A Neural Network Approach for Efficiently Answering Most Probable Explanation Queries in Probabilistic Models

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Abstract

We propose a novel neural networks based approach to efficiently answer arbitrary Most Probable Explanation (MPE) queries—a well-known NP-hard task—in large probabilistic models such as Bayesian and Markov networks, probabilistic circuits, and neural auto-regressive models. By arbitrary MPE queries, we mean that there is no predefined partition of variables into evidence and non-evidence variables. The key idea is to distill all MPE queries over a given probabilistic model into a neural network and then use the latter for answering queries, eliminating the need for time-consuming inference algorithms that operate directly on the probabilistic model. We improve upon this idea by incorporating inference-time optimization with self-supervised loss to iteratively improve the solutions and employ a teacher-student framework that provides a better initial network, which in turn, helps reduce the number of inference-time optimization steps. The teacher network utilizes a self-supervised loss function optimized for getting the exact MPE solution, while the student network learns from the teacher's near-optimal outputs through supervised loss. We demonstrate the efficacy and scalability of our approach on various datasets and a broad class of probabilistic models, showcasing its practical effectiveness.

1 Introduction

Probabilistic representations such as Probabilistic Circuits (PCs) [8], graphical models [26] such as Bayesian Networks (BNs) and Markov Networks (MNs), and Neural Autoregressive Models (NAMs) [50] are widely used to model large, multi-dimensional probability distributions. However, they face a significant challenge: as the complexity of these distributions increases, solving practically relevant NP-hard inference tasks such as finding the Most Probable Explanation (MPE) via exact inference techniques [35, 36] becomes increasingly difficult and time-consuming. In particular, although various exact and approximate solvers exist for the MPE task in PCs, BNs and MNs, exact solvers are often too slow for practical use, and approximate solvers tend to lack the necessary accuracy, particularly in autoregressive models that currently rely on slow hill-climbing/beam search methods.

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In recent work, Arya et al. [4] proposed a method to overcome the limitations of existing approximate methods by using neural networks (NNs) to solve the MPE task in PCs.[1] Their method draws inspiration from the learning to optimize literature [12, 15, 29, 42, 55]. Given a PC and a *predefined partition of variables into query and evidence sets*, the core idea is to train a NN that takes an assignment to the evidence variables as input and outputs the most likely assignment to the query variables w.r.t. the distribution defined by the PC. Arya et al. suggest using either supervised or self-supervised learning techniques to train the NN; the former requires access to exact inference schemes, while the latter does not and is therefore more practical.

In this paper, we address a more general and complex version of the MPE task than the one considered by Arya et al. Specifically, we assume that there is *no predefined partition of the variables into evidence and query sets*, which we refer to as the **any-MPE** task. The complexity of the any-MPE task arises from the exponential increase in the number of input configurations, compounded by the exponential number of possible divisions of variables into evidence and query sets. Furthermore, our method applies to a broad class of probabilistic models, including BNs, MNs and NAMs, whereas Arya et al.'s method is limited to PCs. In addition, Arya et al.'s method does not fully exploit the capabilities of self-supervision, and the benefits of combining supervised and self-supervised loss functions.

This paper presents a novel approach that uses a NN for solving the any-MPE task in a broad class of probabilistic models (PMs) and achieves technical advancements in three key aspects:

1. Efficient MPE Inference via Encoding Scheme and Loss Function: We introduce a new encoding scheme that tailors the NN architecture to the specific structure of the input PM. This scheme not only delineates the input and output nodes for the NN but also establishes a methodology for setting input values and extracting the MPE solution from the NN's outputs. Furthermore, we propose a tractable, and differentiable self-supervised loss function, enabling efficient training.

2. Inference Time Optimization with ITSELF: We introduce a novel inference technique called Inference Time Self Supervised Training (**ITSELF**). This technique iteratively refines the MPE solution during the inference process itself. It utilizes gradient descent (*back-propagation*) to update the NN's parameters using our proposed self-supervised loss, leading to continual (anytime) improvement towards near-optimal solutions. ITSELF fully utilizes the power of our self-supervised loss, as it does not require labeled data or an external MPE solver.

3. Two-Phase Pre-training with Teacher-Student Architecture: To address challenges associated with self-supervised learning and ITSELF, we propose a two-phase pre-training strategy that leverages a teacher-student architecture. Self-supervised learning can suffer from overfitting and requires careful regularization. Additionally, ITSELF, especially with random initializations, might necessitate a substantial number of gradient updates to converge on optimal solutions. Our approach addresses these issues using the following methodology: (i) The teacher network first overfits the training data using ITSELF and (ii) The student network is then trained using supervised loss functions (e.g., binary cross-entropy) by treating the teacher network's output as pseudo-labels. This supervised training phase improves and regularizes the parameter learning process of the student network. It also provides a robust starting point for ITSELF, significantly reducing the required optimization steps and leading to substantial performance gains.

Finally, we conduct a detailed experimental comparison of our method with existing approaches on several types of PMs such as PCs, BNs, MNs and NAMs. Our results demonstrate that our method surpasses state-of-the-art approximate inference techniques in terms of both accuracy and speed.

2 Background and Motivation

Without loss of generality, we use binary variables which take values from the set $\{0, 1\}$. We denote a random variable by an uppercase letter (e.g., X), and a value assigned to it by the corresponding lowercase letter (e.g., x). We denote a set of random variables by a bold uppercase letter (e.g., $\mathbf{X}$) and an assignment of values to all variables in the set by the corresponding bold lowercase letter (e.g., $\mathbf{x}$).

[1] Arya et al. [4] developed a NN-based method for solving the *marginal maximum-a-posteriori* (MMAP) task in PCs. In this paper, we focus on the MPE task, also sometimes referred to as the full MAP task, which is a special case of MMAP. Our method can be easily extended for solving the MMAP problem in PCs and tractable graphical models. For simplicity of exposition, we concentrate on the MPE task in this paper.

Throughout the paper when we use the term probabilistic models (PMs), we are referring to a broad class of probabilistic models in which computing the likelihood[2] of an assignment to all variables in the model can be done in polynomial (preferably linear) time in the size of the model. This class includes, among others, Bayesian and Markov networks collectively called probabilistic graphical models (PGMs) [26], smooth and decomposable probabilistic circuits (PCs) [8], and neural autoregressive models (NAMs) such as NADE [50] and MADE [17].

We are interested in solving the most probable explanation (MPE) task in PMs, namely the task of finding the most likely assignment to all unobserved (non-evidence) variables given observations (evidence). Formally, let $\mathcal{M}$ denote a probabilistic model defined over a set of variables $\mathbf{X}$ that represents the distribution $\mathrm{p}_{\mathcal{M}}(\mathbf{x})$. We categorize the variables $\mathbf{X}$ into evidence $\mathbf{E} \subseteq \mathbf{X}$ and query $\mathbf{Q} \subseteq \mathbf{X}$ groups, ensuring that $\mathbf{E} \cap \mathbf{Q} = \emptyset$ and $\mathbf{E} \cup \mathbf{Q} = \mathbf{X}$. Then, given an assignment $\mathbf{e}$ to the set of evidence variables $\mathbf{E}$, the MPE task can be formulated as:

$$\texttt{MPE}(\mathbf{Q}, \mathbf{e}) = \operatorname*{argmax}_{\mathbf{q}} \mathrm{p}_{\mathcal{M}}(\mathbf{q}|\mathbf{e}) = \operatorname*{argmax}_{\mathbf{q}} \{\log \mathrm{p}_{\mathcal{M}}(\mathbf{q}, \mathbf{e})\} \tag{1}$$

It is known that the MPE task is NP-hard in general and even hard to approximate [9, 11, 38, 41, 44].

Motivation: The goal of this paper is to develop a method that trains a NN for a given PM and, at test time, serves as an approximate MPE solver for any-MPE query posed over the PM. By any-MPE, we mean that the NN can take an assignment to an arbitrary subset of variables (evidence) as input and output the most likely assignments to the remaining (query) variables. Recently, Arya et al. [4] proposed a NN-based solution for solving the MPE task in PCs under the constraint that the partition of the variables into evidence and query sets *is known before training the NN*. This constraint is highly restrictive because, for generative models, it is unlikely that such a partition of variables is known in advance. In such cases, one would typically train a discriminative model rather than a generative one. Unlike Arya et al.'s method, our approach yields an any-MPE solver. Additionally, Arya et al.'s approach has several limitations in that it does not fully exploit the benefits of self-supervision during inference time and requires the use of relatively large NNs to achieve good performance in practice. Our proposed approach, described next, addresses these limitations.

3 A Self-Supervised Neural Approximator for any-MPE

In this section, we develop a neural network (NN) based approach for solving the *any-MPE* task. Specifically, given a PM, we develop an input encoding (see Section 3.1) that determines the number of input nodes of the NN and sets their values for the given MPE query. We also develop an output encoding that determines the number of output nodes for the given PM and allows us to recover the MPE solution from the outputs. For training the NN, we introduce a tractable and differentiable self-supervised loss function (see Section 3.2), whose global minima aligns with the MPE solutions to efficiently learn the parameters of the NN given *unlabeled data*.

3.1 An Encoding For any-MPE Instances

Since NNs require fixed-sized inputs and outputs, we introduce input and output encodings that generate fixed-length input and output vectors for each PM from a given MPE problem instance $\texttt{MPE}(\mathbf{Q}, \mathbf{e})$. To encode the input, for each variable $X_i \in \mathbf{X}$, we associate two input nodes in the NN, denoted by $\hat{X}_i$ and $\bar{X}_i$. Thus for a PM having n (namely, $|\mathbf{X}| = n$) variables, the corresponding NN has $2n$ input nodes. Given a query MPE$(\mathbf{Q}, \mathbf{e})$, we set the values of the input nodes as follows: (1) If $X_i \in \mathbf{E}$ and $X_i = 0$ is in $\mathbf{e}$, then we set $\hat{X}_i = 0$ and $\bar{X}_i = 1$; (2) If $X_i \in \mathbf{E}$ and $X_i = 1$ is in $\mathbf{e}$, then we set $\hat{X}_i = 1$ and $\bar{X}_i = 0$; and (3) If $X_i \in \mathbf{Q}$ then we set $\hat{X}_i = 0$ and $\bar{X}_i = 0$. (The assignment $\hat{X}_i = 1$ and $\bar{X}_i = 1$ is not used.) It is easy to see that the input encoding described above yields an *injective* mapping between the set of all possible MPE queries over the given PM and the set $\{0, 1\}^{2n}$. This means that each unique MPE query $(\mathbf{Q}, \mathbf{e})$ will yield a unique 0-1 input vector of size $2n$.

The output of the neural network comprises of n nodes with sigmoid activation, where each output node is associated with a variable $X_i \in \mathbf{X}$. We ignore the outputs corresponding to the evidence variables and define a loss function over the outputs corresponding to the query variables in the set $\mathbf{Q}$. The MPE solution can be reconstructed from the output nodes of the NN by thresholding the

[2] or a value proportional to it such as the unnormalized probability in Markov networks.

output nodes corresponding to the query variables appropriately (e.g., if the value of the output node is greater than 0.5, then the query variable is assigned the value 1; otherwise it is assigned to 0).

3.2 A Self-Supervised Loss Function for any-MPE

Since the output nodes of our proposed NN use sigmoid activation, each output is continuous and lies in the range $[0, 1]$. Given an MPE query $\texttt{MPE}(\mathbf{Q}, \mathbf{e})$, let $\mathbf{q}^c \in [0, 1]^{|\mathbf{Q}|}$ denote the (continuous) *Most Probable Explanation* (MPE) assignment predicted by the NN. In MPE inference, given $\mathbf{e}$, we want to find an assignment $\mathbf{q}$ such that $\log \mathrm{p}_{\mathcal{M}}(\mathbf{q}, \mathbf{e})$ is maximized, namely, $-\log \mathrm{p}_{\mathcal{M}}(\mathbf{q}, \mathbf{e})$ is minimized. Thus, a natural loss function that we can use is $-\log \mathrm{p}_{\mathcal{M}}(\mathbf{q}, \mathbf{e})$. Unfortunately, the NN outputs a continuous vector $\mathbf{q}^c$ and as a result $\mathrm{p}_{\mathcal{M}}(\mathbf{q}^c, \mathbf{e})$ is not defined.

Next, we describe how to solve the above problem by leveraging the following property of the class of PMs that we consider in this paper—specifically BNs, MNs, PCs and NAMs. In these PMs, the function $\ell(\mathbf{q}, \mathbf{e}) = -\log \mathrm{p}_{\mathcal{M}}(\mathbf{e}, \mathbf{q})$, which is a function from $\{0, 1\}^n \to \mathbb{R}$ is either a multi-linear polynomial or a neural network, and can be computed in linear time in the size of the PM. To facilitate the use of continuous outputs, we define a loss function $\ell^c(\mathbf{q}^c, \mathbf{e}) : [0, 1]^n \to \mathbb{R}$ such that ℓ^c coincides with ℓ on $\{0, 1\}^n$. For PGMs and PCs, ℓ is a multi-linear function and ℓ^c is obtained by substituting each occurrence of a discrete variable $q_i \in \mathbf{q}$ with the corresponding continuous variable $q_i^c \in \mathbf{q}^c$ where $q_i^c \in [0, 1]$. In NAMs, ℓ is a NN and we can perform a similar substitution—we substitute each binary input q_i in the NN with a continuous variable $q_i^c \in [0, 1]$. This substitution transforms the discrete NN into a continuous function while preserving its functional form.

An important property of ℓ^c is that it can be evaluated and differentiated in polynomial time. Moreover, when ℓ is defined by either a neural network (in NAMs) or a multilinear function (in BNs, MNs and PCs), the minimum value of ℓ^c over the domain $[0, 1]^n$ is less than or equal to the minimum value of the original function ℓ over the discrete domain $\{0, 1\}^n$. Formally,

Proposition 1. *Let $l(\mathbf{q}, \mathbf{e}) : \{0, 1\}^n \to \mathbb{R}$ be either a neural network or a multilinear function, and let $l^c(\mathbf{q}^c, \mathbf{e}) : [0, 1]^n \to \mathbb{R}$ be its continuous extension obtained by substituting each binary input q_i with a continuous variable $q_i^c \in [0, 1]$. Then,*

$$\min_{\mathbf{q}^c \in [0,1]^n} \ell^c(\mathbf{q}^c, \mathbf{e}) \leq \min_{\mathbf{q} \in \{0,1\}^n} \ell(\mathbf{q}, \mathbf{e})$$

Following Arya et al. [4], we propose to improve the quality of the loss function by tightening the lower bound given in proposition 1 with an entropy-based penalty (ℓ_E), governed by $\alpha > 0$.

$$\ell_E(\mathbf{q}^c, \alpha) = -\alpha \sum_{j=1}^{|\mathbf{Q}|} \left[q_j^c \log(q_j^c) + (1 - q_j^c) \log(1 - q_j^c) \right] \tag{2}$$

This penalty encourages discrete solutions by preferring q_j^c values close to 0 or 1, where α modulates the trade-off. Setting α to 0 yields the continuous approximation; conversely, an α value of ∞ results exclusively in discrete outcomes. From proposition 1 and by using the theory of Lagrange multipliers, we can show that for any $\alpha > 0$, the use of the entropy penalty yields a tighter lower bound:

Proposition 2.

$$\min_{\mathbf{q}^c \in [0,1]^n} \ell^c(\mathbf{q}^c, \mathbf{e}) \leq \min_{\mathbf{q}^c \in [0,1]^n} \ell^c(\mathbf{q}^c, \mathbf{e}) + \ell_E(\mathbf{q}^c, \alpha) \leq \min_{\mathbf{q} \in \{0,1\}^n} \ell(\mathbf{q}, \mathbf{e})$$

How to use the Loss Function: Given a PM defined over n variables, we can use the self-supervised loss function $\ell^c(\mathbf{q}^c, \mathbf{e}) + \ell_E(\mathbf{q}^c, \alpha)$ (treating α as a hyper-parameter) to train any neural network (NN) architecture that has $2n$ input nodes and n output nodes. This trained NN can then be used to answer any arbitrary MPE query posed over the PM. The training data for the neural network consists of assignments (evidence $\mathbf{e}$) to a subset of the variables. Each training example can be generated using the following three-step process. We first sample a full assignment $\mathbf{x}$ to all variables in the PM using techniques like Gibbs sampling or perfect sampling for tractable distributions such as PCs and BNs. Second, we choose an integer k uniformly at random from the range $\{1, \ldots, n\}$ and designate k randomly selected variables as evidence variables $\mathbf{E}$, and the remaining $n - k$ as query variables $\mathbf{Q}$. Finally, we project the full assignment $\mathbf{x}$ on $\mathbf{E}$. The primary advantage of using the self-supervised loss function is that it eliminates the need for access to a dedicated MPE solver to provide supervision during training; gradient-based training of the neural network provides the necessary supervision.

3.3 Inference-Time Neural Optimization using Self-Supervised Loss

At a high level, assuming that the NN is over-parameterized, if we use the self-supervised loss and repeatedly run (stochastic) gradient updates over the NN for a given dataset, theoretical results [2, 13] as well as prior experimental work [46, 56] suggest that the parameters of the NN will converge to a point near the global minimum of the self-supervised loss function. This means that through gradient updates, the network will find a near-optimal MPE assignment for each training example. This strategy of performing gradient updates over the NN can also be used *during inference (test) time to iteratively improve the MPE solution*, thereby maximizing the benefits of self-supervision.

Specifically, at test time, given a test dataset (or example), we initialize the NN either randomly or using a pre-trained model and then run gradient-based updates over the NN iteratively until convergence. The gradient is computed w.r.t. to the self-supervised loss function $\ell^c(\mathbf{q}^c, \mathbf{e}) + \ell_E(\mathbf{q}^c, \alpha)$. We call the resulting algorithm ITSELF (Inference Time Optimization using SELF-Supervised Loss). The performance of ITSELF typically improves with each iteration until the loss converges.

Our proposed method, ITSELF, is closely related to test-time training approaches which are widely used to solve problems in deep learning [1, 10, 19, 30–32, 40, 49, 51, 57]. Our method differs from these previous approaches in that the global minima of our proposed self-supervised loss correspond to the MPE solutions, provided that the penalty α is sufficiently large.

4 Supervised Knowledge Transfer from ITSELF

A drawback of our self-supervised loss function is that, unlike supervised loss functions such as binary cross entropy, it is a non-convex function of the NN outputs[3]. As a result, it has a significantly larger number of local minima compared to the supervised loss function, but also a potentially exponential number of global minima, because an MPE problem can have multiple optimal solutions [37], all of which have the same loss function value. Thus, optimizing and regularizing using self-supervised loss is difficult compared to supervised loss, especially when the number of training examples is large.

Moreover, our experiments show that large datasets necessitate large, over-parameterized neural networks (NNs) to achieve near-optimal MPE solutions for all examples. However, when the training data is limited and the NN is sufficiently over-parameterized, our preliminary findings, along with theoretical and empirical results from prior studies [3, 6, 23, 27, 28], suggest that the NN is more likely to approach the global optima. Specifically, with a reasonably sized NN and a small dataset, the algorithm ITSELF tends to yield near-optimal MPE solutions. A further challenge with ITSELF is that even for small datasets, achieving convergence from a random initialization requires numerous iterations of gradient descent, rendering the training process inefficient and slow.

4.1 Teacher-Student Strategy

To address these challenges (using small datasets with ITSELF; designing better initialization for it; and using non-convex loss functions for training), we propose a two-network teacher-student strategy [7, 16, 20–22, 24, 39, 47, 52–54], where we have two networks with the same structure that are trained via mini-batch gradient updates. The teacher network is overfitted to the mini-batch using our self-supervised loss via the algorithm ITSELF, and the student network is subsequently trained with a supervised loss function such as binary cross entropy. By overfitting the teacher network via ITSELF on the mini-batch, we ensure that it finds near-optimal MPE assignments for all (unlabeled) examples in the mini-batch and eventually over the whole training dataset.

The student network then learns from the teacher's outputs, using them as soft labels in a supervised learning framework. This transfer of knowledge mitigates the optimization difficulties associated with the non-convex self-supervised loss, allowing the student network to achieve faster convergence and better generalization with a more manageable model size. Additionally, this strategy reduces the need for severe over-parameterization and extensive training iterations for the teacher network because it is operating on a smaller dataset. It also helps achieve better initialization for ITSELF.

[3] Note that we are referring to convexity with respect to the outputs, not the parameters of the NN.

Algorithm 1 GUided Iterative Dual LEarning with Self-supervised Teacher ($\mathcal{GUIDE}$)

Input: Training data $\mathcal{D}$, teacher $\mathcal{T}$ and student $\mathcal{S}$ having the same structure
Output: Trained student network $\mathcal{S}$
▷ Database DB stores the best MPE assignment and loss value for each example in $\mathcal{D}$
Initialize: Randomly initialize $\mathcal{T}$, $\mathcal{S}$, and DB
for each epoch **do**
  Sample a mini-batch $\mathcal{D}'$ from $\mathcal{D}$
  Update the parameters of $\mathcal{T}$ using the algorithm ITSELF (self-supervised loss) with Dataset $\mathcal{D}'$
  for each example $\mathbf{e}_i$ in $\mathcal{D}'$ **do**
    Make a forward-pass over $\mathcal{T}$ to get an MPE assignment $\mathbf{q}_i$ for $\mathbf{e}_i$
    Update the entry in DB for $\mathbf{e}_i$ with $\mathbf{q}_i$ if it has a lower loss value than the current entry
  end for
  Update the parameters of $\mathcal{S}$ using the mini-batch $\mathcal{D}'$ and labels from DB and a supervised loss
  $\mathcal{T} \leftarrow \mathcal{S}$ ▷ Initialize $\mathcal{T}$ with $\mathcal{S}$ for the next epoch
end for

4.2 Training Procedure

Our proposed training procedure, which we call $\mathcal{GUIDE}$, is detailed in Algorithm 1. The algorithm trains a two-network system comprising a teacher network ($\mathcal{T}$) and a student network ($\mathcal{S}$) with the same structure. The goal is to train the student network using a combination of self-supervised and supervised learning strategies. The algorithm takes as input the training data $\mathcal{D}$, along with the teacher and student networks, $\mathcal{T}$ and $\mathcal{S}$, respectively and outputs a trained network $\mathcal{S}$. A database (DB) is utilized to store the best MPE assignment and corresponding loss value for each example in $\mathcal{D}$. The parameters of $\mathcal{T}$ and $\mathcal{S}$, and the entries in DB, are randomly initialized at the start.

In each epoch, a mini-batch $\mathcal{D}'$ is sampled from the training data $\mathcal{D}$. The parameters of the teacher network $\mathcal{T}$ are then updated using the algorithm ITSELF (which uses a self-supervised loss), applied to the mini-batch $\mathcal{D}'$ (the mini-batch helps address large data issues associated with ITSELF). For each example $\mathbf{e}_i$ in $\mathcal{D}'$, we perform a forward-pass over $\mathcal{T}$ to obtain an MPE assignment $\mathbf{q}_i$. The database DB is subsequently updated with $\mathbf{q}_i$ if it has a lower loss value than the current entry for $\mathbf{e}_i$.

Following this, the parameters of the student network $\mathcal{S}$ are updated using the mini-batch $\mathcal{D}'$, the labels from DB, and a supervised loss function such as Binary Cross Entropy or $L2$ loss. Finally, the parameters of the teacher network $\mathcal{T}$ are reinitialized with the updated parameters of the student network $\mathcal{S}$ to prepare for the next epoch (addressing the initialization issue associated with ITSELF).

Thus, at a high level, Algorithm 1 leverages the strengths of both self-supervised and supervised learning to improve training efficiency and reduce the model complexity, yielding a student network $\mathcal{S}$. Moreover, at test time, the student network can serve as an initialization for ITSELF.

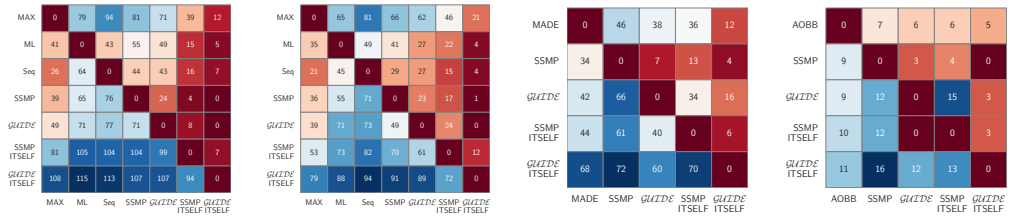
5 Experiments

This section evaluates the ITSELF method (see section 3.3), the $\mathcal{GUIDE}$ teacher-student training method (see section 4) and the method that uses only self-supervised training, which we call SSMP (see section 3.2). We benchmark these against various baselines, including neural network-based and traditional polynomial-time algorithms that directly operate on the probabilistic model. We begin by detailing our experimental framework, including competing methods, evaluation metrics, neural network architectures, and datasets.

5.1 Datasets and Graphical Models

We used twenty binary datasets extensively used in tractable probabilistic models literature [5, 18, 34, 50]—referred to as TPM datasets—for evaluating Probabilistic Circuits (PC)s and Neural Auto-Regressive Model (NAM). For the purpose of evaluating Probabilistic Graphical Models (PGM)s, we utilized high treewidth models from previous UAI inference competitions [14].

To train Sum Product Networks (SPNs), our choice of PCs, we employed the DeeProb-kit library [33], with SPN sizes ranging from 46 to 9666 nodes. For NAM, Masked Autoencoder for Distribution



(a) PCs: Initial Solutions (b) PCs: Hill-Climbing (c) NAMs (d) PGMs

Figure 1: Contingency Tables: Comparing Methods for MPE Problems Across PMs

Estimation (MADE) models were trained using PyTorch as described in [17]. In the case of Markov Networks (MNs), a specific category of PGMs, we utilize Gibbs Sampling, generating 8000, 1000, and 1000 examples for the training, testing, and validation sets, respectively. The query ratio (qr) is defined as the fraction of variables in the query set. For each PM, we varied qr with values from the set $\{0.1, 0.3, 0.5, 0.7, 0.8, 0.9\}$.

5.2 Baseline Methods and Evaluation Criteria

PCs - We employed three polynomial-time baseline methods from the PC and PGM literature as initial benchmarks [41, 45]. **MAX Approximation (MAX)** [45] transforms sum nodes into max nodes. During the upward pass, max nodes output the highest weighted value from their children. The downward pass, starting from the root, selects the child with the highest value at each max node and includes all children of product nodes. **Maximum Likelihood Approximation (ML)** [41] computes the marginal distribution $p_{\mathcal{M}}(Q_i|\mathbf{e})$ for each variable $Q_i \in \mathbf{Q}$, setting Q_i to its most likely value. **Sequential Approximation (Seq)** [41] iteratively assigns query variables according to an order o. At each step j, it selects the j-th query variable Q_j in o and assigns to it a value q_j such that $\mathrm{p}_{\mathcal{M}}(q_j|\mathbf{e}, \mathbf{y})$ is maximized, where $\mathbf{y}$ is an assignment of values to all query variables from 1 to $j-1$. Our study further assessed the impact of initializing stochastic hill climbing searches using solutions from all baseline approaches and our proposed methods for MPE inference, conducting 60-second searches for each MPE problem in our experiments, as detailed in Park and Darwiche [41].

NAMs - As a baseline, we used the stochastic hill-climbing search (HC). Similarly to the PC procedure, for each test example, we conducted a 60-second hill-climbing search, initializing query variables randomly and setting evidence variables based on the example.

PGMs - As a baseline we utilize the AND/OR Branch-and-Bound (AOBB)[36], employing the implementation described in Marinescu [35]. Given that AOBB is an anytime scheme, for each test example, we designated a 60-second time limit for the inference process.

Neural Baselines - Arya et al. [4] introduced Self-Supervised learning based MMAP solver for PCs (SSMP), which trains a neural network to handle queries on a fixed partition of variables on PCs. We proposed an extension of this approach for solving the any-MPE task in PMs (see section 3.2), where a single neural network is trained to answer any-MPE query. We use it as another neural baseline.

Evaluation Criteria - Competing approaches were compared using log-likelihood (LL) scores, calculated as $\ln p_{\mathcal{M}}(\mathbf{e}, \mathbf{q})$, and inference times for a given evidence $\mathbf{e}$ and query output $\mathbf{q}$.

5.3 Neural Network-Based Approaches

For each PM and query ratio, we implemented two neural network training protocols: SSMP and $\mathcal{GUIDE}$. We subjected each model to 20 training epochs, adhering to the established procedures for SSMP as delineated by Arya et al. [4]. Both protocols employed two distinct inference strategies, thus forming four neural-based variants. The first strategy consisted of a single forward pass through the network to estimate query variable values, as specified by Arya et al. [4]. The second strategy utilized our novel test-time optimization-based **ITSELF** approach for inference. For **ITSELF**, we undertook 100 optimization iterations or terminated earlier upon achieving loss convergence, applicable to both PCs and PGMs. In cases involving NAMs, the optimization iterations extended to 1,000, or concluded upon convergence.

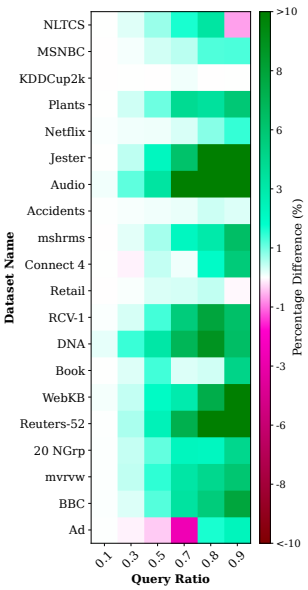
We standardized network architectures for PMs across all experiments. For PCs, we used a fully connected Neural Networks (NN) with three hidden layers (128, 256, 512 nodes). For NAMs and PGMs, a single hidden layer of 512 nodes was employed. All hidden layers featured ReLU activation, while the output layers used sigmoid functions with dropout for regularization [48]. Optimization was performed using the Adam optimizer [25], and models were implemented in PyTorch [43] on an NVIDIA A40 GPU.

Results for PCs: We compare methods—including three polynomial-time baselines, neural network-based SSMP, and our **ITSELF** and $\mathcal{GUIDE}$ methods—on 20 TPM datasets as shown in the contingency table in figure 1a (detailed results in the supplementary materials). We generated 120 test datasets for the MPE task using 20 PCs across 6 query ratios (qr). Each cell (i, j) in the table represents how often (out of 120) the method in row i outperformed the method in column j based on average log-likelihood scores. Any difference between 120 and the combined frequencies of cells (i, j) and (j, i) indicates cases where the compared methods achieved similar scores.

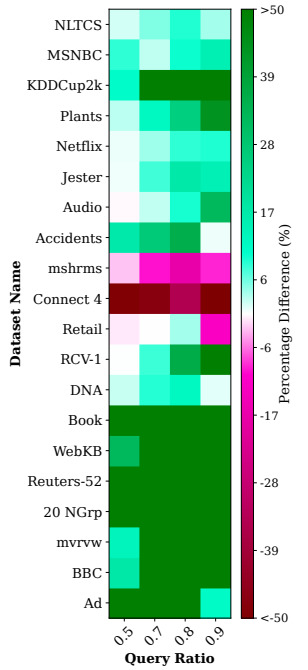
The contingency table for PC shows that the **ITSELF** methods outperform polynomial-time and traditional neural baselines. Specifically, $\mathcal{GUIDE}$ + **ITSELF** is superior to all the other methods in almost two-thirds of the 120 cases, while SSMP + **ITSELF** is better than both SSMP and $\mathcal{GUIDE}$ without **ITSELF**. However, the polynomial-time baseline MAX is better than both SSMP and $\mathcal{GUIDE}$ (note that these methods were used in Arya et al. [4]), highlighting **ITSELF**'s significant role in boosting model performance for the complex *any-MPE* task.

We compare MAX and $\mathcal{GUIDE}$ + **ITSELF** using a heatmap in Figure 2a. The y-axis presents datasets by variable count and the x-axis by query ratio. Each cell displays the percentage difference in mean LL scores between the methods, calculated as $\%\text{Diff.} = 100 \times (ll_{nn} - ll_{max})/|ll_{max}|$. From the heatmap in Figure 2a for PCs, we observe that $\mathcal{GUIDE}$ + **ITSELF** exhibit performance comparable to the MAX approximation when the query set size is small. As the problem complexity increases with an increase in query set size, our new method consistently outperforms MAX across all datasets, except for NLTCS and Tretail. Even when $\mathcal{GUIDE}$ + **ITSELF** underperforms compared to MAX (noted in 12 instances out of 120) the performance gap is very small, evidenced by sparse red cells in the heatmaps.

Further analysis in Figure 1b compares the performance of our proposed methods with various baselines as initialization strategies for Hill Climbing Search. The goal is to assess whether ITSELF and $\mathcal{GUIDE}$ enhance *anytime methods* to outperform other heuristic initialization techniques, with methods utilizing **ITSELF** proving superior in initializing local search-based algorithms.



(a) PC: $\mathcal{GUIDE}$ + **ITSELF** vs. MAX



(b) NAM: $\mathcal{GUIDE}$ + **ITSELF** vs. HC

Figure 2: Heatmaps showing LL Percentage Differences: Top—PC; Bottom—MADE.

Results for NAMs: Our evaluation, detailed in the contingency table in Figure 1c, examines the performance of several methods for NAM, including HC and two neural network methods, SSMP and $\mathcal{GUIDE}$, each with two inference schemes. We tested four neural-based schemes on 20 TPM datasets, generating 80 test datasets for the MPE task using 20 MADEs across four query ratios (qr).

Similar to the results observed with PC, the $\mathcal{GUIDE}$ + **ITSELF** method exhibits superior performance over the baselines and other neural inference schemes. HC outperforms SSMP, while $\mathcal{GUIDE}$ and SSMP + **ITSELF** are superior to HC.

The heatmaps in Figure 2b highlight the superior performance of $\mathcal{GUIDE}$ + **ITSELF** for NAMs, particularly in larger datasets where it outperforms the HC baseline by over 50% in most cases, as indicated by the dark green cells. The integration of $\mathcal{GUIDE}$-based learning with **ITSELF**-based inference consistently outperforms the baseline across most scenarios, with exceptions only in the Mushrooms, Connect 4, and Retail datasets. Thus, the $\mathcal{GUIDE}$ + **ITSELF** approach significantly enhances MPE query answering in NAM models.

Results for PGMs: In our evaluation, as detailed in the contingency table in 1d, we assessed the efficacy of various methods for PGMs, including AOBB and four neural-network-based methods, across four high-treewidth networks (details of these networks are provided in the supplement). To accomplish this, we constructed 16 test datasets for the MPE task by employing four PGMs across four query ratios (qr).

Similar to the outcomes observed with previous PMs, the methods employing **ITSELF** for inference consistently demonstrate enhanced performance compared to the baseline methods AOBB and SSMP in most scenarios. Both $\mathcal{GUIDE}$ and SSMP outperform AOBB in at least 50 percent of the tests.

Is Teacher Student Training Better than A Single Network Trained with Self-Supervised Loss? (SSMP versus $\mathcal{GUIDE}$): In our comparative analysis between SSMP and $\mathcal{GUIDE}$ across different models, we aim to evaluate the performance of $\mathcal{GUIDE}$ against the traditional neural network training methods used in SSMP. Using traditional inference schemes (i.e., one forward pass through the network), $\mathcal{GUIDE}$ consistently outperforms SSMP, demonstrating its superiority in 60% of scenarios for PCs, more than 80% for NAM models, and 75% for PGM models. When employing **ITSELF** for inference over the trained models, $\mathcal{GUIDE}$ continues to outperform SSMP, achieving better results in more than 75%, 85%, and 80% for PCs, NAMs, and PGMs, respectively.

Does Inference Time Optimization help? (One Pass versus Multiple Passes): Comparative analyses reveal that **ITSELF** consistently outperforms traditional single forward pass inference across various PMs. **ITSELF** with SSMP training outperforms the other methods in over 85% of PC cases, and more than 75% for NAM and PGM models. When trained using $\mathcal{GUIDE}$, **ITSELF** demonstrates even better results, achieving superior performance in nearly 90% of PC cases and 75% for both NAMs and PGMs. $\mathcal{GUIDE}$ with the **ITSELF** inference scheme emerges as the best method across all our experiments.

Finally, we present inference times in the supplement. For all the PMs, the neural based method that utilizes traditional inference are the quickest. For MADE, the method employing a $\mathcal{GUIDE}$-trained model with **ITSELF** is the second fastest. Similarly, in PGMs, the $\mathcal{GUIDE}$ + **ITSELF** method emerges as the third fastest, after SSMP + **ITSELF**; in PCs, MAX leads, slightly ahead of both $\mathcal{GUIDE}$ + **ITSELF** and SSMP + **ITSELF**, while ML and Seq record the longest inference times.

Summary: Our experiments demonstrate that $\mathcal{GUIDE}$ + **ITSELF** outperforms both polynomial-time and neural-based baselines across various PMs, as evidenced by higher log-likelihood scores. Specifically, **ITSELF** exceeds the capabilities of traditional forward pass inference in addressing the challenging task of answering *any-MPE* queries within a probabilistic model, highlighting the necessity of Inference Time Optimization. Additionally, the superiority of models trained with $\mathcal{GUIDE}$ over SSMP underscores the effectiveness of using a dual network approach that utilizes two loss functions to enhance the initial model quality and provide an optimal starting point for **ITSELF**.

6 Conclusion and Future Work

We introduced novel methods for answering Most Probable Explanation (MPE) queries in probabilistic models. Our approach employs self-supervised loss functions to represent MPE objectives, enabling tractable loss and gradient computations during neural network training. We also proposed a new inference time optimization technique, **ITSELF**, which iteratively improves the solution to the MPE problem via gradient updates. Additionally, we introduced a dual-network-based strategy that combines supervised and unsupervised training which we call $\mathcal{GUIDE}$ to provide better initialization for **ITSELF** and addressing various challenges associated with self-supervised training. Our method was tested on various benchmarks, including probabilistic circuits, MADE, and PGMs, using 20 binary datasets and high tree-width networks. It outperformed polytime baselines and other neural

methods, substantially in some cases. Additionally, it improved the effectiveness of stochastic hill climbing (local) search strategies.

Future work includes solving complex queries in Probabilistic Models (PM)s with constraints; training neural networks with losses from multiple PMs to embed their inference mechanisms; boosting performance by developing advanced encoding strategies for similar tasks; implementing sophisticated neural architectures tailored to PMs; etc.

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