Simple and Effective Graph Autoencoders with One-Hop Linear Models

Guillaume Salha\(^1,2\), Romain Hennequin\(^1\) and Michalis Vaziriannis\(^2,3\)
\(^1\)Deezer Research, Paris, France
\(^2\)LIX, Ecole Polytechnique, Palaiseau, France
\(^3\)Athens University of Economics and Business, Athens, Greece
research@deezer.com

Abstract

Graph autoencoders (AE) and variational autoencoders (VAE) recently emerged as powerful node embedding methods, with promising performances on challenging tasks such as link prediction and node clustering. Graph AE, VAE and most of their extensions rely on graph convolutional networks (GCN) encoders to learn vector space representations of nodes. In this paper, we propose to replace the GCN encoder by a significantly simpler linear model w.r.t. the direct neighborhood (one-hop) adjacency matrix of the graph. For the two aforementioned tasks, we show that this approach consistently reaches competitive performances w.r.t. GCN-based models for numerous real-world graphs, including all benchmark datasets commonly used to evaluate graph AE and VAE. We question the relevance of repeatedly using these datasets to compare complex graph AE and VAE. We also emphasize the effectiveness of the proposed encoding scheme, that appears as a simpler and faster alternative to GCN encoders for many real-world applications.

1 Introduction

Graphs have become ubiquitous, due to the proliferation of data representing relationships or interactions among entities [Hamilton et al., 2017a; Wu et al., 2019b]. Extracting relevant information from these entities, called the nodes of the graph, is crucial to effectively tackle numerous machine learning tasks, such as link prediction or node clustering. While traditional approaches mainly focused on hand-engineered features [Liben-Nowell and Kleinberg, 2007; Bhagat et al., 2011], significant improvements were recently achieved by methods aiming at directly learning node representations that summarize the graph structure (see [Hamilton et al., 2017a] for a review). In a nutshell, these representation learning methods aim at embedding nodes as vectors in a low-dimensional vector space in which nodes with structural proximity in the graph should be close, e.g. by leveraging random walk strategies [Grover and Leskovec, 2016], matrix factorization [Cao et al., 2015] or graph neural networks [Kipf and Welling, 2016a; Hamilton et al., 2017b].

In particular, graph autoencoders (AE) [Tian et al., 2014; Wang et al., 2016; Kipf and Welling, 2016b] and variational autoencoders (VAE) [Kipf and Welling, 2016b] recently emerged as powerful node embedding methods. Based on encoding-decoding schemes, i.e. on the design of low dimensional vector space representations of nodes (encoding) from which reconstructing the graph (decoding) is possible, graph AE and VAE models have been successfully applied to address several challenging learning tasks, with competitive results w.r.t. popular baselines such as [Perozzi et al., 2014; Grover and Leskovec, 2016]. These tasks include link prediction [Kipf and Welling, 2016b; Pan et al., 2018; Tran, 2018; Grover et al., 2019; Salha et al., 2019c], node clustering [Wang et al., 2017; Pan et al., 2018; Salha et al., 2019a], matrix completion for inference and recommendation [Berg et al., 2018; Do, 2019] and molecular graph generation [Jin et al., 2018; Ma et al., 2018]. Existing models usually rely on graph neural networks (GNN) to encode nodes into embeddings. More precisely, most of them implement graph convolutional networks (GCN) encoders [Kipf and Welling, 2016b; Pan et al., 2018; Do, 2019; Grover et al., 2019; Hasanzadeh et al., 2019; Huang et al., 2019; Salha et al., 2019a; Salha et al., 2019c; Shi et al., 2020], a model originally introduced in [Kipf and Welling, 2016a].

However, despite the prevalent use of GCN encoders in recent literature, the relevance of this design choice has never been thoroughly studied nor challenged. The actual benefit of incorporating GCNs in graph AE/VAE w.r.t. significantly simpler encoding strategies remains unclear. In this paper\(^1\), we propose to tackle this important aspect, showing that GCN-based graph AE/VAE are often unnecessarily complex for numerous applications. Our work falls into a family of recent efforts questioning the systematic use of complex deep learning methods without clear comparison to less fancy but simpler baselines [Dacrema et al., 2019; Lin, 2019]. More precisely, our contribution is threefold:

- We introduce simpler versions of graph AE and VAE, replacing GCNs by linear models w.r.t. the direct neighborhood (one-hop) adjacency matrix of the graph, involving a unique weight matrix to tune, fewer operations and no activation function.

\(^1\)A preliminary version of this work has been presented at a NeurIPS 2019 workshop without proceedings [Salha et al., 2019b].
Through an extensive empirical analysis on 17 real-world graphs with various sizes and characteristics, we show that our models consistently reach competitive performances w.r.t. GCN-based graph AE and VAE on link prediction and node clustering tasks. We identify settings where simple linear encoders appear as a suitable alternative to GCNs and a first relevant baseline to implement before diving into more complex models, and we question the relevance of current benchmark datasets used to evaluate and compare graph AE and VAE.

We publicly release the code\(^{3}\) of these experiments, for reproducibility and easier future usages.

This paper is organized as follows. After reviewing key concepts in Section 2, we introduce our simplified graph AE and VAE models in Section 3. We present and interpret our experiments in Section 4, and we conclude in Section 5.

2 Preliminaries

We consider an undirected graph \(G = (V, E)\) with \(|V| = n\) nodes and \(|E| = m\) edges. \(A\) is the direct neighborhood (i.e. one-hop) adjacency matrix of \(G\), and is binary or weighted.

2.1 Graph Autoencoders

Graph autoencoders (AE) [Tian et al., 2014; Wang et al., 2016; Kipf and Welling, 2016] are a family of models aiming at mapping (encoding) each node \(i \in V\) of the graph to a low-dimensional vector \(z_i \in \mathbb{R}^d\), with \(d \ll n\), from which reconstructing (decoding) the graph should be possible. The intuition of this encoding-decoding scheme is the following: if, starting from the node embedding, the model is able to reconstruct an adjacency matrix \(\hat{A}\) close to the true one, then the low-dimensional vectors \(z_i\) should capture some important characteristics of the original graph structure.

Formally, the \(n \times d\) matrix \(Z\), whose rows are the \(z_i\) vectors, is usually the output of a graph neural network (GNN) [Bruna et al., 2014; Defferrard et al., 2016; Kipf and Welling, 2016a] processing \(A\). To reconstruct the graph, most models [Kipf and Welling, 2016b] stack an inner product decoder to this GNN, i.e. we have \(\hat{A}_{ij} = \sigma(z_i^T z_j)\) for all node pairs \((i, j)\), with \(\sigma(\cdot)\) denoting the sigmoid function: \(\sigma(x) = 1/(1 + e^{-x})\). Therefore, the larger the inner product \(z_i^T z_j\) in the embedding, the more likely nodes \(i\) and \(j\) are connected in \(G\) according to the AE. In a nutshell, we have:

\[
\hat{A} = \sigma(ZZ^T) \quad \text{with} \quad Z = \text{GNN}(A).
\]

Several recent works [Grover et al., 2019; Salha et al., 2019c; Shi et al., 2020] considered other decoders, that we also implement in Section 4. GNN weights are tuned by gradient descent, to minimize a reconstruction loss capturing the similarity of \(A\) and \(\hat{A}\), formulated as a weighted cross entropy loss [Kipf and Welling, 2016b].

2.2 Graph Variational Autoencoders

[Kipf and Welling, 2016b] also extended the variational autoencoder (VAE) framework [Kingma and Welling, 2014] to graph structures. Authors designed a probabilistic model involving a latent variable \(z_i\) of dimension \(d \ll n\) for each node \(i \in V\), interpreted as node representations in a \(d\)-dimensional embedding space. The inference model, i.e. the encoding part of the VAE, is defined as:

\[
q(Z|A) = \prod_{i=1}^{n} q(z_i|A) \quad \text{with} \quad q(z_i|A) = \mathcal{N}(z_i|\mu, \text{diag}(\sigma^2)).
\]

Gaussian means and variances parameters are learned using a GNN for each one, i.e. \(\mu = \text{GNN}_\mu(A)\), with \(\mu\) the matrix stacking up mean vectors \(\mu_i\); likewise, \(\log \sigma = \text{GNN}_\sigma(A)\). Latent vectors \(z_i\) are samples drawn from these distributions. Then, a generative model aims at reconstructing (decoding) \(A\), leveraging inner products:

\[
p(A|Z) = \prod_{i=1}^{n} \prod_{j=1}^{n} p(A_{ij}|z_i, z_j), \quad p(A_{ij} = 1|z_i, z_j) = \sigma(z_i^T z_j).
\]

During training, GNN weights are tuned by maximizing a tractable variational lower bound (ELBO) of the model’s likelihood [Kipf and Welling, 2016b]:

\[
\mathcal{L} = \mathbb{E}_q(Z|A) \left[ \log p(A|Z) \right] - D_{KL}(q(Z|A)||p(Z)),
\]

by gradient descent, with a Gaussian prior on the distribution of latent vectors, and using the reparameterization trick from [Kingma and Welling, 2014]. \(D_{KL}(\cdot||\cdot)\) denotes the Kullback-Leibler divergence.

2.3 Graph Convolutional Networks

While the term GNN encoder is generic, a majority of successful applications of graph AE and VAE actually relied on graph convolutional networks (GCN) [Kipf and Welling, 2016a] to encode nodes. This includes the seminal graph AE and VAE models from [Kipf and Welling, 2016b] as well as numerous extensions [Kipf and Welling, 2016b; Pan et al., 2018; Do, 2019; Grover et al., 2019; Hasanzadeh et al., 2019; Huang et al., 2019; Salha et al., 2019a; Salha et al., 2019c; Shi et al., 2020]. In a GCN with \(L\) layers (\(L \geq 2\)), with input layer \(H^{(0)} = I_n\) and output layer \(H^{(L)}\) (with \(H^{(L)} = Z\) for AE, and \(H^{(L)} = \mu\) or \(\log \sigma\) for VAE), embedding vectors are iteratively updated, as follows:

\[
H^{(l)} = \text{ReLU}(\hat{A}H^{(l-1)}W^{(l-1)}), \quad l \in \{1, \ldots, L - 1\}
\]

\[
H^{(L)} = \hat{A}H^{(L-1)}W^{(L-1)}
\]

where \(\hat{A} = D^{-1/2}(A + I_n)D^{-1/2}\), \(D\) is the diagonal degree matrix of \(A + I_n\), and \(\hat{A}\) is therefore its symmetric normalization. At each layer, each node averages representations from its neighbors (that, from layer 2, have aggregated representations from their own neighbors), with a ReLU activation: \(\text{ReLU}(x) = \max(x, 0)\). Matrices \(W^{(0)}, \ldots, W^{(L-1)}\), whose dimensions can vary, are weight matrices to tune.

GCNs became a popular encoding scheme for graph AE and VAE, thanks to its reduced complexity w.r.t. other GNNs [Bruna et al., 2014; Defferrard et al., 2016], and notably the linear time complexity w.r.t. \(m\) of evaluating each layer [Kipf and Welling, 2016a]. Last, GCN models can also leverage node-level features, summarized in an \(n \times f\) matrix \(X\), in addition to the graph structure. In such setting, the input layer becomes \(H^{(0)} = X\) instead of the identity matrix \(I_n\).
3 Simplifying Graph AE and VAE with One-Hop Linear Encoders

Graph AE and VAE emerged as powerful node embedding methods with promising performances. However, while almost all recent efforts from the literature implement GCN (or another GNN) encoders, the question of the actual benefit of such complex encoding schemes w.r.t. much simpler strategies remains widely open. In the following two sections, we tackle this important problem, arguing that GCN encoders often bring unnecessary complexity and redundancy. We propose alternative versions of graph AE and VAE, learning node embeddings from linear models, i.e. from significantly simpler and more interpretable encoders, involving fewer parameters, fewer computations and no activation function.

3.1 Linear Graph AE

In this paper, we propose to replace the GCN encoder by a simple linear model w.r.t. the normalized one-hop adjacency matrix of the graph. In the AE framework, we have:

\[ Z = \hat{A}W, \text{ then } \hat{A} = \sigma(ZZ^T). \]

We refer to this model as linear graph AE. Embedding vectors are obtained by multiplying the \( n \times n \) normalized adjacency matrix \( \hat{A} \) by a unique \( n \times d \) weight matrix \( W \). We tune this matrix in a similar fashion w.r.t. graph AE [Kipf and Welling, 2016b], i.e. by iteratively minimizing a weighted cross-entropy loss capturing the quality of the reconstruction \( \hat{A} \) w.r.t. the original matrix \( A \), by gradient descent.

This encoder is a straightforward linear mapping. Each element of \( z_i \) is a weighted average from node \( i \)'s direct one-hop connections. Contrary to GCN encoders (as \( L \geq 2 \)), it ignores higher-order (k-hop with \( k > 1 \)) information. Also, the encoder does not include any non-linear activation function.

In Section 4, we will highlight the very limited impact of these two restrictions on empirical performances.

Our encoder runs in a linear time w.r.t. \( m \) using a sparse representation for \( \hat{A} \), and involves fewer operations than a GCN. It includes \( nd \) parameters i.e. slightly fewer than the \( nd + (L-1)d^2 \) parameters required by a \( L \)-layer GCN with \( d \)-dim layers. However, we stress out that, as for standard graph AE, the inner-product decoder has a quadratic \( O(dn^2) \) complexity, as it involves the multiplication of the two dense matrices \( \hat{Z} \) and \( \hat{Z}^T \).

We discuss scalability strategies in Section 4, where we also implement two alternative decoders.

Our linear graph AE can also leverage graph datasets that include node-level features vectors of dimension \( f \), stacked up in the \( n \times f \) matrix \( X \). The encoding step becomes:

\[ Z = \hat{A}XW, \]

where the weight matrix \( W \) is then of dimension \( f \times d \).

3.2 Linear Graph VAE

We adopt the same approach to replace the two GCNs of graph VAE by:

\[ \mu = \hat{A}W_\mu \text{ and } \log \sigma = \hat{A}W_\sigma, \]

with \( n \times d \) weight matrices \( W_\mu \) and \( W_\sigma \). Then:

\[ \forall i \in V, z_i \sim \mathcal{N}(\mu_i, \text{diag}(\sigma_i^2)), \]

with similar decoder w.r.t. standard graph VAE. We refer to this simpler model as linear graph VAE. During the learning phase, as standard graph VAE, we iteratively optimize the ELBO bound [Kipf and Welling, 2016b] w.r.t. \( W_\mu \) and \( W_\sigma \), by gradient descent. To include features \( X \), we compute:

\[ \mu = \hat{A}XW_\mu \text{ and } \log \sigma = \hat{A}XW_\sigma, \]

and weight matrices \( W_\mu \) and \( W_\sigma \) are then of dimension \( f \times d \).

3.3 Related Work

Our work falls into a family of research efforts aiming at challenging and questioning the prevalent use of complex deep learning methods without clear comparison to simpler baselines (see e.g. [Dacrema et al., 2019; Lin, 2019]). In particular, [Wu et al., 2019a] recently proposed to simplify GCNs, notably by removing non-linearities between layers and collapsing some weight matrices during training. Their simplified model empirically rivals standard GCNs on several large-scale classification tasks. While our work also focuses on GCNs, we argue that the two papers actually tackle very different and complementary problems:

- [Wu et al., 2019a] focus on supervised and semi-supervised settings. They consider the GCN as the model itself, optimized to classify node-level labels. On the contrary, we consider two unsupervised settings, in which GCNs are only a building part (the encoder) of a larger framework (the AE or the VAE), and where we optimize reconstruction losses from GCN-based embedding vectors (for AE) or from vectors drawn from distributions learned through two GCNs (for VAE).

- Our encoders only capture one-hop interactions: nodes only aggregate information from their direct neighbors. On the contrary, [Wu et al., 2019a] still rely on a stacked layers design that, although simplified, allows learning from higher-order interactions. Contrary to us, considering such relationships is crucial in their model for good performances (we explain in Section 4 that, in our settings, it would mostly increase running times).

4 Empirical Analysis and Discussion

In this section, we propose an in-depth experimental evaluation of our simplified graph AE and VAE models.

4.1 Experimental Setting

Tasks. We consider two learning tasks. Firstly, we focus on link prediction, as in [Kipf and Welling, 2016b] and most subsequent works. We train models on incomplete versions of graphs where \( 15\% \) of edges were randomly removed. Then, we create validation and test sets from removed edges (resp. from \( 5\% \) and \( 10\% \) of edges) and from the same number of randomly sampled pairs of unconnected nodes. We evaluate the model’s ability to classify edges from non-edges, using the mean Area Under the Receiver Operating Characteristic (ROC) Curve (AUC) and Average Precision (AP) scores on test sets, averaged over 100 runs with random train/validation/test splits. As a second task, we perform node clustering from \( z_i \) vectors. When datasets include node-level ground-truth communities, we train models on complete
graphs, then run $k$-means algorithms in embedding spaces. We compare output clusters to communities via the mean Adjusted Mutual Information (AMI) scores over 100 runs.

Datasets. We provide experiments on 17 publicly available real-world graphs. For each graph, Tables 1 and 2 report the adjusted Mutual Information (AMI) scores over 100 runs.

- We first consider the Cora, Citeseer and Pubmed citation graphs$^3$, with and without node features corresponding to $f$-dimensional bag-of-words vectors. These three graphs were used in the original experiments of [Kipf and Welling, 2016b] and then in the wide majority of recent works [Wang et al., 2017; Pan et al., 2018; Tran, 2018; Grover et al., 2019; Hasanzadeh et al., 2019; Huang et al., 2019; Park et al., 2019; Salha et al., 2019a; Salha et al., 2019c; Shi et al., 2020], becoming the de facto benchmark datasets for evaluating graph AE and VAE. Therefore, comparing linear and GCN-based models on these graphs was essential.

- We also report results on 14 alternative graphs. We consider four other citation networks: DBLP$^4$, Arxiv-HepTh$^4$, Patent$^4$ and a larger version of Cora$^3$, that we denote Cora-larger. We add the WebKD$^5$, Blogs$^5$ and Stanford$^5$ web graphs, where hyperlinks connect web pages, as well as two Google web graphs (a medium-size one$^5$, denoted Google, and a larger one$^5$, denoted Google-large). We complete the list with two social networks (Hamsterster$^5$ and LiveMocha$^5$), the Flickr$^5$ image graph (nodes represent images, connected when sharing metadata), the Proteins$^5$ network of proteins interactions and the Amazon$^5$ products co-purchase network. We span a wide variety of real-world graphs of various natures, characteristics and sizes (from 877 to 2.7 million nodes, from 1 608 to 13.9 million edges).

Models. In all experiments, we compare our models to 2-layer and 3-layer GCN-based graph AE/VAE. We do not report performances of deeper models, due to significant scores deterioration. For a comparison to non-AE/VAE methods, which is out of the scope of this study, we refer to [Kipf and Welling, 2016b; Salha et al., 2019a]. All models were trained for 200 epochs (resp. 300 epochs) for graphs with $n < 100 000$ (resp. $n \geq 100 000$). We thoroughly checked the convergence of all models for these epochs numbers. As [Kipf and Welling, 2016b], we ignored edges directions when initial graphs were directed. For Cora, Citeseer and Pubmed, we set identical hyperparameters w.r.t. [Kipf and Welling, 2016b] to reproduce their results, i.e. we had $d = 16$, 32-dim hidden layer(s) for GCNs, and we used Adam optimizer [Kingma and Ba, 2015] with a learning rate of 0.01. For other datasets, we tuned hyperparameters by performing grid search on the validation set. We adopted a learning rate of 0.1 for Arxiv-HepTh, Patent and Stanford; of 0.05 for Amazon, Flickr, LiveMocha and Google-large, of 0.01 for Blogs, Cora-larger, DBLP, Google and Hamsterster and Proteins (AE models); of 0.005 for WebKD (except linear AE and VAE where we used 0.001 and 0.01) and Proteins (VAE models). We set $d = 16$ (but we reached similar conclusions with $d = 32$ and 64), with 32-dim hidden layer(s) and without dropout. Last, due to the prohibitive quadratic cost of reconstructing (decoding) the exact $A$ for large graphs (with $n \geq 100 000$), we adopted a simple stochastic sampling strategy for these graphs: at each training iteration, we estimated losses by re-sampling a subgraph of 10 000 randomly picked nodes.

### 4.2 Results

| Model            | Cora, with features | Citeeser, with features | Pubmed, with features |
|------------------|---------------------|-------------------------|-----------------------|
|                  | (n = 2 708, m = 5 429) | (n = 3 327, m = 4 732) | (n = 19 717, m = 44 338) |
|                  | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) |
| Linear AE (ours) | 83.19 ± 1.13 | 87.57 ± 0.95 | 77.06 ± 1.81 | 83.05 ± 1.25 | 81.85 ± 0.32 | 87.54 ± 0.28 |
| 2-layer GCN AE   | 84.79 ± 1.10 | 88.45 ± 0.82 | 78.25 ± 1.69 | 83.79 ± 1.24 | 82.51 ± 0.64 | 87.42 ± 0.38 |
| 3-layer GCN AE   | 84.61 ± 1.22 | 87.65 ± 1.11 | 78.62 ± 1.74 | 82.81 ± 1.43 | 83.37 ± 0.98 | 87.62 ± 0.68 |
| Linear VAE (ours) | 84.70 ± 1.24 | 88.24 ± 1.02 | 78.87 ± 1.34 | 83.34 ± 0.99 | 84.03 ± 0.28 | 87.98 ± 0.25 |
| 2-layer GCN VAE  | 84.19 ± 1.07 | 87.68 ± 0.93 | 78.08 ± 1.40 | 83.31 ± 1.31 | 82.63 ± 0.45 | 87.45 ± 0.34 |
| 3-layer GCN VAE  | 84.48 ± 1.42 | 87.61 ± 1.08 | 79.27 ± 1.78 | 83.73 ± 1.13 | 84.07 ± 0.47 | 88.18 ± 0.31 |

Table 1: Link prediction on Cora, Citeseer and Pubmed benchmark datasets. Cells are grayed when linear graph AE/VAE are reaching

3https://linqs.soe.ucsc.edu/data
4http://snap.stanford.edu/data/index.html
5http://konect.uni-koblenz.de/networks/
models consistently reach competitive performances w.r.t. 2 and 3-layer GCN encoders, i.e. they are at least as good ± 1 standard deviation. In some settings, linear graph AE/VAE are even slightly better (e.g. +1.25 points in AUC for linear graph VAE on RealWeb with features). These results emphasize the effectiveness of the proposed simple encoding scheme on these datasets, where the empirical benefit of GCNs is very limited. In Table 3, we consolidate our results by showing similar results on the node clustering task. Nodes are documents clustered in respectively 6, 7 and 3 topic classes, acting as communities. In almost all settings, linear graph AE and VAE rival their GCN-based counterparts.

**Alternative graph datasets.** Table 2 reports link prediction results for the 14 other graphs. Our linear graph AE is competitive in 13 cases out of 15, while our linear graph VAE rivals GCN-based models in 10 cases out of 15. Overall, linear graph AE/VAE also achieve very close results w.r.t. GCN-based models in all remaining datasets. This confirms the empirical effectiveness of simple node encoding schemes, that appear as a suitable alternative to complex encoders for many real-world applications. Regarding node clustering (Table 3), linear AE and VAE models are competitive on the Cora-larger graph, in which nodes are documents clustered in 70 topic classes. However, 2-layer and 3-layer GCN-based models are significantly outperforming on the Blogs graph, where political blogs are classified as either left-leaning or right-leaning.

**When (not) to use GCN encoders?** Linear graph AE and VAE reach strong empirical results on all graphs, and rival or outperform GCN-based graph AE and VAE in a majority of experiments. Our models are also significantly simpler and more interpretable, each element of $\varepsilon_i$ being interpreted as a weighted average from node i’s direct neighborhood. Therefore, we recommend the systematic use of linear graph AE/VAE as a first baseline, before diving into more complex encoding schemes whose actual benefit might be unclear. Moreover, from our experiments, we also conjecture that GCN encoders can bring a slight empirical advantage when dealing with graphs with intrinsic non-trivial high-order interactions. Notable examples of such graphs include the Amazon co-purchase graph (+5.61 AUC points for 2-layer GCN VAE) and web graphs such as Blogs, Google and Stanford, in which two-hop hyperlinks connections of pages usually include relevant information on the global network structure. On such graphs, capturing this additional information tends to improve results, especially 1) for the probabilistic VAE framework, and 2) when evaluating embeddings via the node clustering task (20+ AMI points on Blogs for 2-layer GCN AE/VAE) which is, by design, a more global learning task than the quite local link prediction problem. On the contrary, in citation graphs, the relevance of two-hop links is limited. Indeed, if a reference A in an article B cited by some authors is relevant to their work, authors will likely also cite this reference A, thus creating a one-hop link. Last, while the impact of the graph size is unclear in our experiments (linear models achieve strong results even on large graphs, such as Patent), we note that graphs where GCN encoders outperform are all relatively dense. To conclude, we conjecture that denser graphs with intrinsic high-order interactions (e.g. web graphs) should be better suited that the sparse Cora, Citeseer and Pubmed citation networks, to compare complex graph...
### Table 3: Node Clustering on graphs with communities. Cells are grayed when linear graph AE/VAE are reaching competitive results w.r.t. GCN-based models from Kipf and Welling (2016b) (i.e. at least as good ± 1 standard deviation).

| Model          | Cora (n = 2,708, m = 5,429) | Cora with features (n = 2,708, m = 5,429, f = 1,433) | Citeseer (n = 3,327, m = 4,712) | Citeseer with features (n = 3,327, m = 4,732, f = 2,703) | Pubmed (n = 19,171, m = 44,338, f = 5,500) | Pubmed with features (n = 19,171, m = 44,338, f = 5,500) | Blogs (n = 1,214, m = 19,025) |
|----------------|-------------------------------|------------------------------------------------------|--------------------------------|-----------------------------------------------------|---------------------------------|-----------------------------------------------------|-------------------------------|
|                | AUC (in %)    | AP (in %)    | AUC (in %)    | AP (in %)    | AUC (in %)    | AP (in %)    | AUC (in %)    | AP (in %)    | AUC (in %)    | AP (in %)    | AUC (in %)    | AP (in %)    |
| Linear AE (ours) | 87.54 ± 0.88 | 9.03 ± 0.09 | 86.29 ± 0.88 | 8.70 ± 0.09 | 90.28 ± 0.88 | 9.42 ± 0.09 | 90.16 ± 0.88 | 9.11 ± 0.09 | 85.33 ± 0.88 | 8.16 ± 0.09 | 94.76 ± 0.88 | 9.89 ± 0.09 |
| 2-layer Graph AE | 86.29 ± 0.88 | 8.70 ± 0.09 | 85.33 ± 0.88 | 8.16 ± 0.09 | 94.76 ± 0.88 | 9.89 ± 0.09 | 90.28 ± 0.88 | 9.42 ± 0.09 | 86.29 ± 0.88 | 9.03 ± 0.09 | 88.01 ± 0.88 | 9.42 ± 0.09 |
| 3-layer Graph AE | 85.33 ± 0.88 | 8.16 ± 0.09 | 94.76 ± 0.88 | 9.89 ± 0.09 | 90.28 ± 0.88 | 9.42 ± 0.09 | 86.29 ± 0.88 | 9.03 ± 0.09 | 85.33 ± 0.88 | 8.70 ± 0.09 | 94.76 ± 0.88 | 9.89 ± 0.09 |

### Table 4: Link prediction with Graphite and Gravity alternative decoding schemes. Cells are grayed when linear graph AE/VAE are reaching competitive results w.r.t. GCN-based models (i.e. at least as good ± 1 standard deviation).

| Model          | Cora (n = 2,708, m = 5,429) | Citeseer (n = 3,327, m = 4,732) | Pubmed (n = 19,171, m = 44,338, f = 5,500) | Google (n = 15,573, m = 171,206) |
|----------------|-------------------------------|--------------------------------|---------------------------------|--------------------------------|
|                | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) | AUC (in %) | AP (in %) |
| Linear Graphite AE (ours) | 83.42 ± 0.17 | 78.32 ± 0.17 | 82.88 ± 0.17 | 78.32 ± 0.17 | 85.51 ± 0.17 | 82.88 ± 0.17 | 85.51 ± 0.17 | 82.88 ± 0.17 | 85.51 ± 0.17 | 82.88 ± 0.17 |
| 2-layer Graphite AE | 81.20 ± 0.21 | 75.11 ± 0.21 | 78.92 ± 0.21 | 75.11 ± 0.21 | 84.88 ± 0.21 | 78.92 ± 0.21 | 84.88 ± 0.21 | 78.92 ± 0.21 | 84.88 ± 0.21 | 78.92 ± 0.21 |
| 3-layer Graphite AE | 79.06 ± 0.22 | 71.97 ± 0.22 | 75.92 ± 0.22 | 71.97 ± 0.22 | 83.23 ± 0.22 | 75.92 ± 0.22 | 83.23 ± 0.22 | 75.92 ± 0.22 | 83.23 ± 0.22 | 75.92 ± 0.22 |

AE/VAE, especially on global tasks such as node clustering.

### On more complex decoders.

So far, we compared different encoders but the (standard) inner-product decoder was fixed. As a robustness check, in Table 4, we report complementary link prediction experiments, on variants of graph AE/VAE with two more complex decoders from existing literature: the Graphite model from [Grover et al., 2019] and the gravity-inspired asymmetric decoder from [Salha et al., 2019c]. We draw similar conclusions w.r.t. Tables 1 and 2, consolidating our conclusions. For brevity, we only report results for the Cora, Citeseer and Pubmed graphs, where linear models are competitive, and for the Google graph, where GCN-based graph AE and VAE are slightly outperforming. We stress out that scores from Graphite and gravity-inspired models are not directly comparable, as the former ignores edges directionalities while the latter processes directed graphs.

### On k-hop linear encoders.

While we only learn from direct neighbors interactions, variants of our models could capture higher-order links by considering polynomials of the matrix $A$. For instance, we could learn embeddings from one-hop and two-hop links by replacing $A$ by the normalized version of $A + \alpha A^2$ (with $\alpha > 0$), or simply $A^2$, in the linear encoders of Section 3. While our online implementation proposes such alternative, we observed few to no improvement on most of our graphs, consistently with our claim on the effectiveness of simple one-hop strategies. We underline that such variants significantly increase running times w.r.t. our models (see below), as $A^2$ is usually much denser than $A$.

### On running times.

While this work put the emphasis on performance, we also note that linear AE and VAE models are 10% to 15% faster than their GCN-based counterparts. For instance, on an NVIDIA GTX 1080 GPU, we report a 6.03 seconds (vs 6.73 seconds) mean running time for linear graph VAE (vs 2-layer GCN graph VAE) on the featureless Citeseer dataset, and 791 seconds (vs 880 seconds) on the Pubmed dataset, using our sampling strategy from Section 4.1. This gain comes from the slightly fewer parameters and matrix operations required by our linear encoders and from the sparsity of the one-hop matrix $A$ for most real-world graphs. Nonetheless, as an opening, we point out that the problem of scalable graph autoencoders remains quite open. Despite advances on the encoder, the standard inner-product decoder still suffer from a $O(dn^2)$ time complexity. Our very simple sampling strategy to overcome this quadratic cost on large graphs (randomly sampling subgraphs to reconstruct) might not be optimal. Future works will tackle these issues, aiming at providing efficient strategies to scale graph AE and VAE.

### 5 Conclusion

We highlighted that, despite their prevalent use in recent literature, GCN-based graph AE and VAE are often unnecessarily complex, and that significantly simpler and more interpretable versions of these models achieve comparable performances on numerous real-world datasets. In this direction, we introduced simplified yet effective encoding schemes limiting to one-hop linear strategies, that we recommend to use as baselines to assess the actual benefit of complex encoders.
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