# Variational Graph Normalized AutoEncoders

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#### **ABSTRACT**

Link prediction is one of the key problems for graph-structured data. With the advancement of graph neural networks, graph autoencoders (GAEs) and variational graph autoencoders (VGAEs) have been proposed to learn graph embeddings in an unsupervised way. It has been shown that these methods are effective for link prediction tasks. However, they do not work well in link predictions when a node whose degree is zero (i.g., isolated node) is involved. We have found that GAEs/VGAEs make embeddings of isolated nodes close to zero regardless of their content features. In this paper, we propose a novel Variational Graph Normalized AutoEncoder (VGNAE) that utilize  $L_2$ -normalization to derive better embeddings for isolated nodes. We show that our VGNAEs outperform the existing state-of-the-art models for link prediction tasks. The code is available at https://github.com/SeongJinAhn/VGNAE.

## **CCS CONCEPTS**

• Computing methodologies → Neural networks; Unsupervised learning; Learning latent representations.

#### **KEYWORDS**

Link Prediction, Graph Embedding, Graph Convolutional Networks, Normalization

#### **ACM Reference Format:**

Seong Jin Ahn and MyoungHo Kim. 2021. Variational Graph Normalized AutoEncoders. In *Proceedings of the 30th ACM International Conference on Information and Knowledge Management (CIKM '21), November 1–5, 2021, Virtual Event, QLD, Australia.* ACM, New York, NY, USA, 5 pages. https://doi.org/10.1145/3459637.3482215

## 1 INTRODUCTION

Link prediction in the graph is to determine whether there is an unknown relationship between nodes in the incomplete original graph. For example, it can be used to predict a link indicating if a specific substance in a biological network has a positive effect on the treatment of a specific disease, or if a specific literature or patent belongs to a certain author.

With the advancement of deep learning techniques, graph embedding models have been widely used in solving various problems

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CIKM '21, November 1–5, 2021, Virtual Event, QLD, Australia

© 2021 Association for Computing Machinery. ACM ISBN 978-1-4503-8446-9/21/11...\$15.00 https://doi.org/10.1145/3459637.3482215 in graphs. Graph embedding models generate low-dimensional vectors for nodes in the graph, called node embeddings, and learn these vector representations according to their purpose. Among graph embedding technologies, Graph Convolutional Networks (GCNs) are known to outperform other graph embedding models [Bruna et al. 2013; Defferrard et al. 2016; Kipf and Welling 2016a]. GCNs utilize information of neighborhood to embed nodes by fusing features of the node itself and its neighbors. In link prediction tasks, a Graph Autoencoder (GAE) [Kipf and Welling 2016b] is used to learn node embeddings generated by the GCN-encoder via the reconstruction loss. Since then, numerous GAE/VGAE variants have been proposed to achieve improved performance of link prediction [Di et al. 2020; Mavromatis and Karypis 2020; Pan et al. 2018; Salha et al. 2020].

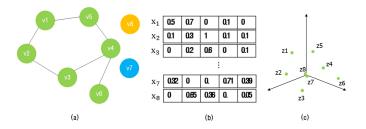


Figure 1: (a) A graph with isolated nodes ( $v_7$  and  $v_8$ ), (b) content features of nodes and (c) embedding space of latent vectors corresponding to node  $v_i$  (i=1,2.....8)

In many applications, there occur nodes in a graph that have no connection with other nodes. In this paper, we call such nodes, i.e., nodes with no connection *isolated nodes*. For example, consider the following scenario. There is a high school that maintains a social network G among members (e.g., students, professors, and staffs) where nodes are members and an edge between two members represents a "friendship" relation. Suppose the school has a number of freshmen. Here "Find out friends of students" can be considered a link prediction task where new nodes (freshmen) are involved. Such new nodes do not have any connection initially, and hence are isolated nodes in G when link prediction tasks are performed. Since there are no connectivity information of this case, feature contents of isolated nodes (e.g. the circles or hobby of students) play a major role in link prediction.

We have found that existing GAEs do not properly handle feature contents of isolated nodes. GAEs learn to make a low similarity of embeddings between a pair of unconnected nodes. Consider a graph consisting of eight nodes in Figure 1 (a). Figure 1 (c) shows vectors in an embedding space of the graph in Figure 1 (a) where  $z_i$  (i=1, 2, ..., 8) is a latent vector corresponding to node  $v_i$  (i=1, 2, ..., 8).

Relative positions of  $z_i$  are determined based on the content information and the connectivity information in Figure 1 (a). Now consider two isolated nodes  $v_7$  and  $v_8$ . Since  $v_7$  and  $v_8$  are not connected with other nodes, similarities between their embeddings and all other nodes should be low. We have found that GAEs tend to make the Euclidean norm of embedding vectors of isolated nodes small in order to reduce similarities between embeddings of isolated nodes and all the other nodes. As a result, the embeddings of isolated nodes go close to zero regardless of their content features.

In this paper, we propose a novel graph embedding technique, called Variational Graph Normalized AutoEncoder (VGNAE) for link prediction where the aforementioned problem of isolated nodes is properly handled. We propose a Graph Normalized Convolutional Network (GNCN) that effectively use  $L_2$ -normalization to prevent embeddings of isolated nodes from going near zero. Our VGNAE is a VGAE model where a GNCN is used to derive the mean and a GCN is used to derive the variance. We show through extensive experiments that our proposed VGNAE effectively handles the problem of isolated nodes, and outperforms other existing state-of-the-art link prediction models.

## 2 PRELIMINARIES

A graph G can be represented as G = (V, E, X) where V is a set of vertices,  $E \subset V \times V$  is a set of edges, and X is a feature matrix of V. N(v) denotes a set of neighbors of  $v \in V$ , n = |V| denotes the number of vertices, and  $A \in \mathbb{R}^{n \times n}$  is an adjacency matrix of G. Let  $\vec{z_v}$  be a vector that is an embedding of a node v, and  $||\vec{x}||$  denotes an euclidean norm  $(L_2$ -norm) of vector  $\vec{x}$ .

# 2.1 Graph Convolutional Networks

Graph Convolutional Networks (GCNs) generalize the convolution operations to the graph domain. The SpectralCNN [Bruna et al. 2013] first proposes convolutional networks to the graph domains using the graph fourier transform. The ChebyConv [Defferrard et al. 2016] parameterizes the graph convolution with chebyshev polynomials for efficient and localized filters. The GCN [Kipf and Welling 2016a] simplifies ChebyConv by using a normalization trick. Some unsupervised learning methods using GCNs have been proposed. Kipf et al. [Kipf and Welling 2016b] propose two graph auto-encoders (GAEs and VGAEs) that reconstruct the adjacency matrix by node embeddings generated by GCNs. LGAE [Salha et al. 2020] is a simple and interpretable linear models leveraging one-hop linear encoding. ARGA and ARVGA [Pan et al. 2018] are two variants of adversarial approaches to learn robust embeddings. GraphInfoClust [Mavromatis and Karypis 2020] captures richer information and nodal interaction by maximizing the mutual information between nodes of a same cluster. sGraphite-VAE [Di et al. 2020] extends the GNNs by exploring the aggregation using mutual information.

## 2.2 $L_2$ -normalization

Certain properties about the norm of the embedding of the object  $(||\vec{z_o}||)$  have been addressed in several studies. In neural translation models, an infrequent word is prone to have a embedding with a low  $L_2$ -norm  $(||\vec{w}||)$  [Arefyev et al. 2018; Kobayashi et al. 2020; Nguyen and Chiang 2017; Nguyen and Salazar 2019; Schakel and

Wilson 2015]. In image recognition models, an embedding representing poor quality image has a low  $L_2$ -norm and vice versa [Liu et al. 2017; Wang et al. 2018]. Also in image search, methods in [Eghbali and Tahvildari 2019; Wu et al. 2017] normalizes the embedding to minimize the quantization error in high-resolution image search. They and their subsequent studies use  $L_2$ -normalization [Ranjan et al. 2017; Wang et al. 2017; Zheng et al. 2018] to minimize errors caused by the imbalance between norms. In addition, some works [Merrill et al. 2020; Nguyen and Salazar 2019] show that the magnitude of the parameter continues (norm) to increase during gradient descent. Zhang et al. [Zhang et al. 2020] turns out that the imbalance between norms causes an unstable direction update and uses  $L_2$ -normalization to resolve the problem.

As far as we know, PairNorm [Zhao and Akoglu 2019] and MSG-Norm [Li et al. 2020] are the only approach that use  $L_2$ -normalization in GCNs. However, they are proposed to solve the over-smoothing problem, not for the problem caused by isolated nodes.

## 3 OUR APPROACH

## 3.1 Norm-zero tendency of isolated nodes

For node  $v \in \{v_1, v_2, ..., v_n\}$  in a graph, there are certain relationships between the norm of nodes  $||\vec{z_v}||$  from GAEs and degrees  $d_v$ . Figure 2 (a) shows node embeddings from a GAE for the Cora and CiteSeer datasets in a 2-dimensional embedding space. Figure 2 (b) shows the norms of node embeddings  $||\vec{z_v}||$  from the GAE with respect to degrees of nodes for the Cora and CiteSeer datasets. As shown in Figure 2 (a), embeddings of isolated nodes are around  $\vec{0}$ . The norm of those vectors will be close to zero. In Figure 2 (b), we can find out the norms of an embedding vectors of isolated nodes tend to be close to zero. This also happens with the mean vector of VGAEs. We call this phenomenon "norm-zero tendency of isolated nodes", which is an extreme case of the imbalance between norms. This tendency makes embeddings of isolated nodes indistinguishable regardless of values of their content features.

## 3.2 Graph Normalized Convolutional Network

We propose a novel graph neural network called a Graph Normalized Convolutional Network (GNCN) that uses  $L_2$ -normalization before propagation. Consider a feature matrix  $X = [\vec{x_1}, \vec{x_2}, ..., \vec{x_n}]^T$  where  $\vec{x_i} \in R^m$  is a content feature vector of node  $v_i$  and n is the number of nodes. A GNCN first generates the feature transformed vectors  $(\vec{h} \in R^f)$  with a learnable matrix  $W \in R^{m \times f}$ .

$$\vec{h_i} = \vec{x_i} W \tag{1}$$

Let  $s \in R$  be a scaling constant that represents a norm of the hidden feature being propagated. Our proposed GNCN generates the normalized feature transformed vectors  $(\vec{n} \in R^f)$  and propagates the normalized vector to generates node embeddings  $(\vec{z} \in R^f)$ .

$$\vec{n_i} = s \frac{\vec{h_i}}{||\vec{h_i}||} \tag{2}$$

$$\vec{z}_i = \frac{1}{d_i + 1} \vec{n}_i + \sum_{j \in N(i)} \frac{1}{\sqrt{d_i + 1} \sqrt{d_j + 1}} \vec{n}_j \quad \text{where} \quad i \in \{1, 2, ..., n\}$$

(3)

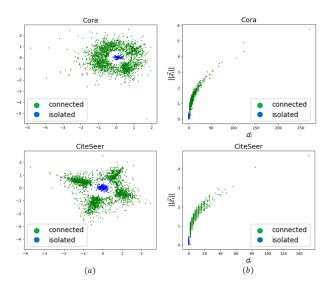


Figure 2: (a) A 2-dimensional embedding space of a GAE in the Cora and the CiteSeer dataset (b) a degree of nodes d(v) and their norms of node embeddings  $||\vec{z_v}||$  from a GAE in the Cora and the CiteSeer dataset.

Now, for a feature matrix  $X \in \mathbb{R}^{n \times m}$  and an adjacency matrix A, GNCN(X, A, s) is defined as follows:

$$GNCN(X, A, s) = s\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}g(XW)$$
 (4)

Here  $g([\vec{h_1},\vec{h_2},...,\vec{h_n}]^T)=[\frac{\vec{h_1}}{||\vec{h_1}||},\frac{\vec{h_2}}{||\vec{h_2}||},...,\frac{\vec{h_n}}{||\vec{h_n}||}]^T$ ,  $Z=[\vec{z_1},\vec{z_2},...,\vec{z_n}]^T\in\mathbb{R}^{n\times f}$  is a node embedding matrix,  $W\in\mathbb{R}^{m\times f}$  is a trainable matrix,  $\tilde{A}=A+I_N,\tilde{D}$  is a degree matrix of  $\tilde{A}$ , and s is a scaling constant. We will show that our proposed GNCN properly handles the norm-zero tendency of isolated nodes through experiments in Sec 4.4.1.

## 3.3 Variational Graph Normalized AutoEncoder

In this paper, we propose two variants of graph autoencoder called Graph Normalized AutoEncoder (GNAE) and Variational Graph Normalized AutoEncoder (VGNAE). For each node  $v \in \{1, 2, ..., n\}$ , GNAE encodes the local structure information and node feature information of its neighborhood to derive latent variables  $\vec{z_v} \in R^f$ . To generate  $Z = [\vec{z_1}, \vec{z_2}, ..., \vec{z_n}]^T \in R^{n \times f}$ , GNAE uses a GNCN encoder that avoids the norm-zero tendency of isolated nodes. GNAE uses a inner-product decoder to create the reconstructed adjacent matrix  $\hat{A}$  from Z as follows:

$$\hat{A} = \sigma(Z^T Z), \text{ with } Z = GNCN(X, A, s)$$
 (5)

where  $\sigma$  is a sigmoid function.

We also propose a Variational Graph Normalized AutoEncoder (VGNAE). Since mean vectors in VGAEs also have norm-zero tendency of isolated nodes, we derive mean vectors of VGNAE with a GNCN encoder. Our VNGAE takes a simple inference model by using the mean field approximation to define the variational family

Table 1: The statistics of the benchmark graph datasets

Dataset	Type	#Nodes	#Edges	#Features	
Cora CiteSeer PubMed CS	Citation Citation Citation Coauthor	2,708 3,327 19,717 18,333	5,429 4,732 44,338 81,894	1,433 3,703 500 6,805	
Photo	Co-purchase	7,487	119,043	745	

as follows:

$$q(Z|X,A) = \prod_{i=1}^{n} q(z_i|X,A) \quad \text{with} \quad q(z_i|X,A) = N(z_i|\mu_i, diag(\sigma_i^2))$$
(6)

where  $\mu = [\mu_1, \mu_2, ..., \mu_n]^T = GNCN(X, A, c)$  is the matrix of mean vectors  $\mu_i$ ; similarly  $log\sigma = [log\sigma_1, ..., log\sigma_i]^T = GCN(X, A)$ .

Our generative model reconstructs graph structure A by using a simple inner product decoder.

$$p(A|Z) = \prod_{i=1}^{n} \prod_{j=1}^{n} p(A_{ij}|\vec{z}_i, \vec{z}_j) \quad \text{with} \quad p(A_{ij} = 1|Z) = \sigma(\vec{z}_i^T \vec{z}_j)$$
(7

For GNAE, we minimize the reconstruction error of  $\hat{A}$ . For VG-NAE, optimization is made by maximizing a tractable variational lower bound (ELBO) as follows:

$$L_{ELBO} = E_{q(Z|X,A)}[logp(A|Z)] - KL(q(Z|X,A)||p(Z))$$
 (8)

where  $KL(q||p) = \sum_j Q_j log(\frac{Q_j}{P_j})$  is the Kullback-Leibler divergence between q and p. We use a Gaussian prior  $p(Z) = \prod_{i=1}^n N(z_i|0,I)$ .

#### 4 EXPERIMENTS

We conduct various experiments to show performance improvements of our proposed VGNAEs in link prediction when isolated nodes are involved. First, we show the performance improvement of our GNCN by comparing the AUC scores of isolated nodes in various types of graph structured networks. Then, we evaluate our GAE/VGNAE employing the GNCN.

## 4.1 Datasets

We use various types of attributed graphs. First, we use three citation network datasets (Cora, Citeseer, and Pubmed). Second, we use a coauthor network Coauthor CS [Shchur et al. 2018]. Third, we use a co-purchase graph Amazon Photo [Shchur et al. 2018]. Statistics about datasets are described in Table 1.

#### 4.2 Setup

We use the Adam optimizer [Kingma and Ba 2014] with a learning rate of 0.005. We train all models for a maximum of 300 epochs and early stopping with a window size of 50. In all the experiments, 64 dimensions are used for node embeddings. A scaling constant (s) in GNCN is set as 1.8. For GCN [Kipf and Welling 2016a], we use a two-layer GCN with the dimension of hidden embeddings is set to 128. For GraphHeat [Xu et al. 2020] and APPNP [Klicpera et al. 2018], the optimal hyper-parameters (e.g. scaling parameter s and

teleport rate *t*) are chosen through validation set. For GraphHeat [Xu et al. 2020], 0.4 is used for the coeffient *s*. For APPNP [Klicpera et al. 2018], 0.15 is used for the teleport rate and 10 is used for the number of propagations. The link prediction models are evaluated by the area under the ROC curve (AUC) and average precision (AP) scores.

#### 4.3 Results

4.3.1 GNCN: Power of normalization for isolated nodes. In this section, we present that performance of GAEs with existing GCN encoders degrades when isolated nodes are involved. We also present that GAEs using our proposed GNCN encoders effectively encode isolated nodes. We compare the performance of GAEs using various GCN-based encoders for isolated nodes and connected nodes on Cora, CiteSeer, CS and, Photo datasets. The compared GCN-based encoders are GCN [Kipf and Welling 2016a], GAT [Veličković et al. 2017], SGCN [Wu et al. 2019], SuperGAT [Kim and Oh 2020], APPNP [Klicpera et al. 2018], GraphHeat [Xu et al. 2020], PairNorm [Zhao and Akoglu 2019], and MSGNorm [Li et al. 2020].

For every dataset, we use a training set 60%, a validation set 10%, and a test set 30% among all edges. We add the same number of randomly sampled negative edges to the valid set and test set. We measured the AUC score for isolated nodes and connected nodes in test sets. The results are shown in Figures 3. Figure 3 shows that the AUC scores of GAEs with other GCN encoders of isolated nodes is significantly lower than that of connected nodes (10  $\sim$  20%) for all types of graphs. Experimental results on graphs of various types show that the degrade of performance in isolated nodes occurs in general graphs. In addition, it can be seen that the accuracy at the isolated nodes for each GCN varies depending on the type of dataset. We confirmed that existing GCNs are not suitable encoders of GAEs when isolated nodes are involved. The methods using proposed GNCN ensured the highest performance of the isolated nodes for all graphs without compromising the performance of the connected nodes.

4.3.2 Performance Comparision of GNAE/VGNAE with state-of-the-art methods. We conduct experiments on citation networks (Cora, CiteSeer, and PubMed) to compare the performance of GNAE/VGNAE with state-of-the-art link prediction models, i.e., LGAE [Salha et al. 2020], ARGA [Pan et al. 2018], ARGVA [Pan et al. 2018], Graph InfoClust (GIC) [Mavromatis and Karypis 2020], and sGraphite-VAE [Di et al. 2020]. For all datasets, 20%, 40%, and 80% of edges are used for training sets. For the remaining edges, the ratio of 1 to 3 are used for valiatdation sets and test sets. We add the same number of randomly sampled negative edges for each valid and test set. For each dataset divided in this way, the AUC and AP scores are measured. The results of link prediction in the dataset are shown in Table 2.

As can be seen in Table 2, our GNAE/VGNAE show superior results compared to other methods in all divisions. Also we can observe that the fewer observed edges (the smaller the ratio of the training rate), the better the performance of our proposed method compared to other SOTA models. This is because as the ratio of unobserved edges increase, the number of isolated nodes also increases.

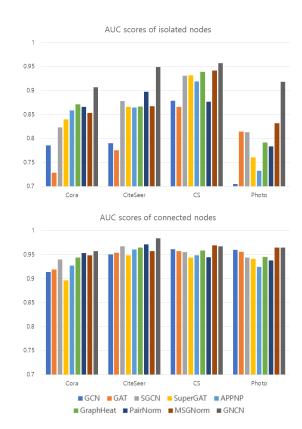


Figure 3: AUC scores of isolated nodes and connected nodes

Table 2: Experiment results for citation datasets on link prediction task

Data	Metric	Train	GAE	LGAE	ARGA	GIC	sGraph	GNAE	VGNAE
	AUC	20%	0.782	0.866	0.795	0.880	0.845	0.887	0.890
		40%	0.856	0.908	0.844	0.914	0.840	0.926	0.929
Cora		80%	0.922	0.938	0.919	0.933	0.885	0.956	0.954
Cora	AP	20%	0.793	0.878	0.806	0.881	0.829	0.901	0.901
		40%	0.861	0.915	0.856	0.911	0.828	0.936	0.933
		80%	0.930	0.945	0.927	0.929	0.867	0.957	0.958
	AUC	20%	0.786	0.906	0.750	0.930	0.928	0.946	0.941
		40%	0.836	0.925	0.832	0.936	0.936	0.956	0.961
CiteSeer		80%	0.894	0.955	0.904	0.962	0.963	0.965	0.970
Citeseer	AP	20%	0.797	0.913	0.777	0.934	0.897	0.953	0.948
		40%	0.850	0.929	0.844	0.938	0.910	0.958	0.966
		80%	0.903	0.959	0.915	0.966	0.943	0.970	0.971
	AUC	20%	0.937	0.946	0.936	0.950	0.837	0.950	0.951
		40%	0.959	0.962	0.955	0.958	0.876	0.963	0.964
PubMed		80%	0.967	0.974	0.973	0.960	0.896	0.975	0.976
i ubivieu	AP	20%	0.940	0.947	0.941	0.947	0.859	0.950	0.949
		40%	0.961	0.961	0.959	0.956	0.879	0.961	0.963
		80%	0.967	0.975	0.976	0.965	0.902	0.975	0.976

## 5 CONCLUSIONS

We have presented that in GAE and VGAE embeddings of isolated nodes tends to go to zero regardless of their content features on various graph-structured networks. This tendency can significantly degrade accuracy of link prediction when many isolated nodes are involved. We have argued that the  $L_2$ -normalization is an effective technique to generate proper embeddings of isolated nodes in the link prediction task. We have shown through extensive experiments that our proposed VGNAE performs better than other existing methods.

#### **ACKNOWLEDGEMENTS**

This work was supported by the Bio-Synergy Research Project of the MSIT (No. 2013M3A9C4078137), the National Research Foundation of Korea(NRF) grant (No. 2020R1A2C1004032), and the ITRC support program (IITP-2020-2020-0-01795) supervised by the IITP.

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