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A Variational Approach for Combinatorial Optimization Problems on Graphs

Abstract

Combinatorial Optimization (CO) problems are often NP-hard, thereby hindering the collection of solutions for supervised learning. Probabilistic method can provide an unsupervised framework, however, inference on it is intractable in general, and the objective is typically non-convex. Our work proposes an unsupervised method to learn a variational distribution for a graphical model, from which we can efficiently sample good solutions for CO problems. We show that our designed graphical model is guaranteed to concentrate on good solutions in both constrained and unconstrained scenarios. Additionally, the graphical model naturally introduces a temperature with which we are able to ease the learning by avoiding (encouraging) local optima during the beginning (ending) of training. We demonstrate our unsupervised learning framework on three CO problems on both synthetic and real-world graphs. The results show that our method achieves performance significantly better than other unsupervised neural methods as well as classical methods and integer solvers.

1 Introduction

Combinatorial Optimization (CO) problems occur whenever there is a requirement to select the best option from a finite set of alternatives. They arise in a wide range of application areas including business, medicine, and engineering (Paschos 2013). Many CO problems are NP-complete (Karp 1972; Garey and Johnson 1979). Thus, excluding the use of exact algorithms to find the optimal solution (Padberg and Rinaldi 1991; Wolsey and Nemhauser 1999), different heuristic methods are utilized to find good solutions in a reasonable amount of time (Nemhauser, Wolsey, and Fisher 1978; Dorigo, Birattari, and Stutzle 2006; Hopfield and Tank 1985; Kirkpatrick, Gelatt, and Vecchi 1983).

Recently, learning algorithms for CO problems has shown much promise, including supervised (Khalil et al. 2016; Gasse et al. 2019; Li, Chen, and Koltun 2018; Selsam et al. 2018; Nair et al. 2020), unsupervised (Karalias and Loukas 2020; Toenshoff et al. 2021), and reinforcement learning (Dai et al. 2017; Sun et al. 2020; Yolcu and Póczos 2019; Chen and Tian 2019) The success of supervised learning relies on labeled data, which could be computationally prohibitive to obtain for difficult problems (Yehuda, Gabel, and Schuster 2020). Reinforcement learning, suffering from its larger state space and lack of fully-differentiability, tends to be harder and more time consuming to train.

Unsupervised learning models the CO problem with a differentiable objective function whose minima represent discrete solutions (Hopfield and Tank 1985; Smith 1999). Naturally, this framework allows for efficient learning on large, unlabeled datasets. However, it also brings two challenges. First, in the absence of the labels, the objective function is typically non-convex (Mezard and Montanari 2009). This means that the learning can fall into local minima which results in the algorithm failing to find optimal solutions. Second, decoding good solutions from the soft assignments learned in unsupervised learning is not easy, especially when the CO problem is constrained (Toenshoff et al. 2021; Karalias and Loukas 2020).

To address those challenges, we propose a method to learn a variational distribution from which we can draw good solutions. Specifically, given a CO problem, we consider a graphical model $P \propto e^{-f(\mathbf{x})/\tau}$ such that the energy function f is designed to have higher values on non-optimal or infeasible solutions, and that is guaranteed to concentrate on good solutions

We train a graph neural network (GNN) to predict the variational distribution Q approximating P. In order to ease the learning, we employ *annealing training* and *forward iteration*. Annealing means beginning with a high temperature τ and decreasing the temperature gradually during the process (Kirkpatrick, Gelatt, and Vecchi 1983; Dowsland and Thompson 2012; Bilbro et al. 1988). The *annealing training* initially gives P a smooth landscape and ultimately focuses P on optimal solutions. In effect, it prevents Q from falling into local minima in the early stage of learning. Although local minima are undesirable in the early stages of learning, the learned Q should be at a local optimum at the end. Hence, we apply differentiable *forward iteration* on top of the GNN to force a local optimality for Q. It not only introduces a prior knowledge to regulate Q, but also does not affect the easy end-to-end training. After obtaining Q, we employ a recurrent sampling strategy that sequentially decodes a solution based on the conditional distribution of the variables (Raghavan and Tompson 1987).

In our experiments, we demonstrate our unsupervised learning framework on three NP-hard graph CO problems:

minimum vertex cover (MVC), weighted max cut (MaxCut), and minimum dominating set (MDS). On both synthetic and real-world graphs, our method achieves significantly better performance compared to other unsupervised neural methods (Toenshoff et al. 2021; Karalias and Loukas 2020), classical algorithms (Aarts, Aarts, and Lenstra 2003; Bilbro et al. 1988; Wang, Chang, and Kolter 2017), and integer solvers (Achterberg 2009; Gurobi Optimization 2020). We also have an ablation study to validate our annealing training schedule and forward iteration. The results show that our variational learning framework offers a substantial improvement for unsupervised learning for CO problems on graphs.

In summary, our work has the following contributions:

- We propose a variational learning framework for generic unsupervised learning on combinatorial optimization problems.
- We exploit annealing training and forward iteration to address the non-convex problem in training and empirically justify our solutions in ablation study.
- We demonstrate the performance of our method on three NP-hard graph combinatorial problems and show that our method can achieve better performance compared to other unsupervised neural methods, classical methods, and integer solvers.

2 Related Work

Recently, there is a surge of interest in learning algorithms for CO problems (Bengio, Lodi, and Prouvost 2020). Supervised learning is widely used. Numerous works have combined GNNs with search procedures to solve classical CO problems, such as travelling salesman problem (Vinyals, Fortunato, and Jaitly 2015; Joshi, Laurent, and Bresson 2019; Prates et al. 2019), graph matching (Wang, Yan, and Yang 2019, 2020), quadratic assignments (Nowak et al. 2017), graph coloring (Lemos et al. 2019), and maximum independent set (Li, Chen, and Koltun 2018). Another fruitful direction is combining learning with existing solvers. For example, in the branch and bound algorithm, He, Daume III, and Eisner (2014); Khalil et al. (2016); Gasse et al. (2019); Nair et al. (2020) learn the variable selection policy by imitating the decision of oracle or rules designed by human experts. However, the success of supervised learning relies on large datasets with already solved instances, which is hard to efficiently generate in an unbiased and representative manner (Yehuda, Gabel, and Schuster 2020),

Many works, therefore, choose to use reinforcement learning instead. Dai et al. (2017) combines Q-learning with greedy algorithms to solve CO problems on graphs. Q-learning is also used in (Bai et al. 2020) for maximum subgraph problem. Sun et al. (2020) uses evolutionary strategy to learn variable selection in the branch and bound algorithm. Yolcu and Póczos (2019) employs REINFORCE algorithm to learn local heuristics for SAT problem. Chen and Tian (2019) uses actor-critic learning to learn a local rewriting algorithm. Despite being a promising approach that avoids using labelled data, reinforcement learning has its limitations. For example, reinforcement learning is typically sample inefficient and notoriously unstable to train, due to poor gradient estimations, correlations present in the sequence of observations, and hard explorations (Espeholt et al. 2018; Tang et al. 2017).

Works in unsupervised learning show promising results. Yao, Bandeira, and Villar (2019) train GNN for the max-cut problem by optimizing a relaxation of the cut objective, Toenshoff et al. (2021) trains RNN for maximum-SAT via maximizing the probability of its prediction. Karalias and Loukas (2020) summarize them as a probabilistic method to learn a distribution g_θ, on which the objective $\min L = \mathbb{E}_{\mathbf{x}\sim g(\cdot)}[f(\mathbf{x})]$. The probabilistic method provides a good framework for unsupervised learning. However, optimizing the distribution is typically non-convex (Mezard and Montanari 2009). Differentiating through combinatorial structures is an important problem in machine learning (Paulus et al. 2020; Indelman and Hazan 2021; Pogančić et al. 2019; Paulus et al. 2021). In this work, to address this problem, we formulate the unsupervised learning as learning an annealed graphical model. Fruitful algorithms are designed for inference on graphical models, including linear relaxation (Raghavan and Tompson 1987), mean field approximation (Peterson 1993; ANDERSON 1988; Peterson and Söderberg 1989; Bilbro et al. 1988), message passing (Wainwright and Jordan 2008; Ravanbakhsh 2015), survey propagation (Braunstein, Mézard, and Zecchina 2005; Braunstein et al. 2006), and sub-problem decomposition (Vontobel and Koetter 2005; Elidan and Koller 2007; Kolmogorov and Wainwright 2012; Rouhani, Rahman, and Gogate 2020). The difference is the propagation in our method is automatically learned.

3 Method

In this section, we introduce our **V**ariational **G**raph **N**eural **N**etwork (VGNN) method.

3.1 Graphical Model

Before defining the variational distribution, we show how to transform a CO problem into a graphical model. First, let's consider an unconstrained problem:

$$\arg\min_{\mathbf{x}\in\{0,1\}^n} c(\mathbf{x}) \tag{1}$$

where $c(\cdot)$ is the objective function. We can define the probability of an assignment $\mathbf{x}$ as $P_\tau(\mathbf{x}) \propto e^{-c(\mathbf{x})/\tau}$, where $\tau > 0$ is the temperature that controls the sharpness of the distribution. Since optimal solutions have lower objective values, as τ approaches zero, P gradually converges to a uniform distribution on optimal solutions.

For a constrained problem with m constraints:

$$\arg\min_{\mathbf{x}\in\{0,1\}^n} c(\mathbf{x}) \quad \text{s.t. } \psi_i(\mathbf{x}) = 0, \quad i = 1, ..., m \tag{2}$$

where $\psi_i : \{0,1\}^n \to \{0,1\}$ is a membership function that maps an assignment $\mathbf{x}$ to 0 if the constraint is not violated, and to 1 otherwise. We first rewrite the constrained problem into an equivalent unconstrained form:

$$\arg\min_{\mathbf{x}\in\{0,1\}^n} f(\mathbf{x}) := c(\mathbf{x}) + \sum_{i=1}^{m} \beta_i \psi_i(\mathbf{x}), \quad \beta_i \geq 0 \tag{3}$$

Using $f(\mathbf{x})$ as energy function, we can define the graphical model:

$$P_\tau(\mathbf{x}) \propto e^{-f(\mathbf{x})/\tau} \tag{4}$$

For the energy function Eq. 3 and graphical model Eq. 4, we have following properties

Property 1. *Assume β_i is sufficiently large and the CO problem Eq. 2 has a feasible solution. Then for any infeasible assignment $\mathbf{x}$, we can always find a $\mathbf{x}'$ feasible for Eq. 2 and $f(\mathbf{x}') < f(\mathbf{x})$.*

Proof. Consider we have a feasible solution x and an infeasible solution y. By definition, there exists i such that $\psi_i(y) = 1$. Hence,

$$\begin{aligned} f(x) &= c(x) + \sum_{i=1}^{m} \beta_i \psi_i(x) = c(x) \leq \frac{1}{2}\beta_j \\ &\leq c(y) + \beta_j \leq c(y) + \sum_{i=1}^{m} \beta_i \psi_i(y) \\ &= f(y) \end{aligned}$$

□

Property 2. *When τ decreases to zero, P_τ in Eq. 4 converges to optimal solutions for Eq. 3*

Proof. Consider the set of optimal solutions is $\mathcal{X}$ and its completion $\mathcal{X}^\perp = \{0,1\}^n \backslash \mathcal{X}$. WLOG, we assume the $f(x^*) = 0, \forall x^* \in \mathcal{X}$. The probability that a state at graphical model P_τ is not optimal can be characterized as a function of τ:

$$F(\tau) = \frac{\sum_{x \in \mathcal{X}^\perp} e^{-f(x)/\tau}}{|\mathcal{X}| + \sum_{x \in \mathcal{X}^\perp} e^{-f(x)/\tau}}$$

As 1) $f(x) > 0, \forall x \in \mathcal{X}^\perp$ and 2) $\mathcal{X}^\perp$ is a finite set, there exists a $\delta > 0$ and $f(x) > \delta, \forall x \in \mathcal{X}^\perp$. We can see the numerator will decrease to 0 when τ goes to zero. The denominator is always larger than $|\mathcal{X}|$. Hence, we have the

$$\lim_{\tau \to 0} F(\tau) = 0$$

and this means the graphical model will converge to the optimal states as long as $\mathcal{X}$ is not empty. □

With a more sophisticated selection of penalty β_i, P will have a smoother landscape. We leave the discussion about our selection of β_i for each problem type in case study. Without causing confusion, we will abuse notation and let $f(\mathbf{x})$ denote either $c(\mathbf{x})$ or $c(\mathbf{x}) + \sum_{i=1}^{m} \beta_i \psi_i(\mathbf{x})$.

3.2 Variational Distribution and Annealing

Although the graphical model will focus on optimal solutions, drawing samples from it could still be difficult (Murray 2007). To address this problem, we use a simple variational distribution Q to approximate P_τ by minimizing the KL-divergence between the two distributions. Unfortunately, the loss function $D_{\mathrm{KL}}(Q||P_\tau)$ is non-convex w.r.t. Q in general (Mezard and Montanari 2009). The fa hindering the learning. We propose an annealing training schedule to resolve this issue. Specifically, we begin training with a high temperature τ. In this case, P_τ has a smooth landscape with shallow local optima such that avoid Q being trapped in local optima. Throughout the training process, we gradually decrease the temperature τ. Consequently, the target distribution P_τ as well as Q can gradually concentrate to the optimal solutions. When the annealing ultimately stops at a threshold, the learned Q becomes a good approximation of optimal solutions.

The Anneal training is not only effective but also very simple to implement. Consider the KL-divergence between Q and P:

$$D_{\mathrm{KL}}(Q||P_\tau) = \int Q(\mathbf{x}) \log Q(\mathbf{x}) d\mathbf{x} \tag{5}$$

$$- \int Q(\mathbf{x}) \log \frac{e^{-f(\mathbf{x})/\tau}}{\sum_{\mathbf{x} \in \{0,1\}^n} e^{-f(\mathbf{x})/\tau}} d\mathbf{x} \tag{6}$$

$$= \frac{1}{\tau} \mathbb{E}_{\mathbf{x} \sim Q(\cdot)}[f(\mathbf{x})] - H(Q) + \log \sum_{\mathbf{x} \in \{0,1\}^n} e^{-f(\mathbf{x})/\tau} \tag{7}$$

where $H(\cdot)$ represents the entropy of a distribution and the last term in Eq. 7 is constant. Assume Q is parameterized by θ, our loss function is defined as:

$$L_\tau(\theta) = \mathbb{E}_{\mathbf{x} \sim Q_\theta(\cdot)}[f(\mathbf{x})] - \tau H(Q_\theta) \tag{8}$$

In this way, the annealing training schedule can be easily implemented by decreasing the weight of the entropy. In addition, when we set the temperature τ to zero, we have:

$$L_0(\theta) = \mathbb{E}_{\mathbf{x} \sim Q_\theta(\cdot)}[f(\mathbf{x})] \geq \min_{\mathbf{x} \in \{0,1\}^n} f(\mathbf{x}) \tag{9}$$

It shows L_0 is an upper bound on the optimal value and the equality is achieved when Q is supported on optimal solutions. One thing needs to be noticed is, although we use a non-zero temperature in training, we still use zero temperature loss L_0 in validation for model selection. For notation, when θ is determined by parameter ϕ and energy function is determined by instance I, we also write the loss function as $L_\tau(\phi, I)$. The algorithm for annealing training is summarized in Alg. 1.

3.3 Parameterization and Forward Iteration

In this work, we consider the simplest form of variational distribution

$$Q_\theta(\mathbf{x}) = \prod_{i=1}^{n} \theta_i^{x_i} (1 - \theta_i)^{1 - x_i} \tag{10}$$

which means all the variables are independent Bernoulli random variables with probability θ_i. Instead of letting a GNN G_ϕ directly predict θ_i, we add additional forward iteration to force the local optimality. Specifically, though we try to avoid local optima in the early stage of training, in the end, the parameter θ should be a local optimum, thereby each entry should satisfy:

$$\theta_i = \arg\min_{\theta_i} L_\tau(\theta_{-i}, \theta_i) \tag{11}$$

where θ_{-i} represents all the entries except θ_i in θ. Though the local optimality is naturally satisfied when we directly optimize θ in Eq. 8, this is not case when we train G_ϕ to predict θ. In order to encourage the local optimality, we apply forward iterations on top of G_ϕ. That's to say, when G_ϕ gives probability $p_i^{(0)}$ for each variable x_i, we run forward iteration for T times:

$$p_i^{(t+1)} = \arg\min_{p_i} L_\tau(p_{-i}^{(t)}, p_i) \tag{12}$$

and define $\theta_i = p_i^{(T)}$. A key point here is, when the temperature $\tau > 0$, the forward iteration is differentiable and we can still train G_ϕ end to end. Since we use independent Bernoulli random variables to parameterize our variational distribution, the forward iteration has simple close-form expression and we elaborate it for each problem type in case study.

3.4 Decoding

After obtaining variational distribution Q_θ, we can easily sample binary solutions from it. In this work, we adopt a conditional decoding strategy (Raghavan 1988). Specifically, consider we decode the variables in an order π, WLOG, we say $\pi = (1, 2, ..., n)$. Assume we have already fixed the value of $x_1 = \hat{x}_1, ..., x_k = \hat{x}_k$, we decode x_{k+1} as:

$$\hat{x}_{k+1} = \arg\min_{x_{k+1} \in \{0,1\}} \mathbb{E}_{\mathbf{x} \sim Q(\cdot|\hat{x}_{1:k}, x_{k+1})}[f(\mathbf{x})] \tag{13}$$

that's to say, we select the value of x_{k+1} such that the expectation of the loss function on conditional distribution $Q(\cdot|\hat{x}_{1:k}, x_{k+1})$ is minimized. In this way, the expectation is non-decreasing during decoding and it guarantees to find solution $\hat{\mathbf{x}}$ bounded by the expected loss on Q.

$$f(\hat{\mathbf{x}}) = \mathbb{E}_{\mathbf{x} \sim Q(\cdot|\hat{\mathbf{x}}_{1:n})}[f(\mathbf{x})] \leq \mathbb{E}_{\mathbf{x} \sim Q}[f(\mathbf{x})] \tag{14}$$

As the decoded solution is determined by the order, we propose two strategies to decode solutions with different variable order:

- *Deterministic*: sample one solution and the variables are ordered by decreasing confidence f_i, which equals to $|2\theta_i - 1|$ for variable x_i.
- *Stochastic*: sample multiple solutions, where the variables are ordered by decreasing confidence in the first run and randomly sampled for the remaining runs.

As the *deterministic* version only requires one run, it is able to find a good solution in milliseconds on large graphs with 1000 nodes and 4000 edges. The *stochastic* version requires more time, but in return, it is able to significantly improve the solution quality. In our parameterization, the conditional decoding in Eq. 13 is equivalent with an asynchronous forward iteration in zero temperature, thus can be implemented very efficiently. We elaborate it for each problem type in case study.

Algorithm 1: Annealing Training

Input: Initial temperature τ_0, decay rate α, threshold temperature τ_{th}, GNN G_ϕ, epoch T, batch size b, training data I_{train}, valid data I_{valid}
Output: ϕ_{out}
Initialize $\tau \leftarrow \tau_0$, $\phi_{\text{out}} \leftarrow \phi$, $L_{\text{best}} \leftarrow L_0(\phi, I_{\text{valid}})$
for $t = 1, ..., T$ **do**
  for batch B in I_{train} **do**
    batch gradient $d\phi \leftarrow \frac{\partial L_\tau(\phi, B)}{\partial \phi}$
    update ϕ by gradient descent
  end for
  if $L' = L_0(\phi, I_{\text{valid}}) < L_{\text{best}}$ **then**
    $\phi_{\text{out}} \leftarrow \phi$, $L_{\text{bext}} \leftarrow L'$
  end if
  update temperature $\tau \leftarrow \max\{\alpha\tau, \tau_{\text{th}}\}$.
end for

4 Case Study

We focus on three NP-hard problems in this work: minimum vertex cover (MVC), maximum cut (Max-Cut) and minimum dominating set (MDS). Consider a graph $G = (V, E, w)$, where V is the set of vertices, E is the set of edges, $w : E \to \mathbb{R}_+$ is the edge weight function. Let $n = |V|$, $m = |E|$, we show energy function for these three problems and their forward iteration as well as conditional decoding. The details of the derivation and complexity analysis are given in appendix.

4.1 Minimum Vertex Cover

A vertex cover of a graph is a set of vertices that includes at least one endpoint of every edge of the graph. To find a minimum cover, the original objective function is $c(\mathbf{x}) = \sum_{v \in V} x_v$. Considering constraints, we set the penalty coefficient $\beta_i = 2$ and define the energy function as:

$$f(\mathbf{x}) = \sum_{v \in V} x_v + 2 \sum_{(u,v) \in E} (1 - x_u)(1 - x_v) \tag{15}$$

If an edge $e = (u_0, v_0)$ is not covered, we can always set an endpoint as 1 to reduce the objective. Hence, every local minimum is feasible and the global minimum is an optimal solution of the original problem. Given a temperature τ, the close-form expression of the forward iteration is:

$$p_i^{(t+1)} = 1/(\exp([2 \sum_{j:(i,j) \in E} (1 - p_j^{(t)}) - 1]/\tau) + 1)$$

In conditional decoding, this means we decode $x_i = 0$ if $2 \sum_{j:(i,j) \in E} (1 - p_j^{(t)}) < 1$, and $x_i = 1$ if $2 \sum_{j:(i,j) \in E} (1 - p_j^{(t)}) > 1$. The complexity of this decoding is $O(m + n)$.

4.2 Max Cut

A cut partitions the graph's vertices into two complementary sets S and T. We aim to find a cut such that the weighted edge sum between S and T is maximized. Since max-cut is unconstrained, we can directly define the energy function

Table 1: Evaluation MVC on 1000 random graphs

Size	256-300		512-600		1024-1100	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
Greedy	1.0330 ± 0.0125	$1.53e^{-4}$	1.0345 ± 0.0086	$5.78e^{-4}$	1.0353 ± 0.0064	$1.49e^{-3}$
MFA	1.0109 ± 0.0074	$9.50e^{-3}$	1.0115 ± 0.0054	$1.65e^{-2}$	1.0124 ± 0.0040	$3.11e^{-2}$
RUN-CSP	1.0117 ± 0.0076	$4.41e^{-2}$	1.0138 ± 0.0059	$6.07e^{-2}$	1.0153 ± 0.0034	$9.81e^{-2}$
Erdos(d)	1.0147 ± 0.0085	$4.19e^{-3}$	1.0153 ± 0.0059	$4.34e^{-3}$	1.0159 ± 0.0044	$4.72e^{-3}$
Erdos(s)	1.0145 ± 0.0084	$1.12e^{-2}$	1.0151 ± 0.0058	$1.96e^{-2}$	1.0156 ± 0.0043	$3.27e^{-2}$
BP	1.0604 ± 0.0162	$1.60e^{-1}$	1.0616 ± 0.0114	$8.10e^{-2}$	1.0630 ± 0.0084	$1.2e^{-1}$
PBP	1.0675 ± 0.0183	$2.05e^{-1}$	1.0632 ± 0.0198	$1.17e^{-1}$	1.0592 ± 0.0072	$1.57e^{-1}$
VGNN(d)	1.0087 ± 0.0066	$5.89e^{-3}$	1.0108 ± 0.0046	$6.67e^{-3}$	1.0099 ± 0.0036	$6.90e^{-3}$
VGNN(s)	1.0052 ± 0.0052	$1.26e^{-2}$	$\mathbf{1.0063 \pm 0.0039}$	$2.26e^{-2}$	$\mathbf{1.0074 \pm 0.0032}$	$3.44e^{-2}$
SCIP(0.1s)	1.0265 ± 0.0117	$1.00e^{-1}$	1.0278 ± 0.0080	$1.02e^{-1}$	1.1857 ± 0.8189	$1.00e^{-1}$
Gurobi(0.1s)	$\mathbf{1.0026 \pm 0.0068}$	$1.38e^{-1}$	1.0795 ± 0.1088	$1.91e^{-1}$	1.3261 ± 0.0244	$2.32e^{-1}$

equals to its objective function

$$f(\mathbf{x}) = c(\mathbf{x}) = \sum_{(u,v)\in E} w(u,v)(x_u + x_v - 2x_u x_v) \quad (16)$$

Given a temperature τ, the close-form expression of the forward iteration is:

$$p_i^{(t+1)} = 1/(\exp(\sum_{j:(i,j)\in E} w(i,j)(2p_j^{(t)} - 1)/\tau) + 1)$$

In conditional decoding, this means we decode $x_i = 0$ if $\sum_{j:(i,j)\in E} w(i,j)(2p_j^{(t)} - 1) > 0$, and $x_i = 1$ if $\sum_{j:(i,j)\in E} w(i,j)(2p_j^{(t)} - 1) < 0$. The complexity of decoding is $O(m+n)$.

4.3 Minimum Dominating Set

A dominating set D is a subset of V such that every vertex not in D is adjacent to at least one member of D. To minimize the size of D the original objective function is $c(\mathbf{x}) = \sum_{v\in V} x_v$. Considering constraints, we set the penalty coefficient $\beta_i = 2$ and define the energy function as:

$$f(\mathbf{x}) = \sum_{v\in V} x_v + 2\sum_{v\in V}(1 - x_v) \prod_{j:(i,j)\in E} (1 - x_j) \quad (17)$$

It can be noticed that, if a vertex v is not dominated, we can set v or one of its neighbor as 1 to reduce the objective. Hence, every local minimum is feasible and the global minimum is an optimal solution of the original problem. Define the augmented neighbor $N_i := \{j : j = i \text{ or } (i,j) \in E\}$ and $N_i^k := \{j : j \neq k, j = i \text{ or } (i,j) \in E\}$, given a temperature τ, the close-form expression of the forward iteration is:

$$p_i^{(t+1)} = 1/(\exp((\sum_{j\in N_i} 2 \prod_{k\in N_j^i} (1 - p_k^{(t)}) - 1)/\tau) + 1)$$

In conditional decoding, this means we decode $x_i = 0$ if $\sum_{j\in N_i} 2\prod_{k\in N_j^i}(1 - p_k^{(t)}) < 1$, and $x_i = 1$ if $\sum_{j\in N_i} 2\prod_{k\in N_j^i}(1-p_k^{(t)}) > 1$. The complexity of decoding is $O(m+n)$.

5 Experiments

We now present comparative experiments against classical algorithms, unsupervised neural methods, and integer solvers to justify our variational method. We also give an ablation study to validate the benefits from annealing training and forward iteration.

5.1 Setup

Dataset: We focus on minimum vertex cover (MVC), weighted maximum cut (MaxCut), and minimum dominating set (MDS) in our experiments. We use both synthetic and real-world graph as our dataset. For synthetic dataset, we use Barabasi-Albert (BA) (Barabási and Albert 1999) with attachment 4 to generate random graphs in sizes {32-40, 64-75, 128-150, 256-300, 512-600, 1024-1100}. For Maxcut, we assign edge weights as uniform distribution between $[0, 1]$. For real-world dataset, we use social network *Github* (Morris et al. 2020) and *Memetracker* (Dai et al. 2017). Since *Github* is unweighted, we assign weight 1 to all edges when we solve Maxcut.

Implementation: We denote VGNN with *deterministic* and *stochastic* decoding strategies as VGNN(d) and VGNN(s), respectively. The details of the implementation are given in Appendix.

Baseline: We compare against several unsupervised neural methods, classical algorithms, and integer solvers. The unsupervised neural methods include Erdos-GNN (Karalias and Loukas 2020) and RUN-CSP (Toenshoff et al. 2021). Erdos-GNN is equivalent to a special case of our VGNN with temperature $\tau = 0$ and forward iteration $T = 0$. Erdos-GNN with *deterministic* and *stochastic* decoding strategies are denoted as Erdos(d) and Erdos(s), respectively. RUN-CSP is only capable solving MVC as it is designed for unweighted graph with binary constraints. We train it using the default setting in (Toenshoff et al. 2021) and for evaluation, we run it multiple times until a large time budget is met and return the optimal solution (Karalias and Loukas 2020). For classical algorithms, we use greedy (Greedy), belief propagation, disturbed belief propagation(Ravanbakhsh 2015), and mean filed annealing algorithms (MFA) (Bilbro et al.

Table 2: Evaluation MaxCut on 1000 random graphs

Size	256-300		512-600		1024-1100	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
Greedy	1.0626 ± 0.0136	$8.90e^{-4}$	1.0545 ± 0.0105	$3.62e^{-3}$	1.0461 ± 0.0077	$1.49e^{-2}$
MFA	1.0209 ± 0.0088	$1.60e^{-2}$	1.0126 ± 0.0080	$3.34e^{-2}$	$\mathbf{1.0043 \pm 0.0056}$	$6.59e^{-2}$
Mixing	1.0529 ± 0.0150	$3.91e^{-2}$	1.0417 ± 0.0115	$1.34e^{-1}$	1.0323 ± 0.0085	$4.50e^{-1}$
Erdos(d)	1.0324 ± 0.0104	$4.63e^{-3}$	1.0237 ± 0.0088	$4.96e^{-3}$	1.0156 ± 0.0061	$5.45e^{-3}$
Erdos(s)	1.0307 ± 0.0100	$1.95e^{-2}$	1.0218 ± 0.0087	$3.71e^{-2}$	1.0133 ± 0.0059	$7.35e^{-2}$
PBP	1.0468 ± 0.0123	$1.68e^{-1}$	1.0365 ± 0.0098	$3.92e^{-2}$	1.0272 ± 0.0068	$3.98e^{-1}$
BP	1.0453 ± 0.0123	$1.97e^{-1}$	1.0359 ± 0.0100	$4.35e^{-2}$	1.0251 ± 0.0071	$4.62e^{-1}$
VGNN(d)	1.0253 ± 0.0095	$5.36e^{-3}$	1.0164 ± 0.0082	$5.76e^{-3}$	1.0105 ± 0.0057	$6.19e^{-3}$
VGNN(s)	$\mathbf{1.0159 \pm 0.0081}$	$2.36e^{-2}$	$\mathbf{1.0104 \pm 0.0073}$	$4.47e^{-2}$	1.0048 ± 0.0055	$8.68e^{-2}$
SCIP(5.0s)	1.1203 ± 0.0152	$5.00e^{0}$	1.1170 ± 0.0156	$5.00e^{0}$	1.1056 ± 0.0105	$5.00e^{0}$
Gurobi(5.0s)	1.1052 ± 0.0249	$5.07e^{0}$	1.1340 ± 0.0357	$5.10e^{0}$	1.1310 ± 0.0257	$5.14e^{0}$

Table 3: Excess ratio on real-world graphs

Data	Github			Memetracker		
	MVC	MaxCut	MDS	MVC	MaxCut	MDS
Greedy	$5.61e^{-3}$	$2.02e^{-2}$	$6.24e^{-3}$	$1.81e^{-2}$	$5.33e{-}2$	$2.38e^{-2}$
MFA	$2.20e^{-4}$	$9.97e^{-3}$	$3.02e^{-5}$	$1.37e^{-3}$	$4.32e{-}2$	$1.68e^{-4}$
Erdos(s)	$7.81e^{-4}$	$6.56e^{-3}$	$1.28e^{-4}$	$9.22e^{-4}$	$2.79e{-}2$	$5.66e^{-5}$
VGNN(s)	$\mathbf{3.52e^{-5}}$	$\mathbf{4.45e^{-3}}$	$\mathbf{1.51e^{-5}}$	$\mathbf{6.60e^{-5}}$	$\mathbf{2.18e^{-2}}$	$\mathbf{3.37e^{-5}}$

1988) for each problem. For greedy algorithms, we use node greedy for MVC, local adjustment greedy for Maxcut and sequential coverage greedy for MDS. MFA combines mean field approximation (ANDERSON 1988) and simulated annealing (SA) (Kirkpatrick, Gelatt, and Vecchi 1983), is able to achieve comparable performance with SA in around fifty times faster speed. We set its initial temperature to $\tau_0 = 5.0$, decay rate to $\alpha = 0.99$, and final temperature to the same as the threshold temperature of VGNN in each problem type. We also use semi-definite programming (Mixing) (Wang, Chang, and Kolter 2017) to solve MaxCut problem. For integer solvers, we use SCIP 7.0.2 (SCIP) (Achterberg 2009) and Gurobi 9.1 (Gurobi) (Gurobi Optimization 2020), the SotA open source and commericial solver, respectively.

Metric: The metric we use to evaluate the solution quality is the *ratio* $r(\cdot)$. In MVC and MDS, $r(\mathbf{x}) := f(\mathbf{x})/f(\mathbf{x}^*)$ and in Max-Cut, $r(\mathbf{x}) := f(\mathbf{x}^*)/f(\mathbf{x})$. The smaller the ratio, the better the solution is. In practice, the optimal value could be hard to find, so we used Gurobi with 3,600 second time limit and used its solution as a substitute.

5.2 Performance on Random Graphs

For each problem type, we generate {50k, 10k} graphs with {256-300} nodes for training and validation. Then, we generate 1k graphs with {256-300, 512-600, 1024-1100} nodes for evaluation. In evaluation, we use the sample size $n = 200$. That's to say, for LS, MFA, Erdos(s), and VGNN(s), we sample 200 solutions and report the best ratio for each method. The results of average *ratio* and average solving time (in seconds) on 1000 random graphs with size are summarized in Table 1, Table 2, Table 4 for MVC, MaxCut, and MDS, respectively. We bold the leading ratios among classical algorithms and neural methods, excluding integer solvers as they are much slower.

We can see that our VGNN achieves the best performance among all heuristic mwethods except for having similar performance with MFA on MaxCut (1024-1100) and MDS (256-300). Also, we are able to find better solutions and use less time than integer solvers SCIP and Gurobi. It is interesting to observe that VGNN always has better ratios than Erdos. This means, although Erdos is trying to approximate a better target distribution P_0, the difficulty in learning suppress its actual performance. Another phenomenon is that VGNN obtains more improvements from *stochastic* decoding than Erdos did, especially in MVC. The reason is that, under non-zero temperature, the Q learned by VGNN has larger entropy so as to avoid concentrating on a single point.

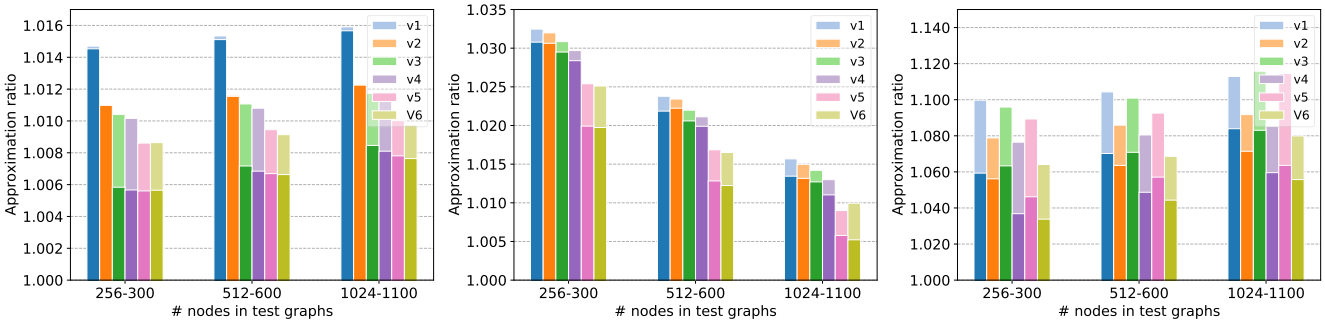
5.3 Performance on Real World Graphs

For *Github*, we split the dataset with ratio 6:2:2. We use 7635 graphs for training, 2545 graphs for validation, and 2545 graphs for evaluation. For *Memetracker*, we use the widely-adopted Independent Cascade model and sample a diffusion cascade from the full graph with constant set to 7, and consider the largest connected component in the graph as a single graph instance. We use 10000 graphs for training, 1000 graphs for valid, and 1000 graphs for testing. Since the *ratio* is fairly small on real-world graphs, we report the

Table 4: Evaluation MDS on 1000 random graphs

Size	256-300		512-600		1024-1100	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
Greedy	1.0877 ± 0.0395	$1.14e^{-4}$	1.0925 ± 0.0261	$4.56e^{-4}$	1.0971 ± 0.0191	$1.21e^{-3}$
MFA	$\mathbf{1.0311 \pm 0.0216}$	$4.63e^{-2}$	1.0431 ± 0.0164	$9.43e^{-2}$	1.0584 ± 0.0124	$1.81e^{-1}$
Erdos(d)	1.0997 ± 0.0409	$4.34e^{-3}$	1.1042 ± 0.0277	$4.62e^{-3}$	1.1129 ± 0.0574	$5.43e^{-3}$
Erdos(s)	1.0593 ± 0.0298	$3.63e^{-2}$	1.0702 ± 0.0210	$6.79e^{-2}$	1.0839 ± 0.0337	$1.14e^{-1}$
VGNN(d)	1.0664 ± 0.0317	$4.89e^{-3}$	1.0686 ± 0.0225	$5.18e^{-3}$	1.0799 ± 0.0325	$6.29e^{-3}$
VGNN(s)	1.0319 ± 0.0234	$5.13e^{-2}$	$\mathbf{1.0410 \pm 0.0177}$	$9.58e^{-2}$	$\mathbf{1.0557 \pm 0.0139}$	$1.79e^{-1}$
SCIP(0.5s)	1.0787 ± 0.0376	$4.96e^{-1}$	1.0854 ± 0.0247	$5.02e^{-1}$	1.0919 ± 0.0883	$5.00e^{-1}$
Gurobi(0.5s)	1.0065 ± 0.0136	$4.52e^{-1}$	1.0211 ± 0.0162	$5.95e^{-1}$	1.0611 ± 0.0307	$6.69e^{-1}$

Figure 1: Ablation results with VGNN, comparing the performance for six different versions.



MVC MaxCut MDS

excess ratio $\tilde{r}(\cdot) := r(\cdot) - 1$ instead. From the results in Table 3, we can see that VGNN still achieves significantly better ratios than all the other methods, meaning our method can successfully apply to real-wrold graphs.

5.4 Ablation Study

In this section, we present an ablation study for the annealing training and forward iteration. We compare six versions of VGNN indexed by the vector $v = (\tau_0, \tau_{\text{th}}, T)$,

- $v_1 = (0.0, 0.0, 0)$: nothing.
- $v_2 = (1.0, 0.0, 0)$: annealing.
- $v_3 = (0.2, 0.2, 0)$: threshold temperature.
- $v_4 = (1.0, 0.2, 0)$: annealing, threshold temperature.
- $v_5 = (0.2, 0.2, 1)$: forward iteration, threshold temperature.
- $v_6 = (1.0, 0.2, 1)$: forward iteration, annealing, threshold temperature.

We show the *ratios* for these six VGNN in Fig. 1. The light bars represent the *ratio* by deterministic decoding and the dark bars represent the *ratio* by *stochastic* decoding with 100 samples. The results strongly support our method. In MVC, v_3, v_4, v_5, v_6 are significantly better than v_1, v_2, showing the importance of non-zero temperature. In MaxCut, v_5, v_6 are significantly better than v_1, v_2, v_3, v_4, showing the importance of forward iteration. In MDS, v_4, v_6 are significantly better than v_1, v_2, v_3, v_5, showing the importance of annealing training schedule.

These phenomenons are directly related to the property for each problem. MVC has a lot of shallow local optima, hence using a non-zero temperature can significantly improve the performance. On the contrary, MDS has deeper local optima. Consequently, the annealing training is crucially needed to prevent being trapped in local optima. Differing from MVC and MDS having variables that tend strongly towards either 0 or 1, the optimal solutions on MaxCut are symmetric, i.e. flipping all variables does not affect the partition. As a result, the predicted Q tends to collapse and give a neutral probability close to one half. Thus, the forward iteration can significantly improve the ratio on MaxCut.

6 Conclusion

In this paper, we propose a generic unsupervised learning framework for constrained or unconstrained CO problems. We introduce two methods, annealing training and forward iteration, naturally arisen from our framework, to help the learning of GNN. We have quantitatively verified our approach compared to other methods on both synthetic and real-world graphs. Further work includes employing more flexible varitional distributions and more sophisticated annealing schedules. In summary, we believe this work provides a new perspective for learning algorithms for CO problems.

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A Technical Details

A.1 Case Study

In this section, we elaborate on the derivation for each problem type, including the forward iteration, conditional decoding, and the complexity.

Minimum Vertex Cover: Given temperature τ, we have the loss function

$$\begin{aligned} L_\tau(\mathbf{p}) = &\sum_{i=1}^{n} p_i + 2 \sum_{(i,j)\in E} (1-p_i)(1-p_j) \\ &+\tau \sum_{i=1}^{n} p_i \log p_i + (1-p_i)\log(1-p_i) \end{aligned} \tag{18}$$

The gradient at local optima should be zero; hence, we have:

$$\frac{\partial L_\tau(\mathbf{p})}{\partial p_i} = 1 - 2 \sum_{j:(i,j)\in E} (1-p_j) + \tau \log \frac{p_i}{1-p_i} = 0 \tag{19}$$

which gives the closed form solution:

$$p_i^{(t+1)} = 1/(\exp([2 \sum_{j:(i,j)\in E} (1-p_j^{(t)}) - 1]/\tau) + 1) \tag{20}$$

In conditional decoding, we have:

$$\hat{\theta}_k = \arg\min_{\theta_k \in \{0,1\}} \mathbb{E}_{\mathbf{x}\sim Q(\cdot|\hat{\theta}_{-k},\hat{\theta}_k)}[f(\mathbf{x})] \tag{21}$$

$$= \arg\min_{\theta_k \in \{0,1\}} L_0(\hat{\theta}_{-k}, \theta_k) \tag{22}$$

$$= \arg\min_{\theta_k \in \{0,1\}} \theta_k [1 - 2 \sum_{j:(i,j)\in E} (1-\hat{\theta}_j)] + C \tag{23}$$

where C is a constant that does not depend on θ_k. Thus, we have $\hat{\theta}_k = 1$ if $1 - 2\sum_{j:(i,j)\in E}(1-p_j) < 0$ and $\hat{\theta}_k = 0$ if $1 - 2\sum_{j:(i,j)\in E}(1-p_j) > 0$. The algorithm for decoding is given in Alg. 2. Line 3 and lines 6-11 both require $O(n)$ computation, and line 5 requires $O(m)$ computation. Therefore, the complexity of this algorithm is $O(m+n)$.

Algorithm 2: Conditional Decoding for Minimum Vertex Cover

1: **Input**: graph $G = (V, E)$, variable order π, Bernoulli probability θ
2: **Output**: cover size c.
3: Initialize $\hat{\theta} = \theta$, $c = 0$
4: **for** k in π **do**
5: Compute local field $F_k = 1 - 2\sum_{j:(k,j)\in E}(1-\hat{\theta}_j)$
6: **if** $F_k > 0$ **then**
7: $\hat{\theta}_k \leftarrow 0$
8: **else**
9: $\hat{\theta}_k \leftarrow 1$
10: $c \leftarrow c + 1$
11: **end if**
12: **end for**

Weighted Maximum Cut: Given temperature τ, we have the loss function

$$\begin{aligned} L_\tau(\mathbf{p}) = &\sum_{(i,j)\in E} w(i,j)(p_i + p_j - 2p_ip_j) \\ &+\tau \sum_{i=1}^{n} p_i \log p_i + (1-p_i)\log(1-p_i) \end{aligned} \tag{24}$$

The gradient at local optima should be zero; hence, we have:

$$\frac{\partial L_\tau(\mathbf{p})}{\partial p_i} = \sum_{j:(i,j)\in E} w(i,j)(1-2p_j) + \tau \log \frac{p_i}{1-p_i} = 0 \tag{25}$$

which gives the close form solution:

$$p_i^{(t+1)} = 1/(\exp(\sum_{j:(i,j)\in E} w(i,j)(2p_j^{(t)} - 1)/\tau) + 1) \tag{26}$$

In conditional decoding, we have:

$$\hat{\theta}_k = \arg\min_{\theta_k \in \{0,1\}} \mathbb{E}_{\mathbf{x}\sim Q(\cdot|\hat{\theta}_{-k},\hat{\theta}_k)}[f(\mathbf{x})] \tag{27}$$

$$= \arg\min_{\theta_k \in \{0,1\}} L_0(\hat{\theta}_{-k}, \theta_k) \tag{28}$$

$$= \arg\min_{\theta_k \in \{0,1\}} \theta_k [\sum_{j:(i,j)\in E} w(i,j)(1-2\hat{\theta}_j)] + C \tag{29}$$

where C is a constant that does not depend on θ_k. So, we have $\hat{\theta}_k = 1$ if $\sum_{j:(i,j)\in E} w(i,j)(1-2p_j) > 0$ and $\hat{\theta}_k = 0$ if $\sum_{j:(i,j)\in E} w(i,j)(1-2p_j) < 0$. The algorithm for decoding is given in Alg. 3. Line 3 and line 6-11 require $O(n)$ computation, line 5 and line 12-16 require $O(m)$ computation, hence the complexity of this algorithm is $O(m+n)$.

Algorithm 3: Conditional Decoding for Weighted Maximum Cut

1: **Input**: graph $G = (V, E, w)$, variable order π, Bernoulli probability θ
2: **Output**: cut size c.
3: Initialize $\hat{\theta} = \theta$, $c = 0$
4: **for** k in π **do**
5: Compute local field $F_k = \sum_{j:(k,j)\in E} w(i,j)(1 - 2\hat{\theta}_j)$
6: **if** $F_k > 0$ **then**
7: $\hat{\theta}_k \leftarrow 1$
8: **else**
9: $\hat{\theta}_k \leftarrow 0$
10: **end if**
11: **end for**
12: **for** (i,j) in E **do**
13: **if** $\hat{\theta}_i != \hat{\theta}_j$ **then**
14: $c \leftarrow c + w(i,j)$
15: **end if**
16: **end for**

Table 5: Evaluation MVC on Large Problem Sizes

Size	2048-2200		4096-4400		8192-8800	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
Greedy	1196 ± 26	$5.6e^{-3}$	2387 ± 50	$2.7e^{-2}$	4769 ± 102	$1.3e^{-1}$
Erdos(s)	1174 ± 26	$6.5e^{-2}$	2348 ± 49	$1.6e^{-1}$	4753 ± 118	$3.2e^{-1}$
VGNN(s)	$\mathbf{1164 \pm 25}$	$6.5e^{-2}$	$\mathbf{2325 \pm 48}$	$1.6e^{-1}$	$\mathbf{4651 \pm 99}$	$3.2e^{-1}$
Gurobi	1205 ± 26	$1.2e^{-1}$	2403 ± 59	$5.3e^{0}$	5331 ± 656	$5.5e^{0}$

Table 6: Evaluation MDS w/ Time Adjusted

Size	256-300		512-600		1024-1100	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
VGNN(s)	$\mathbf{1.0319 \pm 0.0234}$	$5.13e^{-2}$	$\mathbf{1.0410 \pm 0.0177}$	$9.58e^{-2}$	$\mathbf{1.0557 \pm 0.0139}$	$1.79e^{-1}$
Gurobi	1.0698 ± 0.0136	$1.12e^{-1}$	1.1192 ± 0.0414	$2.14e^{-1}$	1.0611 ± 0.0307	$6.69e^{-1}$

Minimum Dominating Set Given temperature τ, we have the loss function

$$L_\tau(\mathbf{p}) = \sum_i p_i + 2\sum_i (1-p_i) \prod_{j:(i,j)\in E} (1-p_j) + \tau \sum_{i=1}^{n} p_i \log p_i + (1-p_i)\log(1-p_i)$$

The gradient at local optima should be zero, hence we have:

$$\frac{\partial L_\tau(\mathbf{p})}{\partial p_i} = 1 - 2\sum_{j\in N_i} \prod_{k\in N_j^i} (1-p_k) + \tau \log \frac{p_i}{1-p_i} = 0 \tag{30}$$

which gives the closed form solution:

$$p_i^{(t+1)} = 1/(\exp((\sum_{j\in N_i} 2 \prod_{k\in N_j^i} (1-p_k^{(t)}) - 1)/\tau) + 1) \tag{31}$$

In conditional decoding, we have:

$$\hat{\theta}_k = \arg\min_{\theta_k\in\{0,1\}} \mathbb{E}_{\mathbf{x}\sim Q(\cdot|\hat{\theta}_{-k},\hat{\theta}_k)}[f(\mathbf{x})] \tag{32}$$

$$= \arg\min_{\theta_k\in\{0,1\}} L_0(\hat{\theta}_{-k}, \theta_k) \tag{33}$$

$$= \arg\min_{\theta_k\in\{0,1\}} \theta_k[1 - 2\sum_{j\in N_i} \prod_{k\in N_j^i} (1-p_k)] + C \tag{34}$$

where C is a constant that does not depend on θ_k. Therefore, we have $\hat{\theta}_k = 1$ if $1 - 2\sum_{j\in N_i} \prod_{k\in N_j^i}(1-p_k) < 0$ and $\hat{\theta}_k = 0$ if $1 - 2\sum_{j\in N_i} \prod_{k\in N_j^i}(1-p_k) > 0$. The algorithm for decoding is given in Alg. 4. We need to enumerate all nodes twice: once for initializing $\hat{\theta}$ in line 3 and once for updating $\hat{\theta}$ in the for-loop in line 7-21. We need to enumerate all edges three times: once for initializing the covers in line 4-6, once for computing the local field in line 8, and once for updating the cover in line 9-20. Hence, the complexity of this algorithm is $O(m+n)$.

Algorithm 4: Conditional Decoding for Minimum Dominate Set

1: **Input**: graph $G = (V, E)$, variable order π, Bernoulli probability θ
2: **Output**: cover size c.
3: Initialize $\hat{\theta} = \theta$, $c = 0$
4: **for** $i = 1, ..., n$ **do**
5: Compute cover $C_i = \prod_{j\in N_i}(1-\hat{\theta}_j)$
6: **end for**
7: **for** k in π **do**
8: Compute local field $F_k = 1 - \sum_{j\in N_i} C_j/(1-\hat{\theta}_j)$
9: **if** $F_k > 0$ **then**
10: **for** j in N_k **do**
11: $C_j \leftarrow C_j/(1-\hat{\theta}_k)$
12: **end for**
13: $\hat{\theta}_k \leftarrow 0$
14: **else**
15: **for** j in N_k **do**
16: $C_j \leftarrow 0$
17: **end for**
18: $\hat{\theta}_k \leftarrow 1$
19: $c \leftarrow c + 1$
20: **end if**
21: **end for**

A.2 Implementation

We run our experiments on a machine with Intel(R) Xeon(R) Gold 5215 CPU @ 2.50GHz, 8 RTX6000, 377G memory, Ubuntu 18.04.5 LTS (GNU/Linux 5.4.0-62-generic x86_64). With the VGNN, we use initial temperature $\tau_0 = 1$, decay rate $\alpha = 0.99$, and forward iteration $T = 1$. More forward iterations can slightly improve the performance on MaxCut but not on MVC and MDS. We select the temperature threshold τ_{th} as 0.2, 0.5, 0.3 for MVC, MaxCut, and MDS, respectively. The GNN G_ϕ comprises of 6 layers of the Graph Isomorphism Network (GIN) (Xu et al. 2018a) with hidden dimension $h = 128$, equipped with skip connections (Xu et al. 2018b), and batch normalization (Ioffe and Szegedy 2015). Our GNN is implemented by PyTorch

Table 7: Evaluation MVC w/ Time Adjusted

Size	256-300		512-600		1024-1100	
Method	*ratio*	avg time (s)	*ratio*	avg time (s)	*ratio*	avg time (s)
VGNN(s)	$\mathbf{1.0052 \pm 0.0052}$	$1.26e^{-2}$	$\mathbf{1.0063 \pm 0.0039}$	$2.26e^{-2}$	$\mathbf{1.0074 \pm 0.0032}$	$3.44e^{-2}$
Gurobi	1.0184 ± 0.0031	$9.6e^{-2}$	1.0795 ± 0.0051	$1.91e^{-1}$	1.0310 ± 0.0193	$6.22e^{-1}$

Geometric (Fey and Lenssen 2019) and trained using gradient descent with batch size 200 for $T = 500$ epochs using the default Adam (Kingma and Ba 2014) with weight decay 0.995. In training, we compute the loss and gradient w.r.t. L_τ on training data and finally select the model that minimizes L_0 on the validation data.

A.3 Results on Larger Minimum Vertex Cover Instances

With the Minimum Vertex Cover problem, the difference in performance between our algorithm and others becomes even clearer as the problem size increases as evident by Table 5. VGNN outperforms the other baselines significantly on these larger instances. Not only does it have the best optimal ratio but it also has the most stable results in terms of standard deviation.

A.4 Results on Minimum Vertex Cover with Time Adjusted

Our algorithm performs better than Gurobi on MVC problems even when given less time. When the amount of time given to Gurobi to solve MVC problems is restricted further to be closer to the amount of time allotted to VGNNe, the difference between the optimal ratio of the VGNN and Gurobi becomes even more significant as evident by Table 7.

A.5 Results on Minimum Dominating Set

Given similar time constraints, our algorithm also outperforms Gurobi on large Minimum Dominating Set problems as evident by Table 6.

B Cover Letter

We revise the presenting our paper to make it more easier to understand. We summary the response to reviewers and the corresponding update in the main paper.

B.1 6pyR

The reviewer wants us to add experiments. We add comparison with baselines: BP, perturbed BP, and CMPE. The results are updated in Table 1, Table 2, Table 4.

B.2 a6Tn

The reviewer concerns about the writing of the paper. We have revised the writing according to the the reviewers suggestions. Here is the list of our response to reviewer's concerns:

1. **graph and graphical model**. The CO problems (vertex cover, max cut, dominate set) studied in this work are defined on a graph G. This gives us the graph. Combining the distribution P_tau defined in equation (4), we defined our graphical model (G, P_τ).

2. θ **in equation (8) and (9)**. For equation (8), what we tried to say is: if the variational distribution Q is parameterized by θ, then the loss function w.r.t. θ is defined as equation (8). In revision, we will add the statement "Q is parameterized by θ. For equation (9), what we meant is, as a function of θ, L_τ pointwise converges to an upper bound of the optimal value. We omit θ as we wanted to stress the validness of this upper bound does not rely on the value of θ.

3. **converges to the optimal solution**. We give the proof here: Consider the set of optimal solutions is $\mathcal{X}$ and its completion $\mathcal{X}^\perp = \{0,1\}^n \backslash \mathcal{X}$. WLOG, we assume the $f(x^*) = 0, \forall x^* \in \mathcal{X}$. The probability that a state at graphical model P_τ is not optimal can be characterized as a function of τ:

$$F(\tau) = \frac{\sum_{x\in\mathcal{X}^\perp} e^{-f(x)/\tau}}{|\mathcal{X}| + \sum_{x\in\mathcal{X}^\perp} e^{-f(x)/\tau}}$$

   As 1) $f(x) > 0, \forall x \in \mathcal{X}^\perp$ and 2) $\mathcal{X}^\perp$ is a finite set, there exists a $\delta > 0$ and $f(x) > \delta, \forall x \in \mathcal{X}^\perp$. We can see the numerator will decrease to 0 when τ goes to zero. The denominator is always larger than $|\mathcal{X}|$. Hence, we have the

$$\lim_{\tau\to 0} F(\tau) = 0$$

   and this means the graphical model will converge to the optimal states as long as $\mathcal{X}$ is not empty.

4. **Lines 117 - 119, for any infeasible solution, we can always find a feasible solution better than it w.r.t.** $f(x)$ **in equation (4)**: Consider we have a feasible solution x and an infeasible solution y. By definition, there exists i such that $\psi_i(y) = 1$. Hence,

$$\begin{aligned} f(x) &= c(x) + \sum_{i=1}^m \beta_i \psi_i(x) \\ &= c(x) \\ &\leq \frac{1}{2}\beta_j \leq c(y) + \beta_j \\ &\leq c(y) + \sum_{i=1}^m \beta_i \psi_i(y) \\ &= f(y) \end{aligned}$$

5. **Lines 129-131 smooth landscape** What we meant is, with a high temperature τ, the target distribution P_τ has a smooth landscape and, as a result, the loss function (KL-divergence) becomes smoother w.r.t. Q. For example, for equation $f(\mathbf{x}) = \sum_{v\in V} x_v + 2\sum_{(u,v)\in E}(1 - x_u)(1 - x_v)$ in equation (15) and $f(\mathbf{x}) = c(\mathbf{x}) = \sum_{(u,v)\in E} w(u,v)(x_u + x_v - 2x_u x_v)$ in equation (17), we can see the Hessian matrix is twice of the adjacency matrix. Hence, when the temperature τ is larger than the spectrum radius of the graph, the loss function becomes strongly convex. Even if τ is small, it can effectively smooth L_τ w.r.t. θ.

6. **Lines 141 - 142**: The definition of support is support$(Q) = \{x : Q(x) \neq 0\}$. If we manage to find a Q that supported on optimal solutions, we have the set $\mathcal{Z} = \{x : f(x) - \min_x f(x) \neq 0\}$ which has zero measure w.r.t. Q, indicating $\mathbb{E}_{x\sim Q}[f(x) - \min_x f(x)] = 0$. Hence, we have:

$$\begin{aligned} \mathbb{E}_{x\sim Q}[f(x)] &= \mathbb{E}_{x\sim Q}[f(x)] - \mathbb{E}_{x\sim Q}[f(x) - \min_x f(x)] \\ &= \mathbb{E}_{x\sim Q}[\min_x f(x)] \\ &= \min_x f(x) \end{aligned}$$

7. **Algorithm 1, Differentiable**: In our parameterization of Q_θ, the loss function L_θ is differentiable w.r.t θ. Also, θ, as an output of a neural network parameterized by ϕ, is differentiable w.r.t. ϕ. Hence, $\frac{\partial L_\tau}{\partial \phi} = \frac{\partial L_\tau}{\theta}\frac{\partial \theta}{\partial \phi}$ exists. After obtaining the gradient $d\phi$, we update ϕ using Adam [Kingma & Ba, 2014] as we mentioned in the appendix.

8. **Algorithm 1, Data**: Every data $D_i = (G_i, C_i, c_i)$ we use for {minimum vertex cover, weighted max cut, minimum dominated set} is a graph G_i with its constraints C_i as well as its objective function $c_i(\cdot)$. We say it is unsupervised as we don't need the optimal solution x_i^* corresponding to D_i. We use unsupervised learning since finding x_i^* for those NP-hard problem could be expensive.

9. **Line 143, Model Selection**: The model selection here means that, during the gradient descent training, we obtain a parameter ϕ_t at every epoch t. We select our final parameter

$$\hat{\phi} := \arg\min_t L_0(\phi_t, I_{\text{valid}})$$

   according to their loss on the valid data.

B.3 gpEy

The reviewer believes the improvement of our methods is not significant. We conduct experiments on larger instances and add the results in Table 5, Table 7, and Table 6.

B.4 oiCr

The reviwer thinks our paper is good.

B.5 Original Version

We give the original version for NeurIPS submission as following.