Efficient distributed representations beyond negative sampling

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Abstract

This article describes an efficient method to learn distributed representations, also known as <code>embeddings</code>. This is accomplished minimizing an objective function similar to the one introduced in the <code>Word2Vec</code> algorithm and later adopted in several works. The optimization computational bottleneck is the calculation of the <code>softmax</code> normalization constants for which a number of operations scaling quadratically with the sample size is required. This complexity is unsuited for large datasets and <code>negative sampling</code> is a popular workaround, allowing one to obtain distributed representations in linear time with respect to the sample size. Negative sampling consists, however, in a change of the loss function and hence solves a different optimization problem from the one originally proposed. Our contribution is to show that the sotfmax normalization constants can be estimated in linear time, allowing us to design an efficient optimization strategy to learn distributed representations. We test our approximation on two popular applications related to word and node embeddings. The results evidence competing performance in terms of accuracy with respect to negative sampling with a remarkably lower computational time.

Keywords: Representation learning, softmax approximation, negative sampling, Word2Vec, Node2Vec

1 Introduction

The ability of assessing the similarity of objects is one of the most crucial roles of machine learning (Bellet et al., 2015). This task is particularly hard to accomplish when dealing with complex entities – such as the words appearing in a text – that do not have an easily defined encoding. Distributed representations (or *embeddings*) allow one to map them into points of a high dimensional space, providing an answer to this problem (Bengio et al., 2013). In the aforementioned example, an effective representation maps *similar* words into nearby vectors.

A very relevant contribution to the field is the Word2Vec algorithm proposed by Mikolov et al. in (Mikolov et al., 2013) that owes its success to the efficiency, scalability and flexibility. Since its proposal, in fact, several works improved it (Bojanowski et al., 2017) or drew inspiration from it to learn distributed representations of sentences and documents (Mikolov et al., 2013), graphs (Perozzi et al., 2014; Grover and Leskovec, 2016; Gao et al., 2019; Rozemberczki et al., 2019; Nickel and Kiela, 2017; Narayanan et al., 2017), time (Kazemi et al., 2019), temporal contact sequences (Goyal et al., 2020; Rahman et al., 2018; Nguyen et al., 2018; Sato et al., 2021; Torricelli et al., 2020), biological entities (Du et al., 2019; Ng, 2017), tweets (Dhingra et al., 2016) and higher order interactions (Billings et al., 2019) among

others. These algorithms build upon two steps: (1) for each $i \in \mathcal{V}$ – the set of entities – a sample $\mathcal{S}_i \subseteq \mathcal{V}$ is defined; (2) the set of embedding vectors $\{x\}$ in \mathbb{R}^d is obtained maximizing the log-likelihood \mathcal{L} ,

$$\mathcal{L}(\{\boldsymbol{x}\}) = \sum_{i \in \mathcal{V}} \sum_{j \in \mathcal{S}_i} \log p_{\boldsymbol{x}}(j|i)$$

$$p_{\boldsymbol{x}}(j|i) = \frac{e^{\boldsymbol{x}_i^T \boldsymbol{x}_j}}{\sum_{k \in \mathcal{V}} e^{\boldsymbol{x}_i^T \boldsymbol{x}_k}} := \frac{e^{\boldsymbol{x}_i^T \boldsymbol{x}_j}}{Z_i}.$$
(1)

Intuitively, if j is often sampled from i, then the probability $p_{\boldsymbol{x}}(j|i)$ is large and the embedding vectors $\boldsymbol{x}_i, \boldsymbol{x}_j$ become closer, obtaining a similar representation to related entities. The known limitation of the optimization of this cost function resides in the partition function Z_i , requiring $\mathcal{O}(n)$ operations to be computed, where $n = |\mathcal{V}|$ is the number of items to be embedded. Since Z_i has to be computed for all $i \in \mathcal{V}$, optimizing \mathcal{L} requires $\mathcal{O}(n^2)$ operations, making it unsuited to approach large datasets. One of the most commonly adopted workarounds is negative sampling (Mikolov et al., 2013) consisting in replacing \mathcal{L} with the cost function $\tilde{\mathcal{L}}$ of a weighted logistic principal component analysis (Landgraf and Bellay, 2017). Its minima should be close to those of \mathcal{L} but it has the advantage of being computed in a linear time with respect to n. Negative sampling has been extensively adopted but, to date, it is still only poorly understood from a theoretical standpoint and some studies evidenced its potential weaknesses (Chen et al., 2018; Qin et al., 2016; Landgraf and Bellay, 2017; Mimno and Thompson, 2017; Kamigaito and Hayashi, 2021).

In this paper we propose an approximation method that allows one to estimate all the Z_i 's in $\mathcal{O}(n)$ operations. Adding a regularization term to the loss function of Equation (1), we formulate the problem in a very general way so that our proposed algorithm can be easily adopted in a variety of contexts. In particular, we suppose there exists a set of sparse sampling probability vectors $\{\boldsymbol{p}^{(i)}\}_{i\in\mathcal{V}}$ in \mathbb{R}^n encoding a measure of proximity between i and the other elements of \mathcal{V} . For instance, in the case of words, $p_j^{(i)}$ may indicate the probability that j is in the same sentence as i. The design of the set $\{\boldsymbol{p}^{(i)}\}_{i\in\mathcal{V}}$ is problem-dependent and beyond the scope of this article in which we describe an efficient framework to create a distributed entity representation given the probability set. Our main contributions are:

- 1. We provide a theoretical framework showing that all the partition functions $\{Z_i\}_{i\in\mathcal{V}}$ can be accurately estimated in $\mathcal{O}(n)$ operations. Based on this result, we describe an efficient strategy to obtain distributed representations.
- 2. We show that the pure Python implementation of our algorithm is competitive or outperforms in terms of speed an optimized $\tt C$ implementation of $\tt Word2Vec.^1$
- 3. We display two use cases of our algorithm applied to node and words embeddings, proving its efficacy also in terms of accuracy.
- 4. We provide Python version of our algorithm at github.com/lorenzodallamico/EDRep.

^{1.} We refer to the *Gensim* implementation (Rehurek and Sojka, 2011), available at radimrehurek.com/gensim/run in parallel on 8 cores.

NOTATIONS

- Sets are denoted with the font A. The cardinality of a set is denoted with |A|.
- Matrices are denoted with a standard capital letter, A. The identity matrix of size n is denoted with I_n .
- The notation $a_n = O_n(b_n)$ implies that there exists a finite c so that $\lim_{n \to \infty} \frac{a_n}{b_n} = c$. Similarly $a_n = o_n(b_n)$ implies that $\lim_{n \to \infty} \frac{a_n}{b_n} = 0$.
- Vectors are indicated in boldface (e.g. a), while vector elements and scalars in standard font (e.g. a_i). The all-ones vector of size n is denoted with $\mathbf{1}_n$.

2 Main result

2.1 Problem position

Consider a set of items \mathcal{V} with $n = |\mathcal{V}|$. For all $i \in \mathcal{V}$, we let $\mathbf{p}^{(i)} \in \mathbb{R}^n$ be a probability distribution defined on \mathcal{V} , encoding similarity: a large $p_j^{(i)}$ implies high affinity between i and j. We further define $\mathbf{p}_0 \in \mathbb{R}^n$ as a baseline $\mathbf{p}^{(i)}$ should be compared to. We aim at giving a distributed representation of $\{\mathbf{p}^{(i)}\}_{i \in \mathcal{V}}$, i.e. a vector embedding $\{x_i\}_{i \in \mathcal{V}}$ that preserves structural properties encoded in the probability distributions. We equivalently denote the set $\{x_i\}_{i \in \mathcal{V}}$ as $X \in \mathbb{R}^{n \times d}$, a matrix storing the embedding vectors in its rows. We define X as the solution to the following optimization problem:

$$X = \underset{Y \in \mathcal{C}_{n \times d}}{\operatorname{arg min}} \sum_{i \in \mathcal{V}} \left[D_{\mathrm{KL}} \left(\boldsymbol{p}^{(i)} \| \boldsymbol{q}_{Y}^{(i)} \right) - D_{\mathrm{KL}} \left(\boldsymbol{p}_{0} \| \boldsymbol{q}_{Y}^{(i)} \right) \right]$$

$$C_{n \times d} = \left\{ Y \in \mathbb{R}^{n \times d} : \| \boldsymbol{y}_{i} \| = f_{i} \ \forall \ i \in \mathcal{V} \right\}$$

$$q_{Y,j}^{(i)} = \frac{1}{Z_{i}} e^{\boldsymbol{y}_{i}^{T} \boldsymbol{y}_{j}}; \qquad Z_{i} := \sum_{k \in \mathcal{V}} e^{\boldsymbol{y}_{i}^{T} \boldsymbol{y}_{k}}, \tag{2}$$

where D_{KL} denotes the Kullback-Leibler divergence between two distributions and $\{f_i\}_{i\in\mathcal{V}}$ are inputs of the optimization problem. In words, we adopt a variational approach, approximating $\boldsymbol{p}^{(i)}$ with the distribution $\boldsymbol{q}_Y^{(i)}$ and optimize over the embeddings under the constraint that they have a predefined norm, $f_i \in \mathbb{R}^+$. The term $D_{\mathrm{KL}}(\boldsymbol{p}_0 || \boldsymbol{q}_Y^{(i)})$ serves as a regularizer and "promotes" only the probability part exceeding the baseline, thus preventing the embedding to encode a trivial piece of information. This type of approach is – for instance to define the modularity (Newman, 2006) – to encode a null model.

Remark 1 (Extension to an asymmetric setting). In Equation (2) and in the remainder, we only consider distributions $\mathbf{p}^{(i)}$ that are defined and indexed over the same set, \mathcal{V} . It is however possible to consider an asymmetric scenario in which the entries $p_a^{(i)}$ are defined for $i \in \mathcal{V}$ and $a \in \mathcal{W}$. In this case, one needs to define two embedding matrices $X \in \mathbb{R}^{|\mathcal{V}| \times d}$ and $Y \in \mathbb{R}^{|\mathcal{V}| \times d}$ and let

$$q_{X,Y,a}^{(i)} = \frac{1}{Z_i} e^{\boldsymbol{x}_i^T \boldsymbol{y}_a}; \qquad Z_i = \sum_{a \in \mathcal{W}} e^{\boldsymbol{x}_i^T \boldsymbol{y}_a}.$$

All the framework described below has a straightforward generalization to this setting.

Given Equation (2) our goal is to efficiently compute Z_i for all $i \in \mathcal{V}$ to obtain the embedding X that solves the optimization problem. We now proceed describing our main result on an efficient way to estimate the normalization constants.

2.2 Efficient estimation of Z_i

In the following, we interpret the vectors $\{x_i\}_{i\in\mathcal{V}}$ as random variables. Under proper assumptions, Z_i/n is concentrated around its expected value.² We then determine the condition ensuring its concentration that only relies on the distribution of the embedding vector norms.³ To compute the expectation of Z_i , an analytical expression thereof is needed and we empirically show that a good approximation can be obtained assuming that $x_i^T x_j$ is distributed as a mixture of κ Gaussians, where κ is a input of our estimation algorithm. Finally, we describe a practical way to efficiently compute Z_i based on our results and detail an algorithm to solve the optimization problem of Equation (2).

Let us first set sufficient conditions for the concentration of Z_i/n to its expected value.

Proposition 1 (Concentration of Z_i). Let $X \in \mathbb{R}^{n \times d}$ be a random matrix so that $\|\mathbf{x}_i\| = f_i$ where $f_i \in \mathbb{R}^+$ are random i.i.d. variables distributed $f_i \sim p_f$. Suppose that the expected value of $f_i = O_n(1)$ and that for all ω there is a $t^* > 0$ so that for $t > t^*$, $p_f(x > t) < 2e^{-\omega t}$. Then, under these hypotheses, for all large n, Z_i/n is concentrated around its expected value.

The Proof of Proposition 1 is given in Appendix A. This result requires that the distribution of the embedding vectors should not be too broad to guarantee concentration. Making some mild assumptions on the distribution of the $\{x_i\}_{i\in\mathcal{V}}$ vectors, we now provide our main result to approximate the Z_i values.

Proposition 2 (Approximation of Z_i). Let $\{x_i\}_{i\in\mathcal{V}}$ be a set of random vectors in \mathbb{R}^d and let $\ell: \mathcal{V} \to [\kappa]$ be a labeling function. Suppose that for all $j \in \mathcal{V}$ so that $\ell(j) = a$ the corresponding embedding vectors are distributed as $x_i \stackrel{\text{i.i.d}}{\sim} P_a(\mu_a, \Omega_a)$, where $\mu_a \in \mathbb{R}^d$ and $\Omega_a \in \mathbb{R}^{d \times d}$ are the mean and covariance matrix of P_a . Then, for i fixed and $\ell(j) = a$,

$$oldsymbol{x}_i^T oldsymbol{x}_i \sim \mathcal{N}(oldsymbol{x}_i^T oldsymbol{\mu}_a, oldsymbol{x}_i^T \Omega_a oldsymbol{x}_i),$$

where \mathcal{N} is a Gaussian random variable. Letting π_a be the fraction of items in class a, we get

$$\frac{Z_i}{n} \approx \sum_{a=1}^{\kappa} \pi_a e^{\boldsymbol{x}_i^T \boldsymbol{\mu}_a + \frac{1}{2}, \boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i}.$$
 (3)

To best understand Proposition 2, let us comment both its hypotheses and conclusion. Since we do not have an explicit expression of the embedding vectors $\{x_i\}_{i\in\mathcal{V}}$ distribution, we suppose that we can write it as a mixture of distributions with finite norm and covariance. If this conditions is verified, then $x_i^T x_j$ is distributed as a Gaussian random variable, for which the expectation can be computed analytically. Under general hypotheses, we did not

^{2.} A random variable Z is said to be concentrated around the pivot a if $\forall t > 0 : \mathbb{P}(|Z - a| > t) \leq \alpha(t)$, where $\alpha : \mathbb{R}^+ \to [0,1]$ is a non-increasing left continuous function (Louart and Couillet, 2018).

^{3.} Note that the f_i values are fixed but they can be seen as a realization of a random variable.

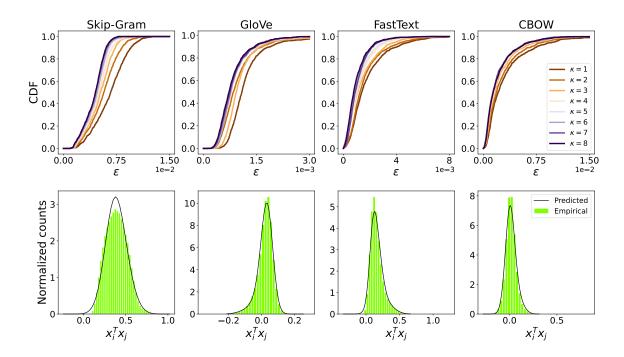


Figure 1: **Empirical validation of Proposition 2**. Top row: cumulative density function (CDF) of the relative error ϵ between the true an estimated value of Z_i for 1000 randomly selected indices i and the order of the mixture of Gaussian distribution $\kappa = 1, \ldots, 8$, color-encoded. Bottom row: histogram of $\mathbf{x}_i^T \mathbf{x}_j$ for a fixed i in green and in black the mixture of Gaussian fit, obtained for $\kappa = 5$.

prove the scalar product to converge towards a Gaussian distribution but, in Appendix A, however, we provide a theoretical support to this claim, further assuming that all embedding dimensions are independent. The consequence of Proposition 2 is that we can efficiently compute all the Z_i with $\mathcal{O}(n\kappa d^2)$ operations: $\mathcal{O}(n\kappa d)$ operations are needed to compute a label assignment with k-means (Lloyd, 1982; Christopher D. Manning, 2010), for instance, while the Z_i 's, given the parameters $\{\mu_a, \Omega_a, \pi_a\}_{a=1,\dots,\kappa}$ are obtained in $\mathcal{O}(n\kappa d^2)$ operations.

We now proceed giving an empirical validation to Proposition 2. We considered 4 datasets taken from the NLPL word embeddings repository (Kutuzov et al., 2017), representing word embeddings obtained with different algorithms:

- 0. British National Corpus, trained with Continuous Skip-Gram (Mikolov et al., 2013), n = 163.473, d = 300;
- 7. English Wikipedia Dump 02/2017, trained with Global Vectors (Pennington et al., 2014), n = 273.930, d = 300;
- 9. English Wikipedia Dump of 02/2017, trained with fastText Skipgram (Joulin et al., 2017), n = 273.930, d = 300;
- 224. Ukrainian CoNLL17 corpus, trained with Continuous Bag-of-Words (Mikolov et al., 2013), n = 99.884, d = 200.

For each of these datasets we (1) set the average of the embedding norm to 1, (2) sample at random 1000 words and (3) compute the corresponding exact and the estimated Z_i values for different approximation orders κ . Figure 1 shows the results of this procedure: in the top row the cumulative density function (CDF) of the relative error is displayed for several values of κ . As expected, the precision is an increasing function of κ , but very good approximations are obtained on all datasets for $\kappa = 1$ already. Note that in this case, the clustering step can be omitted and is, therefore, of particular interest. The bottom row shows the empirical and the predicted distribution of the $\boldsymbol{x}_i^T \boldsymbol{x}_j$ for a randomly chosen fixed i and confirms the goodness of the approximation.

As a remark, the computational complexity of our proposed method scales quadratically with d because we need to compute the covariance matrix Ω_a for all a. If one assumes that all dimensions are independent, then the set of Ω_a becomes diagonal and it can be computed in $\mathcal{O}(n\kappa d)$ operations. We empirically verified that under this assumption results are worse but, for the 4 considered datasets, we still obtain good approximations, with a relative error of the order of 1% or smaller for most items. Let us further point out that in the random matrix regime in which n and d are comparable, the empirical covariance matrix is not a good estimator and more sophisticated techniques should be adopted (Tiomoko et al., 2019). In the code we provide, however, we only implement the sample covariance matrix to estimate the set of Ω_a since in no case n and d are comparable in our settings. On the other hand, we let the user choose whether to compute the full covariance matrix or only its diagonal.

2.3 EDRep: efficient distributed representations

Let us now detail the main steps needed to translate the result of Proposition 2 into a practical algorithm to produce efficient distributed representations.

OPTIMIZATION STRATEGY

According to Equation (2), the embedding matrix $X \in \mathbb{R}^{n \times d}$ is obtained by optimizing a cost function $\mathcal{L}(X)$ that, after some trivial calculations, can be rewritten in the following form:

$$\mathcal{L}(X) = -\sum_{i \in \mathcal{V}} \left[\sum_{j \in \mathcal{V}} \left(p_j^{(i)} - p_{0,j} \right) oldsymbol{x}_i^T oldsymbol{x}_j + \log(Z_i)
ight].$$

We now exploit the result of Proposition 2 and make the notation more compact. Let $P \in \mathbb{R}^{n \times n}$ be a matrix so that $P_{ij} = p_j^{(i)}$. Then, $\mathcal{L}(X)$ can be rewritten as:

$$\mathcal{L}(X) = -\text{tr}\left[X^{T}\left(P - \mathbf{1}_{n}\boldsymbol{p}_{0}^{T}\right)X\right] + \sum_{i \in \mathcal{V}} \log \sum_{a=1}^{\kappa} \underbrace{\pi_{a} \exp\left\{\boldsymbol{x}_{i}^{T}\boldsymbol{\mu}_{a} + \frac{1}{2}\boldsymbol{x}_{i}^{T}\Omega_{a}\boldsymbol{x}_{i}\right\}}_{Z_{ia}}$$

$$:= -\text{tr}\left[X^{T}\left(P - \mathbf{1}_{n}\boldsymbol{p}_{0}^{T}\right)X\right] + \sum_{i \in \mathcal{V}} \log (Z\mathbf{1}_{\kappa})_{i} \tag{4}$$

where we also introduced the matrix $Z \in \mathbb{R}^{n \times \kappa}$ with elements Z_{ia} for convenience. The proposed strategy to optimize \mathcal{L} is summarized in Algorithm 1 and consists of alternating a

Algorithm 1: EDRep optimization

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Input: \{p^{(i)}\}_{i\in\mathcal{V}}, set of probabilities; p_0\in\mathbb{R}^n null model probability; d, embedding dimension; f vector of embedding norms; \ell\in\{1,\ldots,\kappa\}^n node label vector; \eta, largest learning rate; \mathbf{n}_epochs, number of training epochs

Output: X^{n\times d}, embedding matrix

begin

X\leftarrow initialize the embedding matrix; for 1\leq i\leq n_epochs do

\mu_{a=1,\ldots,\kappa}, \Omega_{a=1,\ldots,\kappa}\leftarrow update the parameters; G\leftarrow gradient matrix as in Equation (4); \eta_c\leftarrow largest learing rate so that \forall i, \mathbf{x}_i^T(t+1)\mathbf{x}_i(t)>0 (Equation 6); X\leftarrow(1-\eta_c)X-\eta_cG; gradient descent step; \|\mathbf{x}_i\|\leftarrow f_i\;\forall i; normalize the embedding vectors end
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gradient descent step with a forgetting factor and the normalization. Letting $M \in \mathbb{R}^{d \times \kappa}$ have the $\{\mu_a\}_{a=1,\dots,\kappa}$ values in its rows, the $i \in \mathcal{V}$ and $\alpha \in \{1,\dots,d\}$ gradient component reads

$$G_{i\alpha} = -[(P + P^T)X]_{i\alpha} + [\mathbf{1}_n(\boldsymbol{p}_0^T X) + \boldsymbol{p}_0(\mathbf{1}_n^T X)]_{i\alpha} + \frac{1}{Z_i} \left([ZM]_{i\alpha} + \sum_{a=1}^{\kappa} Z_{ia}[X\Omega_a]_{i\alpha} \right).$$
(5)

At each iteration, the embedding learns only from the gradient component which is orthogonal to the current embedding. As the minimum is approached, this component decreases in magnitude, hence determining the algorithm convergence. To improve the stability, we impose for all i and all t that $\mathbf{x}_i^T(t+1)\mathbf{x}_i(t) > 0$, where $\mathbf{x}_i(t)$ indicates the embedding vector at the t-th iteration. From a straightforward calculation, one can see that, provided $f_i^2 + \mathbf{g}_{it}\mathbf{x}_{it} > 0$, the learning rate η_c must satisfy the following condition for all i:

$$\eta_{\rm c} < \frac{f_i^2}{(f_i^2 + \boldsymbol{g}_{i,t} \boldsymbol{x}_{i,t})}.$$
(6)

If $f_i^2 + g_{it}x_{it} < 0$, any positive η_c can be used, and we preset the value η to be adopted.

Computational complexity of the algorithm

As an important remark, we must mention that Algorithm 1 requires the node labeling vector ℓ as an input which is, generally, not known in advance. To cope with this problem, we run the optimization with $\kappa = 1$ (for which $\ell = \mathbf{1}_n$), obtain an embedding X and compute a new ℓ as the result κ -class clustering on X.

The cost of this optimization procedure requires $\mathcal{O}(n\kappa d)$ operations to compute ℓ , $\mathcal{O}(n\kappa d^2)$ for the "Z part" of the gradient, and $\mathcal{O}(Ed)$ to compute the product PX, where E denotes

the number of non-zero entries of P. This complexity becomes prohibitive when $E \gg n$, but this is not the case in typical settings and the product can be performed very efficiently. Nonetheless, even when E is very large, if P can be written as the product (or sum of products) of sparse matrices, PX can still be computed very efficiently. In fact, let $P = P_m \cdot P_{m-1} \dots P_1$ for some positive m, then PX can be obtained without computing P, simply taking the products from right to left:

$$PX = (P_m \cdot P_{m-1} \cdot \dots \cdot P_1 X),$$

thus speeding up the computational bottleneck of our algorithm. In our implementation we explicitly consider this representation of P as an input. When a non-factorized dense matrix P is provided, one could envision to adopt a method such as the one presented in (Le Magoarou and Gribonval, 2016) to approximate a dense matrix P with the product of sparse matrices to considerably speed up the algorithm.

THE ROLE OF THE VECTOR OF NORMS

The vector of norms f is used as an input of our algorithm and it is necessary to preserve its numerical stability. An effective choice for this parameter depends on how the embedding is used in the successive steps. After convergence is reached, in fact, we may write

$$P_{ij} \approx e^{f_i f_j \cos \operatorname{Sim}(\boldsymbol{x}_i, \boldsymbol{x}_j)},$$

where $\cos \operatorname{Sim}(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x}^T \boldsymbol{y}}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|}$ denotes the cosine similarity between two vectors. P_{ij} , that is the probability to sample j from i, may be large because of their affinity as well as because of the popularity.⁴ If f_i is chosen to be an increasing function of i-th popularity, one allows instances in which P_{ij} may be large for popular items with a low affinity. On the opposite, if it is a decreasing function of popularity, one favors the alignment with popular items. By default, in our implementation, we leave $\boldsymbol{f} = \mathbf{1}_n$.

We now proceed showing two use cases of our algorithm, applied to the generation of node and word distributed representations.

3 Two use cases

In this section we analyze two use cases for two popular applications of distributed representations: node and words embeddings. In the former case, the goal is to determine a distributed representation of the vertices of a graph that preserves its structural properties (Cai et al., 2018; Goyal and Ferrara, 2018). On the other hand, distributed word representations are one of the most popular applications of this class of algorithms that allow one to encode words semantic similarity (Almeida and Xexéo, 2019). In both cases, pairs of *similar* items (nodes or words) should correspond to embedding vectors with a high cosine similarity.

^{4.} For instance, popularity can be the number of times a word appears in a text.

Remark 2. To test our algorithm on practical applications, we must define the set $\{p^{(i)}\}_{i\in\mathcal{V}}$. In the remainder, we adopt simple strategies to obtain this set and show, nonetheless, that the EDRep approach achieves competitive results in terms of performance. We would like to underline, however, that the sampling probabilities choice is a hard and problem-dependent task and addressing it optimally is beyond the scope of this article. Moreover, we formulated EDRep as an offline algorithm while Word2Vec is online. This difference influences the algorithm performances but not the essence our main result – Proposition 2 – that provides an efficient estimation of the partition functions regardless of the details of the implementation strategy.

3.1 Node embeddings

A graph is a tuple $\mathcal{G}(\mathcal{V}, \mathcal{E})$ where \mathcal{V} is the set of nodes and \mathcal{E} the set of edges connecting nodes (Newman, 2003; Borgatti and Halgin, 2011). Graphs are a versatile tool to model interacting systems and have a range spectrum of application, including social networks (Scott, 1988; Wasserman and Faust, 1994), technological networks (Amaral et al., 2000), spatial networks (Barthélemy, 2011), biological networks (Alm and Arkin, 2003) and many others. A graph \mathcal{G} can be easily represented in matrix form with the adjacency matrix $A \in \mathbb{R}^{n \times n}$, so that $A_{ij} = 1$ if $(ij) \in \mathcal{E}$ and equals zero otherwise. Here and in the remainder we only focus on undirected $(A_{ij} = A_{ji})$ and unweighted graphs $(A_{ij} \in [0,1])$. Our algorithm can, however, easily deal with the challenging directed and weighted cases, provided that an appropriate sampling strategy is defined.

One of the most relevant problems in graph learning is community detection that can be informally defined as the task of determining a non-overlapping node partition, unveiling more densely connected groups of nodes (Fortunato and Hric, 2016). In the following – similarly to what done in spectral clustering (Von Luxburg, 2007) – we adopt the EDRep algorithm to produce a node embedding and then perform clustering in the embedded space. Our choice of P in this case is the random-walk Laplacian, obtained from A and imposing that its rows sum up to 1. The entry P_{ij} of this matrix is the limiting probability that a random walker on \mathcal{G} goes from node i to j in one step. We further set $p_0 = \mathbf{1}_n/n$, that is equivalent to comparing $p^{(i)}$ with a uniform prior.

With these choices, we generate a distributed node representation X and then cluster the nodes of \mathcal{G} into groups. To evaluate the accuracy we consider synthetic graphs generated from the *degree-corrected stochastic block model* in which a ground truth label assignment is known and real-world graphs with a class annotation. The accuracy is measured in terms of *normalized mutual information* (NMI), a score that ranges between 0 (random label assignment) and 1 (perfect assignment).

SYNTHETIC GRAPHS

The degree-corrected stochastic block model (DCSBM) (Karrer and Newman, 2011) is a random graph generative model capable to create graphs with a community structure and a arbitrary degree distribution.⁵ This model is convenient to study community detection as it provides a clear definition of communities but it also allows one to model the broad degree distribution, typically observed in real-world graphs (Barabási and Albert, 1999).

^{5.} The degree of a node is its number of connections.

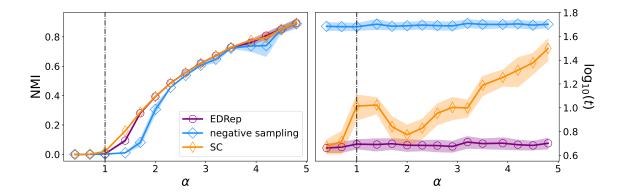


Figure 2: Community detection on synthetic graphs. Left panel: NMI score as a function of α (footnote 6) for a DCSBM graph (Definition 1) with n=30~000, $c=10,~q=4,\kappa=1$ and varying values of $c_{\rm out}$. The three lines correspond to three different embedding techniques. The purple dots are the EDRep algorithm with d=32, the cyan diamonds is DeepWalk with d=32, while the orange narrow diamonds are the spectral clustering algorithm of (Dall'Amico et al., 2021). Right panel: corresponding computational time in logarithmic scale. Both plots: averages are over 10 samples and the error bar width equals the standard deviation.

Definition 1 (DCSBM). Let $\omega : \mathcal{V} \to \{1, \dots, q\}$ be a class labeling function, where q is the number of classes. Let $\mathbb{P}(\omega_i = a) = q^{-1}$ and consider two positive integers satisfying $c_{\text{in}} > c_{\text{out}} \geq 0$. Further Let $\theta \sim p_{\theta}$ be a random variable that encodes the intrinsic node connectivity, so that $\mathbb{E}[\theta] = 1$ and $\mathbb{E}[\theta^2] = O_n(1)$. For all $i \in \mathcal{V}, \theta_i$ is drawn independently at random from p_{θ} . The entries of the graph adjacency matrix are generated independently (up to symmetry) at random with probability

$$\mathbb{P}(A_{ij} = 1) = \frac{\theta_i \theta_j}{n} \cdot \begin{cases} c_{\text{in}} & \text{if } \omega(i) = \omega(j) \\ c_{\text{out}} & \text{else} \end{cases}$$

In words, nodes in the same community $(\omega(i) = \omega(j))$ are connected with a higher probability than nodes in different communities. From a straightforward calculation, the expected degree is $\mathbb{E}[c_i] \propto \theta_i$. For this model, the goal is to infer the node label assignment from a realization of A. It was shown that this is theoretically feasible (in the large n regime) if and only if a function of the model parameters⁶ $\alpha > 1$ (Gulikers et al., 2015, 2017). In left panel of Figure 2 we show the NMI score obtained by different algorithms as a function of α , while the right panel shows the computation time in logarithmic scale. We compare:

• the spectral algorithm of (Dall'Amico et al., 2019, 2021) that was shown to be nearly Bayes-optimal for this task,

^{6.} Letting c be the expected average degree $c = \frac{c_{\text{in}} + (k-1)c_{\text{out}}}{k}$, $\alpha = (c - c_{\text{out}})\sqrt{\frac{\mathbb{E}[\theta^2]}{c}}$.

Name	n	q	${\tt EDRep-NMI}$	NS - NMI	${\tt EDRep}-t$	NS-t
amazon	9 317	232	0.92	0.93	4 s	17 s
youtube	26 931	608	0.60	0.65	12 s	72 s
dblp	60 530	252	0.52	0.51	26 s	180 s
livejournal	64 504	1662	0.92	0.92	34 s	196 s

Table 1: Community detection on real graphs. For each graph we report: 1) the name; 2) the size n; 3) the number of communities q; 4,5) the NMI score for EDRep and negative sampling (NS) and 6,7) the corresponding computational time in seconds. The results are obtained averaging over 5 samples.

- an algorithm combining the EDRep optimization approach with $\kappa = 1$ and k-means. The vector of norms is set to $f_i \propto \sqrt{d_i}g(d_i)$, where $g(d_i)$ is a Gaussian cut-off,
- an algorithm combining DeepWalk (Perozzi et al., 2014) with *k-means*. We used the C++ implementation available at github.com/thibaudmartinez/node2vec. The algorithm is deployed with its default values.

The results show that the EDRep-based algorithm performs almost as well as the optimal algorithm of (Dall'Amico et al., 2021) and a slight mismatch is only observed for hard problems, i.e. for α approaching 1. This is a particularly challenging setting in which few algorithms are capable to retrieve the community structure. The method of (Dall'Amico et al., 2021) was explicitly designed to work well in this regime in which, instead, the spectral algorithm based on the random walk Laplacian (Shi and Malik, 2000) (our choice of P) performs poorly. When compared to the DeepWalk approach, our method generally yields better results for all α .

On top of accuracy, the computational time gives the EDRep approach a decisive advantage with respect to the C++ efficient implementation of DeepWalk being more than 10 times faster with a improvement observed also with respect to the spectral clustering algorithm. The main advantage in this case is however related to the algorithm's computational complexity. The considered spectral clustering algorithm runs in $\mathcal{O}(nq^3)$ operations, while the complexity of EDRep is independent of q. Consequently, for large q, spectral clustering has to pay a significant price in terms of computational efficiency and it becomes unpractical.

Real-world graphs

We further test our algorithm on more realistic data available from the Stanford Network Analysis Platform (Leskovec and Krevl, 2014) that come with a community label annotation. In most cases, for the considered datasets, each node may be associated to more than one community. For simplicity, in order to keep the same framework as the one detailed above,

^{7.} A relevant setting is the one in which $\kappa = q$, i.e. the order of the GMM approximation equals the number of communities. It this case, EDRep's complexity scales as $\mathcal{O}(q^2)$ or $\mathcal{O}(q)$ when considering diagonal matrices Ω . It has to be said, however, that for very large q it seems pointless to set $\kappa = q$ since $\kappa \approx 8$ gave very good estimates in all cases we tested. Actually, while the estimation of Z_i is more accurate for large κ , we did not see any significant gain in the overall performance when choosing $\kappa > 1$.

each node was associated to the largest community it belongs to. In Table 1 we report the results summarizing the network properties, the obtained NMI and the computational time. In this case, spectral clustering is not considered since its complexity does not allow us to obtain a partition in a reasonable time. Similar to what already mentioned for DCSBM-generated graphs, the EDRep algorithm obtains competing performances with respect to negative sampling at a much lower computational time.

3.2 Word embeddings

Word embeddings are one of the most prominent applications for the class of algorithms EDRep belongs to. The goal is to encode in a vector-representation the words semantic similarity as inferred from a text (Selva Birunda and Kanniga Devi, 2021). For instance, the words flower and petal are closely related and should be represented by vectors with a high cosine similarity. This representation is mathematically convenient and opens up to a great span of applications such as those discussed in (Wang et al., 2018; Khattak et al., 2019) to provide some examples.

Unlike graphs, for word representations the matrix P is not given and it has to be built from the text. To do so we define a co-occurrence matrix $W \in \mathbb{R}^{n \times n}$, where n denotes the vocabulary size and W_{ij} is the number of times the word j appeared in the *context* of word i, i.e. within a maximum distance from i. For example, in Albus Dumbledore's sentence

It takes a great deal of bravery to stand up to our enemies, but just as much to stand up to our friends

the words stand, up, to, our, but, just, as, much appear in a context of size 4 around enemies. Given W and normalizing its rows we obtain our choice for the matrix P in which large entries correspond to pairs of words frequently appearing close to one-another. As one can observe in the example above, however, some context-independent words tend to appear with high frequency without carrying much information. This is the case of "to" that has four occurrences in the short sentence. Prior to building the co-occurrence matrix, we first proceed with the standard cleaning procedure introduced in (Mikolov et al., 2013) in which each word is dropped with a probability $1 - \sqrt{e^{-5}/\omega_i}$, where ω_i denotes the number of appearances of word i in the text. For the \mathbf{p}_0 vector, we drew inspiration from negative sampling and used $p_{0,i} \propto \omega_i^{\gamma}$ with $\gamma = 0.75$. The embedding norms are chosen to be a slow increasing function of the word frequency as well and in particular $f_i \propto \log(\omega_i + 1)$.

We trained the EDRep algorithm on three datasets: million, text8 and text9. These files are obtained from a dump of English Wikipedia performed on March $3^{\rm rd}$, 2006 (mattmahoney.net/dc/textdata.html) and represent the first 10^6 words, 10^8 and 10^9 bytes of this dump, respectively. Surprisingly, we observed that a context window of size 1 gives best performances for our algorithm, but in our implementation we leave it as an input parameter. Figure 3.2a shows the histogram of the non-zero entries of the matrix P. As expected (Zipf, 2013), most of them correspond to very rare occurrences. The computational complexity of EDRep scales linearly with the number of non-zero entries and very small values only marginally change the result, but majorly affect efficiency. For this reason we adopted a sparsification strategy, keeping only the 100 largest entries per row in P and observed small losses in the performance.

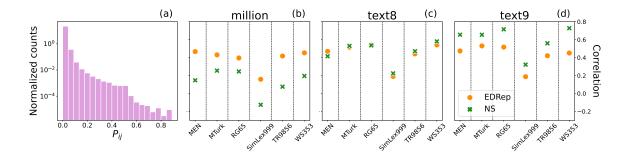


Figure 3: **Test on word embeddings**. (a) distribution of the non-zero entries of the P matrix: the plot is shown for text8 and is plotted in logarithmic scale on the y axis. (b, c, d): performance achieved on different benchmarks indicated on the x axis for the million, text8, text9 datasets. The results of the EDRep algorithm (orange dot) are compared with Word2Vec (green cross). The plotted quantity is average Spearman correlation between the benchmark similarity scores and those obtained with the two embedding methods. Averages are over 20 samples for million and text8 and over 10 samples for text9. Reading the plots from left to right (b, c, d) the online negative sampling approach profits from longer training unlike the offline EDRep method, as detailed in Section 3.2 and motivated in Remark 2.

A standard way to evaluate word embeddings is to check if the cosine similarity between pairs of words relates to its semantic affinity. To obtain a quantitative performance measure, we used the datasets made available by (Jastrzebski et al., 2017) in which a list of pairs of words (a,b) are associated to a score s_{ab} . For each of these pairs, we compute the cosine similarity obtained from the embeddings and use the Spearman correlation coefficient to quantify the agreement between the two measures. Higher correlation values indicate a good match with manually annotated data. The results are compared in Figure 3.2 with the Word2Vec algorithm using d=128 as embedding dimension. In particular, Figure 3.2b evidences a neat advantage of the EDRep approach when dealing with a small text, as it allows us to learn reasonable word representation from a very short text already. Increasing the input file size, in text8 (Figure 3.2c) we observe very similar performances for the two algorithms, while on text9 (Figure 3.2d), higher performances are obtained by Word2Vec on all benchmarks and EDRep performs essentially as well as on text8.

These results can be easily interpreted when looking more closely to the two algorithms. EDRep must first learn a matrix text representation and then a distributed representation thereof. Consequently, the algorithm training time is independent of the text length. On the opposite, Word2Vec, learns the embeddings in an *online* fashion and longer texts imply more training epochs. These two algorithms are indeed different and an online training method may effectively be more powerful than an offline one for this specific task. With this perspective, given that our main result of Proposition 2 would still hold, one could envision to adapt EDRep to different training strategies. Moreover, EDRep's ability to obtain significant

representation from sparse data could be exploited to pre-train the Word2Vec embeddings on a short text to speed up convergence.

Coming to the computation time, we confirm also in this case that our approach is faster on all three texts by approximately a factor 2, even though Word2Vec is run in parallel on all available cores. One can notice that the gain in computational efficiency is smaller than the one obtained in Section 3.1. This is because in that case a graph readily comes with a matrix representation and Node2Vec has to generate a "text" from the graph. Contrariwise, here the matrix must be obtained from the text and, with our implementation, it requires approximately 50% of the total time.

As a final remark, we would like to stress that the scores reported in Figure 3.2 are an only marginally objective way to evaluate a word embedding. In fact, we tried other design choices of the matrix P and in many cases we ended up obtaining larger scores on some benchmarks but lower on others. For this reason, we comfortably state that, once a proper evaluation metric is defined, there is much room for improvement in the design of the P matrix and these results should be interpreted as an algorithm deployment example.

4 Conclusion

In this article we showed that, under proper conditions, an approximation of the normalization constants of softmax can be obtained in linear time. This allowed us to optimize a loss function similar to the one originally proposed in (Mikolov et al., 2013) to efficiently obtain distributed representations. We detailed a theoretical framework justifying our claim that was validated on real data and then translated our result into a practical algorithm. This method relies on the definition of a probability matrix P capable to encode the similarity between the entities to be represented. To foster the impact of our work, we showed two simple examples applied to node and word embeddings.

In both cases, our proposed approach proved to be faster than an optimized negative sampling C implementation. This is a striking result, but we are firmly convinced that there is a lot of room for improvement. In fact, our implementation is fully coded in Python – that is known to be slower than C –, it is not parallelized and it can reasonably gain a considerable advantage if carefully optimized. Moreover, our main result fits in a larger frame than the one described in this paper and can potentially be exploited with other optimization strategies, as we already suggested along the lines.

Negative sampling appeared to be the natural benchmark of comparison of our work, but we would like to stress that it consists in optimizing a different cost function from the one optimized in EDRep. We noticed a remarkable difference between the case in which an affinity matrix representation is given (graphs) from the one in which it is not (texts). In the earlier case all the information related to the corpus (the graph) is represented in the form of a sparse matrix, hence the offline implementation of EDRep works optimally and significantly outperformed Node2Vec both in terms of speed and of accuracy. In the latter case, when encoding the text into a matrix, all the complex relations between the words should be captured by the matrix structure. This is a non-trivial task that might penalize infrequent co-occurrences between pairs of words. We believe, however, that a crucial advantage of our approach lies in its high interpretability. For a given practical deployment of our algorithm,

a practitioner only needs to define a sampling strategy that meaningfully encodes proximity for the problem at hand. The simplicity of our framework makes it also easier to study than negative sampling with the techniques described in (Jaffe et al., 2020), for instance. Moreover, our main result holds in a wider range of settings with respect to the one explored and it can be easily generalized to non symmetric, or non normalized P matrices.

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A Appendix

In this section we provide the proofs of the statements appearing in the main article. Proposition 1 states the sufficient condition to guarantee that Z_i/n is concentrated around its expectation value.

Proposition (1). Let $X \in \mathbb{R}^{n \times d}$ be a random matrix so that $\|\mathbf{x}_i\| = f_i$ where $f_i \in \mathbb{R}^+$ are random i.i.d. variables distributed $f_i \sim p_f$. Suppose that the expected value of $f_i = O_n(1)$ and that for all ω there is a $t^* > 0$ so that for $t > t^*$, $p_f(x > t) < 2e^{-\omega t}$. Then, under these hypotheses, for all large n, Z_i/n is concentrated around its expected value.

Proof. Let $y_k^{(i)} = \exp{\{\|\boldsymbol{x}_i\| \|\boldsymbol{x}_k\| \alpha_{ik}\}}$, where α_{ik} is the cosine-similarity between \boldsymbol{x}_i and \boldsymbol{x}_k . With this notation, Z_i can be written as

$$Z_i = \sum_{k \in \mathcal{V}} y_k^{(i)}.$$

Let us now compute the expectation value of $y_k^{(i)}$. We assume \mathbf{x}_k to be a random variable and \mathbf{x}_i to be fixed and that the α_{ik} is independent from f_k . We then write:

$$\mathbb{E}[y_k^{(i)}] = \int_{-1}^1 d\alpha \ p_X(\alpha) \underbrace{\int_0^\infty d\theta \ p_f(\theta) \ e^{\|\boldsymbol{x}_i\|\theta\alpha}}_{h(\alpha)<\infty} = \int_{-1}^1 d\alpha \ p_X(\alpha) \ h(\alpha) < \infty,$$

where we exploited the fact that p_f goes to zero faster than an exponential distribution. With a similar calculation one sees that, under the same assumption, $\mathbb{E}[(y_k^{(i)})^2]$ is also finite. Chebyshev inequality (Feller, 1968) can then be applied to show that Z_i/n is concentrated around its expected value, in fact

$$\mathbb{P}\left(\left|\frac{Z_i}{n} - \frac{\mathbb{E}[Z_i]}{n}\right| > t\right) \le \frac{\mathbb{V}[Z_i]}{(nt)^2},$$

where \mathbb{V} denotes the variance. The condition that the mean of $\mathbb{E}[f_i] = O_n(1)$ ensures that $\mathbb{V}[Z_i] \propto n$ and hence, that the right hand-side is smaller than 1 for all large n.

Our main result is Proposition 2 that we first recall here.

Proposition (2). Let $\{x_i\}_{i\in\mathcal{V}}$ be a set of random vectors in \mathbb{R}^d and let $\ell: \mathcal{V} \to [\kappa]$ be a labeling function. Suppose that for all $j\in\mathcal{V}$ so that $\ell(j)=a$ the corresponding embedding vectors are distributed as $x_i \overset{\text{i.i.d}}{\sim} P_a(\mu_a, \Omega_a)$, where $\mu_a \in \mathbb{R}^d$ and $\Omega_a \in \mathbb{R}^{d \times d}$ are the mean and covariance matrix of P_a . Then, for i fixed and $\ell(j)=a$,

$$oldsymbol{x}_i^T oldsymbol{x}_j \sim \mathcal{N}(oldsymbol{x}_i^T oldsymbol{\mu}_a, oldsymbol{x}_i^T \Omega_a oldsymbol{x}_i),$$

where N is a Gaussian random variable. Letting π_a be the fraction of items in class a, we get

$$\frac{Z_i}{n} \approx \sum_{a=1}^{\kappa} \pi_a e^{\boldsymbol{x}_i^T \boldsymbol{\mu}_a + \frac{1}{2}, \boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i}.$$

We now proceed with a theoretical justification of our main result.

Proof. The first step to prove Proposition 2 requires to show that $\mathbf{x}_i^T \mathbf{x}_j$ is distributed according to a Gaussian random variable. The intuition is that the scalar product is a sum of random variables with a finite mean and variance. For simplicity, we assume all entries of \mathbf{x}_j to be independent, each one a random variable $R(m_i, v_i)$ with mean m_a and variance v_a . Under this assumption, we may write

$$\mathbf{x}_{i}^{T}\mathbf{x}_{j} = \sum_{a=1}^{d} x_{ia}R(m_{a}, v_{a}) = \sum_{a=1}^{d} R(x_{ia}m_{a}, x_{ia}^{2}v_{a}).$$

This is a sum of independent random variables. To show the convergence towards a Gaussian distribution we use Lyapunov central limit theorem. To apply it, we must first check that the Lyapunov condition holds, as a consequence of the hypotheses of Proposition 1:

$$\sum_{j \in \mathcal{V}} |\boldsymbol{x}_i^T \boldsymbol{x}_j - \mathbb{E}[\boldsymbol{x}_i^T \boldsymbol{x}_j]|^3 \le n \, \max_{j \in \mathcal{V}} \, 2f_j^6 \sim 2n[\log(n)]^6 = o_n(n^{3/2}),$$

where we exploited the fact the maximum of an exponential distribution grows as log(n). From this relation the Lyapunov central limit theorem can be applied to obtain the result of the claim. To finally obtain the estimated value of Z_i , we solve the Gaussian integral:

$$\mathbb{E}\left[\frac{Z_i}{n}\right] = \frac{1}{n} \sum_{j \in \mathcal{V}} \mathbb{E}\left[e^{\boldsymbol{x}_i^T \boldsymbol{x}_j}\right]$$

$$= \frac{1}{n} \sum_{a=1}^k \sum_{j \in \mathcal{V}_a} \mathbb{E}\left[e^{\boldsymbol{x}_i^T \boldsymbol{x}_j}\right]$$

$$= \frac{1}{n} \sum_{a=1}^\kappa \sum_{j \in \mathcal{V}_a} \int_{-\infty}^\infty dt \, \frac{1}{\sqrt{2\pi \boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i}} \cdot \exp\left\{-\frac{(\boldsymbol{x}_i^T \boldsymbol{\mu}_a - t)^2}{2\boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i} + t\right\}$$

$$= \frac{1}{n} \sum_{a=1}^\kappa \sum_{j \in \mathcal{V}_a} e^{\boldsymbol{x}_i^T \boldsymbol{\mu}_a + \frac{1}{2} \boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i}$$

$$= \sum_{a=1}^\kappa \pi_a e^{\boldsymbol{x}_i^T \boldsymbol{\mu}_a + \frac{1}{2} \boldsymbol{x}_i^T \Omega_a \boldsymbol{x}_i}.$$

Given Proposition 1, Z_i/n is concentrated around its expected value.