We show analytically that removing sigmoid transformation in the SGNS objective does not harm the quality of word vectors significantly and at the same time is related to factorizing a binarized PMI matrix, which, in turn, can be treated as an adjacency matrix of a certain graph. Empirically, such graph is a complex network, i.e. it has strong clustering and scale-free degree distribution, and is tightly connected with hyperbolic spaces. In short, we show the connection between static word embeddings and hyperbolic spaces through the binarized PMI matrix using analytical and empirical methods.

1. Introduction

Modern word embedding models (McCann et al. 2017; Peters et al. 2018; Devlin et al. 2019) build vector representations of words in context, i.e. the same word will have different vectors when used in different contexts (sentences). Earlier models (Mikolov et al. 2013b; Pennington, Socher, and Manning 2014) built the so-called static embeddings: each word was represented by a single vector, regardless of the context in which it was used. Despite the fact that static word embeddings are considered obsolete today, they have several advantages compared to contextualized ones. Firstly, static embeddings are trained much faster (few hours instead of few days) and do not require large computing resources (1 consumer-level GPU instead of 8–16 non-consumer GPUs). Secondly, they have been studied theoretically in a number of works (Levy and Goldberg 2014b; Arora et al. 2016; Hashimoto, Alvarez-Melis, and Jaakkola 2016; Gittens, Achlioptas, and Mahoney 2017; Tian, Okazaki, and Inui 2017; Ethayarajh, Duvenaud, and Hirst 2019; Allen, Balazevic, and Hospedales 2019; Assylbekov and Takhanov 2019; Zobnin and Elistratova 2019) but not much has been done for the contextualized embeddings (Reif et al. 2019). Thirdly, static embeddings are still an integral part of deep neural network models that produce contextualized word vectors, because embedding lookup matrices are used at the input and output (softmax) layers of such models. Therefore, we consider it necessary to further study both static and contextualized embeddings. It is noteworthy that with all the abundance of both theoretical and empirical studies on static vectors, they are not fully understood, as this work shows. For instance, it is generally accepted that good quality word vectors are inextricably linked with a low-rank approximation of the pointwise mutual information (PMI) matrix, but we show that vectors of comparable quality can also be obtained from a low-rank approximation of a binarized PMI matrix, which is a rather strong roughening of the original PMI matrix (Section 2). Thus, a binarized PMI matrix is a viable alternative to a standard PMI matrix when it comes to obtaining word vectors. At the same time, it is much easier to interpret the binarized PMI matrix as an adjacency matrix for a certain graph. Studying the properties of such a graph, we come to the conclusion that it is a so-called complex network, i.e. it has a strong clustering property.
and a scale-free degree distribution (Section 3). It is noteworthy that complex networks, in turn, are dual to hyperbolic spaces (Krioukov et al. 2010), which were previously used to train word vectors (Nickel and Kiela 2017; Tifrea, Bécigneul, and Ganea 2018) and have proven their suitability — in hyperbolic space, word vectors need lower dimensionality than in Euclidean space. Thus, to the best of our knowledge, this is the first work that establishes simultaneously a connection between good quality word vectors, a binarized PMI matrix, complex networks, and hyperbolic spaces. Figure 1 summarizes our work and serves as a guide for the reader.

2. BPMI and Word Vectors

A well known skip-gram with negative sampling (SGNS) word embedding model of Mikolov et al. (2013b) maximizes the following objective function

$$\sum_{i \in W} \sum_{j \in W} \#(i,j) \left( \log \sigma(\langle w_i, c_j \rangle) + k \cdot E_{j \sim p}[\log \sigma(-\langle w_i, c_j \rangle)] \right),$$  \hspace{1cm} (1)
where \( \sigma(x) = \frac{1}{1 + e^{-x}} \) is the logistic sigmoid function, \( p \) is a smoothed unigram probability distribution for words\(^1\), and \( k \) is the number of negative samples to be drawn. Interestingly, training SGNS is approximately equivalent to finding a low-rank approximation of a shifted PMI matrix (Levy and Goldberg 2014b) in the form \( \log \frac{p(i,j)}{p(i)p(j)} \approx \langle w_i, c_j \rangle + \log k \), where the left-hand side is the \( ij \)-th element of the \( n \times n \) PMI matrix, and the right-hand side is an element of a matrix with rank \( \leq d \) since \( w_i, c_j \in \mathbb{R}^d \). This approximation was later re-derived by Arora et al. (2016); Assylbekov and Takhanov (2019); Allen, Balazevic, and Hospedales (2019) under different sets of assuptions. In this section we show that constraint optimization of a slightly modified SGNS objective (1) leads to a low-rank approximation of the binarized PMI (BPMI) matrix, defined as \( \text{BPMI}_{ij} := H(\text{PMI}_{ij}) \), where \( H(x) = 1 \) if \( x > 0 \), and \( H(x) = 0 \) otherwise.

**Theorem 1**

Assuming \( 0 < \langle w_i, c_j \rangle < 1 \), the following objective function

\[
\mathcal{L} = \sum_{i \in W} \sum_{j \in W} \#(i,j) \log \langle w_i, c_j \rangle + \sum_{i \in W} \sum_{j \in W} \#(i,j) \mathbb{E}_{j \sim p}[\log(1 - \langle w_i, c_j \rangle)]
\]

reaches its optimum at \( \langle w_i, c_j \rangle \approx \text{BPMI}_{ij} \).

**Proof.** We begin by expanding the sum in (2) as

\[
\mathcal{L} = \sum_{i \in W} \sum_{j \in W} \#(i,j) \log \langle w_i, c_j \rangle + \sum_{i \in W} \sum_{j \in W} \#(i,j) \mathbb{E}_{j \sim p}[\log(1 - \langle w_i, c_j \rangle)]
\]

\[
= \{ \text{the terms in the second sum do not depend on } j \}
\]

\[
= N \sum_{i \in W} \sum_{j \in W} p(i,j) \log \langle w_i, c_j \rangle + N \sum_{i \in W} p(i) \mathbb{E}_{j \sim p}[\log(1 - \langle w_i, c_j \rangle)]
\]

(3)

where we used \( \sum_{j \in W} \#(i,j) = \#(i) \), and \( p(i,j), p(i) \) are empirical probability distributions defined by \( p(i,j) := \frac{\#(i,j)}{N} \), \( p(i) := \frac{\#(i)}{N} \). Next, we use the definition of an expected value:

\[
\mathbb{E}_{j \sim p}[\log(1 - \langle w_i, c_j \rangle)] = \sum_{j' \in W} p(j') \log(1 - \langle w_i, c_{j'} \rangle).
\]

Combining (3) and (4) we have

\[
\mathcal{L} = N \sum_{i \in W} \sum_{j \in W} p(i,j) \log \langle w_i, c_j \rangle + N \sum_{i \in W} \sum_{j' \in W} p(i)p(j') \log(1 - \langle w_i, c_{j'} \rangle)
\]

\[
= N \sum_{i \in W} \sum_{j \in W} p(i,j) \log \langle w_i, c_j \rangle + p(i) \sum_{j \in W} p(j) \log(1 - \langle w_i, c_j \rangle)
\]

(5)

\[\] 
\[1\] The authors of SGNS suggest \( p(i) \propto \#(i)^{3/4} \).
Thus, we can rewrite the individual objective $\ell(w_i, c_j)$ in (2) as

$$\ell = N \left[ p(i, j) \log \langle w_i, c_j \rangle + p(i)p(j) \log(1 - \langle w_i, c_j \rangle) \right].$$

(6)

Differentiating (6) w.r.t. $\langle w_i, c_j \rangle$ we get

$$\frac{\partial \ell}{\partial \langle w_i, c_j \rangle} = N \left[ \frac{p(i, j)}{\langle w_i, c_j \rangle} - \frac{p(i)p(j)}{1 - \langle w_i, c_j \rangle} \right].$$

Setting this derivative to zero gives

$$\frac{p(i, j)}{p(i)p(j)} = \frac{\langle w_i, c_j \rangle}{1 - \langle w_i, c_j \rangle} \Rightarrow \log \frac{p(i, j)}{p(i)p(j)} = \log \frac{\langle w_i, c_j \rangle}{1 - \langle w_i, c_j \rangle}\left[ \frac{p(i, j)}{p(i)p(j)} \right] = \langle w_i, c_j \rangle, \quad (7)$$

where logit$(q) := \log \frac{q}{1 - q}$ is the logit function which is the inverse of the logistic sigmoid function, i.e. $\sigma(\text{logit}(q)) = q$. Since $\sigma(x)$ can be regarded as a smooth approximation of the Heaviside step function $H(x)$, from (7) we have $\text{BPMI}_{ij} := H \left( \log \frac{p(i, j)}{p(i)p(j)} \right) \approx \langle w_i, c_j \rangle$, which concludes the proof.

\[ \square \]

Remark 1

The objective (2) differs from the SGNS objective (1) only in that the former does not use the sigmoid function (keep in mind that $\sigma(-x) = 1 - \sigma(x)$): it is analogous to using raw logits $\langle w, x \rangle$ in the logistic regression instead of the $\sigma(\langle w, x \rangle)$. Thus we will refer to the objective (2) as Logit SGNS.

Direct Matrix Factorization

Optimization of the Logit SGNS (2) is not the only way to obtain a low-rank approximation of the BPMI matrix. A viable alternative is factorizing the BPMI matrix with the singular value decomposition (SVD): $\text{BPMI} = U \Sigma V^\top$, with orthogonal $U, V \in \mathbb{R}^{n \times n}$ and diagonal $\Sigma \in \mathbb{R}^{n \times n}$, and then zeroing out the $n - d$ smallest singular values, i.e.

$$\text{BPMI} \approx U_{1:n,1:d} \Sigma_{1:d,1:d} V_{1:d,1:n}^\top,$$

(8)

where we use $A_{a:b,c:d}$ to denote a submatrix located at the intersection of rows $a, a + 1, \ldots, b$ and columns $c, c + 1, \ldots, d$ of $A$. By the Eckart-Young theorem (Eckart and Young 1936), the right-hand side of (8) is the closest rank-$d$ matrix to the BPMI matrix in Frobenius norm. The word and context embedding matrices can be obtained from (8) by setting $W_{\text{SVD}} := U_{1:n,1:d} \sqrt{\Sigma_{1:d,1:d}}$ and $C_{\text{SVD}} := \sqrt{\Sigma_{1:d,1:d}} V_{1:d,1:n}^\top$. When this is done for a positive PMI matrix (PPMI), the resulting word embeddings are comparable in quality with those from the SGNS (Levy and Goldberg 2014b). Although there are other methods of low-rank matrix approximation (Kishore Kumar and Schneider 2017), a recent study (Sorokina, Karipbayeva, and Assylbekov 2019) shows that two of such methods, rank revealing QR factorization (Chan 1987) and non-negative matrix factorization (Paatero and Tapper 1994), produces word embeddings of worse quality than
the truncated SVD. Thus we will consider only the truncated SVD (8) as an alternative to optimizing the Logit SNGS objective (2).

Empirical Evaluation of the BPMI-based Word Vectors

To evaluate the quality of word vectors resulting from the Logit SNGS objective and BPMI factorization, we use the well-known corpus, text8.\(^2\) We were ignoring words that appeared less than 5 times, resulting in a vocabulary of 71,290 tokens. The SNGS and Logit SNGS embeddings were trained using our custom implementation.\(^3\) The PMI and BPMI matrices were extracted using the HYPERWORDS tool of Levy, Goldberg, and Dagan (2015) and the truncated SVD was performed using the SCIKIT-LEARN library of Pedregosa et al. (2011). The trained embeddings were evaluated on several word similarity and word analogy tasks: WORDSIM (Finkelstein et al. 2002), MEN (Bruni et al. 2012), M.Turk (Radinsky et al. 2011), RARE WORDS (Luong, Socher, and Manning 2013), GOOGLE (Mikolov et al. 2013a), and MSR (Mikolov, Yih, and Zweig 2013). We used the GENSIM tool of Řehůřek and Sojka (2010) for evaluation. We mention here a few key points: (1) Our goal is not to beat state of the art, but to compare PMI-based embeddings (SGNS and PMI+SVD) versus BPMI-based ones (Logit SNGS and BPMI+SVD). (2) For answering analogy questions (a is to b as c is to ?) we use the 3COSADD method of Levy and Goldberg (2014a) and the evaluation metric for the analogy questions is the percentage of correct answers. The results of evaluation are provided in Table 1. As we can see the LogitSNGS embeddings in general underperform the SGNS ones but not by a large margin. SVD is inferior to SGNS/LogitSNGS especially in the analogy tasks. Overall, it is surprising that such aggressive compression as binarization still retains important information on word vectors.

### Table 1

| Method         | WordSim | MEN  | M. Turk | Rare Words | Google | MSR  |
|----------------|---------|------|---------|------------|--------|------|
| SGNS           | .678    | .656 | .690    | .334       | .359   | .394 |
| Logit SNGS     | .649    | .649 | .695    | .299       | .330   | .330 |
| PMI + SVD      | .660    | .651 | .670    | .224       | .285   | .186 |
| BPMI + SVD     | .618    | .540 | .669    | .146       | .129   | .102 |

3. BPMI and Complex Networks

A remarkable feature of the BPMI matrix is that it can be considered as the adjacency matrix of a certain graph. As usually, by a graph \(\mathcal{G}\) we mean a set of vertices \(\mathcal{V}\) and a set of edges \(\mathcal{E}\) which consists of pairs \((i, j)\) with \(i, j \in \mathcal{V}\). It is convenient to represent graph edges by its adjacency matrix \((e_{ij})\), in which \(e_{ij} = 1\) if \((i, j) \in \mathcal{E}\), and \(e_{ij} = 0\) otherwise. The graph with \(\mathcal{V} := \mathcal{W}\) and \(e_{ij} := \text{BPMI}_{ij}\) will be referred to as BPMI Graph.

\(^2\) [http://mattmahoney.net/dc/textdata.html](http://mattmahoney.net/dc/textdata.html).
\(^3\) [https://github.com/zh3nis/BPMI](https://github.com/zh3nis/BPMI)
Figure 2
Spectral distribution of the BPMI-induced graphs (left and middle columns), and of scale-free random graphs with strong clustering property (right top: Goh, Kahng, and Kim (2001), right bottom: Farkas et al. (2001)).

Figure 3
Degree distributions formed by 10,000 most connected words of the BPMI graphs. The axes values are on a logarithmic scale.

Figure 4
Embedding a regular tree into $B^2$.

Table 2
Clustering coefficients of the BPMI graphs.

|        | text8 window = 2 | text8 window = 5 | enwik9 window = 2 | enwik9 window = 5 |
|--------|------------------|------------------|-------------------|-------------------|
| $C$    | .164             | .235             | .190              | .317              |
| $k/n$  | .001             | .002             | .0006             | .001              |

Since $\text{BPMI}_{ij} = 1 \Leftrightarrow \log \frac{p(i,j)}{p(i)p(j)} > 0 \Leftrightarrow p(i,j) > p(i)p(j)$, only those word pairs $(i,j)$ are connected by an edge which co-occur more often than expected when independence between $i$ and $j$ is assumed.
3.1 Spectrum of the BPMI Graph

First of all, we look at the spectral properties of the BPMI Graphs. For this, we extract BPMI matrices from the text8 and enwik9 datasets using the HYPERWORDS tool of Levy, Goldberg, and Dagan (2015). We use the default settings for all hyperparameters, except the word frequency threshold and context window size. We were ignoring words that appeared less than 100 times and 200 times in text8 and enwik9 correspondingly, resulting in vocabularies of 11,815 and 24,294 correspondingly. We additionally experiment with the context window size 5, which by default is set to 2. The eigenvalues of the PMI matrices are calculated using the TENSORFLOW library (Abadi et al. 2016), and the above-mentioned threshold of 200 for enwik9 was chosen to fit the GPU memory (12GB, NVIDIA Titan X Pascal). The eigenvalue distributions are provided in Figure 2. The distributions seem to be symmetric, however, the shapes of distributions are far from resembling the Wigner semicircle law \( x \mapsto \frac{1}{2\sqrt{\pi}} \sqrt{4 - x^2} \), which is the limiting distribution for the eigenvalues of many random symmetric matrices with i.i.d. entries (Wigner 1955, 1958). This means that the entries of a typical BPMI matrix are dependent, otherwise we would observe approximately semicircle distributions for its eigenvalues. Interestingly, there is a striking similarity between the spectral distributions of the BPMI matrices and of the so-called complex networks which arise in physics and network science (Figure 2). In the context of network theory, a complex network is a graph with non-trivial topological features — features that do not occur in simple networks such as lattices or random graphs but often occur in graphs modelling real systems. The study of complex networks is a young and active area of scientific research inspired largely by the empirical study of real-world networks such as computer networks, technological networks, brain networks and social networks. Notice that the connection between human language structure and complex networks was observed previously by Cancho and Solé (2001). A thorough review on approaching human language with complex networks was given by Cong and Liu (2014). In the following subsection we will specify precisely what we mean by a complex network.

3.2 Clustering and Degree Distribution of the BPMI Graph

We will use two statistical properties of a graph — degree distribution and clustering coefficient. The degree of a given vertex \( i \) is the number of edges that connects it with other vertices, i.e. \( \text{deg}(i) = \sum_{j \in V} e_{ij} \). The clustering coefficient measures the average fraction of pairs of neighbors of a vertex that are also neighbors of each other. The precise definition is as follows.

**Definition 1** (Clustering Coefficient)

Let us indicate by \( G_i = \{ j \in V \mid e_{ij} = 1 \} \) the set of nearest neighbors of a vertex \( i \). By setting \( l_i = \sum_{j \in V} e_{ij} \left[ \sum_{k \in G_i; j < k} e_{jk} \right] \), we define the local clustering coefficient as \( C(i) = \frac{l_i}{\binom{\text{deg}(i)}{2}} \), and the clustering coefficient as the average over \( V \): \( C = \frac{1}{n} \sum_{i \in V} C(i) \).

Let \( \bar{k} \) be the average degree per vertex, i.e. \( \bar{k} = \frac{1}{n} \sum_{j \in V} e_{ij} \). For random graphs, i.e. graphs with edges \( e_{ij} \overset{\text{iid}}{\sim} \text{Bernoulli}(p) \), it is well known (Erdős and Rényi 1960) that

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4 We define the graph spectrum as the set of eigenvalues of its adjacency matrix.
A complex network is a graph, for which $C \gg \bar{k} n$ and $p(\deg(i) = k) \propto \frac{1}{k^{\gamma}}$, where $\gamma$ is some constant.

We constructed BPMI Graphs from the text8 and enwik9 datasets using context windows of sizes 2 and 5 (as in Subsection 3.1), and computed their clustering coefficients (Table 2) as well as degree distributions (Figure 3). Due to a large size of the BPMI-graph of enwik9 we partitioned it in batches of 10,000 words each and averaged clustering coefficients over the batches. To ensure the validity of such an approximation we applied it to the BPMI-graph of text8 and obtained .148 and .232 batch clustering coefficient averages, that are close enough to the original .164 and .235 values for window sizes of 2 and 5 respectively. As we see, the BPMI graphs are complex networks, and this brings us to the hyperbolic spaces.

4. Complex Networks and Hyperbolic Geometry

Hyperbolic geometry is a non-Euclidean geometry that studies spaces of constant negative curvature. This, for example, is associated with Minkowski space-time in the special theory of relativity. In network science, hyperbolic spaces have begun to attract attention because they are well suited for modeling hierarchical data. For example, a regular tree can be isometrically embedded into a Poincare disk $\mathbb{B}^2$, which is a model of a Hyperbolic space $\mathbb{H}^2$ (see Figure 4): all connected nodes are spaced equally far apart (i.e., all black line segments have identical hyperbolic length). However, to embed the same tree isometrically into Euclidean space one will need an exponential (in tree depth) number of dimensions. Intuitively, hyperbolic spaces can be thought of as continuous versions of trees or vice versa, trees can be thought of as “discrete hyperbolic spaces”. Moreover, Krioukov et al. (2010) showed that complex networks (as defined in Subsection 3.2) and hyperbolic spaces are highly related to each other: (1) scale-free degree distributions and strong clustering in complex networks emerge naturally as simple reflections of the negative curvature and metric property of the underlying hyperbolic geometry; (2) conversely, if a network has some metric structure (strong clustering), and if the network degree distribution is scale-free, then the network has an effective hyperbolic geometry underneath. The curvature and metric of the hyperbolic space are related to the $\gamma$ and $C$ of the complex network.

5. Conclusion

It is amazing how the seemingly fragmented sections of scientific knowledge can be closely interconnected. In this paper, we have established a chain of connections between word embeddings and hyperbolic geometry, and the key link in this chain is the binarized PMI matrix. Claiming that hyperbolicity underlies word vectors is not novel (Nickel and Kiela 2017; Tifrea, Bécigneul, and Ganea 2018). However, this note is the first attempt to justify the connection between hyperbolic geometry and the word embeddings using analytical and empirical methods.

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