A Deep Generative Model for Graph Layout

Oh-Hyun Kwon, Student Member, IEEE, and Kwan-Liu Ma, Fellow, IEEE

Abstract—As different layouts can characterize different aspects of the same graph, finding a “good” layout of a graph is an important task for graph visualization. In practice, users often visualize a graph in multiple layouts by using different methods and varying parameter settings until they find a layout that best suits the purpose of the visualization. However, this trial-and-error process is often haphazard and time-consuming. To provide users with an intuitive way to navigate the layout design space, we present a technique to systematically visualize a graph in diverse layouts using deep generative models. We design an encoder-decoder architecture to learn a model from a collection of example layouts, where the encoder represents training examples in a latent space and the decoder produces layouts from the latent space. In particular, we train the model to construct a two-dimensional latent space for users to easily explore and generate various layouts. We demonstrate our approach through quantitative and qualitative evaluations of the generated layouts. The results of our evaluations show that our model is capable of learning and generalizing abstract concepts of graph layouts, not just memorizing the training examples. In summary, this paper presents a fundamentally new approach to graph visualization where a machine learning model learns to visualize a graph from examples without manually-defined heuristics.

Index Terms—Graph, network, visualization, layout, machine learning, deep learning, neural network, generative model, autoencoder

1 INTRODUCTION

Graphs are commonly used for representing complex systems, such as interactions between proteins, data communications between computers, and relationships between people. Visualizing a graph can help better understand the relational and structural information in the data that would not be as apparent if presented in a numeric form. The most popular and intuitive way to visualize a graph is a node-link diagram, where the nodes are drawn as points, and the links are rendered as lines.

Drawing a node-link diagram by hand is laborious; since the 1960s, researchers have devised a multitude of methods to automatically lay out a graph. The layouts of the same graph can vary greatly depending on which method is used and the method’s configuration. Since different layouts can highlight different structural characteristics of the same graph, it is important to find a “good” layout.

Finding a good layout of a graph is, however, a challenging task. The “goodness” of a layout is highly subjective and depends on the given circumstances, such as the analysis tasks to be supported by the visualization. Unfortunately, there is no existing method that automatically finds a good layout considering the many different circumstances and/or user preferences. Therefore, in practice, users rely on a trial-and-error process to find a good layout. Until they find a layout that satisfies their requirements, users typically visualize a graph in multiple layouts using different methods and varying parameter settings. This trial-and-error process is generally time-consuming as it often results in a haphazard and tedious exploration of a large number of layouts.

Furthermore, expert knowledge of layout methods is often required to find a good layout. Most layout methods have a number of parameters that can be tweaked to improve the layout of a graph. However,
many layout methods, especially force-directed ones, are very sensitive to the parameter values [65], where the resulting layouts can be incomprehensible or even misleading [22]. A proper selection of the parameter settings for a given graph often requires detailed knowledge of the chosen method. Such knowledge can only be acquired through extensive experience in graph visualization. Thus, novice users are often blindly tweaking the parameters, which might lead to exploring only a fraction of the layout design space, choosing an inadequate layout, or even overlooking critical insights in the graph.

To help users find a layout that best suits their requirements, we present a deep generative model that systematically visualizes a graph in diverse layouts. We design an encoder-decoder architecture to learn a generative model from a collection of example layouts, where the encoder represents training examples in a latent space and the decoder generates layouts from the latent space. In particular, we train the model to construct a two-dimensional latent space for users to intuitively navigate and generate various layouts, even without any expert knowledge of the layout methods.

The results of our evaluations show that our model is capable of learning and generalizing abstract concepts of graph layouts, not just memorizing the training examples. Also, graph neural networks [54,84] and Gromov–Wasserstein distance [64] help the model better learn the complex relationship between the structure and the layouts of a graph. In addition, after training, our model generates new layouts considerably faster than existing layout methods.

In summary, we introduce a fundamentally new approach to graph visualization, where a machine learning model learns to visualize a graph as a node-link diagram from existing examples without manually-defined heuristics. Our work is an example of artificial intelligence augmentation [11], as a machine learning model builds a new type of user interface (i.e., layout latent space) to augment a human intelligence task (i.e., graph visualization design).

2 RELATED WORK

Our work is related to graph visualization, deep generative modeling, and deep learning on graphs. We discuss related work in this section.

2.1 Graph Visualization

A plethora of layout methods has been introduced over the last five decades. In this paper, we focus on two-dimensional layout methods that produce straight-edge drawings, such as force-directed methods [17,23,25,27,50] and dimensionality reduction-based methods [10,42,59], spectral methods [14,58], and multi-level methods [26,29,38,41,44,81]. Many analysts do not have expert knowledge in these layout methods for finding a good layout. Our goal is to learn the layouts produced by the different methods into a single model. In addition, we provide an intuitive way for users to explore and generate diverse layouts of a graph without the need of expert knowledge.

How to effectively find a “good” layout of a graph is still an open problem. However, decades of research in this area have led to several heuristics, often called aesthetic criteria, for improving and evaluating the quality of a layout. For instance, reducing edge crossings has been shown as one of the most effective criteria to improve the quality of a layout [45,52,71,72]. Based on the aesthetic criteria, several metrics have been defined to evaluate layouts quantitatively.

However, even with aesthetic criteria and metrics, human intervention is still needed in the process of selecting a layout for several reasons. First, while each heuristic attempts to enhance certain aspects of a layout, it does not guarantee an overall quality improvement [22,30]. For instance, depending on the given circumstances (e.g., given graph, task, and environment), certain criteria can lead to incomprehensible layouts [7]. Second, there is no consensus on which criteria are the most helpful in a given circumstance [22,30,52]. Third, it is often not feasible to satisfy several aesthetic criteria in one layout because satisfying one may result in violating others [20,21]. Lastly, selecting a good layout is highly subjective, as each person might have varying opinions on what is a “good” layout. For these reasons, there is no existing automatic method to find a good layout of a graph.

To help users find a good layout, several methods have been developed to accelerate the trial-and-error selection process by learning user preferences [23,63,77]. For example, Biedl et al. [6] have introduced the concept of multidrawing, which systematically produces many different layouts of the same graph. Some methods use an evolutionary algorithm [2,3,63] to optimize a layout based on a human-in-the-loop assessment. However, these methods require constant human intervention throughout the optimization process. In addition, the goal of their optimization is to narrow down the search space. This allows the model to create only a limited number of layouts. Hence, multiple learning sessions might be needed to allow users to investigate other possible layouts of the same graph. In contrast to these models, our approach is to train a machine learning model in a fully unsupervised manner to produce diverse layouts, not to narrow the search space.

Recently, several machine learning approaches have been introduced to different tasks in graph visualization, such as previewing large graphs [61], exploring large graphs [12], and evaluating visualizations [39,55]. Unlike these approaches, our goal is to train a model to generate layouts.

2.2 Deep Generative Models

The term “generative model” can be used in different ways. In this paper, we refer to a model that can be trained on unlabeled data and is capable of generating new samples that are similar to, but not the same as, the training data. For example, we can train a model to create synthetic images of handwritten digits by learning from a large collection of real ones [33,52]. Because generating new, realistic samples requires a good understanding of the given data, generative modeling is often considered as a key component of unsupervised learning.

In recent years, parameterizing generative models using deep neural networks and stochastic optimization methods have demonstrated state-of-the-art performance in various applications, such as text generation [45], music generation [75], and drug design [33]. While several approaches have been proposed for deep generative modeling, the two most prominent ones are variational autoencoders (VAEs) [53] and generative adversarial networks (GANs) [54]. VAEs and GANs have their own advantages and disadvantages. GANs generally produce visually sharper results when applied to an image dataset as they can implicitly model a complex distribution. However, training GANs is difficult due to non-convergence and mode collapse [35]. VAEs are easier to train and provide both a generative model and an inference model. However, they tend to produce blurry results when applied to images.

For designing our generative model, we use sliced-Wasserstein autoencoders (SWAEs) [57]. As a variant of VAE, it is easier to train than GANs. In addition, it is capable of learning complex distributions. SWAEs allow us to shape the distribution of the latent space into any samplable probability distribution without training an adversarial network or defining a likelihood function.

2.3 Deep Learning on Graphs

Machine learning approaches to graph-structured data, such as social networks and biological networks, require an effective representation of the graph structure. Recently, many graph neural networks (GNNs) have been proposed for representation learning on graphs, such as graph convolutional networks [54], GraphSAGE [40], graph attention networks [79], and graph isomorphism networks [84]. They have achieved state-of-the-art performance for many tasks, such as graph classification, node classification, and link prediction. We also use GNNs for learning the complex relationship between the structure and the layouts of a graph.

Several generative models have been introduced for graph-structured data using GNNs [14,36,62,76,87]. These models learn to generate whole graphs for tasks that require new samples of graphs, such as de novo drug design. However, generating a graph layout is a different type of task, where the structure of a graph remains the same, but the node attributes (i.e., positions) are different. Thus, we need to design a model that learns to generate different node attributes of the same graph.
3 Approach

Our goal is to learn a generative model that can systematically visualize a graph in diverse layouts from a collection of example layouts. We describe the entire process for building a deep generative model for graph layout, from collecting training data to designing our architecture.

3.1 Training Data Collection

Similar to other machine learning tasks, we need a set of examples to train a generative model. Learning a model using deep neural networks especially requires a large amount of training data. As a data-driven approach, the quality of the training dataset is crucial to build an effective model. For our goal, we need a large and diverse collection of layouts of the input graph.

Grid search is often used for parameter optimization [5], where a set of values is selected for each parameter, and the model is evaluated for each combination of the selected sets of values exhaustively. It is often used for producing multiple layouts of a graph. For example, Haleem et al. [59] have used grid search for producing their training dataset. However, the number of combinations of parameters increases exponentially with each additional parameter. In addition, different sets of parameter values are often required for different graphs. Therefore, it requires expert knowledge of each layout method to carefully define the search space for collecting the training data in a reasonable amount of time.

In this work, we use random search to collect training example layouts, where each layout is computed using randomly assigned parameter values of a method. Random search often outperforms grid search for parameter optimization [5], especially when only a small number of parameters affects the final result. Because the effect of the same parameter can greatly vary depending on the structure of the input graph, we believe random search would produce a more diverse set of layouts than grid search. Moreover, for this approach, we only need to define the interval of values for a continuous parameter, which is a simpler task for non-experts than selecting specific values for grid search.

Computing a large number of layouts would take a considerable amount of time. However, we can start training a model without having the full training dataset, thanks to stochastic optimization methods. For example, we can train a model with stochastic gradient descent [22], where a small batch of training examples (typically a few dozens) are fed to the model at each step. Thus, we can incrementally train the model while generating the training examples simultaneously. This allows the users to use our model as early as possible.

3.2 Layout Feature

Selecting informative, discriminating, and independent features of the input data is also an essential step for building an effective machine learning model. With deep neural networks, we can use low-level features of the input data without handcrafted feature engineering. For example, the red, blue, and green channel values of pixels often are directly used as the input features of an image in deep learning models.

However, what would be a good feature of a graph layout? Although the positions of vertices can be a low-level feature of a layout, using the raw position as a feature of a layout has several issues.

In this paper, we focus on two-dimensional layouts that draw all edges in straight lines, as we have mentioned in Sect. 2.1. This class of graph layouts often uses spatial proximity to encode the similarity between vertices [65], following the Gestalt principle of proximity [83]. For example, several layout methods [10, 42, 50, 59] directly use the spatial proximity to optimize a layout, where they minimize the difference between the Euclidean distance in the layout and the shortest-path distance of the graph. Therefore, the position of a vertex is often a side effect of the layout method; it does not directly encode any attributes or structural properties of a vertex [65].

Moreover, many layout methods are nondeterministic [65], since they employ randomness in the layout process to avoid local minima, such as randomly initializing the positions of vertices. Therefore, the position of a vertex can significantly vary between different runs of the same layout method with the same parameter setting. For these reasons, the positions of vertices are not a reliable feature of a layout.

In this work, we use the pairwise Euclidean distance of vertices in a layout as the feature of the layout. As we focus on graph layouts that use spatial proximity to encode the similarity between vertices, we can directly use the pairwise distance matrices to compare different layouts, without considering the rotation or reflection of the points. Furthermore, we can normalize the pairwise distance matrix of vertices by its mean value for comparing layouts in different scales.

Therefore, for the positions of the vertices (P) of a given layout, we compute the feature of the given layout by $X_l = D/\bar{D}$, where $D$ is the pairwise distance matrix of P and $\bar{D}$ is the mean of D. Each row of $X_l$ is the node-level feature of a layout for each vertex. Other variations of the pairwise distance can be used as a feature, such as the Gaussian kernel from the pairwise distance: $\exp\left(-D^2/2\sigma^2\right)$.

3.3 Structural Equivalence

Two vertices of a graph are said to be structurally equivalent if they have the same set of neighbors. Structurally equivalent vertices (SEVs) of a graph are often placed at different locations, as many layout methods have a procedure to prevent overlapping. For example, the force-directed methods apply repulsive forces between all the vertices of a graph. However, as the layout results are often nondeterministic, the positions of SEVs are mainly determined by the randomness in the layout method. For example, the figure on the right shows two different layout results of the same graph using the same layout method (sfdp [44]) with the same default parameter setting. The blue vertices are the same set of SEVs. However, the arrangements of the blue vertices between the two layouts are quite different. In the top layout, the vertices $\{6, 2, 4\}$ are closer to $\{7, 8\}$ than $\{3, 5, 1\}$. In contrast, in the bottom layout, the vertices $\{5, 3, 4\}$ are closer to $\{7, 8\}$ than $\{2, 6, 1\}$. This presents a challenge because a permutation invariant measure of similarity is needed for the same set of SEVs. In other words, we need a method to permute the same set of SEVs, from one possible arrangement to the other, for visually correct similarity measure.

To address this issue, we compare two different layouts using the Gromov–Wasserstein (GW) distance [64, 69]. The GW distance measures the difference between two metric spaces. For example, we can use the GW distance to measure the difference between two point clouds, invariant to the permutations of the points.

For a more efficient computation, we do not backpropagate through the GW distance in the optimization process of our model. We explain this in more detail in Sect. 3.5.

3.4 Architecture

We design an encoder-decoder architecture that learns a generative model for graph layout. Our architecture and optimization process generally follow the framework of variational autoencoders (VAEs) [53]. The overview of our architecture is shown in Fig. 2.

Preliminaries An autoencoder learns to encode a high-dimensional input object to a lower-dimensional latent space and then decodes the latent representation to reconstruct the input object. A classical autoencoder is typically trained to minimize reconstruction loss, which measures the dissimilarity between the input object and the reconstructed input object. By training an autoencoder to learn significantly lower-dimensional representations than the original dimensionality of the input objects, the model is encouraged to produce highly compressed representations that capture the essence of the input objects.

A classical autoencoder does not have any regularization for the distribution of the latent representation. This leads to an arbitrary distribution of the latent representations, which makes difficult to understand the shape of the latent space. Therefore, if we decode a random area in the latent space, we would get reconstructed objects that do not
look like any of the input objects, as that area has not been used for reconstructing the input objects during the training process. Variational autoencoders (VAEs) extend the classical autoencoders by minimizing variational loss, which measures the difference of the distribution of the input objects’ latent representations and a prior distribution. Minimizing the variational loss encourages VAEs to learn the latent space that follows a predefined structure. This allows us to know which part of the latent space is trained with some input objects. Thus, it is easy for us to decode the learned part of the latent space and to get a reconstructed object similar to some of the input objects.

**Encoder**

For our problem, the input objects are graph layouts, i.e., the positions of vertices ($P$). We first compute the feature of a layout ($X_L$) as discussed in Sect. 3.2 (Fig. 2).

We use graph neural networks (GNNs) to take the structure of a graph into account in the learning process of the latent representation of a layout. Thus, our encoder takes the feature of a layout ($X_L$) and the structure of a graph (the adjacency matrix $A$) as shown in Fig. 2. Each row of $X_L$ is the input feature of each node.

In general, GNNs learn the representation of a node following a recursive neighborhood aggregation (or message passing) scheme, where the representation of a node is derived by recursively aggregating and transforming the representations of its neighbors. After $k$ steps of aggregation, our encoder produces the latent representation of a node, which captures the information within the node’s $k$-hop neighborhood.

Fig. 2 shows an example of 3-layer GNNs, which learn the latent representation of a node by aggregating the information within the node’s 3-hop neighborhood.

The aggregation scheme of GNNs corresponds to the subtree structure rooted at each node, where it learns more global representation of a graph as the number of aggregations steps increases [34]. Therefore, depending on the graph structure, an earlier aggregation step may learn a better representation of a node. To consider all representations at different aggregation steps, we use the outputs of all GNN layers. This is achieved by concatenating the outputs of all GNN layers (Fig. 2) similar to [35].

The graph-level representation of a layout is obtained with a readout function (Fig. 2). A readout function should be permutation invariant to learn the same graph-level representation of a graph, regardless of the vertex ordering. It can be a simple element-wise mean-pooling or a more advanced graph-level pooling, such as DiffPool [86].

For the final output of the encoder, we use multi-layer perceptron (MLP) to produce the final output representation of a layout $Z_L$ (Fig. 2). As our goal is to learn a two-dimensional latent space for users to intuitively navigate the latent space, we define the prior distribution as the uniform distribution in $[-1, 1]^2$ for our encoder. Therefore, our encoder produces a two-dimensional vector representation for each layout ($Z_L$) within $[-1, 1]^2$.

**Fusion Layer**

The encoder produces a graph-level representation of each layout. If we only use this graph-level representation, all vertices will have the same feature value for the decoder. We simply use one-hot encoding of the vertices as the feature of the nodes ($X_V$) for the decoder to distinguish the individual vertices.

To combine the graph-level representation of a layout ($Z_L$) and node-level features ($X_V$), we use a fusion layer [47] that fuses $Z_L$ and $X_V$ by concatenating the graph-level representation with each of the node-level features (Fig. 2).

**Decoder**

Our decoder takes the fused features and learns to reconstruct the input layouts, i.e., it reconstructs the position of the vertices ($P'$). The decoder has a similar architecture to the encoder, except that it does not have a readout function, as the output of the decoder is node-level representations, i.e., the position of the vertices ($P'$).

The feature of the reconstructed layout ($X_L'$) is computed for measuring the reconstruction loss (Fig. 2).

### 3.5 Training

Following the framework of VAEs [33], we learn the parameters of the neural network used in our model by minimizing the reconstruction loss ($L_X$) and the variational loss ($L_Z$).

The reconstruction loss ($L_X$) measures the difference between the input layout ($P$) and its reconstructed layout ($P'$). As we have discussed in Sect. 3.2, we compare the features of the two layouts ($X$ and $X'$) to measure the dissimilarity between them. For example, we can use the $L_1$ loss function for computing the reconstruction loss between the two layouts $L_X = \|X - X'\|_1$.

As we have discussed in Sect. 3.3, for the same set of structurally equivalent vertices (SEVs) in a graph, we use the Gromov–Wasserstein (GW) distance between the two layouts ($P$ and $P'$) for the comparison. However, for a more efficient computation, we do not backpropagate through the GW distance in the optimization process. Computing GW yields a permutation matrix ($T$), as it is based on ideas from mass transportation [80]. We use this permutation matrix to permute the input layout $P = TP$ and compute the feature of the permuted input layout $\hat{X}_L$. Then, we compute the reconstruction loss between the permuted input layout ($\hat{P}$) and the reconstructed layout ($P'$).

For example, if we use the $L_1$ loss, we can compute the reconstruction loss as $L_X = \|X_L - X_L'\|_1$. With this method, we can save computation cost for the backpropagation through the complex GW computation, and we still can compare the different layouts of the SEVs properly.

In this paper, we use the variational loss function defined in sliced-Wasserstein autoencoders (SWAE) [57]. Using sliced-Wasserstein distance for variational loss allows us to shape the distribution of the latent space into any samplable probability distribution without defining a likelihood function or training an adversarial network. Thus, the variational loss is $L_Z = SW(Z_L, Z_P)$, where $SW$ is the sliced-Wasserstein distance defined in [57], and $Z_P$ is a set of samples of the prior distribution.

The optimization objective can be written as:

$$\arg\min_{\theta, \phi} L_X + \beta L_Z,$$

where $E_P$, $D_P$ is the decoder parameterized by $\phi$, and $\beta$ is the relative importance of the two losses.

### 4 Evaluations

The main goal of our evaluations is to see whether our model is capable of learning and generalizing abstract concepts of graph layouts, not just memorizing the training examples. We perform quantitative and qualitative evaluations of the reconstruction of unseen layouts (i.e., the test set), and a qualitative evaluation of the learned latent space.

#### 4.1 Datasets

We use nine real-world graphs and 20,000 layouts per graph in our evaluations. For the quantitative reconstruction evaluation, as we perform 5-fold cross validations, 16,000 layouts are used as the training set, and 4,000 layouts are used as the test set.
Table 1. The nine graphs used in the evaluation. |V|: the number of vertices, |E|: the number of edges, |S|: the number of vertices having structural equivalence, l: average path length.

| Name       | Type          | |V| | |E|/|V| | |S|/|V| | l | Source |
|------------|---------------|-------------------|---|-----------------|-------------------|---|------------------|---|-------------------|
| lesmis     | Co-occurrence | 77                | 254 | 3.30 | 35 | .455 | 2.61 | | | 56 |
| can96      | Mesh structure | 96                | 336 | 3.5  | 0  | 0  | 4.36 | | | 18 |
| football   | Interaction network | 115 | 613 | 5.33 | 0  | 0  | 2.49 | | | 51 |
| raja11     | Circuit simulation | 135 | 276 | 2.04 | 0  | .044 | 5.57 | | | 18 |
| jazz       | Collaboration | 198               | 2,742 | 13.85 | 14 | .071 | 2.22 | | | 32 |
| netsci     | Coauthorship  | 379               | 914 | 2.41 | 183 | .483 | 6.03 | | | 80 |
| dwt419     | Mesh structure | 419               | 1,572 | 3.75 | 32 | .076 | 8.97 | | | 15 |
| asoiaf     | Co-occurrence | 796               | 2,823 | 3.55 | 170 | .214 | 3.41 | | | 87 |
| bus1138    | Power system  | 1,138             | 1,458 | 1.28 | 16 | .014 | 12.71 | | | 18 |

Graphs Table 1 lists the graphs used for our evaluations. These include varying sizes and types of networks. We collected the graphs from publicly available repositories [56, 60]. As disconnected components can be laid out independently, we use the largest component if a graph has multiple disconnected components (netsci and asoiaf). can96 and asoiaf do not have any structurally equivalent vertices. Therefore, we did not use the Gromov–Wasserstein distance [64].

Layouts We collected 20,000 layouts for each graph using the four different layout methods and 5,000 different parameter settings per method following the training data collection process described in Sect. 3.1. The layout methods and their parameter ranges used in the evaluations are listed in Table 2.

While there is a plethora of layout methods, we selected these four layout methods because they are capable of producing diverse layouts by using the wide range of parameter values. Also, their publicly available, robust implementations did not produce any degenerate case in our evaluations. Lastly, these methods are efficient for computing a large number of layouts in a reasonable amount of time.

The resulting 20,000 layouts vary in many ways ranging from aesthetically pleasing looks to incomprehensible ones (e.g., hairballs). We did not remove any layout as we wanted to observe how the models encapsulate the essence of graph layouts from the diverse layouts.

4.2 Models and Configurations

We compare eight different model designs to investigate the effects of graph neural networks (GNNs) and Gromov–Wasserstein (GW) [64] distance in our model. All the models we use have the same architecture as described in Sect. 3.4 except for the GNN layers:

MLP: This model uses 1-layer perceptrons instead of GNNs; it does not consider the structure of the input graph. Thus, the whole model consists of multi-layer perceptrons (MLPs) without any GNNs. This model serves as a baseline for the investigation of the representational power of GNNs.

GCN: This model uses graph convolutional networks (GCN) [54] as the GNN layers. GCN is one of the early works of GNN.

GIN-1: This model uses graph isomorphism networks (GIN) [84] as the GNN layers. 1-layer perceptrons are used as the function approximators (a configuration of GIN) of GINs [84], thus named GIN-1.

GIN-MLP: This model uses GIN [84] as the GNN layers, and MLPs (2 layers) are used as the function approximators of GINs, thus named GIN-MLP. We use the mean aggregator in both of the GIN-1 and GIN-MLP models.

Also, for the models that use the GW distance in the optimization process, we add ‘+GW’ to its model name. For example, GIN-MLP+GW denotes a model uses GIN-MLP as the GNN layers and the GW distance for comparing the structurally equivalent vertices (SEVs) in the optimization process. The models with GW [64] are only used for the graphs having SEVs (all the graphs except can96 and football).

We use varying number of hidden units in each layer depending on the number of vertices of the graph: 32 units for lesmis, can96, football and raja11, 64 units for jazz, netsci, and dwt419, and 128 units for asoiaf and bus1138.

We use the $L_1$ loss function for the reconstruction loss. For the variational loss, we draw the same number of samples as the batch size from the prior distribution and set $p = 2$ to compute the sliced-Wasserstein distances [57]. Also, we set $\beta = 10$ in our optimization objective in Sect. 3.5.

4.3 Implementation

We implemented our models in PyTorch. The machine we used to generate the training data and to conduct the evaluations has an Intel i7-5960X (8 cores at 3.0 GHz) CPU and a NVIDIA Titan X (Maxwell) GPU. The implementation of each layout method used in the evaluations is also shown in Table 2.

4.4 Test Set Reconstruction Loss

We compare the test layout reconstruction to evaluate the models’ generalization capability. Here, a layout reconstruction means the model takes the input layout, encodes it to the latent space, and then reconstructs it from the latent representation. The test reconstruction loss quantifies the generalization ability of a model because it measures the accuracy of generating layouts that the model did not see in the training. We perform 5-fold cross-validations to compare the eight size from the prior distribution and set $p = 2$ to compute the sliced-Wasserstein distances [57]. Also, we set $\beta = 10$ in our optimization objective in Sect. 3.5.

All the models use three GNN layers (or perceptrons in the MLP models), the exponential linear unit (ELU) [15] as the non-linearity, mean-pooling as the readout function in the encoder. The batch size is 1,572 3.75 32 .076 8.97 15

GIN−MLP

GIN−MLP+GW

GIN−1

GIN−1+GW

GIN−1

GCN+GW

GCN

MLP+GW

MLP

a

b

c

d

Table 2. The layout methods and parameter ranges used for producing training data in our experiments. The parameter names follow the documentation of the implementations.

| Method       | Parameter Ranges                                                                 | Implementation                  |
|--------------|----------------------------------------------------------------------------------|---------------------------------|
| DS [9]       | link distance = [1.0, 100.0], charge strength = [−100.0, −1.0], velocity decay = [0.1, 0.7] | 8                               |
| FAZ [49]     | gravity = [1.0, 10.0], scaling ratio = [1.0, 10.0], adjust sizes = {true, false}, linlog = {true, false}, outbound attraction distribution = {true, false}, strong gravity = {true, false} | 4                               |
| FMP [18]     | force model = {new, fr}, galaxy choice = {lower mass, higher mass, uniform}, spring strength = [0.1, 1000.0], repulsive spring strength = [0.1, 1000.0], post spring strength = [0.01, 10.0], post repulsive spring strength = [0.01, 10.0] | 13                              |
| Sfdp [44]    | repulsive force strength (c) = (0.0, 5.0), repulsive force exponent (p) = (0.0, 5.0), attractive force strength (nu) = (0.0, 5.0), attractive force exponent (nu,p) = (0.0, 5.0) | 68                              |

Fig. 3. Average test reconstruction losses. Since the value ranges vary for each graph, we use individual ranges for each graph. The models with Gromov–Wasserstein distance [64] are not used for can96 and football as they do not have any structurally equivalent vertices.
model designs in terms of their test set reconstruction loss. To reduce the effects of the fold assignments, we repeat the experiment 10 times and report the mean losses.

**Results** We compare the eight models in terms of the average reconstruction loss (lower is better) of the test sets, which are the 4,000 layouts that are not used to train the models. The results shown in Fig. 3 are the mean test reconstruction losses of the 10 trials of the 5-fold cross-validations. The standard deviations are not shown as the values are negligible: all standard deviations are less than $3 \times 10^{-4}$.

Overall, the models with GIN-MLP and GW show the lowest test reconstruction loss of all the graphs. The GIN-MLP models show the lowest loss for the graphs that do not have any structurally equivalent vertices (Fig. 3a), where the models with GW are not used. Thus, the GIN-MLP+GW models show the lowest loss for all the other graphs (Fig. 3b–d).

Although the absolute differences vary, the ranking between the models based on the neural network modules is consistent in all the graphs. The ranking of the models with GW is as follows: GIN-MLP+GW, GIN-1+GW, GCN+GW, and MLP+GW. The ranking of the models without GW is as follows: GIN-MLP, GIN-1, GCN, and MLP. In addition, the three different rankings of the models are found for the graphs with structural equivalences (Fig. 3c–d).

**Discussion** For lesmis, netsci, and dwt419 (Fig. 3c), all the models with GW show a lower loss than the models without GW. We have found that a considerable ratio of vertices in the three graphs have structural equivalences as shown as $|S|/|V|$ in Table 1. This shows that the GW in the optimization process is important for graphs that have many sets of structural equivalences.

For jazz and asioaf (Fig. 3d), the models with GIN show better results than the models without GIN. Although they also have a considerable ratio of structural equivalences, GIN-MLP and GIN-1 show lower reconstruction losses than GCN+GW and MLP+GW. Considering the number of vertices as shown in Table 1, we have found that the two graphs (jazz and asioaf) are dense and have a relatively small average path length compared to the other graphs. This suggests the GIN is important for dense and “small-world”-like networks.

For raijat11 and bus1138 (Fig. 3e), the ranking of the models is as follows: GIN-MLP+GW, GIN-MLP, GIN-1+GW, GIN-1, GCN+GW, GCN, MLP+GW, and MLP. We have found that these two graphs are sparse and they have a small ratio of vertices with structural equivalences. This suggests that the representational power of the GNNs has a stronger effect than the usage of GW in such graphs.

### 4.5 Layout Metrics and Test Reconstruction Loss

To investigate our models’ behavior on reconstructing the test sets, we analyze the correlations between the test reconstruction loss and each of the two layout quality metrics of the test layouts: crosslessness [70] and shape-based metric [24]. Crosslessness [70] is a normalized form of the number of edge crossings, where a higher value means fewer edge crossings. Shape-based metric [24] measures the quality of a layout based on the similarity between the graph and its shape graph (a relative neighborhood graph of the positions of the vertices). We use the Gabriel graph [28] as the shape graph of a layout.

We use the models with the lowest test reconstruction loss for each graph from [Sect. 4.3] (GIN-MLP for can96 and football, and GIN-MLP+GW for all the other graphs).

**Results** For all the graphs, the Pearson’s product-moment correlation coefficients show strong negative correlations both between the crosslessness ($c$) and the test loss and between the shape-based metric ($s$) and the test loss. These results are statistically significant as all the $p$-values are less than $2.2 \times 10^{-16}$: lesmis ($c = -0.69355$, $s = -0.69364$), can96 ($c = -0.704$, $s = -0.812$), football ($c = -0.703$, $s = -0.350$), raijat11 ($c = -0.521$, $s = -0.707$), jazz ($c = -0.877$, $s = -0.749$), netsci ($c = -0.488$, $s = -0.630$), dwt419 ($c = -0.586$, $s = -0.715$), asioaf ($c = -0.782$, $s = -0.311$), and bus1138 ($c = -0.517$, $s = -0.706$).

**Discussion** The results show that our models learn better on how to reconstruct the layouts with fewer edge crossings and are similar to its shape graph. In other words, our models tend to generate “good” layouts in terms of the two metrics, even if the models are not trained to do so. We showed detailed examples in [Sect. 4.6].

### 4.6 Qualitative Results

We show the qualitative results of the layout reconstruction and the learned latent space to discuss the behaviors of the models in detail.

**GIN-MLP and GW** The models with GIN-MLP and GW show the lowest test reconstruction loss in [Sect. 4.3]. To further investigate, we compare the reconstructed layouts of the lesmis graph, which has the widest range of losses among the different models. Due to space constraints, we discuss the difference between the four different models (MLP, MLP+GW, GIN-MLP, and GIN-MLP+GW) on lesmis graph.

In Fig. 4 shows the qualitative results of the test reconstruction. The lesmis graph has a number of sets of structurally equivalent vertices (SEVs). In Fig. 4, the vertices with the same color, except gray, are structurally equivalent to each other; they have the same set of neighbors in the graph. The vertices in gray are structurally unique; each of them has a unique relationship to the other vertices in the graph. For example, the blue vertices (1–6) have the same relationship where they are all connected to each other and to the two other vertices (7 and 8).

As described in [Sect. 3.3], the relative locations of SEVs are often not consistent in different layouts. For example, the arrangements of the blue vertices in the D3 layout and the FM² layout are different. In the D3 layout, the blue vertices are placed in the following clockwise order: 2, 1, 5, 3, 4, and 6, where the vertices {2, 1, 5} are closer to {7, 8} than {3, 4, 6}. However, in the FM² layout, the clockwise order of the blue vertices is 4, 2, 5, 1, 6, and 3, where the vertices {4, 2, 5} are closer to {7, 8} than {1, 6, 3}. The arrangements of the SEVs in the reconstructed layouts vary depending on the model. For example, the models with GW are able to lay out the blue vertices in Fig. 4 and e) similar to the input layouts in Fig. 4. However, the models without GW fail to learn this and produce collapsed placements (Fig. 3d). We suspect this is due to the many possible permutations between a set of SEVs. The models without GW tend to place a set of SEVs at the average position of the SEVs to reduce the average loss. However, the models with GW learn about the generalized concept of the blue vertices’ arrangements and produce similar arrangements as the test input layouts in a different permutation of the SEVs.

The other sets of SEVs show similar results (e.g., the orange and green vertices in Fig. 4), where the models without GW produce collapsed arrangements, but the models with GW produce similar arrangements as the test input layouts.

In addition, the placements of the blue vertices are spatially consistent across the different layouts using GIN-MLP+GW (Fig. 4, h, and j) than using MLP+GW (Fig. 4, g and i). This shows that the models with GIN-MLP gains a more stable generalization of the arrangement of SEVs than the models with only MLP. Therefore, using GIN-MLP+GW models, users can generate diverse layouts while preserving their mental map across the different layouts. This is not possible in many existing layout methods due to their nondeterministic results.

There are other examples of the generalization capability of our models. For example, Fig. 4 shows a different arrangement of the blue vertices than Fig. 4, where the layout in Fig. 4 has a star-like arrangement with the vertex 2 in the center. However, the reconstructed layouts in Fig. 4, h) of the layout in Fig. 4 are more similar to the layouts in Fig. 4. We have found that the arrangements like the layouts in Fig. 4 are more dominant in the training set.

Another example is the last row of the Fig. 4 where the input layout is a “hairball” layout. In contrast, the reconstructed layouts using our models are more organized. This also show that the models have a generalized concept of the layouts the graph. This might explain the negative correlations in [Sect. 4.5], as the models do not reconstruct the same hairball layouts.
We report and discuss the layout computation time, model training time, we have described in this paper. The layout computation and layout generation time of each graph using the models with the lowest test reconstruction loss in Sect. 4.4. The layout computation times are the mean seconds for computing one layout per method per graph. The training computation times are the mean seconds for training one epoch (16K samples) per graph. The right chart shows that the average training loss is updated every batch to demonstrate that our models converge quickly.

### Multiple Graphs

To demonstrate our models with more graphs, Fig. 6 shows the qualitative results of five different graphs using the GIN-MLP model for the football graph and the GIN-MLP+GW models for the other graphs. The first three rows show that our models are capable of learning different styles of layouts. The bottom two rows show the models’ behavior on the noisy input layouts. For example, the fourth layout of dwf419 is a twisted mesh, however, the reconstructed layout is not twisted but pinched near the center. The bottom row examples show how the model behaves on “hairball” layouts. We can see that the reconstructed layouts are not hairballs. These hairball examples explain the negative correlations in Sect. 4.5 as the models do not reconstruct the same hairball layouts as the input layouts.

### Latent Space

A common way to qualitatively evaluate a generative model is to show the interpolations between the different latent variables \([34, 37, 53, 57, 75]\). If the transitions between the generated samples based on the interpolation in the latent space are smooth, we can conclude that the generative model has a generalization capability of producing new samples that were not seen in training.

As our models are trained to construct a two-dimensional latent space, we can show a grid of generated samples interpolating throughout the latent space. We show the results of the four different graphs in Fig. 7 and the result of the lesmis in Fig. 1. As we can see, the transitions between the generated samples are smooth. Also, the latent space of can96 is particularly interesting. It seems that the model learned to generate different rotations of the 3D mesh. However, all of the layouts used in this paper are 2D. In addition, the input feature of a layout is the normalized pairwise distance between the vertices, as described in Sect. 3.2, which do not explicitly convey any notion of rotation.

Based on these findings, we conclude that our models are capable of learning and generalizing the abstract concepts of graph layouts. An interactive demo is available in the supplementary material \([1]\) for readers to explore the latent spaces of all the graphs using all the models we have described in this paper.

### 4.7 Computation Time

We report and discuss the layout computation time, model training time, and layout generation time of each graph using the models with the lowest test reconstruction loss in Sect. 4.4. The layout computation time and model training time are shown in Fig. 5.

As we collect a large number of layouts (16K samples per graph for training), computing layouts is the most time-consuming step in building the models. However, we can incrementally generate training examples and train the model simultaneously.

We have found that the training time is related to the (1) number of edges and (2) the number of sets of structurally equivalent vertices (SEVs) of a graph based on \([\text{Fig. 5}]\) and Table 1. The number of edges might be a stronger factor to the computation time than the number of vertices because we have implemented the graph neural networks using sparse matrices. Also, the number of sets of SEVs is directly related to the time complexity of the Gromov–Wasserstein distance \([64]\) computation in our optimization process.

In addition, the models converge quickly as shown in Fig. 5 although the models are trained for 50 epochs for our evaluations, the models are capable of generating diverse layouts less than 10 epochs.

Based on these findings, we expect training a new model for a graph from scratch without any layout examples can be done within a few minutes for a small graph (\(|V| < 200, |E| < 500\)) and a few hours for larger graphs. Although it is a considerable computation time, our model can be trained in a fully unsupervised manner. Thus, it does not require users to be presented during the training.

### Table 1

| Name       | D3 | FA2 | FM3 | sfdp | Epoch |
|------------|----|-----|-----|------|-------|
| lesmis     | 5.39 | .620 | .015 | .229 | 76.7  |
| can96      | 5.46 | .695 | .021 | .329 | 34.7  |
| football   | 5.52 | .845 | .033 | .486 | 43.9  |
| rajat11    | 5.59 | .856 | .044 | .586 | 45.1  |
| jazz       | 5.88 | 1.61 | .116 | 1.18 | 212   |
| netsci     | 6.37 | 2.50 | .236 | 2.59 | 281   |
| dwf419     | 6.45 | 3.08 | .257 | 3.08 | 211   |
| asoiaf     | 8.13 | 9.42 | .620 | 9.16 | 690   |
| bus1138    | 9.42 | 7.88 | 1.07 | 10.3 | 509   |

Fig. 5. Computation time. The left table shows the layout computation time (D3, FA2, FM3, and sfdp) for the collecting training data and the training time (Epoch). The layout computation times are the mean seconds for computing one layout per method per graph. The training computation times are the mean seconds for training one epoch (16K samples) per graph. The right chart shows that the average training loss is updated every batch to demonstrate that our models converge quickly.
we have concluded that our generative model is capable of learning and use a larger batch size for *asoiaf* by the capacity of GPU memory. This is the reason we could not are several limitations we hope to solve in the future work.

As the first approach in a new area, there are many possible layouts for the same graph. As shown in Fig. 1 and Fig. 7, a grid of generated samples shows an aesthetic metrics of the generated samples in high-resolution grids shown in Fig. 1 (center) and Fig. 7 (outer columns), mapping layout about the generated samples onto the latent space. For example, as a valid layout, but it is a rare type of arrangement in the training dataset. Although our model is capable of generalizing for different layouts of the same graph, it does not generalize for both different graphs and different layouts. Therefore, we need to train a new model for each graph. Our model can be trained in a fully unsupervised manner and can be trained incrementally while generating the training samples simultaneously. Still, a better model would learn to generalize across different graphs so that it can be used for any unseen graphs. However, this is a very challenging goal. Most machine learning tasks that require the generalization across different graphs (e.g., graph classifications) aims to learn graph-level representations. But the generalization across both graphs and their layouts in a single model requires to learn the latent representations of nodes across many different graphs. Unfortunately, this is still an open problem in machine learning on graphs.

Our model learns the data distribution of the training set. We have shown several examples of how the models behave on noisy input layouts. However, a valid layout can be ignored in favor of generalizing across different graphs so that it can be used for any unseen graphs. This real-time generation is demonstrated by the capacity of GPU memory. This is the reason we could not use a larger batch size for *asoiaf* and *bus1138* (40 layouts per batch, while 100 layouts per batch for the other graphs). As a sampling-based algorithms that are scalable to millions of vertices has been recently introduced for large graphs, we expect our approach can be applied to much large graphs in the future work.

After training, the mean layout generation time for all the graphs are less than 0.003 seconds. Therefore, users can explore and generate diverse layouts in a real-time. This real-time generation is demonstrated in the supplementary material [1].

### 5 Discussion

Based on the test set reconstruction and the quality of the latent space, we have concluded that our generative model is capable of learning and generalizing many different layouts in a single two-dimensional latent space. Also, the generated layouts are spatially stable, which helps preserve the user’s mental map while visualizing a graph in different layouts. The graph neural networks (GNNs), especially GIN-MLP [84], the Gromov–Wasserstein (GW) distance [64] are helpful for the model to capture the complex relationship between the structure and the layouts of a graph. In addition, after training, our model is able to generate new layouts considerably faster than existing layout methods.

As a VAE, we explicitly define a reconstruction loss for the training. Thus, the model produces a more general arrangement following the user interface with the learned latent space to help users find a good overview of the latent space. Novice users can directly use this sample grid as a WYSIWYG interface for intuitive navigation (40 layouts per batch, while 100 layouts per batch for the other graphs). As a sampling-based algorithms that are scalable to millions of vertices has been recently introduced for large graphs, we expect our approach can be applied to much large graphs in the future work.

Although our model is capable of generalizing for different layouts of the same graph, it does not generalize for both different graphs and different layouts. Therefore, we need to train a new model for each graph. Our model can be trained in a fully unsupervised manner and can be trained incrementally while generating the training samples simultaneously. Still, a better model would learn to generalize across different graphs so that it can be used for any unseen graphs. However, this is a very challenging goal. Most machine learning tasks that require the generalization across different graphs (e.g., graph classifications) aims to learn graph-level representations. But the generalization across both graphs and their layouts in a single model requires to learn the latent representations of nodes across many different graphs. Unfortunately, this is still an open problem in machine learning on graphs.

Our model learns the data distribution of the training set. We have shown several examples of how the models behave on noisy input layouts. However, a valid layout can be ignored in favor of generalization. For example, the arrangement of the blue vertices in Fig. 4f is a valid layout, but it is a rare type of arrangement in the training dataset. The model produces a more general arrangement following the distribution of the training set. As a valid layout can be an outlier in the training dataset, we need an additional measure to not over-generalize valid layouts in the training dataset in the future work.

We have used a sliced-Wasserstein autoencoder [57], a variant of variational autoencoders (VAE) [53], for designing our architecture. As a VAE, we explicitly define a reconstruction loss for the training. However, this was challenging for comparing two different layouts of a set of structurally equivalent vertices. In this paper, we have used the GW distance [64] to address this issue. However, another possible solution is to use generative adversarial networks (GANs), which do not require a explicit reconstruction loss function in the optimization process. While we did not use GANs due to mode collapse and non-convergence [53], we believe it is possible to use GANs for learning a generative model for graph layout.

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1. What You See Is What You Get

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Fig. 6. Qualitative results of the five different graphs. The GIN-MLP model is used for the *football* graph and the GIN-MLP+GW models are used for the other graphs. For each pair of layouts, the left is the test input and the right is the reconstructed layout. The first three rows show the different styles of layouts for each graph, and the bottom two rows shows the reconstruction results of the noisy layouts. The results are discussed in detail in Sect. 4.6.
Fig. 7. Visualization of the latent spaces of the four different graphs. The GIN-MLP model is used for can96. The GIN-MLP+GW models are used for the other graphs. The grids of layouts are the generated samples by the decoding of a 8 × 8 grid in [−1, 1]². Also, Fig. 1 shows the sample grid of lesmis. The smooth transitions between the generated layouts show that the capability of generalization of our models. The outer columns show the color mappings of the four layout metrics of 540 × 540 generated sample layouts in [−1, 1]². The results are discussed in detail in Sect. 4.6. The results of other graphs and models are available in the supplementary material [1].

The learned latent representation of our model is entangled, which means each dimension of latent space is not interpretable. As we can see from the grids of samples in Fig. 1 and Fig. 7, although the transition between the samples are smooth, we cannot interpret the meaning of each dimension. Learning a model that produces interpretable, disentangled representation is an important research direction in generative modeling [43]. With a generative model that can learn a disentangled latent space, we would be able to produce a layout in more interpretable way. For example, one dimension of the latent representation encodes the area of clusters of vertices, so we can directly manipulate a layout. Therefore, instead of using a two-dimensional latent space, we could use a higher-dimensional latent space without losing the intuitiveness of exploring various layouts if we have a model that learns disentangled representations.

6 CONCLUSION

Relational data such as graphs and networks is one of the primary classes of information. Finding a good layout of a graph for visualization is not an easy job. The large number of available layout methods and each method’s associated parameter space confuse even the expert users. The trial-and-error effort required does not promise an optimal layout of the graph. We have introduced a fundamentally new approach to graph visualization, where we train a generative model to learn how to visualize a graph from a collection of examples. As a result, users are presented with a large number of possible layouts (i.e., visualizations) of the graph, and choosing a desired layout becomes an effortless task over an intuitive interface without requiring any knowledge about each layout method and its parameter space.

The generative modeling for image dataset has shown dramatic performance improvement. It took only four years from the first model of generative adversarial networks [34] to an advanced model that can generate high-resolution images [51]. There can be many exciting ways to use generative models for graph visualization, or even other types of data visualization. We hope this paper will encourage others to join this exciting area of study to accelerate designing generative models for revolutionizing the visualization technology.

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