Expressive Modeling Is Insufficient for Offline RL: A Tractable Inference Perspective

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Abstract

A popular paradigm for offline Reinforcement Learning (RL) tasks is to first fit the offline trajectories to a sequence model, and then prompt the model for actions that lead to high expected return. While a common consensus is that more expressive sequence models imply better performance, this paper highlights that *tractability*, the ability to exactly and efficiently answer various probabilistic queries, plays an equally important role. Specifically, due to the fundamental stochasticity from the offline data-collection policies and the environment dynamics, highly non-trivial conditional/constrained generation is required to elicit rewarding actions. While it is still possible to approximate such queries, we observe that such crude estimates significantly undermine the benefits brought by expressive sequence models. To overcome this problem, this paper proposes **Trifle** (**Tr**actable **I**nference for Off**l**in**e** RL), which leverages modern tractable probabilistic models to bridge the gap between good sequence models and high expected returns at evaluation time. Additionally, Trifle benefits significantly from modeling techniques that improve the accuracy of the sequence model. Empirically, Trifle achieves 7 state-of-the-art scores and the highest average scores in 9 Gym-MuJoCo benchmarks against strong baselines. Further, owing to its tractability, Trifle significantly outperforms prior approaches in stochastic environments and safe RL tasks with minimum algorithmic modifications.

1. Introduction

Recent advancements in deep generative models have opened up the possibility of solving offline Reinforcement Learning (RL) (Levine et al., 2020) tasks with sequence modeling techniques (termed RvS approaches). Specifically, we first fit a sequence model to the trajectories provided in an offline dataset. During evaluation, the model is tasked to sample actions with high expected returns given the current state. Leveraging modern deep generative models such as GPTs (Brown et al., 2020) and diffusion models (Ho et al., 2020), RvS algorithms have significantly boosted the performance on various discrete/continuous control problems (Ajay et al., 2022; Chen et al., 2021).

Despite its appealing simplicity, it is still unclear whether expressive modeling alone guarantees good performance of RvS algorithms, and if so, on what types of environments. Perhaps surprisingly, this paper discovers that many common failures of RvS algorithms are not caused by modeling problems. Instead, while useful information is encoded in the model during training, the model is unable to elicit such knowledge during evaluation. Specifically, this issue is reflected in two aspects: (i) *inability to accurately estimate the expected return* of a state and a corresponding action sequence to be executed given near-perfect learned transition dynamics and reward functions; (ii) even when accurate return estimates exist in the offline dataset and are learned by the model, it could still *fail to sample rewarding actions* during evaluation.[1] At the heart of such inferior evaluation-time performance is the fact that highly non-trivial conditional/constrained generation is required to stimulate high-return actions (Paster et al., 2022; Brandfonbrener et al., 2022). Therefore, other than expressiveness, the ability to efficiently and exactly answer various queries (e.g., computing the expected returns), termed *tractability*, plays an equally important role in RvS approaches.

Having observed that the lack of tractability is an essential cause of the underperformance of RvS algorithms, this paper studies *whether we can gain practical benefits from using Tractable Probabilistic Models (TPMs) (Poon & Domingos, 2011; Choi et al., 2020; Kisa et al., 2014), which by design support exact and efficient computation of certain queries?* We answer the question in its affirmative by showing that we can leverage a class of TPMs that support computing

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[1]Both observations are supported by empirical evidence as illustrated in Section 3.

arbitrary marginal probabilities to significantly mitigate the inference-time suboptimality of RvS approaches. The proposed algorithm **Trifle** (**Tr**actable **I**nference for Off**l**in**e** RL) has three main contributions:

Emphasizing the important role of tractable models in offline RL. This is the first paper that demonstrates the possibility of using TPMs on complex offline RL tasks. The superior empirical performance of Trifle suggests that expressive modeling is not the only aspect that determines the performance of RvS algorithms, and motivates the development of better inference-aware RvS approaches.

Competitive empirical performance. Compared against strong offline RL baselines (including RvS, imitation learning, and offline temporal-difference algorithms), Trifle achieves the state-of-the-art result on 7 out of 9 Gym-MuJoCo benchmarks (Fu et al., 2020) and outperforms all baselines in terms of the average score.

Generalizability to stochastic environments and safe-RL tasks. Trifle can be extended to tackle stochastic environments as well as safe RL tasks with minimum algorithmic modifications. Specifically, we evaluate Trifle in 2 stochastic OpenAI-Gym (Brockman et al., 2016) environments and action-space-constrained MuJoCo environments, and demonstrate its superior performance against all baselines.

2. Preliminaries

Offline Reinforcement Learning. In Reinforcement Learning (RL), an agent interacts with an environment that is defined by a Markov Decision Process (MDP) $\langle \mathcal{S}, \mathcal{A}, \mathcal{R}, \mathcal{P}, d_0 \rangle$ to maximize its cumulative reward. Specifically, the $\mathcal{S}$ is the state space, $\mathcal{A}$ is the action space, $\mathcal{R} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is the reward function, $\mathcal{P} : \mathcal{S} \times \mathcal{A} \to \mathcal{S}$ is the transition dynamics, and d_0 is the initial state distribution. Our goal is to learn a policy $\pi(a|s)$ that maximizes the expected return $\mathbb{E}[\sum_{t=0}^{T} \gamma^t r_t]$, where $\gamma \in (0, 1]$ is a discount factor and T is the maximum number of steps.

Offline RL (Levine et al., 2020) aims to solve RL problems where we cannot freely interact with the environment. Instead, we receive a dataset of trajectories collected using unknown policies. An effective learning paradigm for offline RL is to treat it as a sequence modeling problem (termed RL via Sequence Modeling or RvS methods) (Janner et al., 2021; Chen et al., 2021; Emmons et al., 2021). Specifically, we first learn a sequence model on the dataset, and then sample actions conditioned on past states and high future returns. Since the models typically do not encode the entire trajectory, an estimated value or return-to-go (RTG) (i.e., the Monte Carlo estimate of the sum of future rewards) is also included for every state-action pair, allowing the model to estimate the return at any time step.

Tractable Probabilistic Models. Tractable Probabilistic Models (TPMs) are generative models that are designed to efficiently and exactly answer a wide range of probabilistic queries (Poon & Domingos, 2011; Choi et al., 2020; Rahman et al., 2014). One example class of TPMs is Hidden Markov Models (HMMs) (Rabiner & Juang, 1986), which support linear time (w.r.t. model size and input size) computation of marginal probabilities and more. Recent advancements have extensively pushed forward the expressiveness of modern TPMs (Liu et al., 2022; 2023; Correia et al., 2023), leading to competitive likelihoods on natural image and text datasets compared to even strong Variational Autoencoder (Vahdat & Kautz, 2020) and Diffusion model (Kingma et al., 2021) baselines. This paper leverages such advances and explores the benefits brought by TPMs in offline RL tasks.

Probabilistic Circuits. Probabilistic circuits (PCs) (Choi et al., 2020) are a general and unified computational framework for tractable probabilistic modeling, i.e., a wide class of TPMs can be represented as a PC. Similar to neural networks, PCs are also computation graphs containing millions of computation units, where constraints are imposed on their structures to enable efficient computation of various probabilistic queries. Generally, computing probabilistic queries involves executing specific feedforward/backward algorithms over the PC-defined computation graph. More details about TPMs and PCs are in Appx. E and F.

3. Tractability Matters in Offline RL

Practical RvS approaches operate in two main phases – training and evaluation. In the training phase, a sequence model is adopted to learn a joint distribution over trajectories of length T: $\{(s_t, a_t, r_t, \mathrm{RTG}_t)\}_{t=0}^{T}$.[2] During evaluation, at every time step t, the model is tasked to discover an action sequence $a_{t:T} := \{a_\tau\}_{\tau=t}^{T}$ (or just a_t) that has high expected return as well as high probability in the prior policy $p(a_{t:T}|s_t)$, which prevents it from generating out-of-distribution actions:

$$p(a_{t:T}|s_t, \mathbb{E}[V_t] \geq v) := \frac{1}{Z} \cdot \begin{cases} p(a_{t:T}|s_t) & \text{if cond 1,} \\ 0 & \text{otherwise,} \end{cases} \quad (1)$$

where cond 1 is $\mathbb{E}_{V_t \sim p(\cdot|s_t, a_t)}[V_t] \geq v$, Z is a normalizing constant, V_t is an estimate of the value at time step t, and v is a pre-defined scalar chosen to encourage high-return policies. Depending on the problem, V_t could be the labeled RTG from the dataset (e.g., RTG_t) or the sum of future rewards capped with a value estimate (e.g., $\sum_{\tau=t}^{T-1} r_\tau + \mathrm{RTG}_T$) (Emmons et al., 2021; Janner et al., 2021).

The above definition naturally reveals two key challenges in RvS approaches: (i) *training-time optimality* (i.e., "expressivity"): how well can we fit the offline trajectories, and

[2] To minimize computation cost, we only model truncated trajectories of length K ($K < T$) in practice.

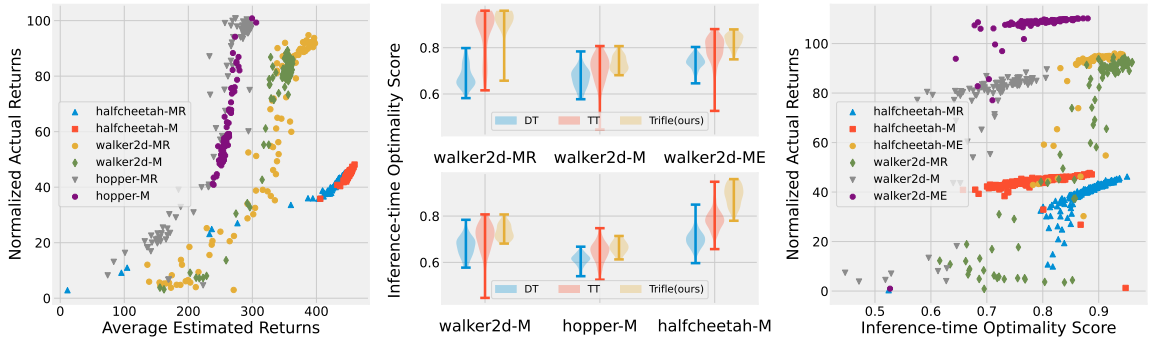


Figure 1: RvS approaches suffer from inference-time suboptimality. **Left:** There is a strong positive correlation between the average estimated returns by Trajectory Transformers (TT) and the actual returns in 6 Gym-MuJoCo environments (MR, M, and ME denote medium-replay, medium, and medium-expert, respectively), which suggests that the sequence model can distinguish rewarding actions from the others. **Middle:** Despite being able to recognize high-return actions, both TT and DT (Chen et al., 2021) fail to consistently sample such action, leading to bad inference-time optimality; Trifle consistently improves the inference-time optimality score. **Right:** We substantiate the relationship between low inference-time optimality scores and unfavorable environmental outcomes by showing a strong positive correlation between them.

(ii) *inference-time optimality*: whether actions can be unbiasedly and efficiently sampled from Equation (1). While extensive breakthroughs have been achieved to improve the training-time optimality (Ajay et al., 2022; Chen et al., 2021; Janner et al., 2021), it remains unclear whether the non-trivial constrained generation task of Equation (1) hinders inference-time optimality. In the following, we present two general scenarios where existing RvS approaches underperform as a result of suboptimal inference-time performance. We attribute such failures to the fact that these models are limited to answering certain query classes (e.g., autoregressive models can only compute next token probabilities), and explore the potential of *tractable* probabilistic models for offline RL tasks in the following sections.

Scenario #1 We first consider the case where the labeled RTG belongs to a (near-)optimal policy. In this case, Equation (1) can be simplified to $p(a_t|s_t, \mathbb{E}[V_t] \geq v)$ (choose $V_t := \text{RTG}_t$) since one-step optimality implies multi-step optimality. In practice, although the RTGs are suboptimal, the predicted values often match well with the actual returns achieved by the agent. Take Trajectory Transformer (TT) (Janner et al., 2021) as an example, Figure 1 (left) demonstrates a strong positive correlation between its predicted returns (x-axis) and the actual cumulative rewards (y-axis) on six MuJoCo (Todorov et al., 2012) benchmarks, suggesting that the model has learned the "goodness" of most actions. In such cases, the performance of RvS algorithms depends mainly on their inference-time optimality, i.e., whether they can efficiently sample actions with high *predicted* returns. Specifically, let a_t be the action taken by a RvS algorithm at state s_t, and $R_t := \mathbb{E}[\text{RTG}_t]$ is the corresponding estimated expected value. We define a proxy of inference-time optimality as the quantile value of R_t in the estimated state-conditioned value distribution $p(V_t|s_t)$.[3] The higher the quantile value, the more frequent the RvS algorithm samples actions with high estimated returns.

We evaluate the inference-time optimality of Decision Transformers (DT) (Chen et al., 2021) and Trajectory Transformers (TT) (Janner et al., 2021), two widely used RvS algorithms, on various environments and offline datasets from the Gym-MuJoCo benchmark suite (Fu et al., 2020). Perhaps surprisingly, as shown in Figure 1 (middle), the inference-time optimality is averaged (only) around 0.7 (the maximum possible value is 1.0) for most settings. And these runs with low inference-time optimality scores receive low environment returns (Fig. 1 (right)).

Scenario #2 Achieving inference-time optimality becomes even harder when the labeled RTGs are suboptimal (e.g., they come from a random policy). In this case, even estimating the expected future return of an action sequence becomes highly intractable, especially when the transition dynamics of the environment are stochastic. Specifically, to evaluate a state-action pair (s_t, a_t), since RTG_t is uninformative, we need to resort to the multi-step estimate $V_t^{\text{m}} := \sum_{\tau=t}^{t'-1} r_\tau + \text{RTG}_{t'}$ $(t' > t)$, where the actions $a_{t:t'}$ are jointly chosen to maximize the expected return. Take autoregressive models as an example. Since the variables are arranged following the sequential order $\ldots, s_t, a_t, r_t, \text{RTG}_t, s_{t+1}, \ldots$, we need to explicitly sample $s_{t+1:t'}$ before proceed to compute the rewards and the RTG in V_t^{m}. In stochastic environments, estimating $\mathbb{E}[V_t^{\text{m}}]$ could suffer from high variance as the stochasticity from the intermediate states accumulates over time.

[3] Due to the large action space, it is impractical to compute $p(V_t|s_t) := \sum_{a_t} p(V_t|s_t, a_t) \cdot p(a_t|s_t)$. Instead, in the following illustrative experiments, we train an additional GPT model $p(V_t|s_t)$ using the offline dataset.

As we shall illustrate in Section 6.2, compared to environments with near-deterministic transition dynamics, estimating the expected returns in stochastic environments using intractable sequence models is hard, and Trifle can significantly mitigate this problem with its ability to marginalize out intermediate states and compute $\mathbb{E}[V_t^{\mathrm{im}}]$ in closed-form.

4. Exploiting Tractable Models

The previous section demonstrates that apart from modeling, inference-time suboptimality is another key factor that causes the underperformance of RvS approaches. Given such observations, a natural follow-up question is *whether/how more tractable models can improve the evaluation-time performance in offline RL tasks?* While there are different types of tractabilities (i.e., the ability to compute different types of queries), this paper focuses on studying the additional benefit of *exactly* computing *arbitrary* marginal/condition probabilities. This strikes a proper balance between learning and inference as we can train such a tractable yet expressive model thanks to recent developments in the TPM community (Liu et al., 2022; Correia et al., 2023). Note that in addition to proposing a competitive RvS algorithm, we aim to highlight the necessity and benefit of using more tractable models for offline RL tasks, and encourage future developments on both inference-aware RvS methods and better TPMs. As a direct response to the two failing scenarios identified in Section 3, in the following, we first demonstrate how tractability could help even when the labeled RTGs are (near-)optimal (Sec. 4.1). We then move on to the more general case where we need to use multi-step return estimates to account for biases in the labeled RTGs (Sec. 4.2).

4.1. From the Single-Step Case...

Consider the case where the RTGs are optimal. Recall from Section 3 that our goal is to sample actions from $p(a_t|s_t, \mathbb{E}[V_t] \geq v)$ (where $V_t := \mathrm{RTG}_t$). Prior works use two typical ways to approximately sample from this distribution. The first approach directly trains a model to generate return-conditioned actions: $p(a_t|s_t, \mathrm{RTG}_t)$ (Chen et al., 2021). However, since the RTG given a state-action pair is stochastic,[4] sampling from this RTG-conditioned policy could result in actions with a small probability of getting a high return, but with a low expected return (Paster et al., 2022; Brandfonbrener et al., 2022).

An alternative approach leverages the ability of sequence models to accurately estimate the expected return (i.e., $\mathbb{E}[\mathrm{RTG}_t]$) of state-action pairs (Janner et al., 2021). Specifically, we first sample from a prior distribution $p(a_t|s_t)$, and then reject actions with low expected returns. Such rejection sampling-based methods typically work well when the action space is small (in which we can enumerate all actions) or the dataset contains many high-rewarding trajectories (in which the rejection rate is low). However, the action could be multi-dimensional and the dataset typically contains many more low-return trajectories in practice, rendering the inference-time optimality score low (cf. Fig. 1).

Having examined the pros and cons of existing approaches, we are left with the question of whether a tractable model can improve sampled actions (in this single-step case). We answer it with a mixture of positive and negative results: while computing $p(a_t|s_t, \mathbb{E}[V_t] \geq v)$ is NP-hard even when $p(a_t, V_t|s_t)$ follows a simple Naive Bayes distribution, we can design an approximation algorithm that samples high-return actions with high probability in practice. We start with the negative result.

Theorem 1. *Let $a_t := \{a_t^i\}_{i=1}^k$ be a set of k boolean variables and V_t be a categorical variables with two categories 0 and 1. For some s_t, assume the joint distribution over a_t and V_t conditioned on s_t follows a Naive Bayes distribution: $p(a_t, V_t|s_t) := p(V_t|s_t) \cdot \prod_{i=1}^k p(a_t^i|V_t, s_t)$, where a_t^i denotes the i^{th} variable of a_t. Computing any marginal over the random variables is tractable yet conditioning on the expectation $p(a_t|s_t, \mathbb{E}[V_t] \geq v)$ is NP-hard.*

The proof is given in Appx. A. While it seems hard to directly draw samples from $p(a_t|s_t, \mathbb{E}[V_t] \geq v)$, we propose to improve the aforementioned rejection sampling-based method by adding a correction term to the original proposal distribution $p(a_t|s_t)$ to reduce the rejection rate. Specifically, the prior is often represented by an autoregressive model such as GPT: $p_{\mathrm{GPT}}(a_t|s_t) := \prod_{i=1}^k p_{\mathrm{GPT}}(a_t^i|s_t, a_t^{<i})$, where k is the number of action variables and a_t^i is the ith variable of a_t. We sample every dimension of a_t autoregressively following:

$$\forall i \in \{1, \ldots, k\} \quad \tilde{p}(a_t^i|s_t, a_t^{<i}; v) := \frac{1}{Z} \cdot p_{\mathrm{GPT}}(a_t^i|s_t, a_t^{<i}) \cdot p_{\mathrm{TPM}}(V_t \geq v|s_t, a_t^{\leq i}), \quad (2)$$

where Z is a normalizing constant and $p_{\mathrm{TPM}}(V_t \geq v|s_t, a_t^{\leq i})$ is a correction term that leverages the ability of the TPM to compute the distribution of V_t given incomplete actions (i.e., evidence on a subset of action variables). Note that while Equation (2) is mathematically identical to $p(a_t|s_t, V_t \geq v)$ when $p = p_{\mathrm{TPM}} = p_{\mathrm{GPT}}$, this formulation gives us the flexibility to use the prior policy (i.e., $p_{\mathrm{GPT}}(a_t^i|s_t, a_t^{<i})$) represented by more expressive autoregressive generative models. Further, as shown in Figure 1 (middle), compared to using $p(a_t|s_t)$ (as done by TT), the inference-time optimality scores increase significantly when using the distribution specified by Equation (2) (as done by Trifle) across various Gym-MuJoCo benchmarks.

[4] This is true unless (i) the policy that generates the offline dataset is deterministic, (ii) the transition dynamics is deterministic, and (iii) the reward function is deterministic.

4.2. ...To the Multi-Step Case

Recall that when the labeled RTGs are suboptimal, our goal is to sample from $p(a_{t:t'}|s_t, \mathbb{E}[V_t^{\mathrm{m}}] \geq v)$ ($t' > t$), where $V_t^{\mathrm{m}} := \sum_{\tau=t}^{t'-1} r_\tau + \mathrm{RTG}_{t'}$ is the multi-step value estimate. However, as elaborated in the second scenario in Section 3, it is hard even to evaluate the expected return of an action sequence due to the inability to marginalize out intermediate states $s_{t+1:t'}$. Empowered by TPMs, we can readily solve this problem by computing the expectation in linear time:

$$\mathbb{E}\big[V_t^{\mathrm{m}}\big] = \sum_{\tau=t}^{t'-1} \mathbb{E}_{r_\tau \sim p(\cdot|s_t, a_{t:t'})}\big[r_\tau\big] + \mathbb{E}_{\mathrm{RTG}_{t'} \sim p(\cdot|s_t, a_{t:t'})}\big[\mathrm{RTG}_{t'}\big].$$

We are now left with the same problem discussed in the single-step case – how to sample actions with high expected returns (i.e., $\mathbb{E}[V_t^{\mathrm{m}}]$). Similar to Equation (2), we add correction terms that bias the action (sequence) distribution towards high expected returns. Specifically, we augment the original (joint) action probability $\prod_{\tau=t}^{t'} p(a_\tau|s_t, a_{<\tau})$ with terms of the form $p(V_t^{\mathrm{m}} \geq v|s_t, a_{\leq\tau})$, which leads to:

$$\tilde{p}(a_{t:t'}|s_t; v) := \prod_{\tau=t}^{t'} \tilde{p}(a_\tau|s_t, a_{<\tau}; v),$$

where $\tilde{p}(a_\tau|s_t, a_{<\tau}; v) \propto p(a_\tau|s_t, a_{<\tau}) \cdot p(V_t^{\mathrm{m}} \geq v|s_t, a_{\leq\tau})$; $a_{<\tau}$ and $a_{\leq\tau}$ represent $a_{t:\tau-1}$ and $a_{t:\tau}$, respectively.[5] In practice, while we compute $p(V_t^{\mathrm{m}} \geq v|s_t, a_{\leq\tau})$ using the TPM, $p(a_\tau|s_t, a_{<\tau}) = \mathbb{E}_{s_{t+1:\tau}}[p(a_\tau|s_{\leq\tau}, a_{<\tau})]$ can either be computed exactly with the TPM or approximated (via Monte Carlo estimation over $s_{t+1:\tau}$) using an autoregressive generative model. In summary, we approximate samples from $p(a_{t:t'}|s_t, \mathbb{E}[V_t] \geq v)$ by first sampling from $\tilde{p}(a_{t:t'}|s_t; v)$, and then rejecting samples whose (predicted) expected return is smaller than v.

5. Practical Implementation with TPMs

The previous section has demonstrated how to efficiently sample from the expected-value-conditioned policy (Eq. 1). Based on this sampling algorithm, this section further introduces the proposed algorithm **Trifle** (**Tr**actable **I**nference for Off**l**in**e** RL). The high-level idea of Trifle is to obtain good action (sequence) candidates from $p(a_t|s_t, \mathbb{E}[V] \geq v)$, and then use beam search to further single out the most rewarding action. Intuitively, by the definition in Equation (1), the candidates are both rewarding and have relatively high likelihoods in the offline dataset, which ensures the actions are within the offline data distribution and prevents overconfident estimates during beam search.

[5] We approximate $p(V_t^{\mathrm{m}} \geq v|s_t, a_{\leq\tau})$ by assuming that the variables $\{r_t, \ldots, r_{t'-1}, \mathrm{RTG}_{t'}\}$ are independent. Specifically, we first compute $\{p(r_\tau|s_t, a_{\leq\tau})\}_{\tau=t}^{t'-1}$ and $p(\mathrm{RTG}_{t'}|s_t, a_{\leq\tau})$, and then sum up the random variables assuming that they are independent. This introduces no error for deterministic environments and remains a decent approximation for stochastic environments.

Beam search maintains a set of N (incomplete) sequences each starting as an empty sequence. For ease of presentation, we assume the current time step is 0. At every time step t, beam search replicates each of the N actions sequences into $\lambda \in \mathbb{Z}^+$ copies and appends an action a_t to every sequence. Specifically, for every partial action sequence $a_{<t}$, we sample an action following $p(a_t|s_0, a_{<t}, \mathbb{E}[V_t] \geq v)$, where V_t can be either the single-step or the multi-step estimate depending on the task. Now that we have $\lambda \cdot N$ trajectories in total, the next step is to evaluate their expected return, which can be computed exactly using the TPM (see Sec. 4.2). The N-best action sequences are kept and proceed to the next time step. After repeating this procedure for H time steps, we return the best action sequence. The first action in the sequence is used to interact with the environment.

Another design choice is the threshold value v. While it is common to use a fixed high return throughout the episode, we follow Ding et al. (2023) and use an adaptive threshold. Specifically, at state s_t, we choose v to be the ϵ-quantile value of $p(V_t|s_t)$, which is computed using the TPM.

Details of the adopted TPM This paper uses Probabilistic Circuits (PCs) (Choi et al., 2020) as an example TPM to demonstrate the effectiveness of Trifle. PCs can compute any marginal or conditional probability in time linear with respect to its size. We use a state-of-the-art PC structure called HCLT (Liu & Van den Broeck, 2021) and optimize its parameters using the latent variable distillation technique (Liu et al., 2022). Additional training/inference details are provided in Appx. F.

6. Experiments

This section takes gradual steps to study whether Trifle can mitigate the inference-time suboptimality problem in different settings. First, in the case where the labeled RTGs are good performance indicators (i.e., the single-step case), we examine whether Trifle can consistently sample more rewarding actions (Sec. 6.1). Next, we further challenge Trifle in highly stochastic environments, where existing RvS algorithms fail catastrophically due to the failure to account for the environmental randomness (Sec. 6.2). Finally, we demonstrate that Trifle can be directly applied to safe RL tasks (with action constraints) by effectively conditioning on the constraints (Sec. 6.3). Collectively, this section highlights the potential of TPMs on offline RL tasks.

6.1. Comparison to the State of the Art

As demonstrated in Section 3 and Figure 1, although the labeled RTGs in the Gym-MuJoCo (Fu et al., 2020) benchmarks are accurate enough to reflect the actual environmental return, existing RvS algorithms fail to effectively sample such actions due to their large and multi-dimensional action space. Figure 1 (middle) has demonstrated that Trifle achieves better inference-time optimality. This section

Table 1: Normalized Scores on the standard Gym-MuJoCo benchmarks. The results of Trifle are averaged over 12 random seeds (For DT-base and DT-Trifle, we adopt the same number of seeds as Chen et al. (2021)). Results of the baselines are acquired from their original papers.

Dataset	Environment	TT		TT(+Q)		DT		DD	IQL	CQL	%BC	TD3(+BC)
		base	Trifle	base	Trifle	base	Trifle					
Med-Expert	HalfCheetah	95.0±0.2	**95.1**±0.3	82.3±6.1	**89.9**±4.6	86.8±1.3	**91.9**±1.9	90.6	86.7	91.6	92.9	90.7
Med-Expert	Hopper	110.0±2.7	**113.0**±0.4	74.7±6.3	**78.5**±6.4	107.6±1.8	/	111.8	91.5	105.4	110.9	98.0
Med-Expert	Walker2d	101.9±6.8	**109.3**±0.1	109.3±2.3	**109.6**±0.2	108.1±0.2	**108.6**±0.3	108.8	109.6	108.8	109.0	110.1
Medium	HalfCheetah	46.9±0.4	**49.5**±0.2	48.7±0.3	**48.9**±0.3	42.6±0.1	**44.2**±0.7	49.1	47.4	44.0	42.5	48.3
Medium	Hopper	61.1±3.6	**67.1**±4.3	55.2±3.8	**57.8**±1.9	67.6±1.0	/	79.3	66.3	58.5	56.9	59.3
Medium	Walker2d	79.0±2.8	**83.1**±0.8	82.2±2.5	**84.7**±1.9	74±1.4	**81.3**±2.3	82.5	78.3	72.5	75.0	83.7
Med-Replay	HalfCheetah	41.9±2.5	**45.0**±0.3	48.2±0.4	**48.9**±0.3	36.6±0.8	**39.2**±0.4	39.3	44.2	45.5	40.6	44.6
Med-Replay	Hopper	91.5±3.6	**97.8**±0.3	83.4±5.6	**87.6**±6.1	82.7±7.0	/	100.0	94.7	95.0	75.9	60.9
Med-Replay	Walker2d	82.6±6.9	**88.3**±3.8	84.6±4.5	**90.6**±4.2	66.6±3.0	**73.5**±0.1	75.0	73.9	77.2	62.5	81.8
Average Score		78.9	**83.1**	74.3	77.4	74.7	/	81.8	77.0	77.6	74.0	75.3

further examines whether higher inference-time optimality scores could consistently lead to better performance when building Trifle on top of different RvS algorithms, i.e., combining p_{TPM} (cf. Eq. 2) with different prior policies p_{GPT} trained by the corresponding RvS algorithm.

Environment setup The Gym-MuJoCo benchmark suite collects trajectories in 3 locomotion environments (HalfCheetah, Hopper, Walker2D) and constructs 3 datasets (Medium-Expert, Medium, Medium-Replay) for every environment, which results in $3 \times 3 = 9$ tasks. For every environment, the main difference between the datasets is the quality of its trajectories. Specifically, the dataset "Medium" records 1 million steps collected from a Soft Actor-Critic (SAC) (Haarnoja et al., 2018) agent. The "Medium-Replay" dataset adopts all samples in the replay buffer recorded during the training process of the SAC agent. The "Medium-Expert" dataset mixes 1 million steps of expert demonstrations and 1 million suboptimal steps generated by a partially trained SAC policy or a random policy. The results are normalized to ensure that the well-trained SAC model has a 100 score and the random policy has a 0 score.

Baselines We build Trifle on top of three effective RvS algorithms: Decision Transformer (DT) (Chen et al., 2021), Trajectory Transformer (TT) (Janner et al., 2021) as well as its variant TT(+Q) where the RTGs estimated by summing up future rewards in the trajectory are replaced by the Q-values generated by a well-trained IQL agent (Kostrikov et al., 2021). In addition to the above base models, we also compare Trifle against many other strong baselines: (i) Decision Diffuser (DD) (Ajay et al., 2022), which is also a competitive RvS method; (ii) Offline TD learning methods IQL (Kostrikov et al., 2021) and CQL (Kumar et al., 2020); (iii) Imitation learning methods like the variant of BC (Pomerleau, 1988) which only uses 10% of trajectories with the highest return, and TD3(+BC) (Fujimoto et al., 2019).

Since the labeled RTGs are informative enough about the "goodness" of actions, we implement Trifle by adopting the single-step value estimate following Section 4.1, where we replace p_{GPT} with the policy of the three adopted base methods, i.e., $p_{\mathrm{TT}}(a_t|s_t)$, $p_{\mathrm{TT(+Q)}}(a_t|s_t)$ and $p_{\mathrm{DT}}(a_t|s_t)$.

Empirical Insights Results are shown in Table 1.[6] First, to examine the benefit brought by TPMs, we compare Trifle with three base policies, as the main algorithmic difference is the use of the improved proposal distribution (Eq. 2) for sampling actions. We can see that Trifle not only achieves a large performance gain over TT and DT in all environments, but also significantly outperforms TT(+Q) where we have access to more accurate labeled values, indicating that Trifle can enhance the inference-time optimality of base policy reliably and benefit from any improvement of the training-time optimality.

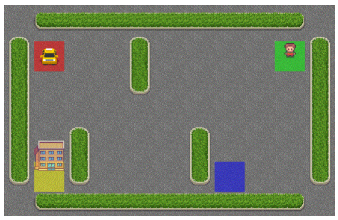
Moreover, compared with all baselines, Trifle achieves the highest average score of 83.1. It also succeeds in achieving 7 state-of-the-art scores out of 9 benchmarks.

6.2. Evaluating Trifle in Stochastic Environments

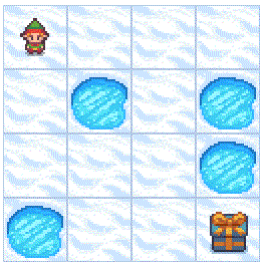
This section further challenges Trifle on stochastic environments with highly suboptimal trajectories as well as labeled RTGs in the offline dataset.As demonstrated in Section 3, in this case, it is even hard to obtain accurate value estimates due to the stochasticity of transition dynamics.Section 4.2 demonstrates the potential of Trifle to more reliably estimate and sample action sequences under suboptimal labeled RTGs and stochastic environments. This section examines this claim by comparing the five following algorithms:

(i) Trifle that adopts $V_t = \mathrm{RTG}_t$ (termed single-step Tri-

[6]When implementing DT-Trifle, we have to modify the output layer of DT to make it combinable with TPM. Specifically, the original DT directly predicts deterministic action while the modified DT outputs categorical action distributions like TT. In the 3 unreported hopper environments, the modified DT fails to achieve the original DT scores.



(a) Stochastic Taxi.



(b) Stochastic FrozenLake.

Methods	Taxi	FrozenLake		
		$\epsilon = 0.3$	$\epsilon = 0.5$	$\epsilon = 0.7$
m-Trifle	-57	0.61	0.59	0.37
s-Trifle	-99	0.62	0.60	0.34
TT	-182	0.63	0.25	0.12
DT	-388	0.51	0.32	0.10
DoC	-146	0.58	0.61	0.23

(c) Empirical performance on the stochastic environment.

Figure 2: Average returns on the stochastic environment. All the reported numbers are averaged over 1000 trials.

fle or **s-Trifle**); (ii) Trifle equipped with $V_t = \sum_{\tau=t}^{t'} r_\tau + \mathrm{RTG}_{t'}$ (termed multi-step Trifle or **m-Trifle**; see Appx. B.2 for additional details); (iii) TT (Janner et al., 2021); (iv) DT (Chen et al., 2021) (v) Dichotomy of Control (DoC) (Yang et al., 2022), an effective framework to deal with highly stochastic environments by designing a mutual information constraint for DT training, which is a representative baseline while orthogonal to our efforts.

We evaluate the above algorithms on two stochastic Gym environments: Taxi and FrozenLake. Here we choose the Taxi benchmark for a detailed analysis of whether and how Trifle could overcome the challenges discussed in Section 4.2. Among the first four algorithms, s-Trifle and DT do not compute the "more accurate" multi-step value, and TT approximates the value by Monte Carlo samples. Therefore, we expect their relative performance to be DT $\approx$ s-Trifle $<$ TT $<$ m-Trifle.

Environment setup We create a stochastic variant of the Gym-Taxi Environment (Dietterich, 2000). As shown in Figure 2a, a taxi resides in a grid world consisting of a passenger and a destination. The taxi is tasked to first navigate to the passenger's position and pick them up, and then drop them off at the destination.There are 6 discrete actions available at every step: (i) 4 navigation actions (North, South, East, or West), (ii) Pick-up, (iii) Drop-off. Whenever the agent attempts to execute a navigation action, it has 0.3 *probability of moving toward a randomly selected unintended direction*. At the beginning of every episode, the location of the taxi, the passenger, and the destination are randomly initialized randomly. The reward function is defined as follows: (i) -1 for each action undertaken; (ii) an additional +20 for successful passenger delivery; (iii) -4 for hitting the walls; (iv) -5 for hitting the boundaries; (v) -10 for executing Pick-up or Drop-off actions unlawfully (e.g., executing Drop-off when the passenger is not in the taxi).

Following the Gym-MuJoCo benchmarks, we collect offline trajectories by running a Q-learning agent (Watkins & Dayan, 1992) in the Taxi environment and recording the first 1000 trajectories that drop off the passenger successfully, which achieves an average return of -128.

Empirical Insights We first examine the accuracy of estimated returns for s-Trifle, m-Trifle, and TT. DT is excluded since it does not explicitly estimate the value of action sequences. Figure 3 illustrates the correlation between predicted and ground-truth returns of the three methods. First, s-Trifle performs the worst since it merely uses the inaccurate RTG_t to approximate the ground-truth return. Next, thanks to its ability to exactly compute the multi-step value estimates, m-Trifle outperforms TT, which approximates the multi-step value with Monte Carlo samples.

We proceed to evaluate their performance in the stochastic Taxi environment. As shown in Figure 2c, the relative performance of the first four algorithms is DT $<$ TT $<$ s-Trifle $<$ m-Trifle, which largely aligns with the anticipated results. The only "surprising" result is the superior performance of s-Trifle compared to TT. One plausible explanation for this behavior is that while TT can better estimate the given actions, the inferior performance is caused by its inability to efficiently sample rewarding actions.

Notably, Trifle also significantly outperforms the strong baseline DoC, demonstrating its potential in handling stochastic transitions. To verify this, we further evaluate Trifle on the stochastic FrozenLake environment. Apart from fixing the stochasticity level $p = \frac{1}{3}$,[7] the experiment design follows the DoC paper Yang et al. (2022). For data collection, we perturb the policy of a well-trained DQN (with an average return of 0.7) with the ϵ-greedy strategy. Here ϵ is a proxy of offline dataset quality and varies from 0.3 to 0.7. As shown in Figure 2c, when the offline dataset contains many successful trials ($\epsilon = 0.3$), all methods perform closely to the optimal policy. As the rollout policy becomes more suboptimal (with the increase of ϵ), the performances of DT and TT drop quickly, while Trifle still works robustly and outperforms all baselines.

6.3. Action-Space-Constrained Gym-MuJoCo Variants

This section demonstrates that Trifle can be readily extended to safe RL tasks by leveraging TPM's ability to compute conditional probabilities. Specifically, besides achieving high expected returns, safe RL tasks require additional con-

[7] When the agent takes an action, it has a probability p of moving in the intended direction and probability $0.5(1-p)$ of slipping to either perpendicular direction.

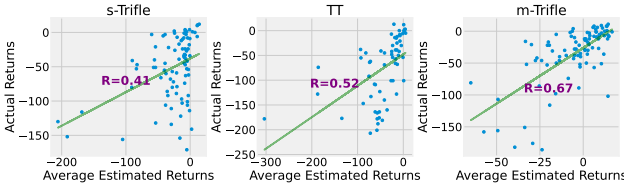


Figure 3: Correlation between average estimated returns and true environmental returns for s-Trifle (w/ single-step value estimates), TT, and m-Trifle (w/ multi-step value estimates) in the stochastic Taxi domain. R denotes the correlation coefficient. The results demonstrate that (i) multi-step value estimates (TT and m-Trifle) are better than single-step estimates (s-Trifle), and (ii) exactly computed multi-step estimates (m-Trifle) are better than approximated ones (TT) in stochastic environments.

straints on the action or states to be satisfied. Therefore, define the constraint as c, our goal is to sample actions from $p(a_t|s_t, \mathbb{E}[V_t] \geq v, c)$, which can be achieved by conditioning on c in the candidate action sampling process.

Environment setup In MuJoCo environments, each dimension of a_t represents the torque applied on a certain rotor of the hinge joints at timestep t. We consider action space constraints in the form of "value of the torque applied to the foot rotor $\leq A$", where $A = 0.5$ is a threshold value, for three MuJoCo environments: Halfcheetah, Hopper, and Walker2d. Note that there are multiple foot joints in Halfcheetah and Walker2d, so the constraint is applied to multiple action dimensions.[8] For all settings, we adopt the "Med-Expert" offline dataset as introduced in Section 6.1.

Empirical Insights The key challenge in these action-constrained tasks is the need to account for the constraints applied to other action dimensions when sampling the value of some action variable. For example, autoregressive models cannot take into account constraints added to variable a_t^{i+1} when sampling a_t^i. Therefore, while enforcing the action constraint is simple, it remains hard to simultaneously guarantee good performance. As shown in Table 2, owing to its ability to exactly condition on the action constraints, Trifle outperforms TT significantly across all three environments.

7. Related Work and Conclusion

In offline reinforcement learning tasks, our goal is to utilize a dataset collected by unknown policies to derive an improved policy without further interactions with the environment. Under this paradigm, we wish to generalize beyond naive imitation learning and stitch good parts of the behavior policy. To pursue such capabilities, many recent works frame offline RL tasks as conditional modeling problems that generate actions with high expected returns

[8]We only add constraints to the front joints in the Halfcheetah environment since the performance degrades significantly for all methods if the constraint is added to all foot joints.

Table 2: Normalized Scores on the Action-Space-Constrained Gym-MuJoCo Variants. The results of Trifle and TT are both averaged over 12 random seeds, with mean and standard deviations reported.

Dataset	Environment	Trifle	TT
Med-Expert	Halfcheetah	**81.9**$\pm$4.8	77.8$\pm$5.4
Med-Expert	Hopper	**109.6**$\pm$2.4	100.0$\pm$4.2
Med-Expert	Walker2d	**105.1**$\pm$2.3	103.6$\pm$4.9

(Chen et al., 2021; Ajay et al., 2022; Ding et al., 2023) or its proxies such as immediate rewards (Kumar et al., 2019; Schmidhuber, 2019; Srivastava et al., 2019). Recent advances in this line of work can be highly credited to the powerful expressivity of modern sequence models, since by accurately fitting past experiences, we can obtain 2 types of information that potentially imply high expected returns: (i) transition dynamics of the environment, which serves as a necessity for planning in model-based fashion (Chua et al., 2018), (ii) a decent policy prior which acts more reasonably than a random policy to improve from (Janner et al., 2021).

While prior works on model-based RL (MBRL) also leverage models of the transition dynamics and the reward function (Kaiser et al., 2019; Heess et al., 2015; Amos et al., 2021), the above-mentioned RvS approaches focus more on directly modeling the correlation between actions and their end-performance. Specifically, MBRL approaches focus on planning *only* with the environment model. Despite being theoretically appealing, MBRL requires heavy machinery to account for the accumulated errors during rollout (Jafferjee et al., 2020; Talvitie, 2017) and out-of-distribution problems (Zhao et al., 2021; Rigter et al., 2022). All these problems add a significant burden on the inference side, which makes MBRL algorithms less appealing in practice. In contrast, while RvS algorithms can mitigate this inference-time burden by directly learning the correlation between actions and returns, the suboptimality of labeled returns could significantly degrade their performance. One potential solution is by combining RvS algorithms with temporal-difference learning methods that can correct errors in the labeled returns (Zheng et al., 2022; Yamagata et al., 2023).

While also aiming to mitigate the problem caused by suboptimal labeled RTGs, our work takes a substantially different route — by leveraging TPMs to mitigate the inference-time computational burden (e.g., by efficiently computing the multi-step estimates). Specifically, we identified two major problems that are caused by the lack of tractability in the sequence models: one regarding estimating expected returns and the other for conditionally sampling actions. We show that with the ability to compute more queries efficiently, we can partially solve both identified problems. In summary, this work provides positive evidence of the potential benefit of tractable models on RvS algorithms, and encourages the development of more inference-aware RvS methods.

8. Impact Statements

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of our work, none of which we feel must be specifically highlighted here.

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Supplementary Material

A. Proof of Theorem 1

To improve the clarity of the proof, we first simplify the notations in Thm. 1: define $\mathbf{X}$ as the boolean action variables $a_t := \{a_t^i\}_{i=1}^k$, and Y as the variable V_t, which is a categorical variable with two categories 0 and 1. We can equivalently interpret Y as a boolean variable where the category 0 corresponds to `F` and 1 corresponds to `T`. Dropping the condition on s_t everywhere for notation simplicity, we have converted the problem into the following one:

Assume boolean variables $\mathbf{X} := \{X_i\}_{i=1}^k$ and Y follow a Naive Bayes distribution: $p(\boldsymbol{x}, y) := p(y) \cdot \prod_i p(x_i|y)$. We want to prove that computing $p(\boldsymbol{x}|\mathbb{E}[y] \geq v)$, which is defined as follows, is NP-hard.

$$p(\boldsymbol{x}|\mathbb{E}[y] \geq v) := \frac{1}{Z} \begin{cases} p(\boldsymbol{x}) & \text{if } \mathbb{E}_{y \sim p(\cdot|\boldsymbol{x})}[y] \geq v, \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

By the definition of Y as a categorical variable with two categories 0 and 1, we have

$$\mathbb{E}_{y \sim p(\cdot|\boldsymbol{x})}[y] = p(y = \texttt{T}|\boldsymbol{x}) \cdot 1 + p(y = \texttt{F}|\boldsymbol{x}) \cdot 0 = p(y = \texttt{T}|\boldsymbol{x}).$$

Therefore, we can rewrite $p(\boldsymbol{x}|\mathbb{E}[y] \geq v)$ as

$$p(\boldsymbol{x}|\mathbb{E}[y] \geq v) := \frac{1}{Z} \cdot p(\boldsymbol{x}) \cdot \mathbb{1}[p(y = \texttt{T}|\boldsymbol{x}) \geq v],$$

where $\mathbb{1}[\cdot]$ is the indicator function. In the following, we show that computing the normalizing constant $Z := \sum_{\boldsymbol{x}} p(\boldsymbol{x}) \cdot \mathbb{1}[p(y = \texttt{T}|\boldsymbol{x}) \geq v]$ is NP-hard by reduction from the number partition problem, which is a known NP-hard problem. Specifically, for a set of k numbers $n_1, \ldots, n_k$ ($\forall i, n_i \in \mathbb{Z}^+$), the number partition problem aims to decide whether there exists a subset $S \subseteq [k]$ (define $[k] := \{1, \ldots, k\}$) that partition the numbers into two sets with equal sums: $\sum_{i \in S} n_i = \sum_{j \notin S} n_j$.

For every number partition problem $\{n_i\}_{i=1}^k$, we define a corresponding Naive Bayes distribution $p(\boldsymbol{x}, y)$ with the following parameterization: $p(y = \texttt{T}) = 0.5$ and[9]

$$\forall i \in [k],\ p(x_i = \texttt{T}|y = \texttt{T}) = \frac{1 - e^{-n_i}}{e^{n_i} - e^{-n_i}} \ \text{ and } \ p(x_i = \texttt{T}|y = \texttt{F}) = e^{n_i} \cdot \frac{1 - e^{-n_i}}{e^{n_i} - e^{-n_i}}.$$

It is easy to verify that the above definitions lead to a valid Naive Bayes distribution. Further, we have

$$\forall i \in [k],\ \log \frac{p(x_i = \texttt{T}|y = \texttt{T})}{p(x_i = \texttt{T}|y = \texttt{F})} = n_i \ \text{ and } \ \log \frac{p(x_i = \texttt{F}|y = \texttt{T})}{p(x_i = \texttt{F}|y = \texttt{F})} = -n_i. \tag{4}$$

We pair every partition S in the number partition problem with an instance $\boldsymbol{x}$ such that $\forall i$, $x_i = \texttt{T}$ if $i \in S$ and $x_i = \texttt{F}$ otherwise. Choose $v = 2/3$, the normalizing constant Z can be written as

$$Z = \sum_{\boldsymbol{x} \in \mathsf{val}(\mathbf{X})} p(\boldsymbol{x}) \cdot \mathbb{1}\big[p(y = \texttt{T}|\boldsymbol{x}) \geq 2/3\big]. \tag{5}$$

Recall the one-to-one correspondence between S and $\boldsymbol{x}$, we rewrite $p(y = \texttt{T}|\boldsymbol{x})$ with the Bayes formula:

$$\begin{aligned} p(y = \texttt{T}|\boldsymbol{x}) &= \frac{p(y = \texttt{T}) \prod_i p(x_i|y = \texttt{T})}{p(y = \texttt{T}) \prod_i p(x_i|y = \texttt{T}) + p(y = \texttt{F}) \prod_i p(x_i|y = \texttt{F})}, \\ &= \frac{1}{1 + e^{-\sum_i \log \frac{p(x_i|y=\texttt{T})}{p(x_i|y=\texttt{F})}}}, \\ &= \frac{1}{1 + e^{-(\sum_{i \in S} n_i - \sum_{j \notin S} n_j)}}, \end{aligned}$$

where the last equation follows from Equation (4). After some simplifications, we have

$$\mathbb{1}\big[p(y = \texttt{T}|\boldsymbol{x}) \geq 2/3\big] = \mathbb{1}\big[\sum_{i \in S} n_i - \sum_{j \notin S} n_j \geq 1\big].$$

Plug back to Equation (5), we have

$$Z = \sum_{S \subseteq [k]} p(\boldsymbol{x}) \cdot \mathbb{1}\big[\sum_{i \in S} n_i - \sum_{j \notin S} n_j \geq 1\big],$$

[9] Note that we assume the naive Bayes model is parameterized using log probabilities.

$$= \frac{1}{2} \sum_{S \subseteq [k]} p(\boldsymbol{x}) \cdot \mathbb{1}\big[\sum_{i \in S} n_i - \sum_{j \notin S} n_j \neq 0\big],$$

where the last equation follows from the fact that (i) if $\boldsymbol{x}$ satisfy $\sum_{i \in S} n_i - \sum_{j \notin S} n_j \geq 1$ then $\bar{\boldsymbol{x}}$ has $\sum_{i \in S} n_i - \sum_{j \notin S} n_j \leq -1$ and vise versa, and (ii) $\sum_{i \in S} n_i - \sum_{j \notin S} n_j$ must be an integer.

Note that for every solution S to the number partition problem, $\sum_{i \in S} n_i - \sum_{j \notin S} n_j = 0$ holds. Therefore, there exists a solution to the defined number partition problem if $Z < \frac{1}{2}$. □

A.1. Training details of the adopted PC

A.1.1. The EM parameter learning algorithm

As mentioned above, a PC takes as input a sample $\boldsymbol{x}$ and outputs the corresponding probability $p_n(\boldsymbol{x})$. Given a dataset $\mathcal{D}$, the PC optimizer takes the PC parameters (consisting of sum edge parameters and input node/distribution parameters) as input and aims to maximize the MLE objective $\sum_{\boldsymbol{x} \in \mathcal{D}} \log p_n(x)$. Since PCs can be deemed as latent variable models with hierarchically nested latent space, the Expectation-Maximization (EM) algorithm is usually the default choice for PC parameter learning. Specifically, considering gradient-based EM, the feedforward computation of PCs which involves computing the log-likelihood $\log p_n(\boldsymbol{x})$ is differentiable and can be modeled by a computation graph. Therefore, we can efficiently compute its gradient w.r.t. each parameter via the backpropagation algorithm. Given a mini-batch of samples, the backpropagation algorithm is used to accumulate gradients for each parameter.

A.1.2. Training PC with Quantile-discretized MuJoCo Dataset

For the PC implemented in Trifle, we adopt the Hidden Chow-Liu Tree (HCLT) structure (Liu & Van den Broeck, 2021) and categorical distributions for its input nodes. We use the same quantile dataset discretized from the original Gym-MuJoCo dataset as TT, where each raw continuous variable is divided into 100 categoricals, and each categorical represents an equal amount of probability mass under the empirical data distribution (Janner et al., 2021).

During training, we first derive an HCLT structure given the data distribution and then utilize the latent variable distillation technique (LVD) to do parameter learning (Liu et al., 2022). Specifically, the neural embeddings used for LVD are acquired by a BERT-like Transformer (Devlin et al., 2018) trained with the Masked Language Model task. To acquire the embeddings of a subset of variables ϕ, we feed the Transformer with all other variables and concatenate the last Transformer layer's output for the variables ϕ. Please refer to the original paper for more details.

B. Additional Algorithmic Details of Trifle

B.1. Gym-MuJoCo

Sampling Details. We take the single-step value estimate by setting $V_t = \mathrm{RTG_t}$ and sample a_t from Equation (2). When training the GPT used for querying $p_{\mathrm{GPT}}(a_t^i | s_t, a_t^{<i})$, we adopt the same model specification and training pipeline as TT or DT. When computing $p_{\mathrm{TPM}}(V_t \geq v | s_t, a_t^{<i})$, we first use the learned PC to estimate $p(V_t | s_t)$ by marginalizing out intermediate actions $a_{t:t'}$ and select the ϵ-quantile value of $p(V_t | s_t)$ as our prediction threshold v for each inference step. Empirically we fixed ϵ for each environment and ϵ ranges from 0.1 to 0.3.

Beam Search Hyperparameters. The maximum beam width N and planning horizon H that Trifle uses across 9 MuJoCo tasks are 15 and 64, respectively.

B.2. Stochastic Taxi Environment

Except for s-Trifle, the sequence length K modeled by TT, DT, and m-Trifle is all equal to 7. The inference algorithm of TT follows that of the MuJoCo experiment and DT follows its implementation in the Atati benchmark. Notably, during evaluation, we condition the pretrained DT on 6 different RTGs ranging from -100 to -350 and choose the best policy resulting from RTG=-300 to report in Figure 2c. Beam width $N = 8$ and planning horizon $H = 3$ hold for TT and m-Trifle.

Table 3: Results on the stochastic Taxi environment. All the reported numbers are averaged over 1000 trials.

Methods	Episode return	# penalty	P(failure)
s-Trifle	-99	0.14	0.11
m-Trifle	**-57**	0.38	**0.02**
TT	-182	2.57	0.34
DT	-388	14.2	0.66
DoC	-146	**0**	0.28
dataset	-128	2.41	0

C. More evaluation metrics on the Taxi benchmark

Besides the episode return, we adopt two metrics to better evaluate the adopted methods: (i) #penalty: the average number of executing illegal actions within an episode; (ii) $P(\texttt{failure})$: the probability of failing to transport the passenger to the destination within 300 steps.

D. Algorithm tables

As introduced in Section 5, Trifle generally works in two phases: rejection sampling for action generation and beam search for action selection. The main algorithm is illustrated in Algorithm 1, where we take the current state s_t as well as the past trajectory $\tau_{<t}$ as input, utilize the specified value estimate f_v as a heuristic to guide beam search, and output the best trajectory. After that, we extract the current action a_t from the output trajectory to execute in the environment.

At the first step of the beam search, we will perform rejection sampling to obtain a candidate action set $\mathbf{a_t}$ (line 4 of Algorithm 1). The concrete rejection sampling procedure for s-Trifle is detailed in Algorithm 2. The major modification of m-Trifle compared to s-Trifle is the adoption of a multi-step value estimate instead of the single-step value estimate, which is also shown in Algorithm 3.

Algorithm 1 Trifle with Beam Search

Input: past trajectory $\tau_{<t}$, current state s_t, beam width N, beam horizon H, scaling ratio λ, sequence model $\mathcal{M}$, value function f_v ▷ $f_v = \mathbb{E}[V_t]$ for s-Trifle and $\mathbb{E}[V_t^m]$ for m-Trifle
Output: The best trajectory
Let $\mathbf{x_t} \leftarrow \texttt{concat}(\tau_{<t}, s_t).\texttt{reshape}(1, -1).\texttt{repeat}(N, \texttt{dim} = 0)$ ▷ Batchify the input trajectory and prepare for the beam search
Perform rejection sampling to obtain $\mathbf{a_t}$ ▷ cf. Algorithm 2
Initialize $X_0 = \texttt{concat}(\mathbf{x_t}, \mathbf{a_t})$
for $t = 1, ..., H$ **do**
  $X_{t-1} \leftarrow X_{t-1}.\texttt{repeat}(\lambda, \texttt{dim} = 0)$ ▷ Scale the number of trajectories from N to λN
  $\mathcal{C}_t \leftarrow \{\texttt{concat}(\mathrm{x}_{t-1}, x) \mid \forall \mathrm{x}_{t-1} \in X_{t-1}, \text{sample } x \sim p_{\mathcal{M}}(\cdot \mid \mathrm{x}_{t-1})\}$ ▷ Candidate next-token prediction
  $X_t \leftarrow \texttt{topk}_{X \in \mathcal{C}_t}\ (f_v(X), \texttt{k} = N)$ ▷ keep N most rewarding trajectories
end for
return $\texttt{argmax}_{X \in X_H}\ f_v(X)$

Algorithm 2 Rejection Sampling with Single-step Value Estimate

Input: past trajectory $\tau_{<t}$, current state s_t, dimension of action k, rejection rate $\delta > 0$
Output: The sampled action $a_t^{1:k}$
Let $x_t \leftarrow \texttt{concat}(\tau_{<t}, s_t)$
for $i = 1, ..., k$ **do**
  Compute $p_{\mathrm{GPT}}(a_t^i \mid x_t, a_t^{<i})$ Note that $a_t^{<1} = \varnothing$.
  Compute $p_{\mathrm{TPM}}(V_t \mid x_t, a_t^{<i}) = \sum_{a_t^{i:k}} p_{\mathrm{TPM}}(V_t \mid x_t, a_t^{1:k})$ ▷ The marginal can be efficiently computed by PC in linear time.
  Compute $v_\delta = \texttt{max}_v\{v \in \texttt{val}(V_t) \mid p_{\mathrm{TPM}}(V_t \geq v \mid x_t, a_t^{<i}) \geq 1 - \delta\}$, for each $a_t^i \in \texttt{val}(A_t^i)$
  Compute $\tilde{p}(a_t^i \mid x_t, a_t^{<i}; v_\delta) = \frac{1}{Z} \cdot p_{\mathrm{GPT}}(a_t^i \mid x_t, a_t^{<i}) \cdot p_{\mathrm{TPM}}(V_t \geq v_\delta \mid x_t, a_t^{\leq i})$ ▷ Apply Equation (2)
  Sample $a_t^i \sim \tilde{p}(a_t^i \mid x_t, a_t^{<i}; v_\delta)$
end for
return $a_t^{1:k}$

Algorithm 3 Multi-step Value Estimate

Input: $\tau_{\leq t} = (s_0, a_0, ..., s_t, a_t)$, sequence model $\mathcal{M}$, terminal timestep $t' > t$, discount γ
Output: The multi-step value estimate $\mathbb{E}\big[V_t^{\mathrm{m}}\big]$
Sample future actions $a_{t+1}, ..., a_{t'}$ from $\mathcal{M}$
Compute $p_{\mathrm{TPM}}(r_h \mid \tau_{\leq t}, a_{t+1:h}) = \sum_{s_{t+1:h}} p_{\mathrm{TPM}}(r_h \mid \tau_{\leq t'})$ for $h \in [t+1, t']$ ▷ Marginalize over intermediate states $s_{t+1:h}$
Compute $p_{\mathrm{TPM}}(\mathrm{RTG}_{t'} \mid \tau_{\leq t}, a_{t+1:t'}) = \sum_{s_{t+1:t'}} p_{\mathrm{TPM}}(\mathrm{RTG}_{t'} \mid \tau_{\leq t'})$
compute $\mathbb{E}\big[V_t^{\mathrm{m}}\big] = \sum_{h=t}^{t'} \gamma^{h-t} \mathbb{E}_{r_h \sim p_{\mathrm{TPM}}(\cdot \mid \tau_{\leq t}, a_{t+1:h})}\big[r_h\big] + \gamma^{t'+1-t} \mathbb{E}_{\mathrm{RTG}_{t'} \sim p_{\mathrm{TPM}}(\cdot \mid \tau_{\leq t}, a_{t+1:t'})}\big[\mathrm{RTG}_{t'}\big]$
return $\mathbb{E}\big[V_t^{\mathrm{m}}\big]$

E. Tractable Probabilistic Models (TPM)

A probabilistic model can be seen as a black box to answer queries about the quantities of interest of the joint probability distribution, such as computing marginal probability and performing maximum-a-posterior inference given some evidence. Tractable probabilistic models provide more guarantees when answering probabilistic queries: (i) it can perform exact inference to the model's distribution and no approximations are required. (ii) the query computation can be carried out efficiently, that is, in time polynomial (linear in many cases) in the size of the model. Notably, tractability is defined for a family of models only w.r.t. a class of queries and not an absolute property. Indeed, a tractable representation for one query class might not admit polynomial time inference for another query class.

F. Probabilistic Circuits (PC)

F.1. Definition of PC

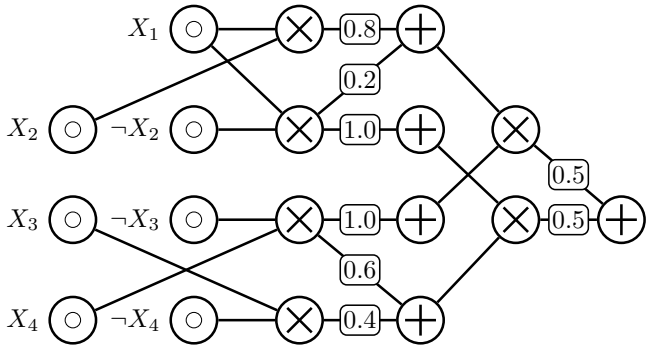

Figure 4: An example PC.

Probabilistic circuits (PCs) represent a wide class of TPMs that model probability distributions with a parameterized directed acyclic computation graph (DAG). Specifically, a PC $p(\mathbf{X})$ defines a joint distribution over a set of random variables $\mathbf{X}$ by a single root node n_r. A PC contains three kinds of computational nodes: *input*, *sum*, and *product*. As illustrated in Figure 4, the example PC in Figure 4 defines a joint distribution over 4 random variables X_1, X_2, X_3, X_4. Each leaf node in the DAG serves as an *input* node that encodes a univariate distribution (e.g., Guassian, Categorical), while *sum* nodes or *product* nodes are inner nodes, distinguished by whether they are doing mixture or factorization over their child distributions (denoted $\mathsf{in}(n)$). A PC defines a probability distribution in the following recursive way:

$$p_n(\boldsymbol{x}) := \begin{cases} f_n(\boldsymbol{x}) & \text{if } n \text{ is an input unit,} \\ \sum_{c \in \mathrm{in}(n)} \theta_{n,c} \cdot p_c(\boldsymbol{x}) & \text{if } n \text{ is a sum unit,} \\ \prod_{c \in \mathrm{in}(n)} p_c(\boldsymbol{x}) & \text{if } n \text{ is a product unit,} \end{cases}$$

where $\theta_{n,c}$ represents the parameter corresponding to edge (n, c) in the DAG. For sum units, we have $\sum_{c \in \mathsf{in}(n)} \theta_{n,c} = 1, \theta_{n,c} \geq 0$, and we assume w.l.o.g. that a PC alternates between the sum and product layers before reaching its inputs.

F.2. Tractability and Expressivity

Definition 1 (Decomposability)**.** A PC is decomposable if for every product unit n, its children have disjoint scopes:

$$\forall c_1, c_2 \in \mathsf{in}(n)\ (c_1 \neq c_2),\ \phi(c_1) \cap \phi(c_2) = \varnothing.$$

Definition 2 (Smoothness)**.** A PC is smooth if for every sum unit n, its children have the same scope:

$$\forall c_1, c_2 \in \mathsf{in}(n),\ \phi(c_1) = \phi(c_2).$$

Similar to neural networks, a large PC contains millions of computation units which enables expressive modeling. However, to guarantee the desired tractability, i.e., the ability to answer numerous probabilistic queries, some properties have to be imposed on their DAG structures. For instance, *smoothness* together with *decomposability* ensure that a PC can compute arbitrary marginal/conditional probabilities in linear time w.r.t. its size, i.e., the number of edges in its DAG. These are properties of the variable scope $\phi(n)$ of PC unit n, that is, the variable set comprising all its descendent nodes. Here we introduce how we execute marginalization inference in practice on a decomposable and smooth PC. Take the example PC in Figure 4 as an example, if we want to acquire $p_n(X_1, X_2, X_3)$ by marginalizing out X_4, we only need to set the output probability of X_4's input nodes to 1 and follow the same forward process as computing $p_n(X_1, X_2, X_3, X_4)$.

Notably, such structural constraints raise higher requirements for PC optimizers to acquire a comparably expressive PC. Thankfully, recent advancement achieved in PC modeling largely bridges this gap and makes it possible to model distributions of more complex data including the offline RL data.