GRADIENT-GUIDED IMPORTANCE SAMPLING FOR LEARNING DISCRETE ENERGY-BASED MODELS

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ABSTRACT

Learning energy-based models (EBMs) is known to be difficult especially on discrete data where gradient-based learning strategies cannot be applied directly. Although ratio matching is a sound method to learn discrete EBMs, it suffers from expensive computation and excessive memory requirement, thereby resulting in difficulties for learning EBMs on high-dimensional data. In this study, we propose ratio matching with gradient-guided importance sampling (RMwGGIS) to alleviate the above limitations. Particularly, we leverage the gradient of the energy function *w.r.t.* the discrete data space to approximately construct the provable optimal proposal distribution, which is subsequently used by importance sampling to efficiently estimate the original ratio matching objective. We perform experiments on density modeling over synthetic discrete data and graph generation to evaluate our proposed method. The experimental results demonstrate that our method can significantly alleviate the limitations of ratio matching and perform more effectively in practice.

1 INTRODUCTION

Energy-Based models (EBMs), also known as unnormalized probabilistic models, model distributions by associating unnormalized probability densities. Such methods have been developed for decades (Hopfield, 1982; Ackley et al., 1985; Cipra, 1987; Dayan et al., 1995; Zhu et al., 1998; Hinton, 2012) and are unified as energy-based models (EBMs) (LeCun et al., 2006) in the machine learning community. EBMs have great simplicity and flexibility since energy functions are not required to integrate or sum to one, thus enabling the usage of various energy functions. In practice, given different data types, we can parameterize the energy function with different neural networks as needed, such as multi-layer perceptrons (MLPs), convolutional neural networks (CNNs) (LeCun et al., 1998), and graph neural networks (GNNs) (Gori et al., 2005; Scarselli et al., 2008). Recently, EBMs have been drawing increasing attention and are demonstrated to be effective in various domains, including images (Ngiam et al., 2011; Xie et al., 2016; Du & Mordatch, 2019), videos (Xie et al., 2017), texts (Deng et al., 2020), 3D objects (Xie et al., 2018), molecules (Liu et al., 2021; Hataya et al., 2021), and proteins (Du et al., 2020b).

Nonetheless, learning (*a.k.a.*, training) EBMs is known to be challenging since we cannot compute the exact likelihood due to the intractable normalization constant. As reviewed in Section 4, many approaches have been proposed to learn EBMs, such as maximum likelihood training with MCMC sampling (Hinton, 2002) and score matching (Hyvärinen & Dayan, 2005). However, most recent advanced methods cannot be applied to discrete data directly since they usually leverage gradients over the continuous data space. For example, for many methods based on maximum likelihood training with MCMC sampling, they use the gradient *w.r.t.* the data space to update samples in each MCMC step. If we update discrete samples using such gradient, the resulting samples are usually invalid in the discrete space. Notably, discrete data is common in our real world, such as texts, graphs, and genome sequences. Therefore, learning EBMs on discrete data remains to be challenging and in demand.

Ratio matching (Hyvärinen, 2007; Lyu, 2009) is proposed to learn discrete EBMs by matching ratios of probabilities between the data distribution and the model distribution, as detailed in Section 2.2. However, as analyzed in Section 3.1, it requires expensive computations and excessive memory usages, which is infeasible if the data is high-dimensional. In this work, we propose to use the gradient of the energy function *w.r.t.* the discrete data space to guide the importance sampling for estimating

the original ratio matching objective. More specifically, we utilize such gradient to approximately construct the provable optimal proposal distribution for importance sampling. Thus, the proposed approach is termed as ratio matching with gradient-guided importance sampling (RMwGGIS). Our RMwGGIS can significantly overcome the limitations of ratio matching. In addition, it is demonstrated to be more effective than the original ratio matching because it can be optimized better in practice. To evaluate our method, we conduct experiments for density modeling on synthetic discrete data and graph generation. Experimental results demonstrate that our RMwGGIS significantly alleviates the limitations of ratio matching and achieves better performance with obvious margins.

2 PRELIMINARIES

2.1 ENERGY-BASED MODELS

Let $\boldsymbol{x}$ be a data point and $E_{\boldsymbol{\theta}}(\boldsymbol{x}) \in \mathbb{R}$ be the corresponding energy, where $\boldsymbol{\theta}$ represents the learnable parameters of the parameterized energy function $E_{\boldsymbol{\theta}}(\cdot)$. The probability density function of the model distribution is given as

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x})}}{Z_{\boldsymbol{\theta}}} \propto e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x})}, \tag{1}$$

where $Z_{\boldsymbol{\theta}} \in \mathbb{R}$ is the normalization constant (*a.k.a.*, partition function). To be specific, $Z_{\boldsymbol{\theta}} = \int e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x})} d\boldsymbol{x}$ if $\boldsymbol{x}$ is in the continuous space and $Z_{\boldsymbol{\theta}} = \sum e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x})}$ for discrete data. Hence, computing $Z_{\boldsymbol{\theta}}$ is usually infeasible due to the intractable integral or summation. Note that $Z_{\boldsymbol{\theta}}$ is a variable depending on $\boldsymbol{\theta}$ but a constant *w.r.t.* $\boldsymbol{x}$.

2.2 RATIO MATCHING

Ratio matching (Hyvärinen, 2007) is developed for learning EBMs on discrete data by matching ratios of probabilities between the data distribution and the model distribution. Note that we focus on d-dimensional binary discrete data $\boldsymbol{x} \in \{0, 1\}^d$ in this work.

Specifically, ratio matching considers the ratio of $p(\boldsymbol{x})$ and $p(\boldsymbol{x}_{-i})$, where $\boldsymbol{x}_{-i} = (x_1, x_2, \cdots, \bar{x}_i, \cdots, x_d)$ denotes a point in the data space obtained by flipping the i-th dimension of $\boldsymbol{x}$. The key idea is to force the ratios $\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}$ defined by the model distribution $p_{\boldsymbol{\theta}}$ to be as close as possible to the ratios $\frac{p_{\mathcal{D}}(\boldsymbol{x})}{p_{\mathcal{D}}(\boldsymbol{x}_{-i})}$ given by the data distribution $p_{\mathcal{D}}$. The benefit of considering ratios of probabilities is that they do not involve the intractable normalization constant $Z_{\boldsymbol{\theta}}$ since $\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})} = \frac{e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x})}}{e^{-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}} = e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}) - E_{\boldsymbol{\theta}}(\boldsymbol{x})}$ according to Eq. (1). To achieve the match between ratios, Hyvärinen (2007) proposes to minimize the objective function

$$\mathcal{J}_{RM}(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{x} \sim p_{\mathcal{D}}(\boldsymbol{x})} \sum_{i=1}^{d} \left[g\left(\frac{p_{\mathcal{D}}(\boldsymbol{x})}{p_{\mathcal{D}}(\boldsymbol{x}_{-i})}\right) - g\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right)\right]^2 + \left[g\left(\frac{p_{\mathcal{D}}(\boldsymbol{x}_{-i})}{p_{\mathcal{D}}(\boldsymbol{x})}\right) - g\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}{p_{\boldsymbol{\theta}}(\boldsymbol{x})}\right)\right]^2. \tag{2}$$

The sum of two square distances with the role of $\boldsymbol{x}$ and $\boldsymbol{x}_{-i}$ switched is specifically designed since it is essential for the following simplification. In addition, the function $g(u) = \frac{1}{1+u}$ is also carefully chosen in order to obtain the subsequent simplification. To compute the objective defined in Eq. (2), it is known that the expectation over data distribution (*i.e.*, $\mathbb{E}_{\boldsymbol{x} \sim p_{\mathcal{D}}(\boldsymbol{x})}$) can be unbiasedly estimated by the empirical mean of samples $\boldsymbol{x} \sim p_{\mathcal{D}}(\boldsymbol{x})$. However, to obtain the ratios between $p_{\mathcal{D}}(\boldsymbol{x})$ and $p_{\mathcal{D}}(\boldsymbol{x}_{-i})$ in Eq. (2), the exact data distribution is required to be known, which is usually impossible.

Fortunately, thanks to the above carefully designed objective, Hyvärinen (2007) demostrates that the objective function in Eq. (2) is equivalent to the following simplified version

$$\mathcal{J}_{RM}(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{x} \sim p_{\mathcal{D}}(\boldsymbol{x})} \sum_{i=1}^{d} \left[g\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right)\right]^2 = \mathbb{E}_{\boldsymbol{x} \sim p_{\mathcal{D}}(\boldsymbol{x})} \sum_{i=1}^{d} \left[g\left(e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}) - E_{\boldsymbol{\theta}}(\boldsymbol{x})}\right)\right]^2, \tag{3}$$

which does not require the data distribution to be known and can be easily computed by evaluating the energy of $\boldsymbol{x}$ and $\boldsymbol{x}_{-i}$. It is proved that the estimator given by Eq. (3) is consistent (Hyvärinen, 2007). That means if it is minimized perfectly, the obtained model distribution will capture the data

distribution exactly. Further, Lyu (2009) shows that the objective function of ratio matching can be reduced to

$$\mathcal{J}_{RM}(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{x}\sim p_{\mathcal{D}}(\boldsymbol{x})} \sum_{i=1}^{d} \left[\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}{p_{\boldsymbol{\theta}}(\boldsymbol{x})} \right]^2 = \mathbb{E}_{\boldsymbol{x}\sim p_{\mathcal{D}}(\boldsymbol{x})} \sum_{i=1}^{d} \left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})} \right]^2. \tag{4}$$

It is obvious that Eq. (3) and Eq. (4) agree with each other since function $g(\cdot)$ decreases monotonically in $[0, +\infty)$, which aligns with the value range of probability ratios $\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}$.

Intuitively, the objective function of ratio matching, as formulated in Eq. (4), can push down the energy of the training sample $\boldsymbol{x}$ and push up the energies of other data points obtained by flipping one dimension of $\boldsymbol{x}$. Thus, this objective faithfully expect that each training sample $\boldsymbol{x}$ has higher probability than its local neighboring points that are hamming distance 1 from $\boldsymbol{x}$.

3 The Proposed Method

In this section, we analyze the limitations of the ratio matching method from the perspective of computational time and memory usage. Then, we describe our proposed method, ratio matching with gradient-guided importance sampling (RMwGGIS), which utilizes the gradient of the energy function *w.r.t.* the discrete input $\boldsymbol{x}$ to guide the importance sampling for estimating the original ratio matching objective. Our approach can alleviate the limitations significantly and is shown to be more effective in practice.

3.1 Analysis of Ratio Matching

Time-intensive computations. According to Eq. (4), for a given training sample $\boldsymbol{x}$, we have to compute the energies for all $\boldsymbol{x}_{-i}$, where $i = 1, \cdots, d$. In other words, we have $\mathcal{O}(d)$ evaluations of the energy function for each training sample. This is computationally intensive, especially when the data dimension d is large.

Excessive memory usages. Besides the expensive computation, the memory usage of ratio matching is another limitation that cannot be ignored, especially when we learn the energy function using modern GPUs with limited memory. As shown in Eq. (4), the objective function consists of d terms for each training sample. When we do backpropagation, computing the gradient of the objective function *w.r.t.* the learnable parameters of the energy function is required. Therefore, in order to compute such gradient, we have to store the whole computational graph and the intermediate tensors for all of the d terms, thereby leading to excessive memory usages especially if the data dimension d is large. Hence, it is challenging to learn EBMs with ratio matching on modern devices, such as GPUs, for high-dimensional discrete data.

3.2 Ratio Matching with Gradient-Guided Importance Sampling

The key idea of our approach is to use the well-known importance sampling technique to reduce the variance of estimating $\mathcal{J}_{RM}(\boldsymbol{\theta})$ with Monte Carlo method. The most critical and challenging part of using the importance sampling technique is choosing a good proposal distribution. In this work, we propose to utilize the gradient of the energy function *w.r.t.* the discrete input $\boldsymbol{x}$ to approximately construct the optimal proposal distribution for importance sampling. We describe the details of our method below.

The objective for each sample $\boldsymbol{x}$, defined by Eq. (4), can be reformulated as

$$\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x}) = d \sum_{i=1}^{d} \frac{1}{d} \left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})} \right]^2 = d\mathbb{E}_{\boldsymbol{x}_{-i}\sim m(\boldsymbol{x}_{-i})} \left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})} \right]^2, \tag{5}$$

where $m(\boldsymbol{x}_{-i}) = \frac{1}{d}$ for $i = 1, \cdots, d$ is a discrete distribution. Thus, the objective of ratio matching for each sample $\boldsymbol{x}$ can be viewed as the expectation of $\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})} \right]^2$ over the discrete distribution $m(\boldsymbol{x}_{-i})$. In the original ratio matching method, as described in Section 2.2, we compute such expectation exactly by considering all possible $\boldsymbol{x}_{-i}$, leading to expensive computations and excessive memory usages as analyzed in Section 3.1. Naturally, we can estimate the desired expectation

with Monte Carlo method by considering fewer terms sampled based on $m(\boldsymbol{x}_{-i})$. However, such estimation usually has a high variance, and is empirically verified to be ineffective by our experiments in Section 5.

Further, we can apply the importance sampling method to reduce the variance of Monte Carlo estimation. Intuitively, certain values have more impact on the expectation than others. Hence, the estimator variance can be reduced if such important values are sampled more frequently than others. To be specific, instead of sampling based on the distribution $m(\boldsymbol{x}_{-i})$, importance sampling aims to sample from another distribution $n(\boldsymbol{x}_{-i})$, namely, proposal distribution. Formally,

$$\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x}) = d\mathbb{E}_{\boldsymbol{x}_{-i}\sim m(\boldsymbol{x}_{-i})}\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2 = d\mathbb{E}_{\boldsymbol{x}_{-i}\sim n(\boldsymbol{x}_{-i})}\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}. \tag{6}$$

The detailed derivation of Eq. (6) is given in Appendix A. Afterwards, we can apply Monte Carlo estimation based on the proposal distribution $n(\boldsymbol{x}_{-i})$. Specifically, we sample s terms, denoted as $\boldsymbol{x}_{-i}^{(1)}, \cdots, \boldsymbol{x}_{-i}^{(s)}$, according to the proposal distribution $n(\boldsymbol{x}_{-i})$. Note that s is usually chosen to be much smaller than d. Then the Monte Carlo estimation for $\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})$ is computed based on these s terms. Formally,

$$\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_n = d\frac{1}{s}\sum_{t=1}^{s}\frac{m(\boldsymbol{x}_{-i}^{(t)})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}^{(t)})}\right]^2}{n(\boldsymbol{x}_{-i}^{(t)})}, \quad \boldsymbol{x}_{-i}^{(t)} \sim n(\boldsymbol{x}_{-i}). \tag{7}$$

It is known that the estimator obtained by Monte Carlo estimation with importance sampling is an unbiased estimator, as the conventional Monte Carlo estimator. The key point of importance sampling is to choose an appropriate proposal distribution $n(\boldsymbol{x}_{-i})$, which determines the variance of the corresponding estimator. The optimal proposal distribution $n^*(\boldsymbol{x}_{-i})$, which yields the minimum variance, is given by the following theorem.

Theorem 1. *Let* $n^*(\boldsymbol{x}_{-i}) = \frac{\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{\sum_{k=1}^{d}\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-k})}\right]^2}$ *be a discrete distribution on* $\boldsymbol{x}_{-i}$*, where* $i = 1, \cdots, d$*. Then for any discrete distribution* $n(\boldsymbol{x}_{-i})$ *on* $\boldsymbol{x}_{-i}$*, where* $i = 1, \cdots, d$*, we have* $Var\left(\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_{n^*}\right) \leq Var\left(\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_n\right)$.

Proof. The proof of Theorem 1 is included in Appendix B. □

To construct the exact optimal proposal distribution $n^*(\boldsymbol{x}_{-i})$ given by Theorem 1, we still have to evaluate the energies of all $\boldsymbol{x}_{-i}$, where $i = 1, \cdots, d$. To avoid such complexity, we propose to leverage the gradient of the energy function *w.r.t.* the discrete input $\boldsymbol{x}$ to approximately construct the optimal proposal distribution. Our approach only needs $\mathcal{O}(1)$ evaluations of the energy function to construct the proposal distribution.

It is observed by Grathwohl et al. (2021) that many discrete distributions are implemented as continuous and differentiable functions, although they are evaluated only in discrete domains. Grathwohl et al. (2021) further proposes a scalable sampling method for discrete distributions by utilizing the gradients of the underlying continuous functions *w.r.t.* the discrete input. In this study, we extend this idea to improve ratio matching. More specifically, in our case, even though our input $\boldsymbol{x}$ is discrete, our parameterized energy function $E_{\boldsymbol{\theta}}(\cdot)$, such as a neural network, is usually continuous and differentiable. Hence, we can use such gradient information to efficiently and approximately construct the optimal proposal distribution given by Theorem 1.

The basic idea is that we can approximate $E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})$ based on the Taylor series of $E_{\boldsymbol{\theta}}(\cdot)$ at $\boldsymbol{x}$, given that $\boldsymbol{x}_{-i}$ is close to $\boldsymbol{x}$ in the data space because they only have differences in one dimension. Formally,

$$E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}) \approx E_{\boldsymbol{\theta}}(\boldsymbol{x}) + (\boldsymbol{x}_{-i} - \boldsymbol{x})^T \nabla_{\boldsymbol{x}} E_{\boldsymbol{\theta}}(\boldsymbol{x}). \tag{8}$$

Thus, we can approximately obtain the desired term $E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})$ in Theorem 1 using Eq. (8). Note that $\nabla_{\boldsymbol{x}} E_{\boldsymbol{\theta}}(\boldsymbol{x}) \in \mathbb{R}^d$ contains the information for approximating all $E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})$, where $i = 1, \cdots, d$. Hence, we can consider the following d-dimensional vector

$$(2\boldsymbol{x} - 1) \odot \nabla_{\boldsymbol{x}} E_{\boldsymbol{\theta}}(\boldsymbol{x}) \quad \in \mathbb{R}^d, \tag{9}$$

Algorithm 1 Ratio Matching with Gradient-Guided Importance Sampling (RMwGGIS)

Input: Observed dataset $\mathcal{D} = \left\{\boldsymbol{x}^{(m)}\right\}_{m=1}^{|\mathcal{D}|}$, parameterized energy function $E_{\boldsymbol{\theta}}(\cdot)$, number of samples s for Monte Carlo estimation with importance sampling

1: **for** $\boldsymbol{x} \sim \mathcal{D}$ **do** ▷ Batch training is applied in practice
2: Compute $E_{\boldsymbol{\theta}}(\boldsymbol{x})$
3: Compute $\nabla_{\boldsymbol{x}} E_{\boldsymbol{\theta}}(\boldsymbol{x})$
4: Compute the proposal distribution $\widetilde{n}^*(\boldsymbol{x}_{-i}) = \frac{\left[e^{2(2\boldsymbol{x}-1)\odot\nabla_{\boldsymbol{x}}E_{\boldsymbol{\theta}}(\boldsymbol{x})}\right]_i}{\sum_{k=1}^{d}\left[e^{2(2\boldsymbol{x}-1)\odot\nabla_{\boldsymbol{x}}E_{\boldsymbol{\theta}}(\boldsymbol{x})}\right]_k}$ ▷ Eq. (11)
5: Sample s terms, denoted as $\boldsymbol{x}_{-i}^{(1)}, \cdots, \boldsymbol{x}_{-i}^{(s)}$, according to $\widetilde{n}^*(\boldsymbol{x}_{-i})$
6: Compute $\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_{\widetilde{n}^*} = d\frac{1}{s}\sum_{t=1}^{s} \frac{m(\boldsymbol{x}_{-i}^{(t)})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}^{(t)})}\right]^2}{\widetilde{n}^*(\boldsymbol{x}_{-i}^{(t)})}$ ▷ Eq. (7) (or Eq. (12))
7: Update $\boldsymbol{\theta}$ based on $\nabla_{\boldsymbol{\theta}}\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_{\widetilde{n}^*}$
8: **end for**

where $\odot$ denotes element-wise multiplication. Note that we have $x_i - \bar{x}_i = -1$ if $x_i = 0$ and $x_i - \bar{x}_i = 1$ if $x_i = 1$, which can be unified as $x_i - \bar{x}_i = 2x_i - 1$. Therefore, we have

$$E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}) \approx \left[(2\boldsymbol{x}-1)\odot\nabla_{\boldsymbol{x}}E_{\boldsymbol{\theta}}(\boldsymbol{x})\right]_i, \quad i = 1, \cdots, d. \tag{10}$$

Afterwards, we can provide a proposal distribution $\widetilde{n}^*(\boldsymbol{x}_{-i})$ as an approximation of the optimal proposal distribution $n^*(\boldsymbol{x}_{-i})$ given by Theorem 1. Formally,

$$\widetilde{n}^*(\boldsymbol{x}_{-i}) = \frac{\left[e^{2(2\boldsymbol{x}-1)\odot\nabla_{\boldsymbol{x}}E_{\boldsymbol{\theta}}(\boldsymbol{x})}\right]_i}{\sum_{k=1}^{d}\left[e^{2(2\boldsymbol{x}-1)\odot\nabla_{\boldsymbol{x}}E_{\boldsymbol{\theta}}(\boldsymbol{x})}\right]_k}, \quad i = 1, \cdots, d. \tag{11}$$

Then $\widetilde{n}^*(\boldsymbol{x}_{-i})$ is used as the proposal distribution for Monte Carlo estimation with importance sampling, as described by Eq. (7). The overall process of our RMwGGIS method is summarized in Algorithm 1.

3.3 Comparison between Ratio Matching and RMwGGIS

Time and memory. Since only s ($s < d$) terms are considered in the objective function of our RMwGGIS, as shown in Eq. (7), we have better computational efficiency and less memory requirement compared to the original ratio matching method. To be specific, our RMwGGIS only needs $\mathcal{O}(s)$ evaluations of the energy function compared with $\mathcal{O}(d)$ in ratio matching, leading to a linear speedup, which is significant especially when the data is high-dimensional. The improvement in terms of memory usage is similar. In Section 5.1, we compare the real running time and memory usage between ratio matching and our proposed RMwGGIS on datasets with different data dimsensions.

Better optimization? In Section 3.2, we propose our RMwGGIS based on the motivation to approximate the objective of ratio matching with fewer terms. Although our RMwGGIS can approximate the original ratio matching objective numerically, our objective only includes s terms compared to d terms in the original ratio matching objective; That is, only s terms are involved in the computational graph, leading to different back-propogated gradients compared to the original ratio matching. In other words, the objective of ratio matching, as shown in Eq. (4), intuitively pushes up the energies of all $\boldsymbol{x}_{-i}$ for $i = 1, \cdots, d$, while our RMwGGIS only considers pushing up energies of s terms among them, as formulated by Eq. (7). Thus, the following question might be raised. *Why can our objective be effective for learning EBMs without pushing up the energies of all d terms?* In practice, we even observe that our RMwGGIS achieves better density modeling performance than ratio matching. We conjecture that this is because our RMwGGIS can be optimized better in practice for the following two properties, which are empirically verified in Section 5.

(1) RMwGGIS introduces stochasticity. Without involving all d terms in the objective function, our method can introduce stochasticity, which could lead to better optimization in practice. This has the same philosophy as the comparison between mini-batch gradient descent and vanilla gradient descent. The gradient is obtained based on each batch in mini-batch gradient descent, while it is computed over the entire dataset in vanilla gradient descent. It is known that the mini-batch gradient

descent usually performs better in practice since the stochasticity introduced by mini-batch training could help to escape from the saddle points in non-convex optimization (Ge et al., 2015). Therefore, the stochasticity introduced by sampling only s terms in RMwGGIS could help the optimization especially when d is large.

(2) RMwGGIS focuses on neighbors with low energies. Even though only energies of s terms are pushed up in our method, these s terms correspond to the neighboring points that have low energies. According to $n^*(\boldsymbol{x}_{-i})$ given by Theorem 1, a neighbor of $\boldsymbol{x}$, denoted as $\boldsymbol{x}_{-i}$, is more likely to be sampled if its corresponding energy value is lower [1]. Hence, we choose to push up the energies of s neighbors according to their current energies. The lower the energy, the more likely it is to be selected. This is intuitively sound because the terms that have low energies are the most offending terms, which should have the higher priorities to be pushed up.

Overall, from the energy dynamics view, for each training sample $\boldsymbol{x}$, RMwGGIS samples s neighbors of $\boldsymbol{x}$ and push up their energies. Note that such sampling process has the above two important properties. Therefore, we further propose the following biased estimation as the objective function by removing the unnecessary coefficients in Eq. (7). Formally,

$$\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_{\widetilde{n}^*}^{biased} = \sum_{t=1}^{s} \left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x}) - E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i}^{(t)})} \right]^2, \quad \boldsymbol{x}_{-i}^{(t)} \sim \widetilde{n}^*(\boldsymbol{x}_{-i}). \tag{12}$$

Note that this objective also samples s neighbors according to their current energies and push up their energies. This biased version is demonstrated to be more effective in practice.

4 Related Works

Learning EBMs has been drawing increasing attention recently. Maximum likelihood training with MCMC sampling, also known as contrastive divergence (Hinton, 2002), is the most representative method. It contrasts samples from training set and samples from the model distribution. To draw samples from the model distribution, we can employ MCMC sampling approaches, such as Langevin dynamics (Welling & Teh, 2011) and Hamiltonian dynamics (Neal et al., 2011). Such methods are further improved and shown to be effective by recent studies (Xie et al., 2016; Gao et al., 2018; Du & Mordatch, 2019; Nijkamp et al., 2019; Grathwohl et al., 2019; Jacob et al., 2020; Qiu et al., 2019; Du et al., 2020a). These methods, however, require the gradient *w.r.t.* the data space to update samples in each MCMC step. Thus, they cannot be applied to discrete data directly. To enable maximum likelihood training with MCMC sampling on discrete data, we can naturally use discrete sampling methods, such as Gibbs sampling and Metropolis-Hastings algorithm (Zanella, 2020), to replace the above gradient-based sampling algorithms. Unfortunately, sampling from a discrete distribution is extremely time-consuming and not scalable. Recently, Dai et al. (2020) develops a learnable sampler parameterized as a local discrete search algorithm to propose negative samples for contrasting. Grathwohl et al. (2021) proposes a scalable sampling method for discrete distributions by surprisingly using the gradient *w.r.t.* the data space, which inspires our work a lot.

Maximum likelihood training with MCMC sampling is computationally expensive since MCMC sampling methods usually require a large number of steps to obtain reasonable samples. An alternative method for learning EBMs is score matching (Hyvärinen & Dayan, 2005; Vincent, 2011; Song et al., 2020; Song & Ermon, 2019), where the scores, *i.e.*, the gradients of the logarithmic probability distribution *w.r.t.* the data space, of the energy function are forced to match the scores of the training data. Ratio matching (Hyvärinen, 2007; Lyu, 2009) is obtained by extending the idea of score matching to discrete data. Our work is motivated by the limitations of ratio matching, as analyzed in Section 3.1. Stochastic ratio matching (Dauphin & Bengio, 2013) also aims to make ratio matching more efficient by considering the sparsity of input data, while our approach uses the gradient of the energy function. Hence, our method is effective for general EBMs, but stochastic ratio matching is limited to sparse data.

There are some other methods for learning EBMs, such as noise contrastive estimation (Gutmann & Hyvärinen, 2010; Bose et al., 2018; Ceylan & Gutmann, 2018; Gao et al., 2020) and learning the stein discrepancy (Grathwohl et al., 2020). We recommend readers to refer to Song & Kingma (2021) for a comprehensive introduction on learning EBMs.

[1] Although this only strictly holds for $n^*(\boldsymbol{x}_{-i})$, this can serve as a relaxed explanation for $\widetilde{n}^*(\boldsymbol{x}_{-i})$ as well since $\widetilde{n}^*(\boldsymbol{x}_{-i})$ is a good approximation of $n^*(\boldsymbol{x}_{-i})$.

Table 1: Results on 32-dimensional synthetic discrete data in terms of MMD. The lower the better. The top two results on each dataset are highlighted as **1st** and **2nd**.

Method	*2spirals*	*8gaussians*	*circles*	*moons*	*pinwheel*	*swissroll*	*checkerboard*
Ratio Matching	0.01514	0.10270	0.11856	**0.02901**	0.31353	0.05820	0.00059
RMwGGIS (unbiased)	**0.01099**	**0.09763**	**0.11017**	0.03111	**0.27885**	**0.05176**	**0.00050**
RMwGGIS (biased)	**0.00876**	**0.08414**	**0.10230**	**0.02787**	**0.26188**	**0.04477**	**0.00026**

5 EXPERIMENTS

5.1 DENSITY MODELING ON SYNTHETIC DISCRETE DATA

Setup. For both quantitative results and qualitative visualization, we follow the experimental setting of Dai et al. (2020) for density modeling on synthetic discrete data. We firstly draw 2D data points from 2D continuous space according to some unknown distribution $\hat{p}$, which can be naturally visualized. Then, we convert each 2D data point $\hat{\boldsymbol{x}} \in \mathbb{R}^2$ to a discrete data point $\boldsymbol{x} \in \{0,1\}^d$, where d is the desired number of data dimensions. To be specific, we transform each dimension of $\hat{\boldsymbol{x}}$, which is a floating-point number, into a $\frac{d}{2}$-bit Gray code[2] and concatenate the results to obtain a d-bit vector $\boldsymbol{x}$. Thus, the unknown distribution in discrete space is $p(\boldsymbol{x}) = \hat{p}\left(\left[\text{GrayToFloat}(\boldsymbol{x}_{1:\frac{d}{2}}), \text{GrayToFloat}(\boldsymbol{x}_{\frac{d}{2}+1:d})\right]\right)$. This density modeling task is challenging since the transformation from $\hat{\boldsymbol{x}}$ to $\boldsymbol{x}$ is non-linear.

To quantitatively evaluate the performance of density modeling, we adopt the maximum mean discrepancy (MMD) (Gretton et al., 2012) with a linear kernel corresponding to *(d-HammingDistance)*. The MMD is commonly used to compare distributions. In our case, particularly, the MMD is computed based on 4000 samples, drawn from the learned energy function via Gibbs sampling, and the same number of samples from the training set. Lower MMD indicates that the distribution defined by the learned energy function is closer to the unknown data distribution. In addition, in order to qualitatively visualize the learned energy function, we firstly uniformly obtain $10k$ data points from 2D continuous space. Afterwards, they are converted into bit vectors and evaluated by the learned energy function. Subsequently, we can visualize the obtained corresponding energies in 2D space.

The energy function is parameterized by a 4-layer MLP with the Swish (Ramachandran et al., 2017) activation and 256 hidden dimensions. The number of samples s involved in the objetive functions of our RMwGGIS method, as formulated in Eq. (7) or Eq. (12), is set to be 10. In the following, we compare our unbiased and biased methods with the original ratio matching method (Hyvärinen, 2007; Lyu, 2009).

Quantitative and qualitative results. The quantitative results on 32-dimensional datasets are shown in Table 1. Our RMwGGIS, especially the biased version, consistently outperforms the original ratio matching by large margins, which demonstrates that it is effective for our proposed gradient-guided importance sampling to stochastically push up neighbors with low energies. This verifies our analysis in Section 3.3. In Figure 1, we qualitatively visualize the learned energy functions of our proposed RMwGGIS. It is observed that EBMs learned by our method can fit the data distribution accurately. Note that we choose $d = 32$ for quantitative evaluation because Gibbs sampling cannot obtain appropriate samples from the learned energy function with an affordable time budget if the data dimension is too high, thus leading to invalid MMD results. We will compare the results on higher-dimensional data in the following by observing the qualitative visualization.

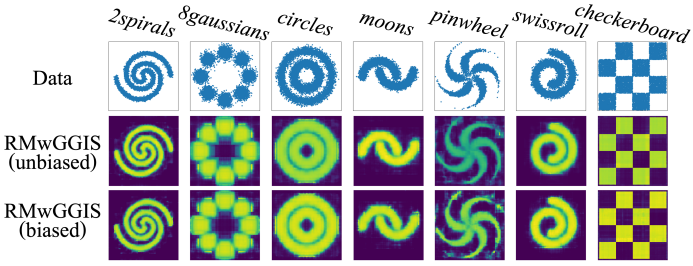


Figure 1: Visualization of learned energy functions on 32-dimensional synthetic discrete datasets.

[2] https://en.wikipedia.org/wiki/Gray_code

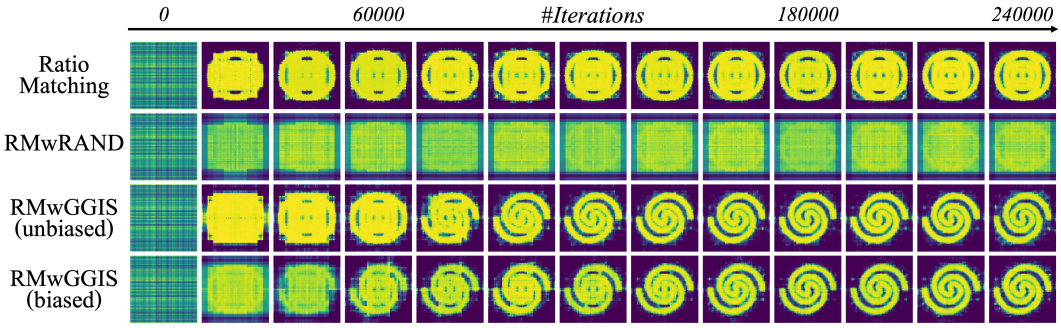


Figure 2: Visualization of learned energy functions *w.r.t.* number of learning iterations on the 256-dimensional *2spirals* dataset.

Table 2: Comparison between ratio matching and our RMwGGIS on *2spirals* datasets with different dimensions in terms of running time and memory usage.

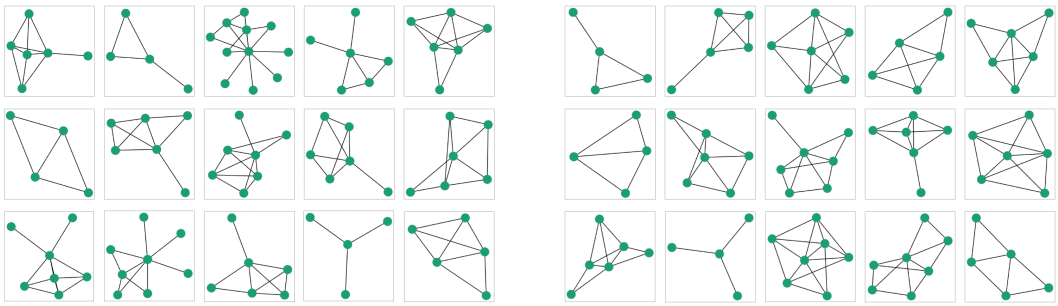
	# Data Dimensions	*32*	*64*	*128*	*256*	*512*	*1024*	*2048*
Time	Ratio Matching	63.9ms	106.5ms	185.6ms	372.9ms	735.2ms	1390.1ms	2684.1ms
	RMwGGIS	**41.2**ms	**47.2**ms	**58.8**ms	**86.9**ms	**137.7**ms	**244.9**ms	**434.1**ms
	Speedup	**1.6**×	**2.3**×	**3.2**×	**4.3**×	**5.3**×	**5.7**×	**6.2**×
Memory	Ratio Matching	957MB	1031MB	1189MB	1545MB	2315MB	4237MB	9633MB
	RMwGGIS	**891**MB	**893**MB	**893**MB	**915**MB	**919**MB	**931**MB	**951**MB
	Memory Saving	**6.9**%	**13.4**%	**24.9**%	**40.8**%	**60.3**%	**78.0**%	**90.1**%

Observations on higher-dimensional data. As analyzed in Section 3.3, the advantages of our approach can be greater on higher-dimensional data. To evaluate this, we conduct experiments on the 256-dimensional *2spirals* dataset, and visualize the learned energy functions corresponding to different learning iterations. We construct a method for ablation study, named as RMwRAND, which estimates the original ratio matching objective by randomly sampling $s = 10$ terms. The only difference between our RMwGGIS method and RMwRAND is that we focus more on the terms corresponding to low energies thanks to our proposed gradient-guided importance sampling.

As shown in Figure 2, our RMwGGIS accurately capture the data distribution, while the original ratio matching method cannot. This further verifies that our RMwGGIS can be optimized better than ratio matching especially when the data dimension is high, as analyzed in Section 3.3. In addition, although RMwRAND can also introduce stochasticity as our RMwGGIS by randomly sampling, it fails to capture the data distribution. This observation is intuitively reasonable since randomly pushing up $s = 10$ terms among $d = 256$ terms leads to large variance and unsatisfactory performance. Instead, our RMwGGIS performs well since we focus on pushing up terms with low energies, which are the most offending terms and should be pushed up first. Overall, these experiments can show the superiority of RMwGGIS endowed by our proposed gradient-guided importance sampling on high-dimensional data.

Running time and memory usage. As analyzed in Section 3.3, our RMwGGIS has better efficiency than ratio matching in terms of computational cost and memory requirement. To empirically verify this, we compare the real running time and memory usage on datasets of various dimensions. Specifically, we construct several *2spirals* datasets with different data dimensions and train parameterized energy functions using ratio matching and our RMwGGIS, respectively. We choose batch size to be 256. The reported time corresponds to the average training time per batch. For RMwGGIS, both the unbiased version and the biased version have almost the same running time and memory usage. Thus, we report the results of the biased version.

As summarized in Table 2, our RMwGGIS is much more efficient in terms of running time and memory usage, compared with the original ratio matching method. In addition, our method can achieve more speedup and save more memory usages with the increasing of data dimension. Specifically, compared with ratio matching, our RMwGGIS can achieve 6.2 times speedup and save 90.1% memory usage on the 2048-dimensional dataset. This shows the efficiency of our RMwGGIS especially for high-dimensional data.



Training data RMwGGIS samples

Figure 3: Visualization of training data and samples drawn from the energy function learned by our RMwGGIS for graph generation.

5.2 Graph Generation

Setup. We further evaluate our RMwGGIS on graph generation using the *Ego-small* dataset (You et al., 2018). It is a set of one-hop ego graphs, where the number of nodes $4 \leq |V| \leq 18$, obtained from the Citeseer network (Sen et al., 2008). Following the experimental setting of You et al. (2018) and Liu et al. (2019), 80% of the graphs are used for training and the rest for testing. To evaluate the graph generation performance based on the generated graphs and the test graphs, we calculate the maximum mean discrepancy (MMD) (Gretton et al., 2012) over three statistics, *i.e.*, degrees, clustering coefficients, and orbit counts, as proposed in You et al. (2018).

Table 3: Graph generation results in terms of MMD. The lower the better. *Avg.* denotes the average over three MMD results. The results of baselines are reported from You et al. (2018), Liu et al. (2019), Niu et al. (2020), Shi et al. (2019), and Luo et al. (2021).

Method	*Degree*	*Cluster*	*Orbit*	*Avg.*
GraphVAE	0.130	0.170	0.050	0.117
DeepGMG	0.040	0.100	0.020	0.053
GraphRNN	0.090	0.220	0.003	0.104
GNF	**0.030**	0.100	**0.001**	0.044
EDP-GNN	0.052	0.093	0.007	0.050
GraphAF	**0.030**	0.110	**0.001**	0.047
GraphDF	0.040	0.130	0.010	0.060
Ratio Matching	0.062	0.066	0.008	0.045
RMwGGIS	0.044	**0.059**	0.013	**0.039**

We parameterize the energy function by a 5-layer R-GCN (Schlichtkrull et al., 2018) model with the Swish (Ramachandran et al., 2017) activation and 32 hidden dimensions, whose input is the upper triangle of the graph adjacency matrix. The number of samples s used in our RMwGGIS objective is 50. We apply our biased version to learn the energy function since it is shown to be more effective in Section 5.1. In addition to ratio matching, we also consider the recent works developed for graph generation as baselines, including GraphVAE (Simonovsky & Komodakis, 2018), DeepGMG (Li et al., 2018), GraphRNN (You et al., 2018), GNF (Liu et al., 2019), EDP-GNN (Niu et al., 2020), GraphAF (Shi et al., 2019), and GraphDF (Luo et al., 2021).

Quantitative and qualitative results. As summarized in Table 3, our RMwGGIS outperforms baselines in terms of the average over three MMD results. This shows that our method can learn EBMs to generate graphs that align with various characteristics of the training graphs. The generated samples are visualized in Figure 4. It can be observed that the generated samples are realistic one-hop ego graphs that have similar characteristics as the training samples. More samples are visualized in Appendix C.

6 Conclusion

We propose ratio matching with gradient-guided importance sampling (RMwGGIS) for learning EBMs on discrete data. In particular, we utilize the gradient of the energy function *w.r.t.* the discrete input space to guide the importance sampling for estimating the original ratio matching objective. Compared to ratio matching, our RMwGGIS is more efficient in terms of computation and memory usage, and shown to be more effective for density modeling. We perform thorough experiments on both synthetic data density modeling and graph generation. The results demonstrate that our RMwGGIS achieves significant improvements over previous methods in terms of both effectiveness and efficiency.

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A THE DETAILED DERIVATION OF EQ. (6)

The detailed derivation of Eq. (6) is as follows.

$$\begin{aligned}
\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x}) &= d\mathbb{E}_{\boldsymbol{x}_{-i}\sim m(\boldsymbol{x}_{-i})}\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2 \\
&= d\sum_{i=1}^{d} m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2 \\
&= d\sum_{i=1}^{d} \frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})} n(\boldsymbol{x}_{-i}) \\
&= d\mathbb{E}_{\boldsymbol{x}_{-i}\sim n(\boldsymbol{x}_{-i})} \frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}.
\end{aligned} \tag{13}$$

B PROOF OF THEOREM 1

Proof. According to Eq. (7), we have

$$Var\left(\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_n\right) = \frac{d^2}{s} Var\left(\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}\right). \tag{14}$$

Then we can compare the variance of the estimator based on $n^*(\boldsymbol{x}_{-i})$ and $n(\boldsymbol{x}_{-i})$. Formally,

$$Var\left(\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}_{n^*}\right) \tag{15}$$

$$= \frac{d^2}{s} Var\left(\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n^*(\boldsymbol{x}_{-i})}\right) \tag{16}$$

$$= \frac{d^2}{s}\left\{\mathbb{E}_{\boldsymbol{x}_{-i}\sim n^*(\boldsymbol{x}_{-i})}\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n^*(\boldsymbol{x}_{-i})}\right]^2 - \left[\mathbb{E}_{\boldsymbol{x}_{-i}\sim n^*(\boldsymbol{x}_{-i})}\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n^*(\boldsymbol{x}_{-i})}\right]^2\right\} \tag{17}$$

$$= \frac{d^2}{s}\left\{\mathbb{E}_{\boldsymbol{x}_{-i}\sim n^*(\boldsymbol{x}_{-i})}\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n^*(\boldsymbol{x}_{-i})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{18}$$

$$= \frac{d^2}{s}\left\{\frac{1}{d}\sum_{i=1}^{d} n^*(\boldsymbol{x}_{-i})\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n^*(\boldsymbol{x}_{-i})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{19}$$

$$= \frac{d^2}{s}\left\{\frac{1}{d}\sum_{i=1}^{d} m^2(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2 \sum_{k=1}^{d}\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-k})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{20}$$

$$= \frac{d^2}{s}\left\{\frac{1}{d}\left[\sum_{i=1}^{d} m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{21}$$

$$= \frac{d^2}{s}\left\{\frac{1}{d}\left[\sum_{i=1}^{d} \frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}\sqrt{n(\boldsymbol{x}_{-i})}\sqrt{n(\boldsymbol{x}_{-i})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{22}$$

$$\leq \frac{d^2}{s}\left\{\frac{1}{d}\sum_{i=1}^{d}\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}\sqrt{n(\boldsymbol{x}_{-i})}\right]^2 \sum_{i=1}^{d} n(\boldsymbol{x}_{-i}) - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{23}$$

$$= \frac{d^2}{s}\left\{\frac{1}{d}\sum_{i=1}^{d} n(\boldsymbol{x}_{-i})\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta}, \boldsymbol{x})}{d}\right]^2\right\} \tag{24}$$

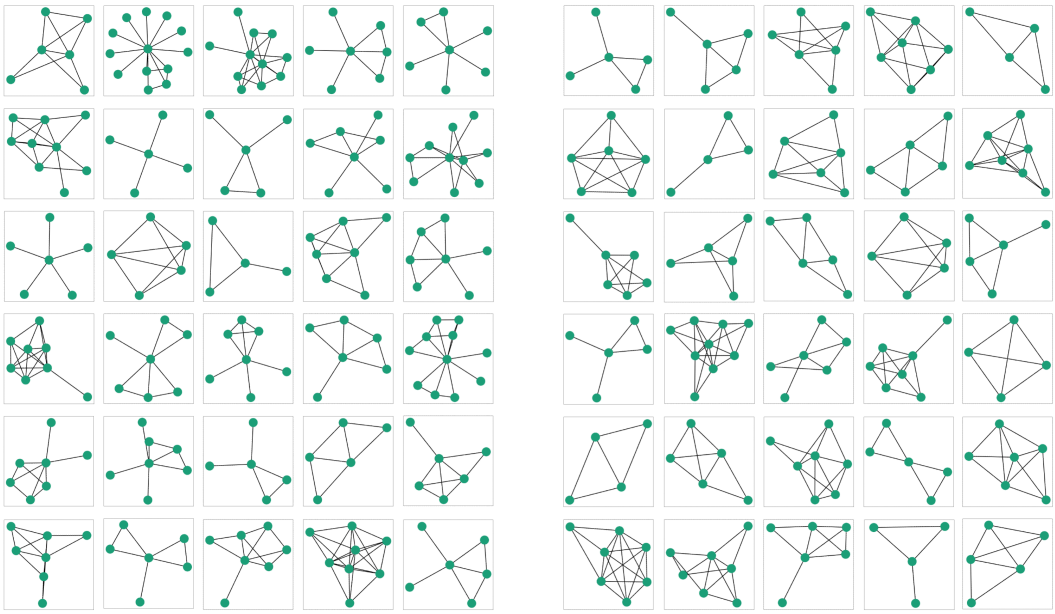
$$= \frac{d^2}{s}\left\{\mathbb{E}_{\boldsymbol{x}_{-i}\sim n(\boldsymbol{x}_{-i})}\left[\frac{m(\boldsymbol{x}_{-i})\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{n(\boldsymbol{x}_{-i})}\right]^2 - \left[\frac{\mathcal{J}_{RM}(\boldsymbol{\theta},\boldsymbol{x})}{d}\right]^2\right\} \tag{25}$$

$$= Var\left(\widehat{\mathcal{J}_{RM}(\boldsymbol{\theta},\boldsymbol{x})}_n\right). \tag{26}$$

Eq. (18) can be derived because the estimator is unbiased no matter what proposal distribution is applied. Eq. (20) is obtained by choosing $n^*(\boldsymbol{x}_{-i}) = \frac{\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-i})}\right]^2}{\sum_{k=1}^{d}\left[e^{E_{\boldsymbol{\theta}}(\boldsymbol{x})-E_{\boldsymbol{\theta}}(\boldsymbol{x}_{-k})}\right]^2}$. Eq. (21) holds since $m(\boldsymbol{x}_{-i}) = \frac{1}{d}$ for $i = 1, \cdots, d$. To derive Eq. (23), we apply the Cauchy-Schwarz inequality $\left(\sum_{i=1}^{d} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{d} a_i^2\right)\left(\sum_{i=1}^{d} b_i^2\right)$. This completes the proof of Theorem 1.

□

C VISUALIZATION OF MORE GENERATED GRAPHS



Training data RMwGGIS samples

Figure 4: Visualization of extra training data and samples drawn from the energy function learned by our RMwGGIS for graph generation.