Representation Learning using Graph Autoencoders with Residual Connections

Indrit Nallbani, Aydin Ayanzadeh, Reyhan Kevser Keser, Nurullah Çalış, and Behçet Uğur Töreyin

1Informatics Institute, Signal Processing for Computational Intelligence (SP4CING) Research Group, Istanbul Technical University
2Department of Biomedical Engineering, Istanbul Medeniyet University

Abstract—Graph autoencoders are very efficient at embedding graph-based complex data sets. However, most of the autoencoders have shallow depths and their efficiency tends to decrease with the increase of layer depth. In this paper, we study the effect of adding residual connections to shallow and deep graph variational and vanilla autoencoders. We show that residual connections improve the accuracy of the deep graph-based autoencoders. Furthermore, we propose Res-VGAE, a graph variational autoencoder with different residual connections. Our experiments show that our model achieves superior results when compared with other autoencoder-based models for the link prediction task.

Index Terms—Variational Graph Autoencoders, Graph Embedding, Residual Connections, Model Depth.

I. INTRODUCTION

Learning-based feature extraction approaches have led to better performance in machine learning tasks, such as computer vision, machine translation, and object detection. As opposed to conventional machine learning approaches, deep learning-based methods utilize a learning-based data-dependent feature extraction scheme. The organization of data determines the type of deep learning-based approach. For non-Euclidean and unstructured data, Graph Neural Networks are preferred. There are various GNN-based techniques in the literature, such as, Recurrent Graph Neural Networks [1], [2], Graph Autoencoders [3], [4] and Spatial-temporal Graph Neural Networks, [5], [6], [7].

Deep learning models based on regular data sets have proven to be very successful in producing data representations that are successfully used in several tasks such as fraud detection [8], recommendation systems [9], churn prediction [10] and drug discovery [11]. However, most real-world data sets are complex and unstructured thus making it difficult for classical deep learning techniques to achieve high accuracy scores.

Therefore, there has been an increasing interest to extend the deep learning techniques into the graph domain. Graph neural networks can efficiently exploit the relationship between data set instances, which cannot be done with regular datasets since we assume that they are independent of each other. The final embeddings are used on three main tasks: node classification, link, prediction [12], [13], [14] and graph classification tasks.

One major drawback of graph-based learning is the depth of the models and there are limited works that study the depth of graph neural network models.

In this paper, we research the accuracy of the models with various layers of depth. Moreover, we propose adding residual connections in both shallow and deep models. We evaluate our models on the link prediction task.

The overall contributions of our study are as follows:

- We propose a graph variational autoencoder model with residual connections and compare it with similar graph autoencoders which have the same depth structure.
- We measure the accuracy of adding residual connections on similar graph-based autoencoders with different depths.

The rest of the paper is organized as follows: The remaining part of Section I-A mentions the related work and our contributions. Section II, we explain in detail the proposed model architectures. In Section III, we show the experimental results of the proposed models. In Section IV, we conclude the paper and propose some suggestions for our future work.

A. Related Work

In recent years several techniques have been proposed to efficiently embed graph data sets. In this section, we discuss the latest models that are able to efficiently embed these data set into meaningful low-dimensional embeddings.

Weng, Z [15] depicts a variational graph auto-encoder that has an attention-based mechanism. To improve the encoder performance, they employ efficient weights for each node of the network and amplify them by analyzing which leads to improvements in the performance of the auto-encoder. The adversarial mechanism is also leveraged to fortify the stability of the distribution of the key variables. Defense VGAE [16] introduces a defensive mechanism in contrast to adversarial attacks with structuring the graph. This model just outperforms the performance of the state-of-the-art in some determined settings and it is not enough generalized and flexible for a wide range of settings. Davidson et al. [17] have proposed hyperspherical variational autoencoders, which uses a von Mises-Fisher (vMF) distribution instead of the standard Gaussian distribution. They state that in low dimensions, Gaussian distribution-based autoencoders force points to be clustered...
in the center. The authors show that their model outperforms every other model on publicly available data sets such as PubMed.

DeepWalk \cite{18}, proposed a specific online learning method that excludes the global information and employs the local information from truncated random walks as an input, in contrast to previous approaches. Node2vec \cite{12}, leveraged to cover the disadvantages of Deepwalk by utilizing the weight on the random walk on the graph. These weights increase the functionality of the method on controlling the path which was not feasible on DeepWalk. To solve the unweighted problem, Node2vec utilizes both Depth-First-Sampling (DFS) and Breadth-Fast-Sampling (BFS) simultaneously, which DeepWalk just applied DFS for the graph embedding step. DVNE \cite{19} utilized as a specific deep variation model to solve the graph embedding application. This method leverages an unsupervised approach for the representation of the network nodes in Wasserstein space which 2-Wasserstein distance measurement has landmark success in the preservation of the transitivity in embedding space in network embedding systems.

Hu, W. \cite{20}, proposed a transfer learning approach for Graph Neural Networks (GNNs) in order to overcome the complication of the pre-training on the graph-based data. They showed that transfer learning has an effective impact on the amount of data set which is labeled pre-training data set in the same domain. The experiment results claim that the pre-training method can satisfy the consistency and better generalization factors in comparison to the approaches without a pre-training mechanism.

Shi \cite{21} proposed an approach that employed a triad-based decoder that leverages on closure property on graph-based networks. The determined VGAE achieves an accomplishment in comparison of baseline methods from graph generation, node clustering, and link prediction perspectives. Most recent works include \cite{22} and \cite{17}.

Mavromatis et al. \cite{22}, have proposed a graph learning method that optimizes node embedding by capturing cluster-level information and maximizing the information between nodes of the same clusters. The authors have managed to obtain significant gains when compared with other methods.

In our previous work \cite{23}, we proposed a novel graph convolutional neural network layer. We showed that our method improves the graph embedding performance of Variational Graph Autoencoders.

In this paper, we propose a novel architecture that combines graph autoencoders and residual connections \cite{24}. We further conduct experiments on architectures with different depths.

A. Graph autoencoders

Graph autoencoders are models whose inputs are instance features and adjacency matrices and whose output is the reconstructed adjacency matrix. These models mainly consist of two components which are the encoder and the decoder. The encoder part transforms the input into a lower-dimensional embedding while the decoder part transforms the embedding into the reconstructed adjacency matrix.

1) Encoder: Let $G = (V, E)$ denote a graph $G$ where $V$ is the set with $N$ nodes and $E$ is the set of edges. Moreover, let $v_i \in V$ denote a node and $e_{ij} = (v_i, v_j)$ denote an edge between two nodes $v_i$ and $v_j$. We define the adjacency matrix $A$ as:

$$A := \begin{cases} 1 & e_{ij} \in E \\ 0 & e_{ij} \notin E \end{cases}$$

and $X$ is the feature matrix of the nodes. For all the encoder architectures, we have used the graph convolutional layer proposed by \cite{25}. The layer follows the propagation rule:

$$H^{(l+1)} = \varphi (\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)})$$

where $\varphi$ is the activation function, $\tilde{D}$ is the degree matrix, $\tilde{A}$ is the normalized adjacency matrix with self-loops and $W^{(l)}$ is the layer’s weight matrix. In a multi-layer model $H^0 = X$ and $H^l$ is the feature map of the $l^{th}$ layer.

Vanilla graph encoders transform the graph into a lower-dimensional embedding, using only graph convolutional layers. The structure of the encoder in vanilla graph autoencoders is given in Figure \cite{1}.

Variational graph encoders transform the graph into a lower-dimensional embedding, using graph convolutional layers and a sampling layer. These graph convolutional layers transform the graph into the desired lower-dimensional space and produces mean and standard deviation values using two layers. Then, the sampling layer takes these mean and deviation values to generate samples from the prior distribution. Hence the generated samples constitute the embedding of the graph.

The final embeddings are encoded as distribution over the latent space which are reparameterized as:

$$q(Z \mid X, A) = \prod_{i=1}^{N} q(z_i \mid X, A)$$

where

$$q(z_i \mid X, A) = \mathcal{N} (\mu_i, \text{diag} (\sigma^2))$$

where $z_i$ is the embedding for node $i$ and $\mu_i$ and $\sigma$ are the graph convolutional layer final outputs of the encoder.

Using this structure provides a graph embedding with the desired distribution. The structure of encoders in variational graph autoencoders is given in Figure \cite{1}.

2) Decoder: For the graph autoencoder models, the decoder is a non-probabilistic model that reconstructs the adjacency matrix by computing the inner product of the latent representations of two nodes:

$$\hat{A} = \varphi (ZZ^T)$$

In all the models, $\varphi(\cdot)$ denotes the activation function.
For the graph variational autoencoder models, the decoder is a probabilistic model that reconstructs the adjacency matrix by computing the probabilistic inner product of the latent representation of nodes:

$$p(\hat{A} | Z) = \prod_{i=1}^{N} \prod_{j=1}^{N} p(\hat{A}_{ij} | z_i, z_j) \quad (6)$$

where

$$p(\hat{A}_{ij} | z_i, z_j) = \phi(\tilde{z}_i^T \tilde{z}_j) \quad (7)$$

3) Losses: Vanilla models are trained by minimizing reconstruction loss:

$$L = \mathbb{E}_{q(Z|X,A)}[\log p(A|Z)] \quad (8)$$

Variational models are optimized by maximizing the variational lower bound while minimizing reconstruction loss:

$$L = \mathbb{E}_{q(Z|X,A)}[\log p(A|Z)] - KL[q(Z|X,A) || p(Z)] \quad (9)$$

where $KL[q(\cdot) || p(\cdot)]$ is the Kullback-Leibler divergence between $q(\cdot)$ and $p(\cdot)$.

B. Proposed method

Our proposed method, Res-VGAE is a variational graph autoencoder with an adjustable number of residual connections. It enhances the encoder part of the variational graph autoencoder. The decoder and loss are the same as variational graph autoencoders. Our work is inspired by the works of [26] and [27].

To improve the performance of the variational graph autoencoder, we propose utilizing residual graph convolutional layers in the encoder. A residual graph convolutional layer can be represented as:

$$H^{(l+1)} = \varphi \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right) + H^{l} \quad (10)$$

where $\varphi$ is the activation function, $\tilde{D}$ is the degree matrix, $\tilde{A}$ is the normalized adjacency matrix with self-loops and $W^{(l)}$ is the layer’s weight matrix. In a multi-layer model $H^{0} = X$ and $H^{l}$ is the feature map of the $l$th layer.

The input and the output sizes of the hidden layers must be the same in order to add residual connections. The number of residual graph convolutional layers can be set as desired. Owing to utilizing this layer, our model is not affected as other types of autoencoders by increasing the depth of the model. The structure of our model is given in Figure 2.

III. EXPERIMENTAL RESULTS

A. Data Sets

We evaluate the models performance on three benchmark data sets: Cora [28], CiteSeer [29] and PubMed [30]. Cora and CiteSeer are networks of computer science publications where the nodes represent the publications and the edges represent the citations. Node features are one-hot encoded random vectors contained in each paper. The PubMed data set is also a citation network that contains a set of articles related to diabetes disease.

All models and data sets in this paper have been used for link prediction tasks and Table I gives a detailed summary of the data sets we used.
Fig. 2. Model architecture of the RGAE and RVGAE. Residual connections start after the first hidden layer since the input and the output size of layers with residual connections must be the same. The encoder takes the adjacency matrix $A$ and the feature matrix $X$ as inputs and outputs the node embeddings $Z$. The decoder takes as input the embedding matrix $Z$ and outputs the reconstructed adjacency matrix $A'$. The blocks in blue indicate the graph convolutional layers that embed the node features into a 32-dimensional matrix and the yellow blocks are graph convolutional layers that embed the hidden layer features into the final 16-dimensional matrix. The upper and below parts of the figure show the variational and vanilla graph autoencoder structures, respectively.

### TABLE I

| Data set  | Type          | Nodes | Edges | Classes | Features |
|-----------|---------------|-------|-------|---------|----------|
| CitesSeer | Citation network | 3,327 | 4,732 | 6       | 3,703    |
| Cora      | Citation network | 2,708 | 5,429 | 7       | 1,433    |
| PubMed    | Citation network | 19,717 | 44,338 | 3       | 500      |

**B. Experimental Settings**

We have evaluated all the models based on the same baseline as in [27]. We use AP and AUC scores to report the mean accuracy of 10 runs with random train, validation, and test splits of the same size, and all the models are trained for 200 epochs. The validation and test sets contain 5% and 10% of the total edges. The size of the hidden layers is 32 and the size of the final layer is 16. The models are optimized using Adam optimizer with a learning rate of 0.01. We have used PyTorch Geometric [31] and our code will be available in our GitHub page.

**C. Results**

Firstly, we show the results of the models with one, five, and eight residual connections. We measured the performances of models using Average Precision (AP) and Area Under Curve (AUC) metrics.

In Table [III] we compared the models with only one residual connection and we observed that models score similar results with each other. In Cora, the Res-VGAE model has the highest AUC and AP scores while we see that the scores of the models are very similar to each other in CiteSeer and PubMed.

Here we see that in shallow networks adding one residual connection has no significant effect on the accuracy score of the models.

In Table [IV], we see the models with five residual layers. We observe that variational graph autoencoders perform better than graph autoencoders and the residual connections improve the results when comparing with non-residual models. In Cora and PubMed, the variational graph autoencoder with residual connections performs better than the other methods, and in the CiteSeer data set the variational autoencoder achieves the highest AP and AUC scores.

When comparing models with one graph layer, we observe that using five graph layers decreases the accuracies of models, and models with residual connections score higher than those without residual connections.

In Table [V] we compared the performances of models with eight graph layers. Here we observe that our model, Res-VGAE performs better than the other models for Cora and CiteSeer data sets. Moreover, the results show that using variational graph autoencoder with residual connections yield significant improvements in accuracy compared to GAE.

Compared with models with one and five residual layers, we see that the accuracy scores decrease significantly for models without residual connections.

Secondly, in Fig. 3, Fig. 4 and Fig. 5 we compare AP scores of the models with a different number of layers starting from one up to eight, for all the data sets. We observe that deep autoencoders score worse when compared to shallow networks. We also observe that adding residual connections significantly improves the accuracy scores of the models with the same architecture.
Table II

Comparison of the models with 1 graph layer

| Method    | Cora AUC | Cora AP | CiteSeer AUC | CiteSeer AP | PubMed AUC | PubMed AP |
|-----------|----------|---------|--------------|-------------|------------|-----------|
| Res-VGAE  | **91.77 ± 1.25** | 92.38 ± 1.10 | 88.28 ± 1.74 | 89.80 ± 1.64 | 96.27 ± 0.25 | 96.78 ± 0.25 |
| VGAE      | 91.36 ± 1.97 | 92.37 ± 1.66 | 89.47 ± 1.31 | **90.29 ± 0.76** | 95.75 ± 0.47 | 96.33 ± 0.34 |
| Res-GAE   | 89.47 ± 0.94 | 90.33 ± 0.99 | 88.32 ± 1.94 | 89.80 ± 1.58 | **96.52 ± 0.23** | **96.98 ± 0.24** |
| GAE       | 91.33 ± 1.12 | 92.14 ± 0.79 | **89.13 ± 2.19** | 90.11 ± 1.53 | 93.76 ± 0.33 | 96.30 ± 0.42 |

Table III

Comparison of the models with 5 graph layers

| Method    | Cora AUC | Cora AP | CiteSeer AUC | CiteSeer AP | PubMed AUC | PubMed AP |
|-----------|----------|---------|--------------|-------------|------------|-----------|
| Res-VGAE  | **89.08 ± 1.55** | 90.00 ± 1.85 | 83.14 ± 3.34 | 85.89 ± 3.50 | **93.81 ± 0.35** | **94.99 ± 0.40** |
| VGAE      | 88.60 ± 1.37 | **90.39 ± 1.25** | **86.27 ± 2.01** | **88.34 ± 1.65** | 88.83 ± 1.41 | 91.77 ± 0.90 |
| Res-GAE   | 88.23 ± 1.81 | 89.50 ± 2.36 | 84.91 ± 1.45 | 87.32 ± 1.46 | 93.14 ± 0.71 | 94.69 ± 0.36 |
| GAE       | 87.80 ± 2.34 | 89.59 ± 2.42 | 83.47 ± 3.54 | 86.14 ± 3.48 | 90.54 ± 1.43 | 92.78 ± 0.91 |

Table IV

Comparison of the models with 8 graph layers

| Method    | Cora AUC | Cora AP | CiteSeer AUC | CiteSeer AP | PubMed AUC | PubMed AP |
|-----------|----------|---------|--------------|-------------|------------|-----------|
| Res-VGAE  | **87.45 ± 1.84** | **89.23 ± 1.61** | **86.62 ± 2.85** | **88.66 ± 2.40** | 91.28 ± 0.80 | 93.19 ± 0.68 |
| VGAE      | 85.92 ± 2.31 | 88.45 ± 2.54 | 83.22 ± 0.77 | 86.41 ± 0.60 | 84.22 ± 0.95 | 88.36 ± 0.60 |
| Res-GAE   | 86.18 ± 3.80 | 87.33 ± 4.14 | 85.29 ± 1.99 | 87.75 ± 1.95 | **92.39 ± 0.46** | **94.04 ± 0.29** |
| GAE       | 83.63 ± 3.79 | 85.99 ± 4.32 | 84.63 ± 1.28 | 87.34 ± 1.17 | 86.10 ± 1.70 | 89.73 ± 0.90 |

Fig. 3. The AP scores of the models with different number of layers for Cora data set. Models with residual connections score higher than those without residual connections.

Fig. 4. The AP scores of the models with different number of layers for CiteSeer data set. Models with residual connections score higher than those without residual connections.

IV. Conclusion

In this paper, we introduce Res-VGAE, a variational graph autoencoder with a different number of residual connections to alleviate the depth problem of graph neural networks. Results demonstrate that our model with 8 graph layers outperforms the vanilla and variational graph autoencoders with the same depth. For future work, we plan to improve our model architecture and experiment with large data sets. We intend to experiment with different decoders and we plan to use different distributions for the graph variational autoencoders.

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Fig. 5. The AP scores of the models with different number of layers for PubMed data set. Models with residual connections score higher than those without residual connections.

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Indrit Nallbani Indrit Nallbani has received his B.S degree in Physics from Middle East Technical University in 2017 and a M.Sc in Applied Informatics from Istanbul Technical University in 2019. His current research focuses on video activity recognition, graph neural networks, computer vision and machine learning.
Aydin Ayanzadeh  
Aydin Ayanzadeh has received his B.S. in Computer Science from the University of Tabriz in 2016 and M.Sc in Applied Informatics from Istanbul Technical University (ITU) in 2020. His research interest includes the Deep Learning, Medical Informatics and Image processing systems.

Reyhan Kevser Keser  
Reyhan Kevser Keser received the B.S and M.S degrees in “Electronics and Communication Engineering” and “Applied Informatics”, respectively, from Istanbul Technical University (ITU), Istanbul, Turkey. She is currently pursuing a Ph.D. degree with the Information and Communications Engineering Department, Informatics Institute, ITU. Her research interests include computer vision and machine learning techniques.

Nurullah Çalış  
Nurullah Çalış received his M.Sc. And a Ph.D. degree in Electronics and Communication Engineering from the Yıldız Technical University, Turkey, in 2013 and 2019, respectively. He was worked as a post-doctoral researcher in Informatics Institute at Istanbul Technical University. He is currently an assistant professor with the Department of Biomedical Engineering, Istanbul Medeniyet University, Turkey. The main research areas are large-scale data analysis, signal and image processing, and AI applications in engineering. His research interests include especially deep learning regression, optimization, and surrogate modeling.

Behçet Uğur Töreyin  
Behçet Uğur Töreyin received the B.S. degree from the Middle East Technical University, Ankara, Turkey in 2001, and the M.S. and Ph.D. degrees from Bilkent University, Ankara, in 2003 and 2009, respectively, all in electrical and electronics engineering. He is now an Associate Professor with the Informatics Institute at Istanbul Technical University. His research interests lie in signal processing and pattern recognition with applications to computational intelligence. He is the head of the Signal Processing for Computational Intelligence Research Group (SP4CING – https://spacing.itu.edu.tr). His research is focused on developing algorithms to analyze and compress signals from sensors, such as visible/infrared/hyperspectral cameras.