

# ReGAE: Graph autoencoder based on recursive neural networks

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**Abstract.** Invertible transformation of large graphs into fixed dimensional vectors (embeddings) remains a challenge. Its overcoming would reduce any operation on graphs to an operation in a vector space. However, most existing methods are limited to graphs with tens of vertices. In this paper we address the above challenge with recursive neural networks – the encoder and the decoder. The encoder network transforms embeddings of subgraphs into embeddings of larger subgraphs, and eventually into the embedding of the input graph. The decoder does the opposite. The dimension of the embeddings is constant regardless of the size of the (sub)graphs. Simulation experiments presented in this paper confirm that our proposed graph autoencoder, ReGAE, can handle graphs with even thousands of vertices.

**Keywords:** Graph Neural Networks · Graph Autoencoders · Graph Embeddings

## 1 Introduction

Graph Neural Networks (Graph NNs, GNNs) [21,27] is an emerging area within artificial intelligence. It addresses operations on graphs such as their generation, representation, classification, as well as operations on their separate nodes or edges such as classification or prediction of their attributes.

In this paper, we design a transformation (encoding) of a set of graphs into vectors of fixed size (embeddings) and inverse transformation (decoding). Our proposed transformations may be applied, among others, to (i) graph classification, with the fixed-size graph embedding fed to an ordinary classifier, (ii) graph evaluation/labeling, with the fixed-size graph embedding fed to a general purpose function approximator, (iii) graph generation, with a noise vector fed to the decoder and (iv) graph transformation without constraints on sizes (of both input and output).

Both proposed transformations are based on feedforward NNs applied recursively to embeddings of subgraphs of the input graph. The encoder recursively aggregates embeddings of subgraphs into embeddings of larger subgraphs. The decoder, conversely, recursively desegregates the embeddings and produces the elements of the adjacency matrix.

In the literature, graphs are typically represented with arrays of embeddings of their vertices. These structures are impossible to handle with methods that accept input of fixed size, such as feedforward neural networks, as they have a different shape depending on the graph size. There are also methods that embed graphs in vectors of fixed size, but they do not enable reconstruction of the graphs from these vectors, hence they lose some information on these graphs.

To the best of our knowledge, our proposed ReGAE is the first one able to represent graphs of arbitrary sizes with embeddings of fixed dimension which enables reconstruction of the source graphs thereby preserving most of the information on these graphs.

The paper is organized as follows. Sec. 2 overviews related literature. Sec. 3 introduces our solution. Sec. 4 presents an experimental study, and Sec. 5 concludes the paper.

*Formal problem description.* We consider undirected graphs. A graph of interest is given by a number of its vertices,  $n \in \mathbb{N}$ , and its adjacency matrix  $A \in \{0, 1\}^{n \times n}$ . Its entry  $A_{i,j}$  indicates if there is an edge between the vertices  $i$  and  $j$ . For a given set of graphs and  $m \in \mathbb{N}$  we seek for a transformation of each graph in this set into a vector in  $\mathbb{R}^m$ , and the inverse transformation.

Our proposed solution in its extended form presented in Sec. 3.4 applies also to more general problems with directed graphs, weighted edges, and labeled edges and vertices.

## 2 Related work

*Graph embeddings in vectors of fixed size and graph classification.* These methods embed graphs in vectors in  $\mathbb{R}^m$  for a fixed  $m$ . Their primary goal is to represent graphs in a set of features to enable their classification. Methods like Graph Kernels [22] or Graph2Vec [14] are inspired by natural language processing techniques and describe graphs with a concentration of specific subgraphs in there. Later methods define NNs that convert graphs into embeddings in  $\mathbb{R}^m$  with a neural network learning directly to optimize the graph classification criterion. In DiffPool [24] the NN operates on a hierarchy of subgraphs. UGraphEmb [1] use multiscale node attention and graph proximity metrics to assure that a distance between graphs corresponds to the distance between their embeddings.

A model able to learn to assign labels to graphs is a convolutional neural network [5]. The SortPooling layer was added to such a network which enables its connection to a traditional NN as an output module [26]. The above classifiers and others were evaluated in an extensive study in [6].

*Graph generation.* There are two generic approaches to graph generation, one based on Generative Adversarial Networks (GAN [7]) and one based on a sequential expansion of the graph.

In NetGAN [2], the adjacency matrix is generated by a biased random walk among the vertices of the graph; the discriminator is an LSTM network that verifies if a walk through the graph is realistic.

[13] proposed a model that learns to assign probabilities to different actions within sequential graph generation, such as adding a vertex, adding an edge, etc. In GraphRNN [25], a recurrent NN is employed to fill in the adjacency matrix. While the previous methods operate recursively, [20] presents a method for one-shot transformation of (random) vectors of fixed size into graphs.

*Graph autoencoders based on embeddings in  $\mathbb{R}^{n \times d}$ .* These architectures implement the general structure of Variational Autoencoder (VAE [11]) and establish transformations  $\text{input\_graph} \rightarrow \text{embedding}$  (encoder) and  $\text{embedding} \rightarrow \text{input\_graph\_reconstruction}$  (decoder). The embedding is in  $\mathbb{R}^{n \times d}$ , with  $n$  being the number of graph’s vertices, and  $d$  being the dimension of a single node embedding.

[12] proposed Graph VAE with an encoder in the form of graph convolutional NN and the decoder in the form of a simple inner product. [15] proposed adversarial regularization for the embeddings to preserve the topological structure of the graph.

Accuracy of graph reproduction is the main problem in graph VAEs. [8] introduced *Graphite*, a graph VAE with a strategy, inspired by low-rank approximations, of graph refinement in its decoder. [16] proposed an autoencoder with graph convolution, Laplacian smoothing of the encoder, and Laplacian sharpening-based decoder.

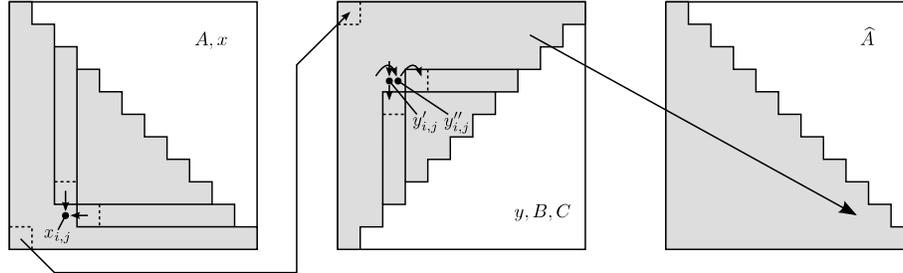
Attention [19] was introduced to graph VAE in [17] as a crucial component of both the encoder and the decoder. [10] proposed a graph VAE aiming to maximize the similarity between the embeddings of neighboring and more distant vertices while minimizing the redundancy between the components of these embeddings.

*Graph autoencoders with embeddings in  $\mathbb{R}^m$ .* Our goal in this paper is to transform graphs of various sizes to embeddings of fixed size,  $m$ , and transform these embeddings back to graphs. A simple way to achieve it is to assume that the number of vertices is bounded by a fixed  $n_{\max}$  and one of the autoencoders from the previous paragraph with an embedding of size  $n_{\max} \times d$  with some kind of padding for smaller graphs. This idea is applied in GraphVAE [18] for small graphs with  $n_{\max}$  up to 38.

[9] introduced MGVAE – an autoencoder whose encoder recursively identifies clusters in the graph, and replace them with nodes of a higher order graph. Eventually the input graph is reduced to a fixed size embedding. The decoder recursively unpacks this embedding to the input graph. MGVAE was shown to process molecular graphs with tens of vertices.

The autoencoder presented in this paper, ReGAE, embed a graph of any size in a vector of a fixed dimension, and recreates it back. In principle, it does not have any limits for the size of the graph, although of course the larger the graph, the more lossy its reconstruction.

### 3 Method



**Fig. 1.** Recursive graph autoencoder. *Left:* The encoder combines embeddings of smaller subgraphs into the embedding of their union. *Middle:* The decoder; for an embedding of a subgraph, it produces half-embeddings for two smaller subgraphs, also an entry in a reindexed adjacency matrix,  $B$ , and an entry in a matrix,  $C$ , which indicates if the main diagonal of  $B$  has been reached. *Right:* By changing indexing in  $y$  we obtain  $\hat{A}$  which is a reconstruction of  $A$ .

We define a **graph embedding** as a vector in  $\mathbb{R}^m$ , where  $m \in \mathbb{N}$  is an even constant. In the course of encoding a graph, embeddings,  $x_{i,j} \in \mathbb{R}^m$ ,  $i > j$ , are produced that approximately represent subgraphs of the given graph limited to its nodes  $j, \dots, i$ . These embeddings are produced recursively and finally,  $x_{n,1}$  represents the whole input graph. The structure of this recursion is presented in the left-hand part of Fig. 1 in reference to the adjacency matrix.

In the process of decoding the graph, embeddings,  $y_{i,j} \in \mathbb{R}^m$ , are recursively produced that represent subgraphs. Eventually, they represent single nodes.  $y$  has its specific indexing because decoding starts from the left lower corner of the adjacency matrix, whose size is initially unknown. In this specific indexing the coordinates of this left lower corner are  $\langle 0, 0 \rangle$ . The decoder recursion is presented in the middle part of Fig. 1. The right-hand part of this figure presents retrieving the original indexing of the adjacency matrix.

The **encoder** is a transformation

$$e : \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R} \mapsto \mathbb{R}^m. \quad (1)$$

To produce  $x_{i,j}$ , the encoder is fed with (i) the embedding  $x_{i,j+1}$ , (ii) the embedding  $x_{i-1,j}$ , (iii) the entry  $A_{i,j}$ . Based on embeddings of two subgraphs, it produces an embedding that represents the union of these subgraphs. Applied recursively according to Algorithm 1, it finally produces  $x_{n,1}$  which represents the entire graph.

The **decoder** is a transformation

$$d : \mathbb{R}^m \mapsto \mathbb{R}^{m/2} \times \mathbb{R}^{m/2} \times \mathbb{R} \times \mathbb{R}. \quad (2)$$

**Algorithm 1** Encoder

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1: Input: Adjacency matrix  $A$ 
2: for  $k = 1, \dots, n - 1$  do
3:    $x_{k+1,k} \leftarrow e(\text{null}, \text{null}, A_{k+1,k})$ 
4: end for
5: for  $i = 1, \dots, n - 1$  do
6:   for  $k = 1, \dots, n - i$  do
7:      $x_{i+k+1,k} \leftarrow e(x_{i+k,k}, x_{i+k+1,k+1}, A_{i+k+1,k})$ 
8:   end for
9: end for
10: return  $x_{n,1}$  // embedding of input graph

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**Algorithm 2** Decoder

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1: Input: Graph embedding  $x$ 
2:  $y_{0,0} \leftarrow x$ 
3: for  $i = 0, \dots$  do
4:   for  $k = 0, \dots, i$  do
5:      $\langle y'_{i+1-k,k}, y''_{i-k,k+1}, B_{i-k,k}, C_{i-k,k} \rangle \leftarrow d(y_{i-k,k})$ 
6:   end for
7:    $y'_{0,i+1} \leftarrow d'(y_{0,i})$ 
8:    $y''_{i+1,0} \leftarrow d''(y_{i,0})$ 
9:   for  $k = 0, \dots, i + 1$  do
10:     $y_{i+1-k,k} \leftarrow \text{concatenate}(y'_{i+1-k,k}, y''_{i+1-k,k})$ 
11:   end for
12:   if the average  $C_{i+1-k,k}$  for  $k \in \{0, \dots, i + 1\}$  is below 0.5 then
13:     set  $n \leftarrow i + 2$  and exit the loop.
14:   end if
15: end for
16: for  $i = 0, \dots, n - 1; j = 0, \dots, n - 1 - i$  do
17:    $\hat{A}_{n-i,j+1} \leftarrow B_{i,j}$ 
18: end for
19: return  $\hat{A}$  // adjacency matrix estimate

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Applied recursively according to Algorithm 2, it reconstructs the adjacency matrix. The input of  $d$  is an embedding,  $y_{i,j}$ , of the subgraph of the target graph limited to its nodes  $j + 1, \dots, n - i$ . When fed with  $y_{i,j}$ ,  $d$  produces (i) the left-hand half of the embedding  $y_{i+1,j}$ , (ii) the right-hand half of the embedding  $y_{i,j+1}$ , (iii) the value  $B_{i,j}$  that later on becomes the entry  $\hat{A}_{n-i,j+1}$  of the resulting adjacency matrix estimate, (iv) the value  $C_{i,j}$  that indicates if  $i + j + 1 = n$ , i.e., if  $(i, j)$  has reached the antidiagonal of the  $B$  matrix (see the middle part of Figure 1).

*Training.* When training the encoder and decoder we require reconstruction of the input graph and a matrix,  $C$ , with ones at appropriate entries, thereby indicating the size of the output graph. That is, we require that

$$B_{i,j} = A_{n-i,j+1}, \quad C_{i,j} = 1 \quad (3)$$

for  $i + j = 0, \dots, n - 2$ , and

$$B_{i,n-1-i} = 0, \quad C_{i,n-1-i} = 0 \quad (4)$$

for  $i = 0, \dots, n - 1$ .

To facilitate the training on large graphs (with thousands of vertices), we utilize the fact that the encoder transforms subgraphs into embeddings, and the decoder transforms embeddings back into the same subgraphs. Therefore, we use subgraphs as training samples for the autoencoder. In subsequent epochs of the training the sizes of these subgraphs grow. We start with short recursion paths and gradually increase their lengths.

*Loss function.* A single graph contributes to the training loss with (i) a sum of cross-entropies for elements of  $A$  equal to 1, (ii) a sum of cross-entropies for elements of  $A$  equal to 0 and (iii) a square of the embedding norm. These components have their constant weights that assure that their contribution is comparable.

*Structure of encoder and decoder.* Our encoder and decoder are inspired by the GRU network [3]. The encoder is designed to combine input embeddings of smaller subgraphs to the output embedding of their union. This combination is based on weighted averaging and additive adjusting. The encoder is based on a feedforward neural network  $f^e$  with a linear output layer, which produces three vectors of size  $m$ :

$$\langle z^0, z^1, \hat{x} \rangle = f^e(x^0, x^1, a). \quad (5)$$

The vectors  $z^0$  and  $z^1$  are applied for weighting input embeddings and  $\hat{x}$  is applied for additive adjusting. The output of the encoder is defined as

$$e(x^0, x^1, a) = (x^0 \circ \sigma(z^0) + x^1 \circ (\mathbf{1} - \sigma(z^0))) \circ \sigma(z^1) + \psi(\hat{x}) \circ (\mathbf{1} - \sigma(z^1)), \quad (6)$$

where  $\mathbf{1}$  is a vector of ones,  $\sigma$  is the logistic sigmoid,  $\psi$  is an activation function, and “ $\circ$ ” denotes the elementwise product.

The decoder is slightly more complex than the encoder, as it needs to combine inputs from two sides and produce outputs in two directions (see the middle part of Fig. 1). The decoder processes an embedding,  $y$ , composed of two half-embeddings,  $y'$  and  $y''$ , of a subgraph and produces two half-embeddings of two smaller subgraphs along with an entry to the adjacency matrix and a marker of reaching the diagonal of this matrix. The output half-embeddings are produced with weighted averaging and additively adjusting the input half-embeddings. The decoder is based on a feedforward neural network,  $f^d$ , with a linear output layer which produces four vectors of size  $m/2$  and two scalars:

$$\langle z', z'', \hat{y}', \hat{y}'', b, c \rangle = f^d(\langle y', y'' \rangle). \quad (7)$$

They are applied to produce the outputs of the decoder as follows:

$$\begin{aligned} d(\langle y', y'' \rangle) &= \langle y' \circ \sigma(z') + \psi(\hat{y}') \circ (\mathbf{1} - \sigma(z')), \\ &\quad y'' \circ \sigma(z'') + \psi(\hat{y}'') \circ (\mathbf{1} - \sigma(z'')), b, c \rangle. \end{aligned} \quad (8)$$

For the upper row and the leftmost column of the  $y$  matrix, there are no half-embeddings that come from above and from the left, respectively. Therefore, we use two additional networks,  $f^{d1}$  and  $f^{d2}$  to produce these embeddings. Those networks proceed as follows:

$$\langle z', \hat{y}' \rangle = f^{d1}(y'), \quad \langle z'', \hat{y}'' \rangle = f^{d2}(y''). \quad (9)$$

The first half-embeddings for the upper row of  $y$  and the second half-embeddings for the leftmost columns are produced, respectively, as follows

$$d'(y') = y' \circ \sigma(z') + \psi(\hat{y}') \circ (\mathbf{1} - \sigma(z')), \quad (10)$$

$$d''(y'') = y'' \circ \sigma(z'') + \psi(\hat{y}'') \circ (\mathbf{1} - \sigma(z'')). \quad (11)$$

### 3.1 Order of vertices and adjacency matrix patches

We apply two known techniques to boost the autoencoder efficiency [17]. Since indexing of vertices is arbitrary, we proceed as follows: The vertices are sorted by their degree in decreasing order. Then, breadth-first search (BFS) runs in the graph starting from the first vertex. Order of occurring of vertices in BFS defines their indexing for the autoencoder. The BFS must accept potentially inconsistent graphs.

Our basic model operates on single entries in the adjacency matrix. However, it may also operate on  $l \times l$  patches of this matrix for  $l \in \mathbb{N}$ . This way, recursion length is reduced  $l$  times, and inputs/outputs of the encoder/decoder become  $l \times l$  matrices rather than scalars. The entries in the patches of  $A$  that reach their diagonal and further are assumed equal to -1. The corresponding entries in the patches of  $C$  are required to be 0. We apply this extension in the experimental study below.

### 3.2 Computational complexity

To encode/decode a graph with  $n$  vertices patch size  $l$ ,  $\lceil n/l \rceil$  layers of calculation are required – for each subgraph size between  $\lceil n/l \rceil$  and 1. The number of basic encodings/decodings is decreasing by one in successive layers, there are an average  $\lceil n/l \rceil / 2$  of them per layer. Consequently, computational complexity of the whole encoding/decoding process is  $O((n/l)^2)$ .

For instance, for  $n = 1000$  and  $l = 10$ , both  $e$  and  $d$  function is applied approximately 5000 times.

### 3.3 Variational Graph Autoencoder

In order to extend ReGAE to the graph VAE, we add two elements:

- A feedforward neural network that transforms graph embeddings,  $x$ , into vectors,  $\rho \in \mathbb{R}^m$ , of logarithms of standard deviations.
- KL-divergence between  $\mathcal{N}(x, \exp(\rho))$  and  $\mathcal{N}(0, I)$  as a part of the training loss.

As in the original VAE [3], when training the graph VAE, the decoder is fed with  $x + \xi \circ \exp(\rho)$ ,  $\xi \sim \mathcal{N}(0, I)$ .

### 3.4 Further extensions

Graphs representing complex systems often have numerical information assigned to their vertices and edges. ReGAE can readily be extended to model and process this information:

- Weighted edges: The weights are inputs to the encoder and outputs of the decoder combined with the adjacency matrix entries.
- Labeled edges: Related to the previous point. The input/output to the encoder/decoder may contain other information than just the graph structure. By treating the entries as vectors instead of scalars, ReGAE could process graphs with labeled edges.
- Labeled vertices: Auxiliary feedforward networks transform the labels into embeddings of single-vertex graphs and back.
- Directed graphs: The encoder is fed with, and the decoder produces, the pair  $\langle A_{i,j}, A_{j,i} \rangle$  instead of just  $A_{i,j}$ .

## 4 Experimental study

### 4.1 Datasets

**Table 1.** Properties of the datasets used in our experiments. *Size* is the number of graphs in the dataset, *AvgNN* is the average number of nodes, *MaxNN* is the maximum number of nodes, *AvgNE* is the average number of edges, *Fill* is the average proportion of the number of edges to the number of entries in the adjacency matrices, and *CIN* is the number of classes.

Dataset	Size	AvgNN	MaxNN	AvgNE	Fill	CIN
GRID-MEDIUM	49	25.0	64	40.0	0.18	-
IMDB-BINARY	1000	19.8	136	96.5	0.52	2
IMDB-MULTI	1500	13.0	89	65.9	0.77	3
COLLAB	5000	74.5	492	2457.5	0.51	3
REDDIT-BINARY	2000	429.6	3782	497.8	0.02	2
REDDIT-MULTI-5K	4999	508.5	3648	594.9	0.01	5
REDDIT-MULTI-12K	11929	391.4	3782	456.9	0.02	11

We use six sets of social graphs from [23]: IMDB-BINARY, IMDB-MULTI, COLLAB, REDDIT-BINARY, REDDIT-MULTI-5K, REDDIT-MULTI-12K and GRID-MEDIUM – a set of synthetic grid-like graphs. Their basic statistics are contained in Table 1.

The datasets are divided 70/15/15 into training, validation, and test subsets. These subsets are augmented by  $N$  random permutations of each graph.  $N = 99$  for GRID-MEDIUM;  $N = 9$  for IMDB-BINARY, IMDB-MULTI and COLLAB;  $N = 0$  for all REDDITs.

## 4.2 Graph autoencoding

We have found two difficulties in comparing ReGAE with the state-of-the-art. Firstly, existing autoencoders are based on embeddings whose size depends on the graph size. Secondly, they usually learn on a single graph, rather than on a set of graphs. A set of graphs can be understood as one graph with a number of separate components. However, an autoencoder trained on such a supergraph is not necessarily applicable to its hypothetical test components. Autoencoders that we have found technically capable of being trained on a set of graphs and tested on separate graphs are GAE, VGAE [12] and Graphite [8].<sup>3</sup> The goal of our experiments is to learn to encode and decode graphs on the training subset. The performance of these operations is verified on the test subset.

When applying GAE, VGAE and Graphite, we used a vertex embedding size,  $d$ , equal to 4 for REDDITs, and 8 for other datasets. The graph embedding size in ReGAE was equal to  $d$  times the average number of vertices in the dataset. Consequently, the graph embedding sizes were on average equal for different methods. These settings gave GAE, VGAE and Graphite an advantage as these algorithms could embed relatively large graphs in accordingly large vectors.

All architectures were trained with early stopping technique and a patience of 20 epochs. We have designated hyperparameters of all methods and datasets with random search and on a number of evaluations specific to the dataset. Values of those hyperparameters are presented in Tab. 2, Tab. 3 and Tab. 4.

**Table 2.** Hyperparameters of ReGAE: emb – embedding size, encoder – sizes of encoder hidden layers, decoder – sizes of decoder hidden layers, patch – patch size, g-c – gradient clipping value, rpb – recall-precision bias i.e., proportion of weights of target 0s and 1s in loss function, higher values favor recall performance by increasing the weights of 1s. For all experiments we set 0.5 as the mask weight and 0.2 as the embedding norm weight for the loss calculation. We use ELU [4] as the activation function.

Dataset	emb	encoder	decoder	patch	lr	g-c	rpb	batch
GRID-M	200	2048	2048	4	0.0003	1.0	0.3	32
IMDB-B	160	1024:768	2048	4	0.0005	1.0	0.5	64
IMDB-M	104	1024	2048	8	0.0005	1.0	0.5	64
COLLAB	604	2048:1536	4096	16	0.0003	0.5	0.3	32
REDDIT-B	1720	4096	6144	64	0.0003	1.0	0.03	32
REDDIT-M-5K	2036	4096	6144	64	0.0003	0.5	0.03	32
REDDIT-M-12K	1564	4096	6144	64	0.0003	0.5	0.03	32

All our experiments are repeated 5 times with different random seeds and on different pre-prepared data splits. We report averaged results.

Tab. 5 presents the F1 score of ones in the adjacency matrix. These statistics were calculated as follows: For each graph, they were averaged over all entries of

<sup>3</sup> Note to reviewers: Unfortunately comparison to MVGAE [9] was not possible. The official implementation of the method is yet incomplete. Moreover, the effective depth of the recursion in this code is 1, which contradicts the idea conveyed in that paper.

**Table 3.** Hyperparameters of GAE/VGAE [12]: hidden – hidden layer size, latent – latent size, recall prec bias – proportion of weights of target 0s and 1s in loss function, higher values favor recall performance by increasing the weights of 1s.

Datasets	hidden	latent	lr	dropout	recall prec bias	batch
GRID-M	512	8	0.005	0.1	0.5	32
IMDBs	512	8	0.005	0.1	0.5	32
COLLAB	4096	8	0.005	0.1	0.5	32
REDDITs	4096	4	0.005	0.1	0.001	32

**Table 4.** Hyperparameters of Graphite [8]: h-enc – hidden layer in encoder size, h-dec – hidden layer in decoder, a-reg – auto-regressive scalar, lat – latent size, d-out – dropout, rpb – recall-precision bias i.e., proportion of weights of target 0s and 1s in loss function, higher values favor recall performance by increasing the weights of 1s.

Datasets	hidden-enc	hidden-dec	auto-reg	lat	lr	d-out	rpb	batch
GRID-M	512	128	0.1	8	0.0005	0.1	0.5	32
IMDBs	512	128	0.1	8	0.0005	0.1	0.5	32
COLLAB	4096	512	0.1	8	0.0005	0.1	0.5	32
REDDITs	4096	512	0.1	4	0.0005	0.1	0.001	32

the adjacency matrix, and then over the test graphs with a weight equal to the number of vertices within a graph. Compared to GAE, VGAE and Graphite, ReGAE yields comparable or better results. On the bigger, more difficult datasets, especially the REDDIT graphs, ReGAE is incomparably more accurate. Neither GAE, VGAE nor Graphite could be trained to provide meaningful output for the harder datasets, often generating only 0s or 1s. Our method is more capable of recognizing the graph structure.

**Table 5.** Autoencoders: F1 score on the test set.

Dataset\method	GAE	VGAE	Graphite-AE	Graphite-VAE	ReGAE
GRID-M	$0.45 \pm 0.09$	$0.45 \pm 0.10$	$0.45 \pm 0.10$	$0.45 \pm 0.10$	$0.70 \pm 0.22$
IMDB-B	$0.91 \pm 0.02$	$0.91 \pm 0.02$	$0.91 \pm 0.02$	$0.90 \pm 0.01$	$0.90 \pm 0.02$
IMDB-M	$0.93 \pm 0.01$	$0.93 \pm 0.01$	$0.91 \pm 0.01$	$0.91 \pm 0.01$	$0.89 \pm 0.01$
COLLAB	$0.80 \pm 0.01$	$0.80 \pm 0.01$	$0.75 \pm 0.01$	$0.75 \pm 0.01$	$0.86 \pm 0.01$
REDDIT-B	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.53 \pm 0.02$
REDDIT-M-5K	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.48 \pm 0.01$
REDDIT-M-12K	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.01 \pm 0.00$	$0.49 \pm 0.01$

Contrary to GAE VGAE and Graphite, ReGAE also learns to properly encode the sizes of graphs, which implies it can make an error related to graph size. As evident in Tab. 6, such errors are generally small in magnitude. For the calculation of F1 score, the graphs of incorrect sizes (either predicted or target) were padded with 0s along the adjacency matrix diagonal, which serves as an added penalty.

**Table 6.** Size accuracy — the number of graphs with correctly designated vertex count over the number of all graphs, Mean size error — the average absolute size difference between the target and predicted graphs over the average target graph size.

Dataset	Size accuracy	Mean size error
GRID-MEDIUM	$0.34 \pm 0.11$	$0.100 \pm 0.039$
IMDB-BINARY	$0.97 \pm 0.03$	$0.003 \pm 0.002$
IMDB-MULTI	$0.97 \pm 0.01$	$0.003 \pm 0.002$
COLLAB	$0.97 \pm 0.01$	$0.001 \pm 0.001$
REDDIT-BINARY	$0.23 \pm 0.04$	$0.029 \pm 0.010$
REDDIT-MULTI-5K	$0.38 \pm 0.10$	$0.006 \pm 0.002$
REDDIT-MULTI-12K	$0.54 \pm 0.15$	$0.021 \pm 0.018$

## 5 Conclusions

In this paper, we have introduced a recursive neural architecture capable of representing graphs of any size in vectors of fixed dimension (embeddings), and capable of reconstructing these graphs from the vectors. The architecture does not impose any structural upper bound on the size of the graph or lower bound on the dimension of the embeddings. In our experiments, we verified the proposed method on 7 datasets with graphs with up to 3782 vertices. Given these experiments, ReGAE is effective and offers a reasonable level of accuracy.

Our proposed graph autoencoder with fixed-size embeddings enables a wide range of further developments such as graph generation, completion, or transformation.

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