_H$ is the Hamming distance. Note that the closure Hamming distance is not a metric, as the distance between two attribute sets sharing the same closure is 0, even though they are not the same. Based on the idea that two attribute sets are similar if they have a small chd, we want to embed the attribute sets into a low-dimensional real-valued space, i.e., two or three dimension. The goal here is that the embedding is approximately an isometric map.

We train a neural network architecture that we call closure2vec to learn the just introduced chd. For this, consider the network depicted in Figure 3. It consists of two input layers $I_L$ and $I'_L$, each of size $|M|$. Then the function $\varphi$ consisting of a linear function and a relu-activation function (see [14]) is used to feed the data into the hidden layers $H_L$ and $H'_L$ respectively, both of size $|G|$. After this the function $\psi$, consisting of a linear function and a relu-activation function is applied to the two “streams” in the network. The result then is input for two output layers $O_L$ and $O'_L$, both of size $|M|$. This, however is not the...
final step of this network model. Finally, the layers $E_L$ and $E'_L$, which consist of either two or three dimensions, are fed from $O_L$ and $O'_L$, respectively, via $\rho$. This function is again build via composing a linear function and another relu-activation function. The output layer $D_L$ consists has size one. Using a fixed function $\delta$ (in our case either the Euclidean distance or cosine distance) we compute a distance between $O_L$ and $O'_L$. By sharing the functions $\varphi$, $\psi$, and $\rho$ between the different layers we ensure that a commutation of the input sets does not lead to a different prediction of the neural network.

The network then is trained by showing it two attribute sets in binary encoding as well as their closure Hamming distance at the output layer. The required loss function for this setup is then the mean squared error. The learning rate of our network is set to 0.001. The training set for our approach is sampled as follows: For some $t \in \mathbb{N}$ take all attribute combinations that contain at most $t$ elements and put them in some set $\mathcal{X} = \{X_1, X_2, \ldots\}$, hence, $X_i \subseteq M$. For each $X_i \in \mathcal{X}$ generate a random attribute $m_i \in M$. Let the set $\mathcal{Y} = \{Y_1, Y_2, \ldots\}$ with

$$Y_i = \begin{cases} X_i \setminus \{m_i\} & \text{if } m_i \in X_i, \\ X_i \cup \{m_i\} & \text{else,} \end{cases}$$

and finally $Z = \{z_i := d(X_i, Y_i)/|M| \mid X_i \in \mathcal{X}, Y_i \in \mathcal{Y}\}$ as the set of pairwise closure Hamming distances. The network is trained by showing it the binary encodings of $X_i$, $Y_i$, and $z_i$. Note, the values of $Z$ are normalized. We will evaluate this setup in Section 5.2 on different data sets and for relevant notions of FCA.

4.2 Object2Vec and Attribute2Vec

The idea of adapting word2vec to non-text mining problems is a common approach these days. Particular examples for that are node2vec [10] and deepwalk [21]. In the realm of networks it was shown that SG based architectures for node embeddings can beat former approaches that use classic graph measures. They significantly enhanced node classification and link prediction [10,21] tasks. To do so, they interpret nodes as words for their vocabulary, random walks through the graphs to generate “sentences”, and then employ word2vec.

Analogously, we transfer word2vec to the realm of formal concept analysis. In the following we present an approach to use the concepts of a given formal context to generate embeddings of the object set or attribute set. Referring to its origin, we name our novel methods object2vec and attribute2vec, respectively. Since both methods will emerge to be dual to each other for obvious reasons we only consider object2vec in the following. The basic idea is to interpret two objects to be more close to each other, if they are included in more concept extents together. Hence, the set of extents of a formal context is used to generate a low dimensional embedding of the object set $G$.

In the following we explain how to adapt the CBoW and the SG architecture to the realm of formal concept analysis. We show how to generate (multi-) sets of training examples from a given formal context. As an analogon for target word context words we introduce target object and context object sets. From this we can draw pairs as already done in CBoW and SG.
SG and CBoW in the Realm of Object2Vec Let $\mathcal{K} := (G, M, I)$ be a (finite) formal context. The vocabulary is given by $G = \{g_1, \ldots, g_n\}$. Furthermore, let $\phi : G \to \mathbb{R}^n, g_i \mapsto e^i$ the one-hot encoding of our vocabulary (objects). We derive our training examples from the set

$$
T(\mathcal{K}) := \{(a, A \setminus \{a\}) \mid a \in A, |G| > |A| > 1, \exists B \subseteq M : (A, B) \in \mathcal{B}(\mathcal{K})\},
$$

where every element is a pair of a target object and some extent in which $a$ is element of. More specifically, we remove $a$ from this extent. We interpret then $A \setminus \{a\}$ as the object context set. The word “context” here refers to the word2vec approach and is not be confused with “formal context”. Note that we do not generate any training examples from the concept $(G, G')$ since the extent $G$ does not provide any information about the formal context.

The Skip-gram Architecture for Object2Vec In the SG model, the input and output training pairs generated from a target object and an object context set, i.e., the elements $(t, C) \in T(\mathcal{K})$, are given by:

$$
T_{SG}(t, C) := \{ (\phi(t), \phi(c)) \mid c \in C \}. \quad (3)
$$

Using this it is possible for some pairs $(t_1, C_1), (t_2, C_2) \in T(\mathcal{K})$ where we have $(t_1, C_1) \neq (t_2, C_2)$ that $T_{SG}(t_1, C_1) \cap T_{SG}(t_2, C_2) \neq \emptyset$. Hence, samples can be generated multiple times in this setup. We account for this in our modeling, as the reader will see in the presentation of the algorithm. To give an impression of our modeling we furnish the following example.

**Example 1.** Consider the classical formal context from [8] called “Living beings and Water”, which we depicted in Figure 4. We map the objects with the one-hot encoding: $\phi : G \to \mathbb{R}^8$, with $\phi(a) = e^1, \phi(b) = e^2, \ldots, \phi(h) = e^8$. Using this we easily find a training sample from $T_{SG}$ which is generated two times. Consider the concepts $(\{a, f, g\}, \{4, 5, 6\})$ and $(\{f, g, h\}, \{5, 6, 7\})$. The first concept generates the pairs of target object and object context sets $(a, \{f, g\})$ as well as $(f, \{a, g\})$ and $(g, \{a, f\})$. The second formal concept generates the pairs $(f, \{g, h\})$, $(g, \{f, h\})$ and $(h, \{f, g\})$. If we train in the SG architecture we derive from the pair $(f, \{a, g\})$ the training examples $(e^6, e^1)$ and $(e^6, e^7)$. Also, from the pair $(f, \{g, h\})$ we derive the examples $(e^6, e^7), (e^7, e^8)$. Hence, the training example $(e^6, e^7)$ is shown to be drawn at least twice per epoch.

The CBoW Architecture for Object2Vec Analogously to the cases of CBoW in word2vec we will use for object2vec a notion of “middle point” for object context sets. More specifically, for a pair of target object and object context set $(t, C) \in T(\mathcal{K})$ the training example is derived as follows:

$$
T_{CBoW}(t, C) := \left( \frac{1}{|C|} \sum_{c \in C} \phi(c), \phi(t) \right)
$$

Hence, in the CBoW model the set of all training examples is given by

$$
T_{CBoW}(\mathcal{K}) := \{ T_{CBoW}(t, C) \mid (t, C) \in T(\mathcal{K}) \}. \quad (4)
$$
Figure 4. Formal context of the classical “Living beings and Water” example from [8].

Lemma 1. The map $T_{\text{CBOW}} : T(\mathbb{K}) \to \mathbb{R}^2, (t, C) \mapsto \left( \frac{1}{|C|} \sum_{c \in C} \phi(c), \phi(t) \right)$ is injective.

Proof. Let $E_n$ be the set of standard basis vectors. We first show that

$$f : 2^{E_n} \to \mathbb{R}^n, E \mapsto \frac{1}{|E|} \sum_{e \in E} e$$

is injective. Let $E_1, E_2 \in 2^{E_n}$ with $E_1 \neq E_2$ where we assume $E_1 \not\subseteq E_2$ w.l.o.g.. Hence, we find $e^i \in E_1 \setminus E_2$. It then follows $f(E_1)_i > 0 = f(E_2)_i$, therefore $f(E_1) \neq f(E_2)$ and $f$ is injective. The function $\phi : G \to E_n$ is also injective, so the map $\Phi : 2^G \to 2^{E_n}, A \mapsto \Phi(A) := \phi[A]$ is also injective. For all $(t, C) \in T(\mathbb{K})$ the equality

$$T_{\text{CBOW}}(t, C) = (f(\Phi(C)), \phi(t))$$

holds. Hence, $T_{\text{CBOW}}$ is injective. \hfill \Box

It follows that the modeling of training samples as set (cf. Equation (4)) is approbate since no training example is derived multiple times from $T(\mathbb{K})$.

Order of the training examples Let $\mathbb{K} := (G, M, I)$ be a formal context. We want to embed the set of objects. Since we model our training examples as sets with frequency (in the case of SG) we need to discuss how to construct a traversable list of training examples for our training procedures. This is not necessary in word2vec where the order is given naturally by the order of the given text. We propose to generate the traversable list in the following manner:

1. For all extents in $A$ of $\mathbb{K}$, construct a list $L_A$ that consists of all elements of $A$. The order in the list $L_A$ should be random.
2. Construct a list $L_{\text{ext}}$ that consists of all lists $L_A$ in a random order.
3. For each $L_A$ use Equation (4) or Equation (3) to add the training examples to the list of all training examples.

We present an algorithmic representation of this course of action in Algorithm 1.
Algorithm 1: The pseudocode of object2vec. The algorithm takes a formal context and an option determining Skip-gram or Continuous Bag of Words. It returns a list of pairs to train the neural network.

**Input**: a formal context \((G, M, I)\) and type \(\in\{SG, CBoW\}\)

**Output**: A list \(L\) of training examples.

1. \(L \leftarrow []\)
2. \(L_{\text{ext}} \leftarrow \text{list-of-extents}(G, M, I)\) in randomized order (excluding \(G\)).
3. \(\forall A \in L_{\text{ext}}\) do
4. \(L_A \leftarrow \text{list}(A)\), with randomized order.
5. \(\forall o \in L_A\) do
6. \(\text{if type} = \text{SG then}\)
7. \(\text{forall } \hat{o} \in L_A: \text{do}\)
8. \(\text{if } o \neq \hat{o} \text{ then}\)
9. \(\text{add } ((\phi(o), \phi(\hat{o}))) \text{ to } L\)
10. \(\text{if type} = \text{CBoW and } |A| > 1 \text{ then}\)
11. \(\text{add } (\frac{1}{|L_A|-1} \sum_{\hat{o} \in L_A, o \neq \hat{o}} \phi(\hat{o}), \phi(o))) \text{ to } L\)
12. return \(L\)

## 5 Experiments

This section contains experimental evaluations for both our research directions. We conduct our experiments on three different data sets. We depict the statistical properties of these data sets in Table 1. A detailed description of each follows.

**wiki44k** The first data set we use in this work is the wiki44k data set taken from [13] and then adapted by [12]. It consists of relational data extracted from Wikidata in December 2014. Even though the it is constructed to be a dense part of the Wikidata knowledge graph, it is relatively sparse for a formal context.

**Mushroom** The Mushroom data set [6, 25] is a well investigated and broadly used data set in machine learning and knowledge representation. It consists of 8124 mushrooms. It has twenty two nominal features that are scaled into 119 different binary attributes to form a formal context. The Mushroom data set, compared to wiki44k, is more dense, and even though it has a smaller number of objects, contains 10 times the concepts of wiki44k.

**ICFCA** To generate the ICFCA context, we use the DBLP dump from 2019-08-01 which can be found at [https://dblp.uni-trier.de/xml/](https://dblp.uni-trier.de/xml/). We exclude authors in the DBLP data that have the type “disambiguation” or “group”. As attributes we use all publications of these authors. By all publications we denote all publications present in DBLP, not restricted to ICFCA proceedings. To exclude publication originating from editing etc (which do not indicate any co-authorship) we discard all publications that are not of the type “article”, “inproceedings”, “book”
Table 1. Comparison of the different data sets used in this work. For ICFCA we do only indicate the specification of the context as used for the training in the link prediction model. To compute the canonical base of the ICFCA data set as is not feasible for the equipment at our research group.

|                     | Wiki44k | Mushroom | ICFCA* |
|---------------------|---------|----------|--------|
| Number of Objects   | 45021   | 8124     | 263    |
| Number of Attributes| 101     | 119      | 8442   |
| Density             | 0.04    | 0.19     | 0.005  |
| Number of Concepts  | 21923   | 238710   | 680    |
| Mean attributes per concept | 7.01    | 16.69    | 33.28  |
| Mean objects per concept | 109.47  | 91.89    | 2.51   |
| Size of the Canonical Base | 7040    | 2323     | ?      |

or “incollection”. We also discarded all publications that are marked with an additional “publtype” such as “withdrawn”, “informal” and “informal withdrawn”. Note that this also excludes works that are solely published on preprint servers. This modeling results in a formal context with 351 objects and 12614 attributes. However, as later indicated in the experiments, for the neural network training we will use only a part of that formal context. This part is derived by omitting all publications after 2015 and then considering the largest component. The specifications of the resulting formal context ICFCA* are depicted in Table 1. The ICFCA data set is available in the conexp-clj software [11] for FCA hosted on GitHub. By the nature of being based on a publication network, it is very sparse and contains only 878 concepts.

5.1 Object2Vec and Attribute2Vec

We evaluate our new approaches object2vec and attribute2vec with two distinct experiments. First, we will study embeddings in the realm of link prediction. For this, we investigate a self created publication network as described in the last section, called ICFCA. In this formal context, consisting of authors as objects and publications as attributes, the incidence relation is then given by $g$ is author of $m$. Link prediction tasks can be split into two categories: decide in a network which links are missing or predict from a given temporal network snapshot which new links will occur in the future. In general this experiment evaluates the ability of object2vec to enhance link prediction.

In our second experiment we present a task that is of more general interest to formal concept analysis concerned research. We investigate a correspondence between the canonical base of implication $\mathcal{L}$ for a given formal context $(G, M, I)$ and our embedding methods. In particular, we cluster the set of attributes $M$ based on attribute2vec using a partitioning procedure and obtain a clustering $\mathcal{C}$. We then count the number of implications $A \rightarrow B$ from $\mathcal{L}$ that are in subset relation with a cluster, i.e., $A \cup B \subseteq C$ for some cluster $C \in \mathcal{C}$. With that we

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5 see https://github.com/tomhanika/conexp-clj
evaluate to which extend attribute2vec embeddings are able to reflect parts of the implicational structure from a formal context.

**Link Prediction using Object2Vec** Network embedding techniques like the prominent node2vec approach have proven their capability to predict links in huge networks [10]. Even though these methods employ low dimensional embeddings for their computations, the actual employed dimension is still incomprehensible high for human understanding, i.e., more than 100. The realm of formal concept analysis is especially interested in interpretable and explainable methods. Hence, we focus on embeddings into \( \mathbb{R}^2 \) and \( \mathbb{R}^3 \).

Using the afore described ICFCA data set our goal for the link prediction task is as follows. For learning an embedding we restrict ICFCA to the largest connected component we discover after we omitted all publications later than 2015. The prediction task then is to find future co-authorships. More specifically, we predict these co-authorships in the time interval from 2016-01-01 until 2019-08-01. We compare the introduced object2vec using both architectures, i.e., CBOW and SG, and compare the results with link prediction computed via node2vec. We may note that the node2vec embeddings are conducted in two and three dimensions as well. Our precise experimental pipeline looks as follows.

**Compute an embedding via object2vec** We first compute an embedding of the formal context with the object2vec approach. For the training of the neural network we use a starting learning rate of 1.0 with linear decrease. We train for 200 epochs. We repeat the embedding process for 30 times.

**Compute the node2vec embedding** The node2vec embedding uses the parameters as used in [10], i.e., 10 walks per node with length 80 and a window size of 10. We use the standard learning rate of 0.025 as well as 1.0 for comparability reasons with respect to object2vec. However, we do not report the results for 1.0 since they were worse for the two and three dimensional case. We also repeat the embedding process for 30 times. The procedure parameters \( p \) and \( q \) of node2vec are chosen by grid search in \( \{0.25, 0.5, 1, 2, 4\} \).

**Edge vector generation** Since link prediction is concerned with edges we need to focus on the edge set. To generate the edge vectors from the node embedding we use the componentwise product of two node vectors. In [10] it was shown that this practice is favorable. Furthermore, in the special case of bibliometric link prediction this is the common approach, cf. [7].

**Training examples** Our learning procedure demands for training examples. The positive training examples are the edges in the co-author graph until (including) 2015. For each positive example, we select one negative example, i.e., two randomly picked nodes without an edge connecting them. This approach leads to 1278 training examples.

**Test examples** The positive examples are the author pairs which have an edge after 2016-01-01, but not before. For each such pair, we choose one negative example of two authors that neither co-authored before or after 2016. Using this we obtain 84 test examples, half of them positive.
Classification For the binary classification problem, we employ logistic regression. In particular, we use the implementation provided by Scikit Learn [19]. Logistic regression is often used in classification emerging from embeddings in the realm of word2vec, e.g., in [10, 21]. To determine the C parameter of the classifier, we do a grid search over \( \{10^{-3}, 10^{-2}, \ldots, 10^2\}\).

The results of our experiments are depicted in Table 2. We observe that in all three indicators, i.e., recall, precision and F1-Score, node2vec is dominated by the object2vec approach. Furthermore, we see that the CBoW architecture performs better compared to SG in almost all cases. However, this benefit is small and well covered in the standard deviation. Finally, we find that embeddings in three dimensions perform in generally better than in two.

Clustering Attributes with Attribute2Vec In FCA, implications on the set of attributes of a formal context are of major interest. While computing the canonical base, i.e., the minimal base of the implicational theory of a formal context, is often infeasible, one could be interested in implications of smaller attribute subsets. This leads naturally to the question of how to identify attribute subsets that cover a large part of the canonical base, as explained in the beginning of Section 5.1. In detail, the resulting task is as follows: Let \((G, M, I)\) be a formal context and \(\mathcal{L}\) the canonical base \((G, M, I)\). Using a simple clustering procedure (in our case \(k\)-means), find a for a given \(k \in \mathbb{N}_0\) partitioning of \(M\) in \(k\) clusters such that the ratio of implications completely contained in one cluster (cf. Section 5.1) is as high as possible. We additionally constraint this task by limiting clusterings in which the largest cluster is significantly smaller than \(|M|\).

We investigate to which extend our proposed approach attribute2vec maps attributes closely that are meaningful for the afore mentioned task. We conduct this research by computing an embedding via attribute2vec and run the \(k\)-means clustering algorithm on top of it. We evaluate our approach on the introduced wiki44k data set. Again, we refer the reader to the collected statistics of this data set in Table 1. The experimental pipeline looks as follows.

Table 2. The result of our classification experiment. We compare node2vec to object2vec with the Skip-gram architecture (O2V-SG) and with the object2vec Continuous Bag of Words architecture (O2V-CBoW). We display the mean value over the 30 rounds of the experiments and also present the sample standard deviation.
Applying attribute2vec on wiki44k We start by computing two and three dimensional vector embeddings of the wiki44k attributes using attribute2vec. We employ both architectures, SG and CBoW. Here we use again the learning rate of 1.0. In contrast to the embeddings of the ICFCA data set we find that 5 training epochs are sufficient for stabilization of the embeddings.

K-means clustering We use the computed embedding to cluster our attributes with the k-means algorithm. As implementation we rely on the Scikit Learn software package. For the initial clustering, we use the so called “k-means++” technique by [3]. The method from Scikit Learn runs internally for ten times with different seeds and returns the best result encountered. We choose k from \{2, 5, 10\}. We denote the resulting clustering with C.

Computation of the intra-cluster implications An implication drawn from the canonical base, i.e., \(A \rightarrow B \in \mathcal{L}\), is called intra-cluster if there is some \(C \in \mathcal{C}\) such that \(A \cup B \subseteq C\). The canonical base of wiki44k has the size 7040. For a clustering \(\mathcal{C}\) we compute the ratio of intra-cluster implications.

Repetition We repeat the steps above for 20 times. Hence, we report the mean as well as the standard deviation of all the results.

Baseline clusterings To evaluate the ratios computed in the last step we use the following baseline approaches. As a first baseline we make use of a random procedure. This results in a random clustering of the attribute set. Using an arbitrary random clustering with respect to cluster sizes is unreasonable for comparison. Hence, for each k-means clustering obtained above we generate 50 random clusterings of the same size and the same cluster size distribution. For those we also compute the intra-cluster implication ratio.

Naive k-means clustering As second baseline we envision a more sophisticated procedure. We call this the “naive” clustering approach. In this setting we encode an attribute \(m\) through a binary vector representation using the objects from \(\{m\}'\) as described in Section 4.1. We then run twenty rounds of k-means and compare the results with the attribute2vec approach. For comparison we use here again \(k \in \{2, 5, 10\}\).

We display our observations from this experiment in Table 3. In there we omit results for the CBoW architecture since they do not exceed the results obtained in the random baseline approach. As our main result we find that the Skip-gram architecture in three dimensions achieves the best intra-cluster ratio. More specifically, SG outperforms for all cluster sizes and all dimension the baseline approach and the naive clustering approach by a large margin. This margin, however, is smaller in the two dimensional case compared to the three dimensional try. For smallest investigated clustering size, i.e., two, naive clustering performs worse than the random baseline. We can report for our experiments the following average maximum cluster sizes. For dimension three we have 54.5 attributes for \(k = 2\), 33.2 attributes for \(k = 5\), and 14.9 attributes for \(k = 10\). We also spot for clustering sizes five and ten that the naive clustering does operate better than the random baseline. Finally, we note that the stability of the SG result in the \(k = 2\) case sticks out compared to the results of the competition.
Table 3. Results of the clustering task. For the dimensions 2 and 3 we show the mean and sample standard deviation values for the Skip-gram architecture and the random clusters with same cluster size distributions as the corresponding Skip-gram clusterings. We also compared our method with the “naive” clustering approach.

| # clusters | 2     | 5     | 10    |
|------------|-------|-------|-------|
| type       | dim   | mean  | stdev | mean  | stdev | mean  | stdev |
| Skip-gram  | 2     | 0.1608| 0.0031| 0.0703| 0.0122| 0.0069| 0.0004|
| Random     | 2     | 0.0534| 0.0412| 0.0084| 0.0088| 0.0010| 0.0007|
| Skip-gram  | 3     | 0.3217| 0.0005| 0.1028| 0.0218| 0.0080| 0.0001|
| Random     | 3     | 0.0219| 0.0107| 0.0036| 0.0027| 0.0007| 0.0004|
| Naive Clustering | - | 0.0158| 0.0000| 0.0055| 0.0042| 0.0035| 0.0002|

Discussion In both our experiments we find that all embedding procedures perform better in dimension three than in dimension two. This is not surprising since a higher embedding dimension posses a higher degree of freedom to represent structure. Furthermore, in both experiments we can show that the object2vec and attribute2vec approaches do succeed and outperform the competition.

The first experiment reveals some particularities. We find that our embedding approach has a big advantage over the also considered node2vec procedure. For the later method one has to perform additional parameter tuning for the $p$ and $q$ parameters \cite{10} to obtain the presented results. Not doing so leads worse to performance. The object2vec embedding procedure, as defined in Section 4.2, needs no parameters for the training example generation. In addition to that is the set of computed training examples deterministic. However, these positive properties come with a high computational cost, i.e., the necessity of computing the set of formal concepts. For the sake of completeness we also report on high dimensional embeddings. When applying node2vec with embedding dimension one hundred we find the results outperforming the so far reported. Still, since such embeddings conflict with the goal in this work, i.e., the human interpretability and explainability of embeddings, we discard them.

The second experiment also unraveled different properties of our novel embedding technique. We witness that the number of learning epochs is much smaller compared to the first experiment. We suspect that this can be attributed to the higher average number of attributes per intent in wiki44k compared to the average number of objects per extent in ICFCA. Furthermore, we think there is an influence by the fact that the absolute number of intents in wiki44k is greater than the absolute number of extents in ICFCA. As application for our attribute2vec approach we envision the computation of parts of the canonical base of a formal context. Taking the average maximum cluster sizes into account we claim that this application is reasonable. We do not consider the then necessary computation of all formal concepts as an disadvantage. The computation of the canonical base is in general far more complex than computing the set of all concepts and our embedding. We are surprised that the naive clustering baseline
performs not significantly better than the random baseline. We presume that the employed distance function from k-means applied to the binary representation vectors is not useful to reflect implicational knowledge in the embedding space. Hence, we admit that more powerful base line comparisons may be considered here. However, so far we are not aware of less computational demanding ones with respect to object2vec and attribute2vec respectively.

5.2 FCA Features Through Closure2Vec

To evaluate the embeddings produced by closure2vec we introduce two FCA related problems: computing the covering relation of a concept lattice and computing the canonical base for a given formal context. The intention here is to rediscover structural features from FCA in low dimensional embeddings. We choose for the dimension two and three in order to respect our overall goal for human interpretability and explainability. We test two different functions $\delta$ for the distance between the output layers $O_L, O'_L$, cf. Section 4.1. More specific, we employ the Euclidean distance and the cosine distance. We conduct our experiments on two larger than average sized formal contexts. Precisely, we test the Wiki44k [12,13] and the well investigated Mushroom data set [6,25]. A comparison of the statistical properties of data sets we use is depicted in Table 1.

Distance of Covering Relation For this experiment we compute first the set of all concepts $B$ of a given formal context $K$. Using the concept order relation $<$ as introduced in Section 3 a covering relation on $B$ is given by: $\prec \subseteq (B \times B)$ with $A \prec B$, if and only if $A < B$ and there is no $C \in B$ such that $A < C < B$. The covering relation is an important tool in ordinal data science. Elements of the covering relation are essential for investigating and understanding order relations and order diagrams. However, in the case of large formal contexts computing the covering relation of the concept lattice can get computationally expensive, as this problem is linked to the transitive reduction of a graph [2].

The experimental setup now is as follows. First we train the neural network architecture as introduced in Section 4.1. Hence, an input element is a binary encoded attribute $X_i$, another binary encoded attribute set $Y_i$ of size $|X_i|\pm 1$, and the closure Hamming distance of them. In our experiment we fix $|X_i|$ to be four or less. Furthermore, we train the network over five epochs using the learning rate 0.001, with batch size 32, and mean-squared-error as loss function.

To evaluate the structural quality of the obtained embedding we computed the covering relation of the concept lattices using 1000 threads on highly parallelized many-core systems, which took about one day. In the following we compare the distances between pairs of concepts in covering relation against concepts that are not in covering relation. The results of these experiments is depicted in Table 4. For all embeddings the expected distance for two concepts in covering relation a significantly smaller than the expected difference of two concepts not in covering relation. This is true for both data sets. However, the observed effect is more notable for the wiki44k data set. The Euclidean distance outperforms the cosine distance in all experiments using two and three dimensions.
Table 4. Distance between concept pairs, that are in covering relation (CR) and that are not in the covering relation (Non-CR).

|                | Wiki44k: |                | Mushrooms: |
|----------------|----------|----------------|------------|
|                | Dim 2    | Dim 3          |            |
|                | Mean: Std.| Mean: Std.     |            |
| Euk: CR:       | 0.17 0.14| 0.16 0.15      |            |
| Non-CR:        | 0.71 0.59| 1.54 1.41      |            |
| Cos: CR:       | 0.63 0.33| 0.15 0.27      |            |
| Non-CR:        | 0.99 0.71| 0.36 0.43      |            |

Distance of Canonical Bases

In this experiment we look at the canonical base of implications for a formal context and try to rediscover this canonical base in the computed embedding. The experiment consists of two different parts. The first part has the following setup. Take an implication of the canonical base, i.e., take \((P, C)\) where \(P \subseteq M\) is the premise and \(C \subseteq M\) is the conclusion. For such an implication, construct all single conclusion implications \((P, c)\) where \(c \in C\). Then, compute the distance (with the same distance functions as used for the embedding process) of \(P\) and the embedding for all \(c\). Additionally, also embed all \(m \in M \setminus C\). Essentially, by doing so, we embedded all \(m \in M\) using our embedding function. We do this for all elements of the canonical base.

Now compute for all implications from the canonical base the following distances. First, the distances between a premise \(P\) and all its singleton conclusions \(c\) of \((P, C)\). Secondly, the distances between \(P\) and \(m \in M \setminus C\). Equipped with all these distances we try to detect a structural difference in favor of the embedded implications in contrast to other combinations of attribute sets, i.e., pairs of premises \(P\) and \(m \in M \setminus C\). When using the cosine distance function we observe minimal to no structural difference. However, when using the Euclidean distance function we detect a significant structural difference. In particular, for pairs of \((P, c)\) with \(c \in C\) the mean of the distances is significantly higher than the mean distance of the distances for some premise \(P\) with all singleton sets \(m \in M \setminus C\).

The observation is even stronger in the case of the Mushroom data set when compared to wiki44k. The results are depicted in Table 5 by the rows S-Imp (for the combinations \((P, c)\)) and Non-S-Imp (for combinations \((P, m)\)).

For the second part we embed both attribute sets, i.e., the premise \(P\) and the conclusion \(C\), for an implication from the canonical base. For every pair we compute the distance of \(P\) and \(C\) and compare them the distance between two randomly generated attribute sets \(X, Y\) with \(|X| = |P|\) and \(|Y| = |C|\). The later
Table 5. Distances of implication premises and conclusions for singleton implications (S-Impl) and implications (Impl) in the computed embeddings.

|             | Wiki44k: |              | Mushrooms: |              |
|-------------|----------|--------------|------------|--------------|
| Dim 2       | Mean: Std.: |              | Mean: Std.: |              |
| Euk: S-Imp: | 0.94 0.28 |              | 0.95 0.41  |              |
| Non-S-Imp:  | 0.73 0.40 |              | 0.45 0.32  |              |
| Imp:        | 0.44 0.33 |              | 0.70 1.01  |              |
| Non-Imp:    | 0.51 0.48 |              | 1.02 0.98  |              |
| Cos: S-Imp: | 1.00 0.69 |              | 1.00 0.65  |              |
| Non-S-Imp:  | 1.00 0.67 |              | 1.00 0.65  |              |
| Imp:        | 1.01 0.70 |              | 1.00 0.69  |              |
| Non-Imp:    | 1.01 0.70 |              | 0.99 0.69  |              |

is set for reasons of comparability. As shown in Table 5 we detect again structural differences for the considered implications and the randomly generated sets using average distances as features. In fact, the distance between the two randomly generated sets is on average larger than the average distance between premises and conclusions from implications drawn from the canonical base.

Discussion In both experiments concerning the closure system embedding we are able to rediscover and infer conceptual structures in the embeddings. In general we find that it is favorable to use for the Euclidean distance case the squares of the closure Hamming distances as output, i.e., for $z_i$. Overall we discovered a significant bias in distances of embedded concepts that are in covering relation. This signal is even stronger for the wiki44k data sets. We suspect that this can be attributed to the lesser density of this data set compared to Mushroom. The observations can be exploited naturally for mining covering relations, or important parts of those, from embedded concept lattices.

For second experiment we can report that the neural network embedding of parts of the closure system allows for rediscovering implicational structures. Since we trained our neural network on attribute sets of size four and smaller,
Dominik Dürrschnabel, Tom Hanika, and Maximilian Stubbemann

Figure 5. Embedding of all concepts of the mushroom dataset into three dimensions. The coloring is done as follows. Left: The edible mushrooms are green, the non-edible mushrooms are red. Middle: The mushrooms with a broad gill are green, the mushrooms with a narrow gill are red. Right: The mushrooms with a crowded gill spacing are green and the mushrooms with a distant gill spacing are red.

we were interested in the number of closures our algorithm encounters. For both data sets we can report that this number is approximately 10% of all closures.

The described a differing behavior for embedding whole implications, i.e., premise and conclusions, and single-conclusion implications. In cases where an attribute is element of the conclusion of some canonical base implication the distance to the premise set is significant. At this point we are unable to provide a rational for that. The same goes for the second part of the experiment where we compare premise-conclusion pairs of canonical base implications with randomly generated pairs of attributes having the same sizes. At this point we are not aware how this observation can improve the computations of the canonical base. This would need a more fundamental investigation of bases of implicational theories with respect to closure system embeddings. For example, one has to investigate if the observed effect is also true for other kinds of bases, e.g., direct basis [1].

As a final remark we report that the Euclidean distance performed in all our experiments better than the cosine distance for both problem settings.

Empirical Structural Observations Additionally to the two experiments above we want to provide some insights we discovered for conceptual structures in our embeddings. We note that concepts sharing attributes seem to result in meaningful clusters. To see this one can consider Figure 5. In there we see the same embedding of all formal concepts of the Mushroom data set in three dimensions for three times. In each case we colored different sets of concepts with red and green. In the first (Figure 5, left) we depict with red the not edible mushrooms and with green the edible ones. Even though we employed a very low dimensional embedding, we can still visually identify the two different classes. Hence, our embedding approach preserved some structure. The same seems true for the other depictions in which we colored broad gill versus narrow gill and crowded gill spacing versus distant gill spacing. Therefore, we are confident that our approach for low dimensional embeddings of closure systems using neural networks is beneficial. Moreover, as this empirical study shows, is the low dimensional representation still visitable by a human data analyst.
6 Conclusion

In this work we presented fca2vec, a first approach for modeling data and conceptual structures from FCA to the realm of embedding techniques based on word2vec. Taken together, the ideas in this paper outline an appealing connection between formal concepts, closure systems, low dimensional embeddings, and neural networks learning procedures. We are confident that future research may draw on the demonstrated first steps, in particular object2vec, attribute2vec and learning closure operator representations. In our investigation we have found convincing theoretical as well as experimental evidence that FCA based methods can profit from word2vec like embedding procedures. We demonstrated that closure operator embeddings that result from simple neural network learning algorithms may capture significant portions of the conceptual structure. Furthermore, we were able to demonstrate that the cover relation of the set of formal concepts may be partially extracted from a low dimensional embedding. Especially when employing conceptual structures in large and complex data this notion is an important step forward. Moreover, we were able to enhance the common embedding approach node2vec in low dimensional cases, i.e., dimension two or three.

All these results were achieved while obeying the constraint for human interpretable and/or explainable embeddings. Applying neural network learning procedures on large and complex data does not necessarily constitute a contradiction to explainability when combined with conceptual notions from FCA. However, our work clearly has some limitations. The ideas for object2vec and attribute2vec do require the computation of the concept lattice. In future work we will investigate if this obligation can be weakened through statistical methods. Despite this we believe that our work could be the standard framework for word2vec like FCA approaches. As a next concrete application we are currently in the process of investigating genealogy graphs in combination with co-authorship networks. These multi-relational data sets are large and complex and do require novel methods, like fca2vec, to draw knowledge from them. Questions for the relation of particular nodes in such data sets may be answered through conceptual embeddings. In this context we do also take Resource Description Framework (RDF) structures into account. Ideas for embedding those is a state of the art approach to knowledge graph structures. Hence, enhancing RDF embeddings using fca2vec as well as discovering conceptual structures in RDF is a fruitful endeavor. Finally, on a more technical note we are interested in characterizing sets of formal context data allowing for particular representations of the closure operator, e.g., closure operators representable by affine maps.

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