Micro and Macro Level Graph Modeling for Graph Variational Auto-Encoders

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Abstract

Generative models for graph data are an important research topic in machine learning. Graph data comprise two levels that are typically analyzed separately: node-level properties such as the existence of a link between a pair of nodes, and global aggregate graph-level statistics, such as motif counts. This paper proposes a new multi-level framework that *jointly* models node-level properties and graph-level statistics, as mutually reinforcing sources of information. We introduce a new micro-macro training objective for graph generation that combines node-level and graph-level losses. We utilize the micro-macro objective to improve graph generation with a GraphVAE [42], a well-established model based on graph-level latent variables, that provides fast training and generation time for medium-sized graphs. Our experiments show that adding micro-macro modeling to the GraphVAE model improves graph quality scores up to 2 orders of magnitude on five benchmark datasets, while maintaining the GraphVAE generation speed advantage.

1 Introduction: multi-level graph modeling

Many datasets contain relational information about entities and their links that can be represented as a graph. Deep generative learning on graphs has become a popular research topic [20], with applications including molecule design [41], and recommendation [12]. It is common in graph analysis to distinguish two levels of information [10, 20]: (1) local node-level properties, such as the existence of a link between two nodes or the attribute of a node [27, 37, 19], and (2) global graph-level statistics (graph statistics for short) that depend on the entire graph, such as node degree distribution or motif counts. Most deep Graph Generative Models (GGMs) are trained with an objective based on local properties (e.g., maximizing the probabilities of observed edges). Figure 1 illustrates the difference between local and global structure. This paper proposes a new perspective on the node/graph level dichotomy: we introduce a principled probabilistic framework that incorporates both local and global graph properties. From the framework we derive a novel micro-macro (MM) objective function for training a GGM to match *both* local and global properties. The term *micro-macro* originates from the philosophy of science and has long been used to refer to scientific frameworks that treat both local and global properties of a system as equally important modeling targets [17].

Motivation Micro-macro modeling increases graph realism and user control. (1) Compared to objective functions that are based on predicting local properties, matching graph statistics serves as a *regularizer* for latent representations that increases the realism of the generated graph structures. (2) O'Bray et al. [35] note that different graph statistics are important for different applications. They therefore advise selecting a GGM based on the graph statistics of interest in the target application. However this entails searching through the space of generative models and their hyperparameters to

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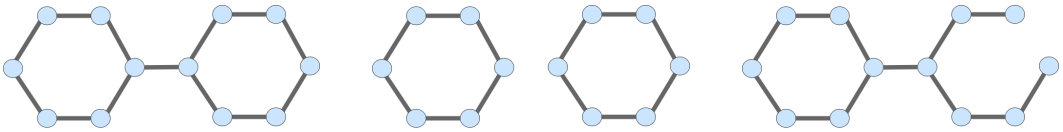

(a) Original Graph (b) Generated Graph 1 (c) Generated Graph 2

Figure 1: To illustrate the difference between local and global properties. The two right graphs (1b), (1c) score the same in terms of number of edges reconstructed from the left graph (1a), a local node-level property. However the right graph (1c), is structurally more similar to (1a), containing the same number of connected components, a global graph-level statistic.

find a good match with target graph statistics. In our MM framework, the user only needs to specify the target graph statistics and learning will automatically select graph models that match them.

Approach We introduce a joint probabilistic model over both local properties and global graph statistics. An MM objective is derived as an ELBO from the joint probability model that can be used with graph encoder-decoder models. Our experiments focus on the GraphVAE (Graph Variational Auto-Encoder) model where the encoder outputs a graph-level latent posterior $\boldsymbol{z}$ (graph embedding) and the decoder maps the graph embedding $\boldsymbol{z}$ to a soft adjacency matrix representing link probabilities [42]. A graph-level embedding supports modeling graph-level statistics. We show how the recent calibrated Gaussian variational auto-encoder [40] can be adapted to model graph statistics with divergent scales. The implementation and datasets are provided at an anonymous repository `https://github.com/ddccbbee/GraphVAE-MM`.

Evaluation Evaluating GGMs has become a research topic of its own [43, 35]; see the related work section below. Proposed metrics quantify how similar a set of generated graphs is to a set of observed graphs. Our assessment focuses on evaluation metrics based on Graph Neural Networks (GNN-based metrics) [43]. To our knowledge, this is the most recent published evaluation method, with state-of-the-art (SOTA) performance shown in extensive experiments. For GraphVAEs, our proposed approach improves both the realism and the diversity of the generated graphs, up to an order of magnitude on GNN-based metrics, while maintaining the efficiency of the GraphVAE model. This is sufficient to reach very competitive graph quality compared to auto-regressive benchmark models [32, 45, 11].

Contributions. Our main contributions can be summarized as follows.

- A new joint probabilistic model over both local graph properties and global graph-level statistics.
- Deriving a joint ELBO as a new micro-macro objective function for training graph encoder-decoder models.
- An adaptation of the GraphVAE architecture [42] to learn graph embeddings using the joint micro-macro objective.

2 Related work

We discuss the most relevant prior work.

Graph Statistics as Modeling Targets. To our knowledge, this is the first work to propose a deep graph generative model with the objective of matching graph statistics. Work on graph moment matching in network statistics [36, 6] has studied theoretical properties of graph moment estimators with increasing graph size. Maximizing the likelihood of exponential random graph models [21] such as Markov Logic Networks is equivalent to maximizing entropy subject to matching a set of graph statistics [28].

Graph Statistics for Evaluating Generative Models. The ability of generative models to match an empirical graph statistic distribution has been assessed in several research papers. This shows the importance of graph statistics and supports our approach of including them in the training objective.

Farnadi et al. [16] compare relational models in terms of matching (expected) motif counts. You et al. [45] and Liao et al. [32] use 4 graph statistics to measure the realism of generated graphs.

The question of how to evaluate a GGM has been studied in recent papers [35, 43]. An evaluation metric quantifies how similar a set of generated graphs $\hat{G}_1, \ldots, \hat{G}_{m_1}$ is to a set of test graphs $G_1, \ldots, G_{m_2}$. From the graphs we can compute corresponding descriptors $\hat{x}_1, \ldots, \hat{x}_{m_1}$ and $x_1, \ldots, x_{m_2}$. The similarity of two descriptor sets can be quantified using Maximum Mean Distance (MMD). O'Bray et al. [35] raise several difficulties with this approach. (1) Given a list of graph statistics, we obtain a list of MMD scores, rather than a single score that can be used to rank GGMs. (2) An MMD score is sensitive to hyper-parameters; different settings can lead to different model rankings even for a single graph statistic. (3) In perturbation studies where observed graphs are corrupted in a controlled manner, MMD scores do not correlate well with degree of perturbation. Thompson et al. [43] develop a recent proposal to address these issues. They utilize a *reference embedding network* GNN $\mathcal{E}$. The embedder $\mathcal{E}$ is obtained from pretraining or from random weights and is therefore independent of any of the models under evaluation. Given m_1 generated and m_2 test graphs, $\mathcal{E}$ provides embeddings $\hat{e}_1, \ldots, \hat{e}_{m_1}$ and $e_1, \ldots, e_{m_2}$ which can be compared using a distance metric such as MMD. Extensive evaluation shows that the GGM scores provided by the reference embedding approach correlate well with perturbation degree and capture the realism and diversity of generated graphs. To our knowledge, the GNN-based approach is the state of the art for evaluating GGMs, so we use it as our main evaluation metric.

Graph Generation Architecture. Our novel contribution is to develop a new kind of objective function, not a new kind of GGM. We therefore follow an AB design where we utilize an existing architecture as is and change only the training objective. Developing GGMs is an on-going topic of research; overviews can be found in [47, 20]. Two major GGM groups are all-at-once and auto-regressive methods [20]. All-at-once generation decodes a latent variable $\boldsymbol{z}$ to generate a (soft) adjacency matrix $\tilde{\boldsymbol{A}}$. Auto-regressive methods [32, 45] generate a graph incrementally. All-at-once methods are faster at graph generation, but tend to generate less realistic graphs. They can use node-level representations or a graph-level latent representation (embedding). We use a graph-level latent representation for two reasons: (1) A natural fit with modeling graph-level statistics. (2) It is known from previous work that node-level representations, while useful for many applications, do not capture enough graph structure to generate realistic graphs. We utilize the well-known GraphVAE architecture for computing graph embeddings [42],[20, Ch.9 Sec.1.2].

For a generative model of graph statistics, we adapt the state-of-the-art calibrated Gaussian variational auto-encoder [40], which has been developed as a generative model for i.i.d. data, but not previously been applied to graph modeling.

3 Data model and micro-macro objective

An attributed graph is a pair $G = (V, E)$ comprising a finite set of N nodes and edges where each node is assigned an d-dimensional attribute $\boldsymbol{X}_i$. An attributed graph can be represented by an $N \times N$ adjacency matrix $\boldsymbol{A}$ with $\{0, 1\}$ entries, together with an $N \times d$ node feature matrix $\boldsymbol{X}$. Following Ma et al. [33], we view the observed adjacency matrix as a sample from an underlying probabilistic adjacency matrix $\tilde{\boldsymbol{A}}$ with $\tilde{\boldsymbol{A}}_{i,j} \in [0, 1]$. The sampling distribution for independent edges is given by

$$P(\boldsymbol{A}|\tilde{\boldsymbol{A}}) = \prod_{i=1}^{N} \prod_{j=1}^{N} \tilde{\boldsymbol{A}}_{i,j}^{\boldsymbol{A}_{i,j}} (1 - \tilde{\boldsymbol{A}}_{i,j})^{1-\boldsymbol{A}_{i,j}}. \tag{1}$$

A **descriptor function** ϕ maps an adjacency matrix $\boldsymbol{A}$ to a l-dimensional **graph statistic** such that $\phi(\boldsymbol{A}) \in \mathbb{R}^l$ [35]. In the following we consider only descriptor functions that are permutation-equivariant [20, Ch.5]. A graph statistic represents a higher-order graph property. Examples include a node degree histogram or motif counts; for discussion and further examples see [20, Sec.2.1.2] and Section 4 below.

3.1 Micro-macro objective

We assume a finite list of descriptor functions $\phi_1, \ldots, \phi_m$ that define **target statistics**. A **micro-macro (MM) loss** is of the form

$$\mathcal{L}_{\boldsymbol{\theta}}(\boldsymbol{A}) = \mathcal{L}^0_{\boldsymbol{\theta}}(\boldsymbol{A}) + \gamma \mathcal{L}^1_{\boldsymbol{\theta}}(\boldsymbol{F}_1, \ldots, \boldsymbol{F}_m)$$

where $\boldsymbol{A}$ is the training graph and $\boldsymbol{F}_u, u = 1, \ldots, m$ is a random variable defined by applying the u-th descriptor function to the training graph. The hyperparameter γ controls the balance between capturing micro and macro aspects of the training graph. The micro loss $\mathcal{L}^0$ decomposes into losses for each node or pair of nodes. Well-known examples include the cross-entropy loss and max-margin loss. In this paper we work with negative log-likelihood losses and a variational approximation based on an encoder-decoder architecture:

$$\mathcal{L}^0_{\boldsymbol{\psi}}(\boldsymbol{A}) = -\ln p^0_{\boldsymbol{\psi}}(\boldsymbol{A}) = -\ln \int P(\boldsymbol{A}|\tilde{\boldsymbol{A}}_{\boldsymbol{z}})p(\boldsymbol{z})d\boldsymbol{z} \tag{2}$$

$$\mathcal{L}^1_{\boldsymbol{\psi},\boldsymbol{\sigma}}(\boldsymbol{F}_1, \ldots, \boldsymbol{F}_m) = -\sum_{u=1}^{m} \frac{1}{|\boldsymbol{F}_u|} \ln p^1_{\boldsymbol{\psi},\boldsymbol{\sigma}}(\boldsymbol{F}_u) \tag{3}$$

$$p^1_{\boldsymbol{\psi},\boldsymbol{\sigma}}(\boldsymbol{F}_u) = \int \mathcal{N}(\boldsymbol{F}_u|\phi_u(\tilde{\boldsymbol{A}}_{\boldsymbol{z}}), \sigma_u^2 I)p(\boldsymbol{z})d\boldsymbol{z} \tag{4}$$

using the following notation.

- $\boldsymbol{z}_{1\times t}$ specifies a latent t-dimensional graph embedding.
- $\tilde{\boldsymbol{A}}_{\boldsymbol{z}}$ is a probabilistic adjacency matrix computed as a trainable deterministic decoder function of graph embedding $\boldsymbol{z}$. The decoder parameters are denoted as $\boldsymbol{\psi}$. The edge reconstruction probability $P(\boldsymbol{A}|\tilde{\boldsymbol{A}}_{\boldsymbol{z}})$ is computed as in Equation (1).
- The distribution of each graph statistic is modeled as a Gaussian $\mathcal{N}$ with diagonal variance parameter σ_u^2.
- $|\boldsymbol{F}_u|$ is the dimensionality of target statistic $\boldsymbol{F}_u$.

Figure 4a in the Appendix shows a generative model diagram for Equations (2)–(4). Normalizing each graph statistic by its dimension is important because their scales can diverge widely. For example, transition matrices have N^2 entries, while the number of triangles is a single scalar. The following proposition provides an ELBO for an MM loss.

Proposition 1 *Let $\mathcal{L}_{\boldsymbol{\theta}}(\boldsymbol{A})$ be a micro-macro loss defined by Equations* (2)– (4)*. Then*

$$\mathcal{L}_{\boldsymbol{\theta}}(\boldsymbol{A}) \leq E_{\boldsymbol{z}\sim q_\varphi(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X})}\big[-\ln p^0_{\boldsymbol{\psi}}(\boldsymbol{A}|\tilde{\boldsymbol{A}}_{\boldsymbol{z}}) - \gamma \sum_{u=1}^{m} \big(\frac{1}{|\boldsymbol{F}_u|} \ln \mathcal{N}(\boldsymbol{F}_u|\phi_u(\tilde{\boldsymbol{A}}_{\boldsymbol{z}}), \sigma_u^2 I)\big] \tag{5}$$
$$+(1+\gamma m)KL(q_\varphi(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X})||p(\boldsymbol{z}))$$

where $q_\varphi(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X}) = q(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X},\boldsymbol{F}_1,\ldots,\boldsymbol{F}_m)$ is an approximate posterior distribution with parameters φ and given node attributes $\boldsymbol{X}$.

The proof is in the Appendix section 8.2. The basic idea is to combine ELBOs for each individual loss term. Adding a hyperparameter β to control the relative importance of the KL-divergence (as in the β-VAE), we obtain the following *training objective* for a set of observed training graphs $\boldsymbol{A}^1, \ldots, \boldsymbol{A}^n$:

$$\arg\min_{\varphi,\boldsymbol{\psi},\boldsymbol{\sigma}} \sum_{j=1}^{n} E_{\boldsymbol{z}\sim q_\varphi(\boldsymbol{z}|\boldsymbol{A}^j)}\big[-\ln p^0_{\boldsymbol{\psi}}(\boldsymbol{A}^j|\tilde{\boldsymbol{A}}_{\boldsymbol{z}}) - \gamma \sum_{u=1}^{m} \frac{1}{|\boldsymbol{F}_u|} \ln \mathcal{N}(\boldsymbol{F}^j_u|\phi_u(\tilde{\boldsymbol{A}}_{\boldsymbol{z}}), \sigma_u^2 I)\big] \tag{6}$$
$$+\beta KL(q_\varphi(\boldsymbol{z}|\boldsymbol{A}^j)||p(\boldsymbol{z}))$$

In this objective, *the graph statistic reconstruction loss, $-\sum_{u=1}^{m} \frac{1}{|\boldsymbol{F}_u|} \ln p^1_{\boldsymbol{\psi},\boldsymbol{\sigma}}(\boldsymbol{F}_u)$, acts as a regularizer with respect to the edge reconstruction loss $-\ln p^0_{\boldsymbol{\psi}}(\boldsymbol{A}^j|\tilde{\boldsymbol{A}}_{\boldsymbol{z}})$.*

3.2 Implementation

We implement the micro-macro ELBO (6) utilizing graph neural networks as follows.

- The prior $p(\boldsymbol{z})$ is a standard normal distribution.
- We limit the encoder input to the observed training graph, so $q(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X},\boldsymbol{F}_1,\ldots,\boldsymbol{F}_m) = q_\varphi(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X})$. Therefore we can use any standard graph encoder with parameters φ. The encoder deterministically maps an input graph $(\boldsymbol{A},\boldsymbol{X})$ to a posterior distribution $q_\varphi(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{X})$.

- The decoder deterministically maps a latent representation $\boldsymbol{z}$ to a probabilistic graph $\tilde{\boldsymbol{A}}_{\boldsymbol{z}}$ with parameters $\boldsymbol{\theta}$. Any standard graph decoder can be used.
- For each graph-level statistic, the diagonal co-variance parameter is computed using the optimal σ-VAE method from the calibrated Gaussian framework [40]. This uses the maximum likelihood estimate given the estimated means with respect to a minibatch of size B:

$$\sigma_u^2 = \frac{1}{B}\sum_{j=1}^{B} MSE(\phi_u(\tilde{\boldsymbol{A}}_{\boldsymbol{z}^j}), \boldsymbol{F}_u^j)), \qquad MSE(\boldsymbol{x}, \boldsymbol{\mu}) = \frac{1}{|\mu|}\sum_{d=1}^{|\mu|}(\boldsymbol{x}_d - \boldsymbol{\mu}_d)^2.$$

Figure 4b plots the architecture. The advantages of the calibrated Gaussian model for generating graph statistics are as follows. (1) In experiments on non-relational data, the calibrated Gaussian model achieves state-of-the-art performance. (2) Learning a variance parameter eliminates hyperparameters compared to user-assigned weights for each graph statistic. (3) The variance values can be interpreted as quantifying the empirical uncertainty of a graph feature. For example, if all training graphs exhibit a similar number of triangles, the corresponding variance parameter will be small.

4 Graph Statistics

The micro-macro ELBO (6) requires user-specified input graph descriptors for computing target graph statistics. In our experiments, we utilize several types of statistics that are easy to interpret. They can be used as defaults to regularize graph embeddings. In an application, they can be combined with other statistics of interest.

Graph descriptors used in network analysis and graph kernels comprise two main groups [20]: (1) Summaries of local node-level properties. We utilize a descriptor derived from the degree histogram, and the number of triangles in a graph.(2) Higher-order proximity relations between nodes. We utilize s-step transition probability matrices, for $s = 1, \ldots 5$ [9, 46]. These descriptors are differentiable with respect to the entries in a reconstructed soft adjacency matrix.

Vector label histogram. For a weighted undirected graph represented by $\tilde{\boldsymbol{A}}$, the **degree** of node v_i is given by $d(v_i) = \sum_j \tilde{\boldsymbol{A}}_{ij}$. We adapt the vector label histogram (VLH) [34]. VLH is based on a soft assignment of points to bins given bin centers and widths. Binning the soft degrees forms a soft degree histogram of graph $\tilde{\boldsymbol{A}}$ comparable to the hard degree histogram. In detail, the bin centers are the possible (hard) node degrees $b = 0, \ldots, N$. All widths are uniformly set to 0.1 (based on experimentation). Then we have

$$\mathbf{d}_{\tilde{\boldsymbol{A}}}(b) \equiv \sum_{i=1}^{N} a(v_i, b), \qquad a(v_i, b) = \max\{0, 1 - 0.1 \cdot |d(v_i) - b|\}.$$

Thus the membership $a(v_i, b)$ of a node in a bin b ranges from 0 to 1 and decreases with the difference between the node's expected degree and the bin center. The VLH assigns to each bin the sum of nodes membership in the bin. In a naive implementation, the computational cost of finding the $\mathbf{d}_{\tilde{\boldsymbol{A}}}(b)$ vector is $O(N^2)$. In our experiments, we use N parallel processors for a near constant time to obtain the soft degree histogram.

S-Step transition probability kernel. The s-step transition probability matrix of adjacency matrix $\tilde{\boldsymbol{A}}$ is a $N \times N$ matrix such that $P^s(\tilde{\boldsymbol{A}})_{i,j}$ is the probability of a transition from node i to node j in a random walk of s steps, where the probability of each transition is the normalized link probability. The transition matrix $P^s(\tilde{\boldsymbol{A}})$ can be computed by $P^s(\tilde{\boldsymbol{A}}) = (D(\tilde{\boldsymbol{A}})^{-1}\tilde{\boldsymbol{A}})^s$ where the degree matrix $D(\tilde{\boldsymbol{A}})$ is a diagonal matrix whose entries $D(\tilde{\boldsymbol{A}})_{ii} \equiv d(i)$ are the expected node degrees defined by Equation (7). The transition probability matrix is usually dense and encodes the connectivity information of the graph. An important difference to the adjacency matrix is that whereas adding or removing an edge changes only one adjacency, it can and often does result in a substantive change in many transition matrix elements. The descriptor $P^s(\tilde{\boldsymbol{A}})$ thus measures the importance of an edge in the graph structure (cf. Figure 1). In our experiments, we compute the transition probability matrix exactly with a runtime cost of $O(N^3)$.

Triangle count. The number of triangles in a simple graph $\boldsymbol{A}$ is computed by $Tri(A) = \sum_i (A^3)_{ii}$ with a runtime cost of $O(N^3)$. The number of triangles is a fundamental graph statistic in network

science [5] with many applications in graph mining [1]. For example it has been used to detect spamming activity and assess content quality in social networks [4], to uncover thematic structure in the world-wide web [14] and for query planning in databases [3]. It is also used extensively in exponential random graph models [21].

5 Experiments

We describe our baseline methods and benchmark datasets, then report comparison results.

5.1 Comparison methods

We examine the effect of micro-macro modeling on a GraphVAE architecture. Our AB methodology is to keep the architecture the same and train the model using the joint MM ELBO (6) that combines both local and global graph properties. We also compare the MM GraphVAE with popular GGMs. As the architectures are not new, we describe them briefly. Our experiments used the public repository and recommended hyperparameter by original creators; the Appendix contains further details.

GraphVAE. A popular model that uses a graph-level latent variable to generate a soft adjacency matrix [33, 42]. Encoder utilizes a Multi-layer Graph Convolutional Network (GCN) followed by a graph level readout and a Fully Connected Layer (FCL) that outputs (μ, σ). Decoder utilizes multi-layer FCL that outputs entries of a probabilistic adjacency matrix $\hat{A}$. To evaluate the reconstruction probability, we use a BFS ordering of nodes [31][20, ch.9.1.2].
GraphVAE–MM. GraphVAE trained with the micro-macro objective 6. *Our new method.*
GraphRNN. Auto-regressive method that generates the adjacency matrix incrementally. Each step generates one entry in the GraphRNN design, or one column in the GraphRNN-S design [45].
GRAN. Auto-regressive method that generates a block of nodes and associated edges at a step [32].
BiGG. Auto-regressive method that leverages graphs sparsity to avoid generating the full adjacency matrix [11]. To our knowledge BiGG achieves SOTA graph quality and generation time.

5.2 Benchmark datasets

Our design closely follows previous experiments on generating realistic graph structures [45, 32]. We utilize 3 synthetic, and 2 real-world datasets. The synthetic Grid and Lobster are from previous studies [45, 32], Triangle Grid is introduced in this paper. Protein and ogbg-molbbbp are real-world datasets from biology with information about proteins and molecules respectively. The Appendix, section 8.4, contains further details. *Train/Test Split.* Following [45, 30, 11] we randomly split the graphs sets into train (70%), validation (10%) and test (20%) sets. We use the same train and test graph sets for all models. To evaluate a trained model, we generate T new graphs to compare with the T graphs in the test set (cf. Section 2). Appendix Figure 5 illustrates the evaluation process and extends the experiments to other real datasets, including MUTAG, PTC [44] and QM9 [38].

Network modeling at the micro-level might be used for surveillance of individuals and communities. Therefore ethical network data collection must take into account issues of consent, privacy, and bias. None of the datasets used in this research study contain personally identifiable information, or offensive/harmful content about either individuals or communities. The *social impact* of our work we expect to be on balance more positive than negative, because our macro model enhances the understanding of global network structure, not the targetting of individuals.

5.3 Evaluation

We empirically verified the effectiveness of micro-macro modeling through different evaluation metrics: Qualitative and quantitative evaluation of graph quality, generation time, and training time.

Qualitative evaluation. Following [45, 32] we compare the generated graphs by visual inspection. Figure 2 provides a visual comparison of randomly selected test graphs and generated graphs. GraphVAE-MM and BiGG achieve the best visual match. The Appendix provides more examples.

Quantitative evaluation. We follow the descriptor-based approach established in previous works (cf. Section 2). As recommended by O'Bray et al. [35], we include scores computed from a 50/50 split of the test set as an ideal score, or lower bound on the GGM scores.

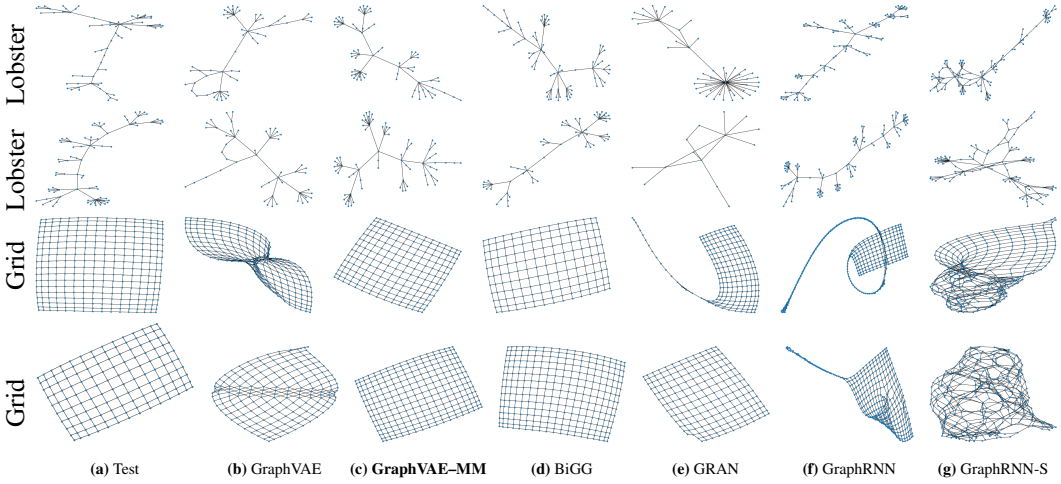

Figure 2: Visualization of generated graphs. The left-most column (2a) shows randomly selected graphs from the test set for each dataset, the other columns show graphs generated by each model from the prior. The generated graphs shown are the two visually most similar samples in the generated set. GraphVAE–MM achieves the best visual match, much better than GraphVAE.

(1) The GNN-based evaluation metrics [43] MMD RBF and F1 PR compare generated and test graph embeddings computed by a reference GNN with randomly initialized weights (Section 2). *The reference embeddings are independent of any target graph statistics used in GraphVAE-MM.* F1 PR stands for "Improved Precision and Recall". Precision is the percentage of generated graph embeddings that fall within the manifold of test graph embeddings, while recall is the percentage of test graph embeddings that fall within the manifold of generated graph embeddings. This metric mainly captures the *diversity* of generated graphs [35]. MMD RBF compares generated graph embeddings and test graph embeddings using an RBF kernel. This metric captures the *realism* of the generated graphs.

(2) The statistics-based evaluation metric [32, 45] compares generated and test graphs using *evaluation statistics*, namely node degree, clustering coefficient, orbit counts, and the spectra of the graphs. We add graph diameter, a statistic commonly studied in network science [29]. The target statistics used to train a GraphVAE-MM model are distinct from the evaluation statistics used to measure graph quality (however, node degree and VLH are closely related). For each statistic, MMD is computed using total variation (TV) distance [32].

Impact on GraphVAE. Table 1 shows a very large improvement from micro-macro modeling for both MMD RBF and F1 PR. The improvement in F1 PR ranges from 8%-40%, achieving a near perfect score. For MMD RBF the reduction ranges from 0.6 to 0.23 which is significant given the low theoretical ideal score. Table 2 shows the results for evaluation graph statistics. Micro-macro modeling reduces MMD by 1-2 orders of magnitude on almost all datasets, which is significant given the low theoretical ideal score. In sum, MM modeling provides a large improvement in the realism and diversity of graphs generated by a GraphVAE architecture.

Lesion studies in the Appendix investigate the effects of each target statistic in isolation (Table 5). No single statistic has the power of all three combined. We also observe that different statistics are more important for different datasets.

Table 1: GNN-based evaluation of micro-macro modeling for GraphVAEs. For each dataset we report the MMD RBF and F1 PR (see text) between the test set graphs (left-most column in Figure 2) and the generated graphs (see other columns in Figure 2). Values reported are the mean $\pm$ std. For MMD RBF smaller values are better, for F1 PR larger values are better.

Method	**Triangle Grid**		**Lobster**		**Grid**		**ogbg-molbbbp**		**Protein**	
	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR
50/50 split	0.03 ± 0.00	98.99 ± 0.00	0.04 ± 0.00	98.58 ± 0.00	0.009 ± 0.00	98.70 ± 0.00	0.002 ± 0.00	98.07 ± 0.00	0.04 ± 0.00	98.67 ± 1.11
GraphVAE	0.23 ± 0.01	75.92 ± 8.96	0.36 ± 0.11	78.48 ± 24.13	0.17 ± 0.01	75.52 ± 2.53	0.20 ± 0.07	54.53 ± 6.15	0.10 ± 0.05	84.11 ± 9.56
GraphVAE-MM	$\mathbf{0.17 \pm 0.01}$	$\mathbf{83.58 \pm 5.50}$	$\mathbf{0.10 \pm 0.00}$	$\mathbf{100.00 \pm 0.00}$	$\mathbf{0.13 \pm 0.01}$	$\mathbf{97.09 \pm 6.33}$	$\mathbf{0.02 \pm 0.01}$	$\mathbf{93.78 \pm 1.33}$	$\mathbf{0.03 \pm 0.01}$	$\mathbf{90.78 \pm 3.76}$

Table 2: Statistics-based evaluation of micro-macro modeling for GraphVAEs. For a named evaluation graph statistic, each column reports the MMD between the test graphs and the generated graphs.

(a) Synthetic Graphs

Method	Triangle Grid					Lobster					Grid				
	Deg.	Clus.	Orbit	Spect	Diam.	Deg.	Clus.	Orbit	Spect	Diam.	Deg.	Clus.	Orbit	Spect	Diam.
50/50 split	$3e^{-5}$	0.002	$8e^{-5}$	0.004	0.014	0.002	0	0.002	0.005	0.032	$1e^{-5}$	0	$2e^{-5}$	0.004	0.014
GraphVAE	0.0821	0.442	0.421	0.020	0.152	0.081	0.739	0.372	0.056	**0.129**	0.062	0.055	0.515	0.018	0.143
GraphVAE-MM	**0.001**	**0.093**	**0.001**	**0.013**	**0.133**	**$2e^{-4}$**	**0**	**0.008**	**0.017**	0.187	**$5e^{-4}$**	**0**	**0.001**	**0.014**	**0.065**

(b) Real Graphs

Method	Protein					ogbg-molbbbp				
	Deg.	Clus.	Orbit.	Spect.	Diam.	Deg.	Clus.	Orbit.	Spect.	Diam.
50/50 split	$4e^{-5}$	0.004	$5e^{-4}$	$4e^{-4}$	0.003	$2e^{-4}$	$2e^{-5}$	$9e^{-5}$	$5e^{-4}$	0.002
GraphVAE	0.022	0.108	0.577	0.016	**0.080**	0.028	0.442	0.047	0.015	0.055
GraphVAE-MM	**0.006**	**0.059**	**0.152**	**0.007**	0.091	**0.001**	**0.005**	**$8e^{-4}$**	**0.005**	**0.018**

Table 3: GNN-based comparison with benchmark GGMs. See table 1 caption. The best result is in bold and the second best is underlined.

Method	Triangle Grid		Lobster		Grid		ogbg-molbbbp		Protein	
	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR	MMD RBF	F1 PR
50/50 split	0.03 ± 0.00	98.58 ± 0.00	0.04 ± 0.00	98.58 ± 0.00	0.009 ± 0.00	98.70 ± 0.00	0.002 ± 0.00	98.07 ± 0.00	0.04 ± 0.00	98.67 ± 1.11
GraphVAE-MM	$\mathbf{0.17 \pm 0.01}$	$\mathbf{83.58 \pm 5.50}$	$\mathbf{0.10 \pm 0.00}$	$\mathbf{100.00 \pm 0.00}$	$\mathbf{0.13 \pm 0.01}$	$\mathbf{97.09 \pm 6.33}$	$\mathbf{0.02 \pm 0.01}$	93.78 ± 1.33	$\mathbf{0.03 \pm 0.01}$	90.78 ± 3.76
GraphRNN-S [45]	0.72 ± 0.17	33.68 ± 19.44	0.98 ± 0.13	58.72 ± 7.55	0.79 ± 0.08	71.18 ± 2.36	0.48 ± 0.02	81.41 ± 0.71	0.28 ± 0.26	72.36 ± 27.63
GraphRNN [45]	0.64 ± 0.11	25.80 ± 11.75	0.87 ± 0.04	61.97 ± 0.00	0.99 ± 0.03	13.22 ± 0.05	1.45 ± 0.19	$\mathbf{98.94 \pm 0.56}$	0.32 ± 0.14	93.94 ± 0.56
GRAN [32]	0.88 ± 0.09	23.71 ± 9.72	0.24 ± 0.04	50.53 ± 12.12	0.40 ± 0.00	78.73 ± 0.02	0.39 ± 0.07	94.06 ± 2.60	$\underline{0.07 \pm 0.00}$	$\underline{98.05 \pm 0.76}$
BiGG [11]	$\underline{0.41 \pm 0.13}$	$\underline{62.08 \pm 0.14}$	$\underline{0.12 \pm 0.00}$	$\underline{99.74 \pm 0.76}$	$\underline{0.35 \pm 0.00}$	$\underline{92.43 \pm 0.00}$	$\underline{0.04 \pm 0.00}$	$\underline{96.16 \pm 0.31}$	0.15 ± 0.00	$\mathbf{98.11 \pm 0.62}$

GraphVAE-MM vs. benchmark GGMs. For benchmarking we include GGMs that are known to generate realistic graphs. Tables 3 shows the GNN-based quality scores. Other than the most recent BiGG method, GraphVAE-MM achieves a much better score, except for GraphRNN on the Molecule dataset. This dataset is unusual in that it comprises only small graphs (average 23 edges). MMD RBF scores and 3 out of 5 F1 PR scores are also better in GraphVAE-MM compared to BiGG. Triangle Grid shows the biggest improvement, which illustrates the usefulness of matching triangle counts for this dataset.

Appendix Table 6 shows the benchmark results of statistics-based evaluation; we summarize them here. On synthetic graphs, the GraphVAE-MM scores are superior to or competitive with the BiGG and GRAN scores. On the real-world graphs, the GraphVAE-MM scores are competitive with the BiGG and GRAN scores, and superior to the other benchmarks. Given the already strong performance of the auto-regressive models, we conclude that GraphVAE-MM generates high-quality graphs.

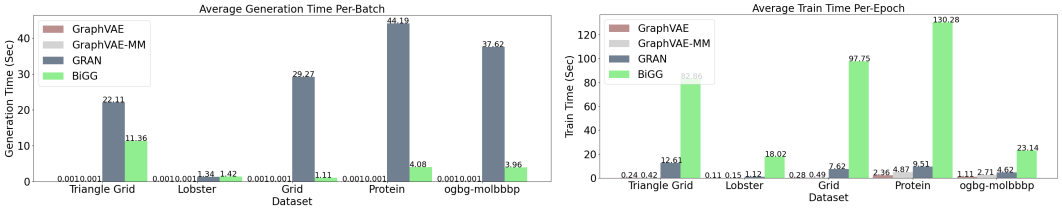

Figure 3: Comparison of benchmark GGMs with GraphVAEs on *generation time* (left) and *training time* (right). For visualization, generation time of GraphVAE and GraphVAE–MM are rounded up to 0.001, the first and second bar of each dataset respectively.

Generation and training time. The code for all models is run on the same system, detailed in Appendix section 8.11. Figure 3 compares GraphVAEs to the fastest auto-regressive methods. The auto-regressive methods require substantially more generation time than GraphVAEs. While MM modeling slows down training for the GraphVAE, the training time is still much less than for the auto-regressive methods. The Appendix table 7 provides time measurements for all methods.

6 Limitations and discussion

We discuss the limitations of our GraphVAE-MM model and options for combining micro-macro modeling with other GGMs.

Strengths and Weaknesses. GraphVAE-MM inherits the strengths of GraphVAE [20, Ch.9.1.2]: expressive power through graph embeddings, and fast generation and training time due to all-at-once parallel edge generation. GraphVAE-MM also inherits the known limitations of GraphVAEs: 1) We need to know a maximum number of nodes before generation. (Smaller graphs can be generated using a mask.) 2) The decoder is an FCL that ouputs $N \times N$ numbers; we need to (implicitly) assume a node ordering to evaluate edge reconstruction probabilities based on the FCL output. The dependence on a node ordering is common to both GraphVAEs and auto-regressive GGMs, and efficient heuristics have been designed whose effectiveness has been confirmed in experiments, including those reported in this paper. We note that MM modeling makes GGM training less dependent on a node ordering because it uses permutation-equivariant graph statistics.

Scalability. For medium-sized graphs all-at-once generation offers fast generation/learning, but a theoretical complexity analysis indicates that scaling GraphVAEs to very large graphs is a challenge. Table 11 in the Appendix presents computational complexity bounds for training/generation of the methods in our experiments. Evaluating the GraphVAE-MM ELBO during training incurs computational overhead compared to the GraphVAE ELBO due to computing graph statistics. Table 10 in the Appendix gives complexity bounds for the different default statistics we use in this paper. We note that evaluating the edge reconstruction probability is already expensive. Approximating graph statistics can reduce the computational cost significantly [24, 15, 31, 39].

Micro-Macro modeling for other GGM architectures. An interesting hybrid architecture combines a graph-level encoder with an auto-regressive decoder [25]. This is an option for leveraging micro-macro modeling in auto-regressive graph generation. An auto-regressive decoder is much more expressive than the all-at-once standard GVAE decoders.

In a graph GAN [7, 8] the generator maps a graph latent $\boldsymbol{z}$ to an adjacency matrix, and the discriminator classifies the adjacency matrix as real or synthetic. A straightforward way to combine MM modeling with GANs is to augment the input to the discriminator with graph statistics computed for both real and generated graphs.

7 Conclusion and future work

The main idea in this paper was to model graph data jointly at two levels: a micro level based on local information (e.g. the existence of a link between two nodes) and a macro level based on aggregate graph statistics. We described a principled joint probabilistic model for both micro and macro levels, and derived an ELBO training objective for graph encoder-decoder models. Compared to previous micro level training objectives, the macro statistics regularize graph embeddings to match global graph statistics. To evaluate our model, we described a set of strong default graph statistics (node degree, number of triangles, transition probabilities). We applied the new training objective to the GraphVAE architecture, a widely used graph generative model based on latent graph representation. Micro-macro (MM) modeling greatly improved the quality of graphs generated by GraphVAE, to match or exceed that of benchmark models. With an efficient computation of graph statistics, MM modeling maintained the speed advantages of edge-parallel all-at-once graph generation for both model training and graph generation.

Micro-macro modeling opens a number of fruitful avenues for future work. i) Investigating which graph statistics are important for generating which types of graphs. This connects with the rich area of graph kernels [34] that are often based on graph statistics. ii) Investigating which graph statistics are important for particular domains. iii) Developing a micro-macro model for other graph generative architectures, such as auto-regression and GANs. iv) Developing a micro-macro modeling for attributed graphs with node or edge features and evaluating its impact on other graph-level tasks, including graph classification and unsupervised deep representation learning.

In sum, modeling both global graph statistics and local information enhances the power of graph generation. Compared to using local information only, graph statistics can be used to regularize graph representations to efficiently generate realistic graphs.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 6 for details.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 5.2 and 8.13 for details.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 3 for details.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Section 3 and Appendix for details.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Code, datasets and library requirements can be found in our anonymous repository, `https://github.com/ddccbbee/GraphVAE-MM`
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Sections 5.2 and Appendix for all experiment settings. We also added all details, including models, generated samples, training logs and library requirements in our public repository.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] The focus of this paper is on the GNN-based metrics, tables 1 and 3, containing error bar information. For all other compared metrics, the proposed approach typically results in 1-2 orders of magnitude of improvement. This evidence seems to be sufficient without error bars.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section 8.11 for machine details.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] Reported datasets and codes are open-source and publicly available. We cited them clearly in Tables and Context
   (b) Did you mention the license of the assets? [Yes] All codes and datasets used in this study are publicly available and clearly mentioned in the Section 5.2 and 5.1. Our implementation is publicly released under MIT license as mentioned in our repository.
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] We included our model implementation and it is publicly available at `https://github.com/ddccbbee/GraphVAE-MM`
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] As mentioned in Section 5.1, we used the original papers' public repository; hence no consent was needed to curate this study. Also all used datasets are open source and publicly available.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [Yes] As mentioned in Section 5.2, None of the datasets used for this research study contain any personally identifiable information or offensive content.
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A] This point is not applicable for this research study.

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A] This point is not applicable for this research study.

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A] No such participants were used for this research study.

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