Policy-Guided Diffusion

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Abstract

In many real-world settings, agents must learn from an *offline* dataset gathered by some prior behavior policy. Such a setting naturally leads to distribution shift between the behavior policy and the target policy being trained—requiring policy conservatism to avoid instability and overestimation bias. Autoregressive world models offer a different solution to this by generating synthetic, on-policy experience. However, in practice, model rollouts must be severely truncated to avoid compounding error. As an alternative, we propose *policy-guided diffusion.* Our method uses diffusion models to generate entire trajectories under the behavior distribution, applying *guidance* from the target policy to move synthetic experience further on-policy. We show that policy-guided diffusion represents a regularized form of the target distribution that balances action likelihood under both the target and behavior policies, leading to plausible trajectories with high target policy probability, while retaining a lower dynamics error than an offline world model baseline. Using synthetic experience from policy-guided diffusion as a drop-in substitute for real data, we demonstrate significant improvements in performance across a range of standard offline reinforcement learning algorithms and environments. Our approach provides an effective alternative to autoregressive offline world models, opening the door to the controllable generation of synthetic training data.

1 Introduction

A key obstacle to the real-world adoption of reinforcement learning (RL, Sutton & Barto, 2018) is its notorious sample inefficiency, preventing agents from being trained on environments with expensive or slow online data collection. A closely related challenge arises in environments where exploration, required by standard RL methods, is inherently dangerous, limiting their applicability. Yet many such settings come with an abundance of pre-collected or offline experience, gathered under one or more *behavior* policies (Yu et al., 2020). These settings enable the application of offline RL (Levine et al., 2020), where a policy is optimized from an offline dataset without access to the environment. However, the distribution shift between the *target* policy (i.e., the policy being optimized) and the collected data poses many challenges (Kumar et al., 2020; Kostrikov et al., 2021; Fujimoto et al., 2019).

In particular, *distribution shift* between the target and behavior policies leads to an out-of-sample issue: since the goal of offline RL is to *exceed* the performance of the behavior policy, the distribution of state-action pairs sampled by the target policy necessarily differs from that of the behavior policy, and its samples are therefore underrepresented (or unavailable) in the offline dataset. However, the maximizing nature of RL classically leads to overestimation bias when generalizing to rarely seen state-action pairs, resulting in an overly optimistic target policy. As a solution, most prior *model-free* work has proposed severe regularization of the target policy—such as penalizing value estimates in uncertain states (Kumar et al., 2020; An et al., 2021) or regularizing it towards the behavior policy (Fujimoto & Gu, 2021)—sacrificing target policy performance for stability.

In this paper, we focus on an alternative class of methods: generating *synthetic experience* to both augment the offline dataset and lessen the out-of-sample issue. Prior methods in this area use a
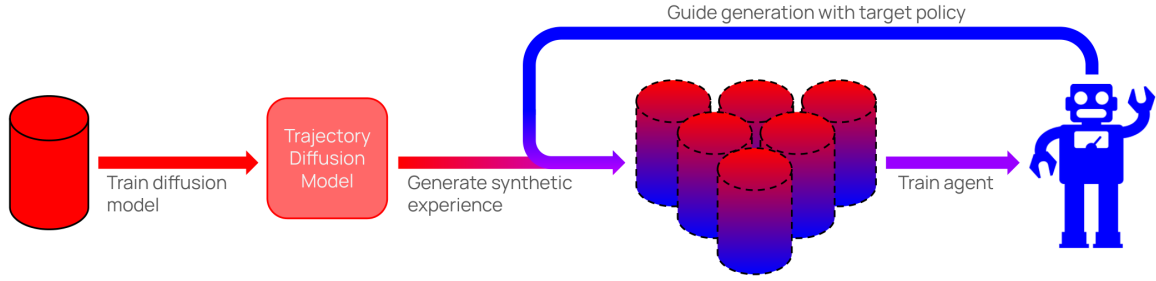
Figure 1: Offline reinforcement learning with policy-guided diffusion. Offline data from a behavior policy is first used to train a trajectory diffusion model. Synthetic experience is then generated with diffusion, guided by the target policy in order to move trajectories further on-policy. An agent is then trained for multiple steps on the synthetic dataset, before it is regenerated.

model-based approach (Yu et al., 2020; Kidambi et al., 2020; Ball et al., 2021, see Section 3.1), in which a single-step world model is learned from the offline dataset, which the target policy interacts with to generate synthetic on-policy training experience. While this allows the target policy to sample synthetic trajectories under its own action distribution, compounding model error forces these methods to severely truncate model rollouts to a handful of interactions. Thus, there are two options which trade off coverage and bias. The first is to roll out from the initial state, which is unbiased but lacks coverage. The second is to roll out from states randomly sampled from the data set, which increases coverage but introduces bias. Neither option fully addresses the difference in observed states between the behavior and target policy when deployed, nor the out-of-sample issue.

Instead, we propose *policy-guided diffusion* (PGD, Figure 1), which avoids compounding error by modeling entire trajectories (Section 3.2) rather than single-step transitions. To achieve this, we train a *diffusion model* on the offline dataset, from which we can sample synthetic trajectories under the behavior policy. However, while this addresses *data sparsity*, these trajectories are still *off-distribution* from our target policy. Therefore, inspired by classifier-guided diffusion (Dhariwal & Nichol, 2021), we apply *guidance* from the target policy to shift the sampling distribution towards that of the target policy. At each diffusion step, our guidance term directly increases the likelihood of synthetic actions under the target policy, while the diffusion model updates the entire trajectory towards those in the dataset. This yields a regularized target distribution that we call the *behavior-augmented target distribution*, ensuring actions do not diverge too far from the behavior policy, limiting generalization error. As a result, PGD does not suffer from compounding error, while also generating synthetic trajectories that are far more representative of the target policy. We illustrate this point in Figure 2.

Our approach results in consistent improvements in offline RL performance for agents trained on policy-guided synthetic data, compared to those trained on unguided synthetic or real data. We evaluate using the standard TD3+BC (Fujimoto & Gu, 2021) and IQL (Kostrikov et al., 2021) algorithms across a variety of D4RL (Fu et al., 2020) datasets. Notably, we see a statistically significant 11.2% improvement in performance for the TD3+BC algorithm aggregated across MuJoCo (Todorov et al., 2012) locomotion tasks compared to training on the real data, with no algorithmic changes. Our results also extend to even larger improvements for the challenging Maze2d navigation environments. Furthermore, we analyze synthetic trajectories generated by PGD and show that it achieves lower dynamics error than PETS (Chua et al., 2018) deep ensembles used by MOPO (Yu et al., 2020)—a prior offline model-based method—while matching the target policy likelihood of PETS. Together, our experiments illustrate the potential of PGD as an effective drop-in replacement for real data—across agents, environments, and behavior policies.

2 Background

2.1 Offline Reinforcement Learning

Formulation We adopt the standard reinforcement learning formulation, in which an agent acts in a Markov Decision Process (MDP, Sutton & Barto, 2018). An MDP is defined as a tuple

$M = \langle \mathcal{S}, \mathcal{A}, p_0, T, R, H \rangle$, where $s \in \mathcal{S}$ and $a \in \mathcal{A}$ are the state and action spaces, $p_0(s_0)$ is a probability distribution over the initial state, $T(s_{t+1}|s_t, a_t)$ is a conditional probability distribution defining the transition dynamics, $R : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is the reward function, γ is the discount factor, and H is the horizon.

In RL, we learn a policy $\pi(a|s)$ that defines a conditional probability distribution over actions for each state, inducing a distribution over trajectories $\boldsymbol{\tau} \coloneqq (s_0, a_1, r_1, s_1, \ldots, s_H)$ given by

$$p_{\pi,M}(\boldsymbol{\tau}) = p_0(s_0) \prod_{t=0}^{H-1} \pi(a_t|s_t) \cdot T(s_{t+1}|s_t, a_t), \tag{1}$$

omitting the reward function throughout our work for conciseness. Our goal is to learn a policy that maximizes the expected return, defined as $\mathbb{E}_{p_{\pi,M}}[V(\boldsymbol{\tau})]$ where $V(\boldsymbol{\tau}) \coloneqq \sum_{t=0}^{H} r_t$ is the return of a trajectory. The *offline RL* setting (Levine et al., 2020) extends this, preventing the agent from interacting with the environment and instead presenting it with a dataset of trajectories $\boldsymbol{\tau} \in \mathcal{D}_{\text{offline}}$ gathered by some behavior policy π_{off}, with which to optimize a target policy π_{target}.

Out-of-Sample Generalization The core challenge of offline RL emerges from the distribution shift between the *behavior distribution* $p_{\pi_{\text{off}},M}(\boldsymbol{\tau})$ and the *target distribution* $p_{\pi_{\text{target}},M}(\boldsymbol{\tau})$, which are otherwise denoted $p_{\text{off}}(\boldsymbol{\tau})$ and $p_{\text{target}}(\boldsymbol{\tau})$ for conciseness. Optimization of π_{target} on $\mathcal{D}$ can lead to catastrophic value overestimation at unobserved actions, a problem termed the *out-of-sample issue* (Kostrikov et al., 2021). As such, model-free offline algorithms typically regularize the policy towards the behavior distribution, either explicitly (Fujimoto & Gu, 2021; Kumar et al., 2020) or implicitly (Kostrikov et al., 2021).

Alternatively, prior work proposes learning a single-step world model $\mathcal{M}$ from $\mathcal{D}$ (Yu et al., 2020; Kidambi et al., 2020; Lu et al., 2022). By rolling out the target policy using $\mathcal{M}$, we generate trajectories $\boldsymbol{\tau} \sim p_{\text{target}}(\boldsymbol{\tau})$, with the aim of avoiding distribution shift. However, in practice, this technique only pushes the generalization issue into the world model. In particular, RL policies are prone to exploiting errors in the world model, which can compound over the course of an episode. This results in value overestimation, when combined with typical argmax operations used in off-policy RL (Sims et al., 2024).

2.2 Diffusion Models

Definition To generate synthetic data, we consider diffusion models (Sohl-Dickstein et al., 2015; Ho et al., 2020), a class of generative model that allows one to sample from a distribution $p(x)$ by iteratively reversing a forward noising process. Karras et al. (2022) present an ODE formulation of diffusion which, given a noise schedule $\sigma(i)$ indexed by i, mutates data according to

$$d\boldsymbol{x} = -\dot{\sigma}(i)\sigma(i)\nabla_{\boldsymbol{x}} \log p\left(\boldsymbol{x}; \sigma(i)\right) di, \tag{2}$$

where $\dot{\sigma} = \frac{d\sigma}{di}$ and $\nabla_{\boldsymbol{x}} \log p\left(\boldsymbol{x}; \sigma(i)\right)$ is the score function (Hyvärinen & Dayan, 2005), which points towards areas of high data density. Intuitively, infinitesimal forward or backward steps of this ODE respectively nudge a sample away from or towards the data. To generate a sample, we start with pure noise at the highest noise level σ_{max}, and iteratively denoise in discrete timesteps under Equation 2.

Classifier Guidance Our method is designed to augment the data-generating process towards on-policy trajectories from the target distribution $p_{\text{target}}(\boldsymbol{\tau})$, rather than the behavior distribution $p_{\text{off}}(\boldsymbol{\tau})$. To achieve this, we take inspiration from classifier guidance (Dhariwal & Nichol, 2021), which leverages a differentiable classifier to augment the score function of a pre-trained diffusion model towards a class-conditional distribution $p(\boldsymbol{x}|y)$. Concretely, this adds a classifier gradient to the score function, giving

$$\nabla_{\boldsymbol{x}} \log p_\lambda\left(\boldsymbol{x}|y; \sigma(i)\right) = \nabla_{\boldsymbol{x}} \log p\left(\boldsymbol{x}; \sigma(i)\right) + \lambda \nabla_{\boldsymbol{x}} \log p_\theta\left(y|\boldsymbol{x}; \sigma(i)\right), \tag{3}$$

where $\nabla_{\boldsymbol{x}} \log p_\theta\left(y|\boldsymbol{x}; \sigma(i)\right)$ is the gradient of the classifier and λ is the guidance weight.
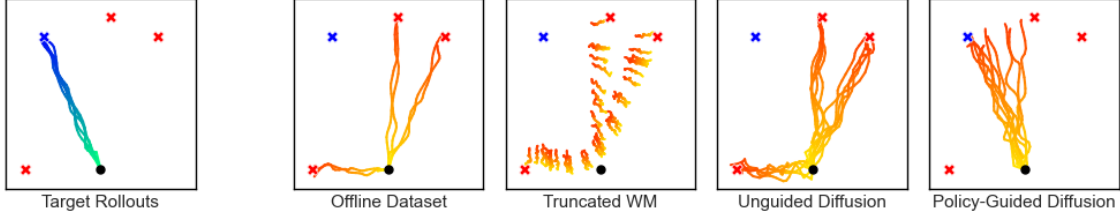
Figure 2: Trajectories from an illustrative 2D environment, in which the start location is indicated by ● and the goals for the behavior and target policies are indicated by × and ×. **Left:** Rollouts from the target policy in the real environment. **Right:** Offline datasets gathered by the behavior policy suffer from distribution shift and limited sample size. Truncated world models (Yu et al., 2020; Kidambi et al., 2020) previously used in offline model-based reinforcement learning offer a partial solution to this problem but suffer from bias due to short rollouts. Meanwhile, unguided diffusion (Lu et al., 2023) can increase the sample size, but maintains the original distribution shift. In contrast, policy-guided diffusion samples from a regularized target distribution, generating entire trajectories with low error but higher likelihood under the target distribution.

3 On-Policy Sampling from Offline Data

Generating synthetic agent experience is a promising approach to solving out-of-sample generalization in offline RL. By generating experience that is unseen in the dataset, the policy may be directly optimized on OOD samples, thereby moving the generalization problem from the policy to the generative model. Some prior work has suggested learning a model from the offline dataset (Lu et al., 2023), thereby sampling synthetic experience from the behavior distribution. While this improves sample coverage, the approach retains many of the original challenges of offline RL. As with the behavior policy, the synthetic trajectories may be suboptimal, and we still require conservative off-policy RL techniques to train the agent.

Instead, we seek to extend this approach by making our generative model sample from the target distribution. This reduces the need for conservatism and generates synthetic trajectories with increasing performance as the agent improves over training. Practically, the effectiveness of this approach depends on how we parameterize each of the terms of the trajectory distribution (Equation 1). In this section, we consider two parameterizations: autoregressive and direct.

3.1 Autoregressive Generation — Model $\mathcal{T}$, Sample $p(s_0)$

The autoregressive—or model-based—approach to generating on-policy data is to use the offline dataset to train a transition model $\mathcal{T}(s_{t+1}|s_t, a_t; \theta)$. In order to generate unbiased sample trajectories from the target distribution, we first sample an initial state (i.e., one that starts an episode) from the offline dataset $s_0 \sim \mathcal{D}_{\text{offline}}$. Next, we roll out our agent in the learned model by iteratively sampling actions from the target policy and approximating environment transitions with the learned dynamics model. However, compounding error from the transition model requires agent rollouts to be much shorter than the environment horizon—such that the agent takes $k \ll H$ steps.[1] Consequently, any states more than k steps away from any initial state cannot be generated in this manner, limiting the applicability of this approach.

As an approximation, autoregressive methods typically sample initial states from any timestep $s_t \sim \mathcal{D}_{\text{offline}}$ in the offline dataset. Given a truncated rollout length k, this may be seen as approximating the sub-trajectory distribution—i.e., the trajectory from time t to $t+k$—given by

$$p_{\text{target}}(\boldsymbol{\tau}_{t:t+k}; \theta) = p_{\text{target}}(s_t) \cdot p_{\text{target}}(\boldsymbol{\tau}_{t:t+k}|s_t; \theta), \tag{4}$$

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[1]Typically $k \leq 5$ (Janner et al., 2019; Yu et al., 2020).

by instead modeling

$$\mathcal{F}(\boldsymbol{\tau}_{t:t+k};\theta) = p_{\text{off}}(s_t) \cdot p_{\text{target}}(\boldsymbol{\tau}_{t:t+k}|s_t;\theta). \tag{5}$$

Here, we denote the stationary state distributions of the target and behavior policies at time t by $p_{\text{target}}(s_t)$ and $p_{\text{off}}(s_t)$ respectively, and define the conditional sub-trajectory distribution as

$$p_{\text{target}}(\boldsymbol{\tau}_{t:t+k}|s_t;\theta) \coloneqq \prod_{j=0}^{k-1} \pi_{\text{target}}(a_{t+j}|s_{t+j}) \cdot \mathcal{T}(s_{t+j+1}|s_{t+j}, a_{t+j};\theta). \tag{6}$$

When generating trajectories from this distribution, the divergence between $p_{\text{target}}(s_t)$ and $p_{\text{off}}(s_t)$ biases the start of rollouts towards states visited by the behavior policy. Furthermore, we still require k to be small to avoid compounding error. In combination, sampling from the offline dataset "anchors" synthetic rollouts to states in the offline dataset, while truncated rollouts prevent synthetic trajectories from moving far from this anchor. Therefore, the practical application of autoregressive generation leads to a strong bias towards the behavior distribution, thereby failing to address the out-of-sample problem.

3.2 Direct Generation — Model $p_{\text{off}}(\boldsymbol{\tau})$

As an alternative to autoregressive generation, we can parameterize the target distribution by *directly modeling* the behavior distribution, as follows:

$$
\begin{aligned}
p_{\text{target}}(\boldsymbol{\tau}) &= p(s_0) \prod_{t=0}^{H-1} \pi_{\text{target}}(a_t|s_t) \cdot \mathcal{T}(s_{t+1}|s_t, a_t) \\
&= p(s_0) \prod_{t=0}^{H-1} \frac{\pi_{\text{target}}(a_t|s_t)}{\pi_{\text{off}}(a_t|s_t)} \cdot \pi_{\text{off}}(a_t|s_t) \cdot \mathcal{T}(s_{t+1}|s_t, a_t) \\
&= p_{\text{off}}(\boldsymbol{\tau}) \prod_{t=0}^{H-1} w_{a_t,s_t} \\
&\approx p_{\text{off}}(\boldsymbol{\tau};\theta) \prod_{t=0}^{H-1} w_{a_t,s_t} = p_{\text{target}}(\boldsymbol{\tau};\theta)
\end{aligned}
\tag{7}
$$

where $w_{a,s} \coloneqq \frac{\pi_{\text{target}}(a|s)}{\pi_{\text{off}}(a|s)}$ denotes the importance sampling weight for (a, s) (Precup, 2000). This directly parameterizes the behavior distribution $p_{\text{off}}(\boldsymbol{\tau};\theta)$—which may be learned by modeling entire trajectories on the offline dataset—and adjusts their likelihoods by the relative probabilities of actions w_{a_t,s_t} under the target and behavior policies. By jointly modeling the initial state distribution, transition function, and behavior policy, such a parameterization is not required to enforce the Markov property. As a result, it can directly generate entire trajectories, thereby *avoiding the compounding model error* suffered by autoregressive methods when iteratively generating transitions.

However, computing w_{a_t,s_t} requires access to the behavior policy $\pi_{\text{off}}(a|s)$, which is not assumed in offline RL. Prior work has explored modeling the behavior policy from the offline dataset and using this to compute importance sampling corrections. However, products of many importance weights can lead to problems with high variance (Precup et al., 2000; Levine et al., 2020).

4 Policy-Guided Diffusion

In this work, we propose a method following the direct generation approach outlined in Section 3.2, named *policy-guided diffusion* (PGD, Algorithm 1). Following the success of diffusion models at generating trajectories (Janner et al., 2022; Lu et al., 2023), we first train a trajectory-level diffusion model on the offline dataset to model the behavior distribution. Then, inspired by classifier-guided

diffusion (Section 2.2), we guide the diffusion process using the target policy. Specifically, during the denoising process, we compute the gradient of the action distribution for each action when conditioned on its corresponding state under the target policy, using it to augment the diffusion process towards high-probability actions. In doing so, we model the *behavior-augmented target distribution*, a regularized target distribution using action likelihoods under the behavior policy, which we define below.

Algorithm 1 Trajectory sampling via policy-guided diffusion — based on Karras et al. (2022); Ma et al. (2023).

1: **Parameters:** Noise schedule σ_n, guidance schedule λ_n, noise level S_{noise}, diffusion steps $N_{\text{diffusion}}$
2: **Required:** Denoiser model D_θ
3: **sample** $\boldsymbol{\tau}_0 \sim \mathcal{N}(\boldsymbol{0}, \sigma_0^2 \boldsymbol{I})$
4: **for** $n = 0$ **to** $N_{\text{diffusion}} - 1$ **do**
5:     **sample** $\epsilon_n \sim \mathcal{N}(\boldsymbol{0}, S_{\text{noise}}^2 \boldsymbol{I})$
6:     $\hat{\sigma}_n \leftarrow \sigma_n + \gamma_n \sigma_n$
7:     $\hat{\boldsymbol{\tau}}_n \leftarrow \boldsymbol{\tau}_n + \sqrt{\hat{\sigma}_n^2 - \sigma_n^2} \epsilon_n$
8:     $\bar{\boldsymbol{\tau}}_n \leftarrow D_\theta(\hat{\boldsymbol{\tau}}_n; \hat{\sigma}_n)$
9:     $\boldsymbol{d}_n \leftarrow (\hat{\boldsymbol{\tau}}_n - \bar{\boldsymbol{\tau}}_n) / \hat{\sigma}_n$
10:     $\boldsymbol{g}_n \leftarrow \nabla_{\bar{\boldsymbol{\tau}}_n^{\text{actions}}} \pi_\phi(\bar{\boldsymbol{\tau}}_n^{\text{actions}} | \bar{\boldsymbol{\tau}}_n^{\text{states}})$
11:     $\hat{\boldsymbol{\tau}}_n^{\text{actions}} \leftarrow \hat{\boldsymbol{\tau}}_n^{\text{actions}} + \lambda_n(\boldsymbol{g}_n / \|\boldsymbol{g}_n\|_2)$
12:     $\boldsymbol{\tau}_{n+1} \leftarrow \hat{\boldsymbol{\tau}}_n + (\sigma_{n+1} - \hat{\sigma}_n) \boldsymbol{d}_n$
13:     **if** $t_{t+1} \neq 0$ **then**
14:         $\boldsymbol{d}_n' \leftarrow (\boldsymbol{\tau}_{n+1} - D_\theta(\boldsymbol{\tau}_{n+1}; \sigma_{n+1})) / \sigma_{n+1}$
15:         $\hat{\boldsymbol{\tau}}_{n+1} \leftarrow \hat{\boldsymbol{\tau}}_n + (\sigma_{n+1} - \hat{\sigma}_n)\left(\frac{1}{2}\boldsymbol{d}_n + \frac{1}{2}\boldsymbol{d}_n'\right)$
16:     **end if**
17: **end for**
18: **return** $\boldsymbol{\tau}_N$

Derivation In order to model the target distribution (Equation 7) with diffusion, we consider the score function for a noised trajectory $\hat{\boldsymbol{\tau}} := (\hat{s}_0, \hat{a}_1, \hat{r}_1, \hat{s}_1, \ldots, \hat{s}_H)$ sampled from the target distribution at a noise level σ,

$$\nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{target}}(\hat{\boldsymbol{\tau}}; \sigma) = \nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{off}}(\hat{\boldsymbol{\tau}}; \sigma) + \sum_{t=0}^{H-1} \left(\nabla_{\hat{a}_t} \log \pi_{\text{target}}(\hat{a}_t | \hat{s}_t) - \nabla_{\hat{a}_t} \log \pi_{\text{off}}(\hat{a}_t | \hat{s}_t) \right). \quad (8)$$

We model the first term (the score function under the behavior distribution) by training a denoiser model on the offline dataset (Section 2.2). Furthermore, we may directly compute the gradient of actions under the target policy we are currently optimizing, giving us the second term.

The third term requires access to the behavior policy, which is unavailable in offline RL. While we could approximate this with behavior cloning to compute the final term, we instead exclude this term as a form of regularization towards the behavior policy. Doing so biases trajectories towards the support of the offline data, preventing the diffusion model from moving too far out-of-distribution and thereby limiting model error. This yields our policy-guided score function

$$\nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{off}}(\hat{\boldsymbol{\tau}}; \sigma) + \sum_{t=0}^{H-1} \nabla_{\hat{\boldsymbol{\tau}}} \log \pi_{\text{target}}(\hat{a}_t | \hat{s}_t) = \nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{off}}(\hat{\boldsymbol{\tau}}; \sigma) + \nabla_{\hat{\boldsymbol{\tau}}} \log \prod_{t=0}^{H-1} \pi_{\text{target}}(\hat{a}_t | \hat{s}_t)$$

$$= \nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{off}}(\hat{\boldsymbol{\tau}}; \sigma) + \nabla_{\hat{\boldsymbol{\tau}}} \log q_{\text{target}}(\hat{\boldsymbol{\tau}}), \quad (9)$$

where $q_{\text{target}}(\hat{\boldsymbol{\tau}}) := \prod_{t=0}^{H-1} \pi_{\text{target}}(\hat{a}_t | \hat{s}_t)$ denotes the product of action probabilities under a policy π_{target}. This has the same form as classifier guidance (Dhariwal & Nichol, 2021), substituting the classifier gradient $\nabla_x \log p(y|x)$ with $\nabla_{\hat{\boldsymbol{\tau}}} \log q_{\text{target}}(\hat{\boldsymbol{\tau}})$. Therefore, applying the same sampling
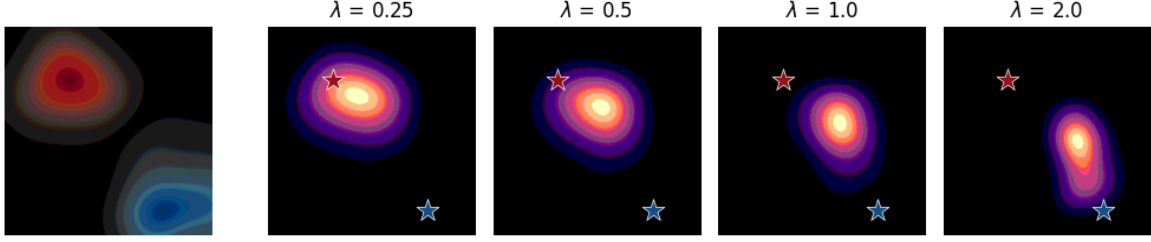
Figure 3: **Left:** Trajectory probability distribution for an example behavior distribution $p_{\text{off}}(\boldsymbol{\tau})$ and target policy likelihood $q_{\text{target}}(\boldsymbol{\tau})$. **Right:** PGD sampling distribution (Equation 12) over a range of policy-guidance coefficients λ. By increasing λ, we transform from the sampling distribution towards the regions of high target policy likelihood, making PGD an effective mechanism for controlling the level of regularization towards the behavior distribution.

procedure with policy guidance models a proxy distribution of the form

$$\mathcal{F}(\boldsymbol{\tau}|\pi_{\text{target}};\theta) \propto p_{\text{off}}(\boldsymbol{\tau};\theta) \prod_{t=0}^{H-1} \pi_{\text{target}}(a_t|s_t)$$
$$\approx p_{\text{off}}(\boldsymbol{\tau}) \cdot q_{\text{target}}(\boldsymbol{\tau}) = p_{\text{target}}(\boldsymbol{\tau}) \cdot q_{\text{off}}(\boldsymbol{\tau}). \tag{10}$$

where $q_{\text{off}}(\boldsymbol{\tau}) \coloneqq \prod_{t=0}^{H-1} \pi_{\text{off}}(a_t|s_t)$. We refer to $\mathcal{F}(\boldsymbol{\tau}|\pi_{\text{target}};\theta)$ as the *behavior-augmented target distribution* and provide further discussion in Appendix B, as well as a summary of PGD against alternative sources of training data in Table 1.

Guidance Coefficient A standard technique from classifier-guided diffusion is the use of guidance coefficients. These augment the guided score function by introducing a coefficient on the guidance term. Applied to Equation 9, this has the form

$$\nabla_{\hat{\boldsymbol{\tau}}} \log p_{\text{off}}(\hat{\boldsymbol{\tau}};\sigma) + \lambda \nabla_{\hat{\boldsymbol{\tau}}} \log q_{\text{target}}(\hat{\boldsymbol{\tau}}), \tag{11}$$

where λ denotes the guidance coefficient. Under the same diffusion procedure, this therefore augments the sampling distribution to

$$\mathcal{F}(\boldsymbol{\tau}|\pi_{\text{target}};\theta,\lambda) \propto p_{\text{off}}(\boldsymbol{\tau}) \cdot q_{\text{target}}(\boldsymbol{\tau})^{\lambda}. \tag{12}$$

Intuitively, λ interpolates the actions in the sampling distribution between the behavior and target distributions. By tuning λ, we can therefore control the strength of guidance towards the target policy, avoiding high dynamics error when the target policy is far from the behavior policy. We visualize this effect in Figure 3 and analyze its impact on target policy likelihood in Figure 5.

Following Ma et al. (2023), we also apply a cosine guidance schedule to the guidance coefficient, defined as

$$\lambda_n = \sigma_n + \beta\sigma_N \cdot \sin(\pi \cdot n/N), \tag{13}$$

where β is the cosine weight, which is set to 0.3 in all experiments. By decreasing the strength of guidance in later steps, we find that this schedule stabilizes guidance and reduces dynamics error.

Estimating Denoised Trajectories for Guidance When under distribution shift, RL policies are known to suffer from poor generalization to unseen states (Kirk et al., 2023). This makes policy guidance challenging, since the policy must operate on noised states, and compute action gradients from noised actions. Similar issues have been studied in classifier-guided diffusion (Ma et al., 2023), where the classifier gradient can be unstable when exposed to out-of-distribution inputs.

Therefore, Bansal et al. (2023), rather than applying guidance to the noised sample at each denoising step, predict and compute guidance from the denoised sample estimated by the denoiser model. By applying this to policy guidance, we avoid generalizing the target policy to noisy states, thereby decreasing the variance of our guidance term, which we find decreases dynamics error.

Table 1: Overview of training experience sources in offline RL—for each, we consider the sampling distribution, expected **error** in transition dynamics, **likelihood** of actions under the target policy, and state space **coverage** beyond the behavior distribution. Policy-guided diffusion provides an effective trade-off between each error, likelihood, and coverage.

Data source	Distribution	Error ($\downarrow$)	Likelihood ($\uparrow$)	Coverage ($\uparrow$)
Offline dataset	$p_{\text{off}}(\boldsymbol{\tau})$	—	Low	Low
Episodic world model	$p_{\text{target}}(\boldsymbol{\tau})$	High	—	High
Truncated world model	Equation 5	Low	—	Low
Unguided diffusion	$p_{\text{off}}(\boldsymbol{\tau})$	Low	Low	High
Policy-guided diffusion	Equation 10	Low	High	High

5 Results

Through our experiments, we first demonstrate that agents trained with synthetic experience from PGD outperform those trained on unguided synthetic data or directly on the offline dataset (Section 5.2). We show that this effect is consistent across agents (TD3+BC and IQL), environments (HalfCheetah, Walker2d, Hopper, and Maze), behavior policies (random, mixed, and medium), and modes of data generation (continuous and periodic). Following this, we demonstrate that tuning the guidance coefficient enables PGD to sample trajectories with high action likelihood across a range of target policies. Finally, we verify that PGD retains low dynamics error despite sampling high-likelihood actions from the policy (Section 5.3).

5.1 Experimental Setup

We evaluate PGD on the MuJoCo and Maze2d continuous control datasets from D4RL (Fu et al., 2020; Todorov et al., 2012). For MuJoCo, we consider the HalfCheetah, Walker2d, and Hopper environments with random (randomly initialized behavior policy), medium (suboptimal behavior policy), and medium-replay (or "mixed", the replay buffer from medium policy training) datasets. For Maze2d we consider the original (sparse reward) instances of the umaze, medium and large layouts. We train 4 trajectory diffusion models on each dataset, for which we detail hyperparameters in Appendix A. In Section 5.3, we conduct analysis of PGD against MOPO-style PETS (Chua et al., 2018) models, an autoregressive world model composed of an ensemble of probabilistic models, for which we use model weights from OfflineRL-Kit (Sun, 2023).

To demonstrate synthetic experience from PGD as a drop-in substitute for the real dataset, we transfer the original hyperparameters for IQL (Kostrikov et al., 2021) and TD3+BC (Fujimoto & Gu, 2021)—as tuned on the real datasets—*without any further tuning.* Policy guidance requires a stochastic target policy, in order to compute the gradient of the action distribution. Since TD3+BC trains a deterministic policy, we perform guidance by modeling the action distribution as a unit Gaussian centered on the deterministic action. We train all agents and diffusion models from scratch in Jax (Bradbury et al., 2018) using our own implementation, which we will release upon publication.

5.2 Offline Reinforcement Learning

For each D4RL dataset, we train two popular model-free offline algorithms, TD3+BC (Fujimoto & Gu, 2021) and IQL (Kostrikov et al., 2021) on synthetic experience generated by trajectory diffusion models with and without policy guidance, as well as on the real dataset. We first consider *periodic generation* of synthetic data, in which the synthetic dataset is regenerated after extended periods of agent training, such that the agent is near convergence on the synthetic dataset at the point it is regenerated with the current policy. Each epoch, we generate a dataset of 2^{14} synthetic trajectories of length 16. Following the notation of Algorithm 2, we set the number of epochs to $N_{\text{epochs}} = 4$

with $N_{\text{policy}} = 250,000$ train steps per epoch, meaning the agent is trained to close to convergence before the dataset is regenerated. This can be viewed as solving a sequence of offline RL tasks with synthetic datasets, in which the behavior policy is the target policy from the previous generation.

Using periodic generation, performance improves significantly across benchmarks for both IQL and TD3+BC (Table 2). In MuJoCo, the most consistent improvement is on mixed datasets, with 4 out of 6 experiments achieving significant performance improvement. This is to be expected, as these datasets contain experience from a mixture of behavior policy levels. In this case, the diffusion model is likely to be able to represent a wide variety of policies, and on-policy guidance would naturally produce higher return trajectories as the target policy improves.

Table 2: Final return of IQL and TD3+BC agents trained on real, unguided ($\lambda = 0$) synthetic and policy-guided ($\lambda = 1$) synthetic data—mean and standard error over 4 seeds (diffusion models and agents) is presented, with significant improvements ($p < 0.05$) shaded.

		IQL			TD3+BC		
		Dataset	**Unguided**	**Guided**	**Dataset**	**Unguided**	**Guided**
Random	HalfCheetah	9.1 ± 2.2	2.6 ± 0.1	6.5 ± 1.7	11.2 ± 0.8	11.0 ± 0.4	21.1 ± 0.9
	Walker2d	4.3 ± 0.5	2.7 ± 0.7	5.3 ± 0.3	0.5 ± 0.3	1.1 ± 1.2	-0.3 ± 0.1
	Hopper	7.4 ± 0.4	5.2 ± 0.9	4.9 ± 1.0	7.4 ± 0.6	4.2 ± 1.4	5.5 ± 2.1
Mixed	HalfCheetah	44.2 ± 0.2	43.6 ± 0.2	43.6 ± 0.2	44.7 ± 0.1	43.1 ± 0.2	46.1 ± 0.3
	Walker2d	81.3 ± 2.0	85.2 ± 0.3	84.9 ± 1.4	82.7 ± 1.3	70.7 ± 10.1	84.0 ± 1.0
	Hopper	82.9 ± 3.5	97.4 ± 2.7	100.5 ± 0.5	58.6 ± 11.2	52.1 ± 1.8	91.9 ± 4.3
Medium	HalfCheetah	48.4 ± 0.1	45.4 ± 0.1	45.1 ± 0.1	48.6 ± 0.1	45.3 ± 0.2	47.6 ± 0.3
	Walker2d	81.7 ± 1.4	82.1 ± 0.9	77.8 ± 3.6	84.8 ± 0.1	85.2 ± 0.2	86.3 ± 0.3
	Hopper	63.6 ± 0.8	59.7 ± 2.0	62.8 ± 1.2	62.4 ± 0.9	57.4 ± 0.4	63.1 ± 0.6
	Total	46.9 ± 0.4	47.0 ± 0.4	47.9 ± 0.3	44.5 ± 1.1	41.1 ± 1.1	49.5 ± 0.9
Maze2d	UMaze	42.6 ± 0.4	42.9 ± 1.8	43.8 ± 3.5	50.0 ± 2.4	33.8 ± 3.0	76.2 ± 17.4
	Medium	38.5 ± 1.9	33.4 ± 3.2	60.0 ± 13.9	32.1 ± 6.8	24.0 ± 4.0	89.6 ± 19.9
	Large	50.9 ± 5.8	23.4 ± 8.0	45.3 ± 14.8	137.2 ± 20.2	93.3 ± 31.0	131.1 ± 37.5
	Total	44.0 ± 2.2	33.2 ± 1.8	49.7 ± 9.5	73.1 ± 6.7	50.4 ± 11.1	99.0 ± 14.5

In order to demonstrate the flexibility of PGD, we also evaluate PGD in a *continuous generation* setting, using a data generation rate closer to that of traditional model-based methods. For this, we set $N_{\text{epochs}} = 100$ and $N_{\text{policy}} = 10,000$, then lower the sample size to match the overall number of synthetic trajectories generated by periodic generation across training. Due to the decrease in sample size, we maintain each generated dataset across epochs in a replay buffer, with each dataset being removed after 10 epochs.

We see similar improvements in performance against real and unguided synthetic data under this approach, with PGD outperforming real data on 2 out of 3 environments and datasets (Figure 4). Periodic generation outperforms continuous generation across environments and behavior policies, which we attribute to training stability, especially when performing guidance early in training. Regardless, both approaches consistently outperform training on real and unguided synthetic data, demonstrating the potential of PGD as a drop-in extension to replay and model-based RL methods.

5.3 Synthetic Trajectory Analysis

We now analyze the quality of trajectories produced by PGD against those from unguided diffusion and autoregressive world model (PETS) rollouts. In principle, we seek to evaluate the divergence of these sampling distributions from the true target distribution. However, this is not tractable to compute directly, so we instead investigate two proxy objectives:
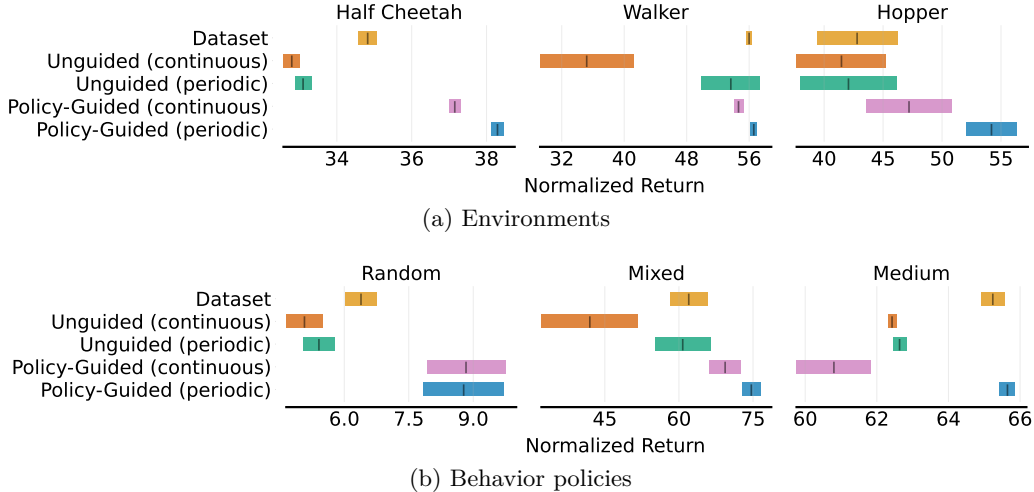
(a) Environments

(b) Behavior policies

Figure 4: Aggregate MuJoCo performance after training on unguided or policy-guided synthetic data under continuous and periodic dataset generation, as well as on the real dataset. For each setting, mean return over TD3+BC and IQL agents is marked, with standard error over 4 seeds (diffusion models and agents) highlighted.

1. **Trajectory likelihood**: mean log-likelihood of actions under the target policy; and

2. **Dynamics error**: mean squared error between states in the synthetic trajectory and real environment, when rolled out with the same initial state and action sequence.

In our experiments, we consider trajectory diffusion and MOPO-style PETS (Chua et al., 2018) models trained on representative datasets from the D4RL (Fu et al., 2020) benchmark that were featured in the previous section. Specifically, we consider the models trained on halfcheetah-medium, before sampling trajectories with IQL target policies trained on the halfcheetah-random, -medium, and -expert. This enables us to test the robustness of these models to target policies far from the behavior policy, both in performance and policy entropy.

Policy guidance increases trajectory likelihood In Figure 5, we present the trajectory likelihood of synthetic trajectories over varying degrees of guidance. Unsurprisingly, unguided diffusion generates low probability trajectories for all target policies, due to it directly modeling the behavior distribution. However, as we increase the guidance coefficient λ, trajectory likelihood increases monotonically under each target policy. Furthermore, this effect is robust across target policies, giving the ability to sample high-probability trajectories with OOD target policies. The value of λ required to achieve the same action likelihood as direct action sampling (PETS) varies with the target policy. Since this threshold increases with target policy performance, we hypothesize that it increases with target policy entropy. Based on this, a promising avenue for future work is automatically tuning λ for hyperparameter-free guidance.

Policy guided diffusion achieves lower error than autoregressive models In Figure 6, we present the dynamics error of synthetic trajectories over 16 rollout steps. For a fair comparison, we fix the guidance coefficient of PGD to $\lambda = 1.0$, since this was sufficient to match the trajectory likelihood of PETS (Figure 5). Over all target policies, PGD achieves significantly lower error than PETS. Furthermore, PGD has similar levels of error across target policies, while PETS suffers from significantly higher error on OOD (random and expert) target policies. This highlights the robustness of PGD to target policy, a critical feature for generating high-likelihood training data throughout tabula rasa policy training.
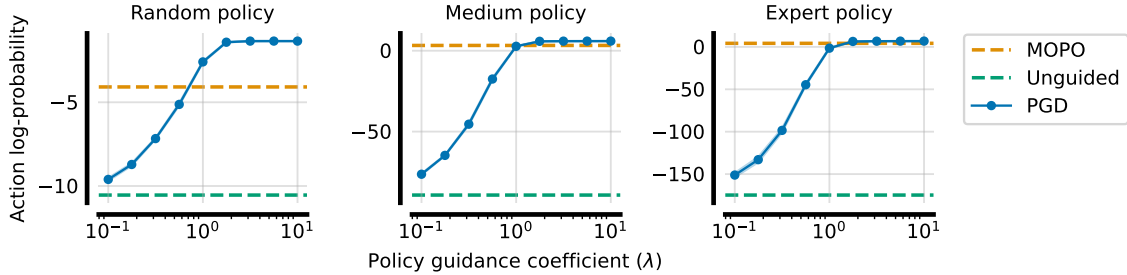
10

Figure 5: Action probability of synthetic trajectories generated by diffusion and PETS models trained on halfcheetah-medium. Target policies are trained on halfcheetah-random, halfcheetah-medium, and halfcheetah-expert datasets, demonstrating robustness to OOD actions. Standard error over 4 diffusion model seeds is shaded, with each generating 2048 synthetic trajectories for analysis.
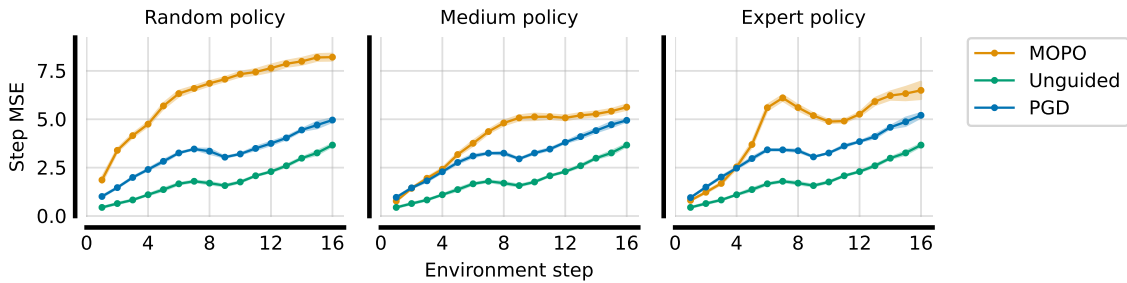

Figure 6: Dynamics mean squared error of synthetic trajectories generated by diffusion and PETS models trained on halfcheetah-medium. Standard error over 4 diffusion model seeds and 3 PETS seeds (via OfflineRL-Kit) is shaded, with each generating 2048 synthetic trajectories for analysis.

6 Related Work

Model-based Offline Reinforcement Learning Model-based methods in offline RL (Yu et al., 2020; Kidambi et al., 2020; Rigter et al., 2022; Lu et al., 2022) are designed to augment the offline buffer with additional on-policy samples in order to mitigate distribution shift. This is typically done by rolling out a policy in a learned world model (Janner et al., 2019) and applying a suitable pessimism term in order to account for dynamics model errors. While these methods share the same overall motivation as our paper, the empirical realization is quite different. In particular, forward dynamics models are liable to compounding errors over long horizons, resulting in model exploitation, whereas our trajectories are generated in a single step.

Model-free Offline Reinforcement Learning Model-free methods in offline RL typically tackle the out-of-sample issue by applying conservatism to the value function or by constraining the policy to remain close to the data. For example, CQL (Kumar et al., 2020) and EDAC (An et al., 2021) both aim to minimize the values of out-of-distribution actions. Meanwhile, BCQ (Fujimoto et al., 2019) ensures that actions used in value targets are in-distribution with the behavioral policy using constrained optimization. We take the opposite approach in this paper: by enabling our diffusion model to generate on-policy samples without diverging from the behavior distribution, we reduce the need for conservatism.

Diffusion in Reinforcement Learning Diffusion models are a flexible method for data augmentation in reinforcement learning. SynthER (Lu et al., 2023) uses unguided diffusion models to upsample offline or online RL datasets, which are then used by model-free off-policy algorithms. While this improves performance, SynthER uses unguided diffusion to model the behavior distribution, resulting

in the same issue of distributional shift. Similarly, MTDiff (He et al., 2023) considers unguided data generation in multitask settings.

Diffusion models have also been used to train world models. Zhang et al. (2023) train a world model for sensor observations by first tokenizing using VQ-VAE and then predicting future observations via discrete diffusion. Alonso et al. (2023) also train a world model using diffusion and demonstrate it can more accurately predict future observations. However, neither of these approaches model the whole trajectory, thereby suffering from compounding error, nor do they apply policy guidance. Parallel to this work, Rigter et al. (2023) use guidance from a policy to augment a diffusion world model for online RL. By contrast, we focus on the offline RL setting, provide a theoretical derivation and motivation for the trajectory distribution modeled by policy guidance, and demonstrate improvements in downstream policy performance.

Diffusion models are also used elsewhere in reinforcement learning. For example, Diffuser (Janner et al., 2022) and Decision Diffuser (Ajay et al., 2023) use trajectory diffusion models for planning and to bias planned trajectories towards high return. By contrast, we use on-policy guidance and train on the generated data. Diffusion models have also been used as an expressive policy class (Wang et al., 2023) for Q-learning, showing improvement over MLPs.

7 Conclusion

We presented policy-guided diffusion, a method for controllable generation of synthetic trajectories in offline RL. We provided a theoretical analysis of existing approaches to synthetic experience generation, identifying the advantages of direct trajectory generation compared to autoregressive methods. Motivated by this, we proposed PGD under the direct approach, deriving the regularized target distribution modeled by policy guidance.

Evaluating against PETS deep ensembles, a state-of-the-art autoregressive approach, we found that PGD can generate synthetic experience at the same target policy likelihood with significantly lower dynamics error. Furthermore, we found consistent improvements in downstream agent performance over a range of environments and behavior policies when trained on policy-guided synthetic data, against real and unguided synthetic experience.

By addressing the out-of-sample issue through synthetic data, we hope that this work enables the development of less conservative algorithms for offline RL. There are a range of promising avenues for future work, including automatically tuning the guidance coefficient for hyperparameter-free guidance, leveraging on-policy RL techniques with policy-guided data, and extending this approach to large-scale video generation models.

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Appendix

A Hyperparameters

A.1 Diffusion model

For the diffusion model, we used a U-Net architecture (Ronneberger et al., 2015) with hyperparameters outlined in Table 3. We transformed the trajectory by stacking the observation, action, reward, and done flags for each transition, before performing 1D convolution across the sequence of transitions.

Table 3: U-Net hyperparameters

Hyperparameter	Value
Trajectory length	16
Kernel size	3
Features	1024
U-Net blocks	3
Batch size	16
Dataset epochs	250
Optimizer	Adam
Learning rate	2×10^{-3}
LR schedule	Cosine decay

A.2 Diffusion sampling

We use EDM (Karras et al., 2022) for diffusion sampling, retaining many of the default hyperparameters from Lu et al. (2023) (Table 4). We tuned the number of diffusion timesteps, finding diminishing improvement in dynamics error beyond 256 timesteps.

Table 4: EDM hyperparameters

Hyperparameter	Value
Diffusion timesteps	256
S_{churn}	80
S_{noise}	1.003
S_{tmax}	50
S_{tmin}	0.05
σ_{max}	80
σ_{min}	0.002

B   Behavior-Augmented Target Distribution

Intuitively, the behavior-augmented target distribution transforms the target distribution by increasing the likelihood of actions under the behavior policy. As is typical in offline RL (Kumar et al., 2020; Fujimoto & Gu, 2021; Fujimoto et al., 2019), regularizing the policy towards the behavior distribution is required in order to avoid out-of-sample states and consequently minimize value overestimation. Rather than regularizing the policy, PGD shifts this regularization to the data generation process, which helps our guided samples remain in-distribution with respect to the diffusion model, and thus less susceptible to model error.

Moreover, we note that this type of regularization is not immediately available for prior autoregressive world models, and thus they typically penalize reward by dynamics error (Yu et al., 2020; Kidambi et al., 2020; Lu et al., 2022) in an ad-hoc fashion in order to avoid model exploitation. In contrast, PGD presents a *natural mechanism for behavioral regularization during data generation*, making offline policy optimization without regularization a promising path for future work.

C   Agent Training with Policy-Guided Diffusion

In Algorithm 2, we present pseudocode for training an agent with synthetic experience generated by PGD. PGD is agnostic to the underlying offline RL algorithm used to train the target policy, making it a drop-in extension to any model-free method.

Algorithm 2 Agent training via policy-guided diffusion.

1: **Parameters:** Number of epochs N_{epochs}, steps per epoch N_{policy}
2: **Required:** Diffusion trajectory sampler $\mathcal{F}(\boldsymbol{\tau}|\pi; \theta, \lambda)$
3: Initialize policy π_ϕ
4: **for** epoch $= 0$ **to** N_{epochs} **do**
5:     Generate synthetic dataset $\mathcal{D}_{\text{epoch}} \sim \mathcal{F}(\boldsymbol{\tau}|\pi_\phi; \theta, \lambda)$
6:     **for** step $= 0$ **to** N_{policy} **do**
7:         Sample mini-batch $\{\boldsymbol{\tau}\} \sim \mathcal{D}_{\text{epoch}}$
8:         Update policy π_ϕ on mini-batch $\{\boldsymbol{\tau}\}$
9:     **end for**
10: **end for**
11: **return** π_ϕ