From Function to Distribution Modeling: A PAC-Generative Approach to Offline Optimization

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Abstract

This paper considers the problem of offline optimization, where the objective function is unknown except for a collection of "offline" data examples. While recent years have seen a flurry of work on applying various machine learning techniques to the offline optimization problem, the majority of these works focused on learning a surrogate of the unknown objective function and then applying existing optimization algorithms. While the idea of modeling the unknown objective function is intuitive and appealing, from the learning point of view it also makes it very difficult to tune the objective of the learner according to the objective of optimization. Instead of learning and then optimizing the unknown objective function, in this paper we take on a less intuitive but more direct view that optimization can be thought of as a process of sampling from a generative model. To learn an effective generative model from the offline data examples, we consider the standard technique of "re-weighting", and our main technical contribution is a probably approximately correct (PAC) lower bound on the natural optimization objective, which allows us to jointly learn a weight function and a score-based generative model from a surrogate loss function. The robustly competitive performance of the proposed approach is demonstrated via empirical studies using the standard offline optimization benchmarks.

1 Introduction

Offline optimization refers to the problem of optimizing an *unknown* real-valued objective function f based only on a collection of "offline" data examples $(\boldsymbol{x}_i, f(\boldsymbol{x}_i)), \forall i \in [m] := \{1, 2, \ldots, m\}$, where each $\boldsymbol{x}_i$ is an independent sample drawn from an *unknown* distribution p_{data}. Aside from these examples, no additional information on the objective function f is available prior to or during the optimization process, and hence the name "offline optimization". This rather restrictive setting is particularly relevant to the optimization scenarios where: i) the objective function is very complex and no structural information is available; and ii) querying the objective function is very expensive.

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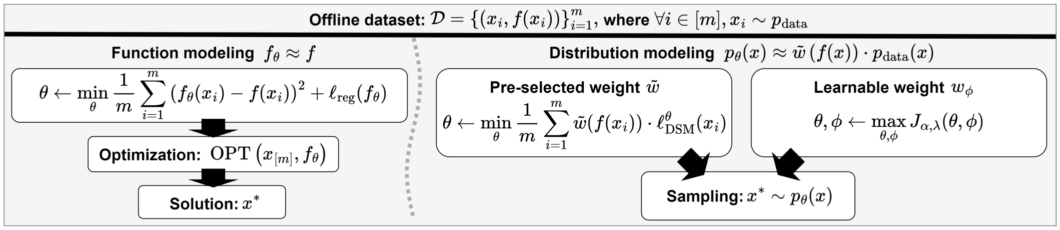

Figure 1: Function vs. distribution modeling for offline optimization.

Obviously, offline optimization is a more challenging setting than standard optimization [6], where *full* structural information on the objective function is available; or black-box optimization [5], where even though no *structural* information on the objective function is available, the objective function can be queried upon during the optimization process. Therefore, instead of aiming at the global optima, for offline optimization we are usually satisfied with finding a few candidates, among which there are *significantly* better [2] solutions than the existing offline observations. Under this lesser objective, a direct application of offline optimization is *experimental design*, for which the candidates are to be efficiently found without querying objective functions through experiments that are often slow or expensive. Applications in the literature include the design of proteins [32], chemical molecules [21], DNA sequences [29], aircraft [25], robots [39], and hardware accelerators [37].

Related work. Traditionally, offline optimization has been mainly approached through the *Bayesian* view, i.e., by endowing the unknown objective function f a *prior* distribution. This has led to a large body of work under the name *Bayesian optimization*; see Fu and Levine [19] and the references therein for the recent progress in this direction. Motivated by the rapid progress in machine learning, recent years have also seen a flurry of work on offline optimization from a *frequentist's* view [11, 22, 35, 45], i.e., by modeling the objective function f as a *deterministic but unknown* function. However, most of these works have been focusing on learning a surrogate of the unknown objective function and then applying existing optimization algorithms (see "Function Modeling" in Figure 1). Prime examples include Trabucco et al. [45], Brookes et al. [11], Gupta and Zou [22], Chen et al. [14].

While the idea of modeling the unknown objective function is intuitive and appealing, from the learning point of view it also makes it very difficult to tune the objective of the learner according to the objective of optimization [45, 11, 22]. As a result, it is very difficult to gauge whether these previous approaches actually come with any theoretical guarantees.

Main contribution. Figure 1 illustrates the key differences between function modeling and distribution modeling for offline optimization. In sharp contrast to function modeling, our approach does *not* explicitly learn a surrogate of the unknown objective function, but directly learns a generative model [3] from the offline examples using a *theoretically-grounded* surrogate of the natural optimization objective: $J_{\text{opt}}(\theta) = \mathbb{E}_{\mathbf{x} \sim p_\theta}[f(\mathbf{x})]$. The main contribution can be summarized as follows:

> We derive a PAC bound on the natural optimization objective, allowing the generative model and weight function to be jointly learned from a *surrogate* loss function that *aligns* the learner's and optimization objectives.

2 The Method

In this paper we take on a less intuitive but more *direct* view of optimization and consider it as a process of *sampling* from a *generative model*. There are two natural advantages to this view. First, through sampling *exploration* is now intrinsic in the optimization process. Second, this view allows us to shift our focus from modeling the objective function to modeling a *target distribution*. Unlike learning a surrogate on the objective function, as we shall see, the objective of learning a generative model can be naturally aligned with the objective of optimization, thus bringing *theoretical guarantees* on the optimization performance.

More specifically, let p_θ be a *generative model* from which sampling can produce, with high probability, samples whose objective values are significantly better than the offline observations. Note that

[2]Throughout the paper, better or superior solutions refer to those with either larger or smaller objective values, depending on whether the goal of optimization is maximizing or minimizing the objective function.

[3]We emphasize here that the idea of leveraging generative models for offline optimization is not entirely new, e.g. Brookes et al. [11], Krishnamoorthy et al. [34, 33].

unlike the traditional generative models, whose purpose to generate samples that are "similar" to the training examples, the goal of our generative model p_θ is to generate samples with *superior* objective values than the offline observations. Relative to the data-generating distribution p_{data}, these targeted samples with superior objective values are the "outliers". Therefore, from the learning perspective, our main challenge here is to learn a generative model that generates *outliers* rather than the norm.

2.1 Learning a Generative Model with a Pre-selected Normalized Weight Function

To facilitate the learning of a desired generative model, in this paper we shall consider the standard technique of "re-weighting" [12]. Roughly speaking, we shall consider a *weight* function that assigns higher weights to the domain points with better objective values and then train a generative model using the *weighted* offline examples. This allows us to tune the generative model towards generating samples with better objective values.

Formally, let $q_{\text{target}}(\boldsymbol{x}) := \tilde{w}(f(\boldsymbol{x})) \cdot p_{\text{data}}(\boldsymbol{x})$ be a *hypothetical* target distribution, where $\tilde{w}$ is a normalized, non-negative *weight* function such that $\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}[\tilde{w}(f(\mathbf{x}))] = 1$, and p_{data} is the (unknown) data-generating distribution from which the offline observations $\boldsymbol{x}_{[m]} := (\boldsymbol{x}_i : i \in [m])$ were drawn. In our approach, the hypothetical target distribution q_{target} plays *dual* roles: On one hand, it serves as the *hypothetical* learning target of the generative model p_θ; on the other hand, it is also connected to the unknown data-generating distribution p_{data} via the normalized weight function $\tilde{w}$ and hence allows a generative model p_θ to be learned from the offline data examples. Operationally, we would like to train a generative model p_θ such that $p_\theta \approx q_{\text{target}}$. But what would be a suitable choice for the normalized weight function $\tilde{w}$?

In this section, we shall focus on training a *score-based* model, which is mainly motivated by the following connection between the *score function* of the hypothetical target distribution q_{target} and the *gradient* of the unknown objective function f:

$$\boldsymbol{s}_{\text{target}}(\boldsymbol{x}) = \nabla_{\boldsymbol{x}} \log q_{\text{target}}(\boldsymbol{x}) = \nabla_{\boldsymbol{x}} \log [\tilde{w}(f(\boldsymbol{x})) p_{\text{data}}(\boldsymbol{x})] = \boldsymbol{s}_{\text{data}}(\boldsymbol{x}) + \frac{\tilde{w}'(f(\boldsymbol{x}))}{\tilde{w}(f(\boldsymbol{x}))} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}),$$

where $\boldsymbol{s}_{\text{target}}$ and $\boldsymbol{s}_{\text{data}}$ are the score functions of q_{target} and p_{data}, respectively. If $\tilde{w}$ is monotone *increasing*, the derivative $\tilde{w}'(f(\boldsymbol{x})) > 0$ for all $\boldsymbol{x} \in \mathcal{X}$. In this case, the score function $\boldsymbol{s}_{\text{target}}$ is aligned with the *gradient* of the objective function f, so sampling along the direction of $\boldsymbol{s}_{\text{target}}$ will naturally produce samples with high objective values.

In practice, the normalized weight function can be either *pre-selected* or *learned* from the offline data examples. In the former case, as we have seen, the generative model p_θ can be learned via a loss function that is simply the *weighted* version of the loss function for training a *standard* generative model. In the latter case, however, *a priori*, it is unclear how to construct a loss function that would allow us to *jointly* learn a generative model p_θ and a normalized weight function $\tilde{w}$.

2.2 Jointly Learning a Generative Model and a Normalized Weight Function

To address the above challenge, in this section we shall start with the following *natural* optimization objective $J_{\text{opt}}(\theta)$ for identifying a desired generative model p_θ. The above natural optimization objective, however, *cannot* be evaluated for any θ, because the objective function f is *unknown*. Instead of trying to learn a surrogate on f and then use it to guide the training of the generative model, here we consider the more learning-theoretic approach of constructing a *probably approximately correct (PAC)* [42] bound on J_{opt}. Unlike J_{opt}, which depends only on θ, the PAC bound depends on both θ and the normalized weight function $\tilde{w}$. As we shall see, not only it captures *both* the utility and learnability considerations for selecting $\tilde{w}$, it will also *naturally* suggest a surrogate loss function, from which both a generative model p_θ and a normalized weight function $\tilde{w}$ can be jointly learned from the offline data examples.

To construct an appropriate loss function, let us assume without loss of generality that our goal of optimization is to *maximize* an unknown objective function f. Our proposed loss function is based on the following PAC *lower* bound on the natural optimization objective $J_{\text{opt}}(\theta)$:

$$\begin{aligned} J_{\text{opt}}(\theta) \geq \underbrace{\hat{J}_{\boldsymbol{x}_{[m]}}(\tilde{w})}_{\text{empirical utility}} - \underbrace{c_0 K \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})}}_{\text{empirical weighted DSM loss}} - \underbrace{c_0 K \sqrt{2\Delta} \sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})}}_{\text{empirical variance}} - \\ c_1 K W_2(\bar{q}_{\text{target}}, \mathcal{N}) - c_0 K \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - O\left(1/\sqrt[8]{m}\right). \end{aligned} \quad (1)$$

Table 1: Experimental results on the benchmark datasets [↑].

	Supercond.	TFBind8	GFP	UTR	Fluores.	Ave. Improv.	#Best
$\mathcal{D}_{\text{best}}$	0.399	0.439	0.789	0.593	0.485		
Grad	0.483±0.021	**0.985±0.007**	0.053±0.002	0.657±0.039	**0.747±0.209**	0.234	2/5
COMs	0.481±0.017	0.918±0.027	0.864±0.000	**0.683±0.009**	**0.740±0.064**	0.414	2/5
CbAS	0.491±0.028	0.868±0.076	0.864±0.000	0.659±0.009	0.574±0.020	0.320	0/5
$\psi = 20$	0.423±0.044	0.903±0.050	**0.865±0.000**	**0.693±0.006**	**0.803±0.057**	0.407	3/5
$\alpha = 0.25$	**0.537±0.045**	0.941±0.034	**0.865±0.000**	**0.693±0.013**	**0.809±0.078**	**0.485**	**4/5**

Incorporating proper changes to the PAC lower bound (1) leads to the following objective for jointly learning a (un-normalized) weight function w_ϕ and a score-function model $\boldsymbol{s}_t^\theta$:

$$J_{\alpha,\lambda}(\theta,\phi) =$$

$$\frac{1}{m}\sum_{i=1}^{m}\frac{w_\phi(f(\boldsymbol{x}_i))f(\boldsymbol{x}_i)}{\hat{Z}_\phi} - \lambda\sqrt{\frac{1}{m}\sum_{i=1}^{m}\frac{w_\phi(f(\boldsymbol{x}_i))\ell_{\text{DSM}}^{\theta}(\boldsymbol{x}_i)}{\hat{Z}_\phi}} - \alpha\sqrt[4]{\frac{1}{m}\sum_{i=1}^{m}\left(\frac{w_\phi(f(\boldsymbol{x}_i))}{\hat{Z}_\phi} - 1\right)^2}. \quad (2)$$

Details regarding the PAC lower bound (1), the surrogate loss function (2), as well as the training and sampling algorithms are elaborated in A.4, A.5, and A.6, respectively.

3 Experimental Results

We assess the performance of the proposed learning algorithm using the four standard tasks (Superconductor, TF Bind 8, GFP, and UTR) from the Design-Bench benchmark [46]. In addition, we have included the “Fluorescence" task from Fannjiang et al. [18] for a comprehensive evaluation.

Evaluation. We generated a total of $N = 128$ designs for each task and subsequently computed the mean and standard deviation of the 100th percentile of the normalized ground truth over eight independent trials.

Results. The results are listed in Table 1, where $\mathcal{D}_{\text{best}}$ denotes the normalized maximum objective value among the initial samples; “Grad" and “COMs" refer to [45]; “CbAS" refers to [11]; “$\psi = 20$" refers to our proposed approach with a pre-selected weight function $w(y) = \exp(\psi y)$ for $\psi = 20$; and “$\alpha = 0.25$" refers to our proposed approach with a learnable weight function and hyper-parameters $\alpha = 0.25$, $\lambda = 0.1$. Results that fall within one standard deviation of the best performance are highlighted in bold.

Note that across all tasks, our proposed approaches demonstrate not only notable improvement over the best initial samples, but also *consistently competitive* performances against the other three prominent offline optimization algorithms. Quantitatively, our proposed approach with a learnable weight function achieves the *highest* average improvement over all five tasks, where the improvement over a specific task is defined as $(y - \mathcal{D}_{\text{best}})/\mathcal{D}_{\text{best}}$. We believe that this superior consistency is rooted in our *modeling* perspective and the *theoretically-grounded* design of the learning algorithm.

4 Conclusion

In this paper, we introduced a novel generative approach to offline optimization by shifting the focus from traditional function modeling to distribution modeling. This approach leverages the concept of sampling from a generative model rather than optimizing a surrogate of the unknown objective function. We proposed a PAC-bound framework that enables the joint learning of a generative model and a weight function, ensuring that the learning process is aligned with the optimization goals. Our empirical results, validated on standard offline optimization benchmarks, demonstrate the robustness and competitive performance of the proposed method. Future research could explore further refinements of the PAC-bound framework and its applications to more diverse optimization problems.

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Appendices

Contents

List of Symbols

The next list describes several symbols that are used within the entire body of the paper.

α, λ	Hyper-parameters (learnable case)
ℓ_{DSM}	Denoising score matching loss function
$\hat{\mathfrak{R}}$	Rademacher complexity
$\mathcal{D}_{\text{best}}$	Maximum objective value within the offline dataset
$\mathcal{N}$	Normal distribution
p_{data}	Data-generating distribution
ψ	Hyper-parameter (pre-selected case)
q_{target}	Target distribution (hypothetical)
$\tilde{w}$	Normalized weight function
$\boldsymbol{x}$	Domain point, Design or Feature vector
$\boldsymbol{x}_{[m]}$	A set of offline domain points $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m\}$
$\boldsymbol{x}_i$	Offline domain point
f	Unknown objective function
$f(\boldsymbol{x}_i)$	Offline objective value
f_θ	Parameterized surrogate objective function
J_{opt}	Natural optimization objective
p_θ	Parameterized generative model
w_ϕ	Parameterized weight function (unnormalized)
W_p	p-Wasserstein distance
y	Objective value, Label or Score

A Technical Details

A.1 The denoising diffusion probabilistic model (DDPM)

For score-based generative models, we are particularly interested in the *denoising diffusion probabilistic model (DDPM)* [44, 24] due to its stability and performance on high-dimensional datasets. Below we first recall a few essential results on the DDPM.

Consider a *forward* process of continuously injecting white Gaussian noise into a signal $\mathbf{x}_t$:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)}d\mathbf{w}_t, \quad t \in [0, 1], \tag{3}$$

where $\beta : [0, 1] \to \mathbb{R}_{++}$ is a positive *noise scheduler*, $\mathbf{w}_t$ is a standard *Wiener* process [28], and time in this process is assumed to flow in the *forward* direction from $t = 0$ to $t = 1$. Denote by q_t the marginal distribution of $\mathbf{x}_t$ from the forward process (3). The DDPM is mainly motivated by the fact that the marginal distributions q_t, $t \in [0, 1]$, can be *recovered* through the following *reverse* process [3]:

$$d\mathbf{x}_t = -\beta(t)\left(\frac{1}{2}\mathbf{x}_t + \boldsymbol{s}_t^\theta(\mathbf{x}_t)\right)dt + \sqrt{\beta(t)}d\bar{\mathbf{w}}_t, \tag{4}$$

where $\boldsymbol{s}_t^\theta$ is a model of the score function of q_t and $\bar{\mathbf{w}}_t$ is (again) a standard *Wiener* process but with time flowing *backward* from $t = 1$ to $t = 0$. More specifically, let p_1 be the initial distribution of $\mathbf{x}_1$ from the reverse process (4) and let p_t^θ be the marginal distribution of $\mathbf{x}_t$, $t \in [0, 1)$ from the reverse process (4). If we let $p_1 = q_1$ and $\boldsymbol{s}_t^\theta$ be the *exact* score function of q_t for all $t \in [0, 1]$, we have $p_t^\theta = q_t$ for *all* $t \in [0, 1)$ [10]. In particular, the initial distribution of the forward process q_0 can be recovered at the end of the reverse process via the score functions of q_t, $t \in [0, 1]$. Thus, to learn the initial distribution of the forward process q_0, it suffices to learn a model $\boldsymbol{s}_t^\theta$ that approximates the score functions of q_t for all $t \in [0, 1]$.

There are several methods [26, 48, 43] that allow a model $\boldsymbol{s}_t^\theta$ to be learned from a training dataset drawn from q_0. Here we focus on the *denoising score matching (DSM)* method due to its scalability to large datasets. For the DSM method, a model $\boldsymbol{s}_t^\theta$ is learned by minimizing the following DSM loss:

$$\mathcal{L}_{\text{DSM}}(\theta; q_0) := \mathbb{E}_{\mathbf{x}\sim q_0}\left[\ell_{\text{DSM}}^\theta(\mathbf{x})\right], \tag{5}$$

where

$$\ell_{\text{DSM}}^\theta(\mathbf{x}) := \int_0^1 \lambda(t)\mathbb{E}_{\mathbf{z}\sim\mathcal{N}(0,\boldsymbol{I})}\left[\left\|\boldsymbol{s}_t^\theta(\mathbf{x}_t) + \frac{\mathbf{z}}{\sigma(t)}\right\|^2\right]dt \tag{6}$$

is the *point-wise* DSM loss, $\mathbf{x}_t = \sqrt{1-\sigma(t)^2}\mathbf{x} + \sigma(t)\mathbf{z}$, $\lambda : [0, 1] \to \mathbb{R}_{++}$ can be any positive function, and $\sigma(t) = \sqrt{1 - \exp\left[-\int_0^t \beta(s)ds\right]}$.

While the previous DSM loss can be easily estimated from a dataset drawn from q_0 and hence is very *conductive* to learning, *a priori* it is unclear how it would connect to any *generative* loss between q_0 and p_0^θ. Interestingly, it was shown in Theorem 2 and Corollary 3 of Kwon et al. [38] that under some (relatively) mild conditions[4] on β, q_0, and $\boldsymbol{s}_\theta$, by choosing $\lambda(t) = \beta(t)$ we have

$$W_2(q_0, p_0^\theta) \leq c_0\sqrt{\mathbb{E}_{\mathbf{x}\sim q_0}\left[\ell_{\text{DSM}}^\theta(\mathbf{x})\right]} + c_1 W_2(q_1, p_1), \tag{7}$$

where $W_2(q, p)$ is the 2-Wasserstein distance [1] between the probability distributions q and p, and c_0 and c_1 are constants that only depend on the choice of the noise scheduler β and some prior knowledge on p_0 and $\boldsymbol{s}_t^\theta$ but is independent of the model parameter θ. In Kwon et al. [38], this result was coined as "score-based generative modeling *secretly* minimizes the Wasserstein distance".

[4]The readers are referred to Section 3.1 of Kwon et al. [38] for the assumptions under which the inequality (7) holds.

A.2 Weighted learning

To learn a generative model $p_\theta \approx q_{\rm target}$, we shall let $q_0 = q_{\rm target}$ and p_1 be the standard multivariate Gaussian distribution $\mathcal{N}$. If we denote q_1 and p_0^θ by $\bar{q}_{\text{target}}$ and p_θ respectively, by (7) we have

$$W_2(q_{\rm target}, p_\theta) \leq c_0 \sqrt{\mathbb{E}_{\mathbf{x}\sim q_{\rm target}}\left[\ell^\theta_{\text{DSM}}(\mathbf{x})\right]} + c_1 W_2(\bar{q}_{\text{target}}, \mathcal{N}). \tag{8}$$

We mention here that the output distribution of the forward process $\bar{q}_{\text{target}}$ is potentially dependent on the choice of $\tilde{w}$, even though this dependency is not explicit from the notation. In practice, however, $\bar{q}_{\text{target}}$ can be made very close to the standard multivariate Gaussian distribution $\mathcal{N}$ with an appropriate choice of the noise scheduler β. Therefore, the Wasserstein distance $W_2(\bar{q}_{\text{target}}, \mathcal{N})$ is very small and is usually disregarded from the learning process.

To estimate the DSM loss $\mathbb{E}_{\mathbf{x}\sim q_{\rm target}}\left[\ell^\theta_{\text{DSM}}(\mathbf{x})\right]$ from the offline data examples, note that by the definition of $q_{\rm target}$, we have

$$\begin{aligned}\mathbb{E}_{\mathbf{x}\sim q_{\rm target}}\left[\ell^\theta_{\text{DSM}}(\mathbf{x})\right] &= \mathbb{E}_{\mathbf{x}\sim p_{\rm data}}\left[\tilde{w}(f(\mathbf{x}))\ell^\theta_{\text{DSM}}(\mathbf{x})\right] &(9)\\ &\approx \frac{1}{m}\sum_{i=1}^{m} \tilde{w}(f(\boldsymbol{x}_i))\ell^\theta_{\text{DSM}}(\boldsymbol{x}_i), &(10)\end{aligned}$$

where (9) is also known as "re-weighting" or *importance sampling* [12]. By (8), minimizing the empirical weighted DSM loss (10) can help to identify a generative model $p_\theta \approx q_{\rm target}$ for a pre-selected normalized weight function $\tilde{w}$.

Finally, we note that scaling the normalized weight function $\tilde{w}$ does *not* change the optimal solution that minimizes the empirical weighted DSM loss (10). Therefore, when using (10) to identify a generative model p_θ, one can use an *un-normalized* weight function instead of a normalized one.

A.3 Trade-off between utility and learnability

Intuitively, there are two considerations for selecting a normalized weight function $\tilde{w}$. On one hand, from the *utility* point of view, we would like to choose $\tilde{w}$ such that the hypothetical target distribution $q_{\rm target}$ focuses most of its densities on the domain points with *superior* objective values. This can be achieved, for example, by choosing $\tilde{w}$ to be heavily *skewed* towards superior objective values. On the other hand, from the *learning* viewpoint, the generative model p_θ is learned from the offline observations, which were generated from the unknown data-generating distribution $p_{\rm data}$. If $\tilde{w}$ is chosen to be heavily skewed, the hypothetical target distribution $q_{\rm target}$ then becomes very *different* from the data-generating distribution $p_{\rm data}$. In this case, learning the generative model p_θ from the offline data examples may be subject to very high *sample* complexity.

A.4 The main theorem

Our proposed loss function is based on the following PAC *lower* bound on the natural optimization objective:

$$J_{\text{opt}}(\theta) = \mathbb{E}_{\mathbf{x}\sim p_\theta}[f(\mathbf{x})]. \tag{11}$$

Theorem A.1. *Assume that: i) the unknown objective function f is K-Lipschitz and satisfies $|f(\boldsymbol{x})| \leq F$ for all $\boldsymbol{x} \in \mathcal{X}$; ii) the generative model p_θ is a DDPM; iii) the point-wise DSM loss ℓ^θ_{DSM} satisfies $0 \leq \ell^\theta_{DSM}(\boldsymbol{x}) \leq \Delta$ for all $\boldsymbol{x} \in \mathcal{X}$ and all $\theta \in \Theta$; and iv) the conditions from Section 3.1 of Kwon et al. [38] on the noise scheduler β, the data-generating distribution $p_{\rm data}$, the normalized weight function $\tilde{w}$, and the score-function model $\boldsymbol{s}^\theta_t$ are satisfied. Let $\tilde{\mathcal{W}}$ be the collection of all normalized weight functions $\tilde{w}$ that are L-Lipschitz and satisfy $0 \leq \tilde{w}(y) \leq B$ for any $y \in [-F, F]$. With probability $\geq 1-\delta$, we have for* any *$\tilde{w} \in \tilde{\mathcal{W}}$ and* any *$\theta \in \Theta$,*

$$\begin{aligned}J_{opt}(\theta) \geq \underbrace{\hat{J}_{\boldsymbol{x}_{[m]}}(\tilde{w})}_{\text{empirical utility}} - \underbrace{c_0 K \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})}}_{\text{empirical weighted DSM loss}} - \underbrace{c_0 K \sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})}}_{\text{empirical variance}} - \\ c_1 K W_2(\bar{q}_{target}, \mathcal{N}) - c_0 K \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - O\left(1/\sqrt[8]{m}\right),\end{aligned} \tag{12}$$

where

$$\hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^{m} \tilde{w}(f(\boldsymbol{x}_i))f(\boldsymbol{x}_i) \tag{13}$$

is the empirical *utility of* $\tilde{w}$*,*

$$\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) = \frac{1}{m}\sum_{i=1}^{m} \tilde{w}(f(\boldsymbol{x}_i))\ell^{\theta}_{DSM}(\boldsymbol{x}_i) \tag{14}$$

is the empirical *weighted DSM loss of* $\boldsymbol{s}^{\theta}_t$*,*

$$\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^{m} (\tilde{w}(f(\boldsymbol{x}_i)) - 1)^2 \tag{15}$$

is the empirical *variance of* $\tilde{w}$*,*

$$\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) = \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta} \frac{1}{m}\sum_{i=1}^{m} \sigma_i \ell^{\theta}_{DSM}(\boldsymbol{x}_i)\right] \tag{16}$$

is the empirical *Rademacher complexity with respect to the parameter family* Θ*, and the last term* $O\left(1/\sqrt[8]{m}\right)$ *is independent of the model parameter* θ *and* $\tilde{w}$*.*

The proof of the above theorem is long and technical and hence is deferred to next section to enhance the flow of the paper. We mention here that the proof utilizes several key technical results including the *duality* theorem of Kantorovich-Rubenstein [2] for the 1-Wasserstein distance [4], the fact that "score-based generative modeling *secretly* minimizes the Wasserstein distance" [38], the Rademacher bound for *bounded* functions [42], the Wasserstein contraction property [9], and the covering bound for *Lipschitz* functions [47].

Note that to maximize the PAC lower bound (1), we need to simultaneously maximize the *utility* of $\tilde{w}$ and minimize the *weighted DSM loss* of $\boldsymbol{s}^{\theta}_t$ and the *variance* of $\tilde{w}$. Therefore, the PAC lower bound (1) captures both the utility and learnability considerations for selecting a normalized weight function $\tilde{w}$.

A.5 From PAC lower bound to surrogate loss function

To jointly learn a generate model p_θ and a normalized function $\tilde{w}$, first note that the last two terms of the PAC lower bound (1) are independent of θ and $\tilde{w}$ and hence can be ignored from the learning objective. The forth term is due to the "initial" sampling error of the reverse process. As discussed previously in Section A.2, while this term is potentially dependent on the normalized weight function $\tilde{w}$, in practice it can be made very small by choosing an appropriate noise scheduler β and hence will be ignored from our learning objective.

To make the first three terms *learnable*, we consider the following two modifications to the bound.

First, the coefficients $c_0 K$ and $c_0 K\sqrt{2\Delta}$ in the second and the third term require some prior knowledge on the unknown data-generating distribution p_{data} and the unknown objective function f. In practice, we replace them by two *hyper-parameters* λ and α, respectively. We mention here that the hyper-parameter α plays a particular important role in the learning objective, as it controls the utility-learnability tradeoff for selecting a normalized weight function $\tilde{w}$.

Second, the weight function $\tilde{w}$ needs to be *normalized* with respect to the unknown data-generating distribution p_{data} and the unknown objective function f. In practice, we let $\tilde{w}(\cdot) = \frac{w_\phi(\cdot)}{Z_\phi}$, where w_ϕ is an *un-normalized* weight function parameterized by a second parameter ϕ, and $Z_\phi = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}[w_\phi(f(\mathbf{x}))]$ is the normalizing constant. While the exact calculation of Z_ϕ again requires the knowledge of p_{data} and f, in practice it can be easily estimated from the offline data examples as $\hat{Z}_\phi = \frac{1}{m}\sum_{i=1}^{m} w_\phi(f(\boldsymbol{x}_i))$.

A.6 Algorithms

Algorithm 1 TRAINING

1: **Input**: Offline examples $(\boldsymbol{x}_i, f(\boldsymbol{x}_i))$; hyper-parameters α, λ; learning-rate parameters η_1, η_2.
2: **General step**:
3: $\phi_0 \leftarrow \arg\max_{\phi\in\Phi} \left\{ \frac{1}{m}\sum_{i=1}^m \frac{w_\phi(f(\boldsymbol{x}_i))f(\boldsymbol{x}_i)}{\hat{Z}_\phi} - \alpha \sqrt[4]{\frac{1}{m}\sum_{i=1}^m \left(\frac{w_\phi(f(\boldsymbol{x}_i))}{\hat{Z}_\phi} - 1\right)^2} \right\}$ ▷ via GD
4: $\theta_0 \leftarrow \arg\min_{\theta\in\Theta} \left\{ \frac{1}{m}\sum_{i=1}^m w_{\phi_0}(f(\boldsymbol{x}_i)) \cdot \ell^{\theta}_{\text{DSM}}(\boldsymbol{x}_i) \right\}$ ▷ via SGD
5: **for** $k = 0$ **to** $K-1$ **do**
6: $\quad\phi_{k+1} \leftarrow \phi_k + \eta_1 \cdot \nabla_\phi J_{\alpha,\lambda}(\theta_k, \phi_k)$ ▷ via GD
7: $\quad\theta_{k+1} \leftarrow \theta_k - \eta_2 \cdot \nabla_\theta \left\{ \frac{1}{m}\sum_{i=1}^m w_{\phi_{k+1}}(f(\boldsymbol{x}_i)) \cdot \ell^{\theta_k}_{\text{DSM}}(\boldsymbol{x}_i) \right\}$ ▷ via SGD
8: **end for**
9: **Output**: Model parameters $(\phi^*, \theta^*) = (\phi_K, \theta_K)$.

Algorithm 2 SAMPLING/OPTIMIZATION

1: **Input**: Score function model $\boldsymbol{s}_t^{\theta^*}(\boldsymbol{x})$, number of samples N, number of steps T, noise scheduler parameters $(\beta_{\min}, \beta_{\max})$, and $\tilde{\beta}(t) = \frac{1}{T}\left[\beta_{\min} + \frac{t}{T}(\beta_{\max} - \beta_{\min})\right]$.
2: **General step**:
3: Draw N samples $\boldsymbol{x}_T^{(1)}, \boldsymbol{x}_T^{(2)}, \ldots, \boldsymbol{x}_T^{(N)} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \boldsymbol{I})$
4: **for** $n = 1$ **to** N **do**
5: $\quad$**for** $t = T$ **to** 1 **do**
6: $\quad\quad\boldsymbol{x}_{t-1}^{(n)} \leftarrow \left(2 - \sqrt{1 - \tilde{\beta}(t)}\right) \cdot \boldsymbol{x}_t^{(n)} + \frac{1}{2}\tilde{\beta}(t) \cdot \boldsymbol{s}_{t/T}^{\theta^*}(\boldsymbol{x}_t^{(n)})$
7: $\quad$**end for**
8: **end for**
9: **Output**: Optimized samples $\boldsymbol{x}_0^{(1)}, \boldsymbol{x}_0^{(2)}, \ldots, \boldsymbol{x}_0^{(N)}$.

B Proof of the Main Theorem

In this section, we introduce a few technical results, which will lead to the proof of the main theorem.

B.1 Wasserstein distance

Let μ and ν be two probability distributions on $\mathbb{R}^d$. A *coupling* γ between μ and ν is a joint distribution on $\mathbb{R}^d \times \mathbb{R}^d$ whose marginals are μ and ν. The p-Wasserstein distance between μ and ν (with respect to the Euclidean norm) is given by [1]:

$$W_p(\mu, \nu) = \left(\inf_{\gamma\in\Gamma(\mu,\nu)} \mathbb{E}_{(\mathbf{x},\tilde{\mathbf{x}})\sim\gamma}\left[\|\mathbf{x} - \tilde{\mathbf{x}}\|^p\right] \right)^{1/p}, \tag{17}$$

where $\Gamma(\mu, \nu)$ is the set of all couplings between μ and ν, and $\|\cdot\|$ denotes the standard Euclidean norm.

The 1-Wasserstein distance, also known as the *earth mover's distance*, has an important equivalent representation that follows from the *duality* theorem of Kantorovich-Rubenstein [2]:

$$W_1(\mu, \nu) = \frac{1}{K} \sup_{\|\tilde{f}\|_{\text{Lip}} \le K} \left\{ \mathbb{E}_{\mathbf{x}\sim\mu}[\tilde{f}(\mathbf{x})] - \mathbb{E}_{\mathbf{x}\sim\nu}[\tilde{f}(\mathbf{x})] \right\}, \tag{18}$$

where $\|\cdot\|_{\text{Lip}}$ denotes the *Lipschitz* norm. In our construction, this *dual* representation of the 1-Wasserstein distance serves as the bridge between the *objective-specific* generative loss and the *generic* generative loss.

By the standard Jensen's inequality [16], we also have

$$W_1(\mu, \nu) \leq W_2(\mu, \nu) \tag{19}$$

for any two distributions μ and ν. As we shall see, this simple relationship between the 1-Wasserstein and 2-Wasserstein distances can help to further connect the *objective-specific* generative loss to the *DSM* loss for training a *score-based* generative model.

B.2 Generalization bound for weighted learning

Let $\ell_\theta : \mathcal{X} \to \mathbb{R}$ be a *bounded* loss function parameterized by $\theta \in \Theta$ such that $0 \leq \ell_\theta(\boldsymbol{x}) \leq \Delta$ for all $\boldsymbol{x} \in \mathcal{X}$ and all $\theta \in \Theta$. Consider the problem of estimating the expected *weighted* loss $\mathcal{L}_p(\theta, \tilde{w}) = \mathbb{E}_{\mathbf{x}\sim p}[\tilde{w}(\mathbf{x})\ell_\theta(\mathbf{x})]$, where $\tilde{w} : \mathcal{X} \to \mathbb{R}_+$ is a normalized, *bounded* weight function such that $\mathbb{E}_{\mathbf{x}\sim p}[\tilde{w}(\mathbf{x})] = 1$ and $0 \leq \tilde{w}(\boldsymbol{x}) \leq B$ for all $\boldsymbol{x} \in \mathcal{X}$. We have the following PAC upper bound, with respect to the parameter family Θ, on the expected weighted loss $\mathcal{L}_p(\theta, \tilde{w})$ for any given $\tilde{w}$.

Lemma B.1. *For any given $\tilde{w}$, with probability $\geq 1 - \delta$ we have for* any $\theta \in \Theta$

$$\mathcal{L}_p(\theta, \tilde{w}) \leq \hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) + 2\Delta\sqrt{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} + 2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) + 3\sqrt{\frac{2B\Delta\log(2/\delta)}{m}}, \tag{20}$$

where $\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) = \frac{1}{m}\sum_{i=1}^m \tilde{w}(\boldsymbol{x}_i)\ell_\theta(\boldsymbol{x}_i)$ is the empirical *weighted loss over the training dataset $\boldsymbol{x}_{[m]}$, $\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^m (\tilde{w}(\boldsymbol{x}_i) - 1)^2$ is the* empirical *variance of $\tilde{w}$ over $\boldsymbol{x}_{[m]}$, and $\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) = \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta} \frac{1}{m}\sum_{i=1}^m \sigma_i\ell_\theta(\boldsymbol{x}_i)\right]$ is the* empirical *Rademacher complexity with respect to the parameter family Θ over $\boldsymbol{x}_{[m]}$.*

Proof. By assumption, we have $0 \leq \tilde{w}(\boldsymbol{x}) \leq B$ for any $\boldsymbol{x} \in \mathcal{X}$ and $0 \leq \ell_\theta(\boldsymbol{x}) \leq \Delta$ for any $\boldsymbol{x} \in \mathcal{X}$ and any $\theta \in \Theta$. It follows immediately that the *weighed* loss function $\tilde{w}(\boldsymbol{x})\ell_\theta(\boldsymbol{x})$ satisfies $0 \leq \tilde{w}(\boldsymbol{x})\ell_\theta(\boldsymbol{x}) \leq B\Delta$ for any $\boldsymbol{x} \in \mathcal{X}$ and any $\theta \in \Theta$. Applying the standard Rademacher bound to the *weighted* loss function class $(\tilde{w}(\boldsymbol{x})\ell_\theta(\boldsymbol{x}) : \theta \in \Theta)$, with probability $\geq 1 - \delta$ we have for any $\theta \in \Theta$

$$\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(\mathbf{x})\ell_\theta(\mathbf{x})\right] \leq \hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) + 2\hat{\mathfrak{R}}^{\tilde{w}}_{\boldsymbol{x}_{[m]}}(\Theta) + 3\sqrt{\frac{2B\Delta\log(2/\delta)}{m}}, \tag{21}$$

where $\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) = \frac{1}{m}\sum_{i=1}^m \tilde{w}(\boldsymbol{x}_i)\ell_\theta(\boldsymbol{x}_i)$ is the empirical weighted loss over $\boldsymbol{x}_{[m]}$, and $\hat{\mathfrak{R}}^{\tilde{w}}_{\boldsymbol{x}_{[m]}}(\Theta) = \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta} \frac{1}{m}\sum_{i=1}^m \sigma_i\tilde{w}(\boldsymbol{x})\ell_\theta(\boldsymbol{x}_i)\right]$ is the empirical *weighted* Rademacher complexity [42] with respect to the parameter family Θ over $\boldsymbol{x}_{[m]}$. The empirical weighted Rademacher complexity $\hat{\mathfrak{R}}^{\tilde{w}}_{\boldsymbol{x}_{[m]}}(\Theta)$ can be further bounded from above as:

$$\begin{aligned}
\hat{\mathfrak{R}}^{\tilde{w}}_{\boldsymbol{x}_{[m]}}(\Theta) &= \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^m \sigma_i\left(w(\boldsymbol{x}_i) - 1 + 1\right)\ell_\theta(\boldsymbol{x}_i)\right] \\
&\leq \mathbb{E}_{\sigma_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^m \sigma_i(\tilde{w}(\boldsymbol{x}_i) - 1)\ell_\theta(\boldsymbol{x}_i)\right] + \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^m \sigma_i\ell_\theta(\boldsymbol{x}_i)\right]
\end{aligned} \tag{22}$$

Further note that

$$\begin{aligned}
\frac{1}{m}\sum_{i=1}^m \sigma_i(\tilde{w}(\boldsymbol{x}_i) - 1)\ell_\theta(\boldsymbol{x}_i) &\leq \sqrt{\frac{\sum_{i=1}^m(\tilde{w}(\boldsymbol{x}_i) - 1)^2}{m}}\sqrt{\frac{\sum_{i=1}^m\left(\sigma_i\ell_\theta(\boldsymbol{x}_i)\right)^2}{m}} \\
&= \sqrt{\frac{\sum_{i=1}^m(\tilde{w}(\boldsymbol{x}_i) - 1)^2}{m}}\sqrt{\frac{\sum_{i=1}^m \ell_\theta^2(\boldsymbol{x}_i)}{m}} \\
&\leq \Delta\sqrt{\frac{\sum_{i=1}^m(\tilde{w}(\boldsymbol{x}_i) - 1)^2}{m}}
\end{aligned}$$

for any $\theta \in \Theta$ and any realization of $\boldsymbol{\sigma}_{[m]}$, where the first inequality follows from the standard Cauchy-Schwarz inequality, the second equality follows from the fact that the square of a Rademacher variable takes a constant value of 1, and the last inequality follows from the assumption that $0 \leq \ell_\theta(\boldsymbol{x}) \leq \Delta$ for any $\boldsymbol{x} \in \mathcal{X}$ and any $\theta \in \Theta$. It follows immediately that

$$\mathbb{E}_{\sigma_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^{m}\sigma_i(\tilde{w}(\boldsymbol{x}_i)-1)\ell_\theta(\boldsymbol{x}_i)\right] \leq \Delta\sqrt{\frac{\sum_{i=1}^{m}(\tilde{w}(\boldsymbol{x}_i)-1)^2}{m}}. \tag{23}$$

Substituting (23) into (22) gives

$$\hat{\mathfrak{R}}^{\tilde{w}}_{\boldsymbol{x}_{[m]}}(\Theta) \leq \Delta\sqrt{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} + \hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta), \tag{24}$$

where $\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^{m}\left(\tilde{w}(\boldsymbol{x}_i)-1\right)^2$ is the empirical variance of $\tilde{w}$ over $\boldsymbol{x}_{[m]}$, and $\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) = \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^{m}\sigma_i\ell_\theta(\boldsymbol{x}_i)\right]$ is the empirical (un-weighted) Rademacher complexity with respect to the parameter family Θ over $\boldsymbol{x}_{[m]}$. Substituting (24) into (21) completes the proof of (20) and hence Lemma B.1. $\square$

The main insight from the above lemma is that the *generalization error* (with respect to the parameter θ) between the expected weighted loss $\mathcal{L}_p(\theta, \tilde{w})$ and the empirical weighted loss $\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})$ can be controlled by controlling the *complexity* of the model class Θ and the *variance* of the normalized weight function $\tilde{w}$.

B.3 A distribution-dependent surrogate on the natural optimization objective

Proposition B.2. *Assume that the unknown objective function f is K-Lipschitz and the generative model p_θ is a DDPM. Under the assumptions from Section 3.1 of Kwon et al. [38] on the noise scheduler β, the data-generating distribution p_{data}, the normalized weight function $\tilde{w}$, and the score-function model $\boldsymbol{s}^\theta_t$, we have*

$$J_{opt}(\theta) \geq \underbrace{\mathbb{E}_{\mathbf{x}\sim p_{\mathrm{data}}}\left[\tilde{w}(f(\mathbf{x}))f(\mathbf{x})\right]}_{\text{expected utility}} - \underbrace{c_0K\sqrt{\mathbb{E}_{\mathbf{x}\sim p_{\mathrm{data}}}\left[\tilde{w}(f(\mathbf{x}))\ell^\theta_{DSM}(\mathbf{x})\right]}}_{\text{expected weighted DSM loss}} - c_1KW_2(\bar{q}_{target}, \mathcal{N}), \tag{25}$$

where ℓ^θ_{DSM} is the point-wise DSM loss of $\boldsymbol{s}^\theta_t$ as defined in (6), $\bar{q}_{target}$ is the output distribution of the forward process (3), Φ is the standard Gaussian distribution, and c_0 and c_1 are constants that are independent of the model parameter θ and $\tilde{w}$.

Proof. We start by writing $J_{\mathrm{opt}}(\theta)$ as:

$$J_{\mathrm{opt}}(\theta) = \mathbb{E}_{\mathbf{x}\sim q_{\mathrm{target}}}[f(\mathbf{x})] - \left\{\mathbb{E}_{\mathbf{x}\sim q_{\mathrm{target}}}[f(\mathbf{x})] - \mathbb{E}_{\mathbf{x}\sim p_\theta}[f(\mathbf{x})]\right\}. \tag{26}$$

By the definition of q_{target}:

$$q_{\mathrm{target}}(\boldsymbol{x}) := \tilde{w}(f(\boldsymbol{x}))\cdot p_{\mathrm{data}}(\boldsymbol{x}), \tag{27}$$

we have

$$\mathbb{E}_{\mathbf{x}\sim q_{\mathrm{target}}}[f(\mathbf{x})] = \mathbb{E}_{\mathbf{x}\sim p_{\mathrm{data}}}\left[\tilde{w}(f(\mathbf{x}))f(\mathbf{x})\right]. \tag{28}$$

Furthermore,

$$\begin{aligned}\mathbb{E}_{\mathbf{x}\sim q_{\mathrm{target}}}[f(\mathbf{x})] - \mathbb{E}_{\mathbf{x}\sim p_\theta}[f(\mathbf{x})] &\leq \sup_{\|\tilde{f}\|_{\mathrm{Lip}}\leq K}\left\{\mathbb{E}_{\mathbf{x}\sim q_{\mathrm{target}}}[\tilde{f}(\mathbf{x})] - \mathbb{E}_{\mathbf{x}\sim p_\theta}[\tilde{f}(\mathbf{x})]\right\} &(29)\\ &= K\cdot W_1(q_{\mathrm{target}}, p_\theta), &(30)\end{aligned}$$

where the first inequality follows directly from the assumption that f is K-Lipschitz, and the second equality follows from the dual representation (30) of the 1-Wasserstein distance.

Under the assumption that p_θ is a DDPM, we can further bound the 1-Wasserstein distance $W_1(q_{\mathrm{target}}, p_\theta)$ as:

$$W_1(q_{\mathrm{target}}, p_\theta) \leq W_2(q_{\mathrm{target}}, p_\theta) \leq c_o\sqrt{\mathbb{E}_{\mathbf{x}\sim p_{\mathrm{data}}}\left[\tilde{w}(f(\mathbf{x}))\ell^\theta_{\mathrm{DSM}}(\mathbf{x})\right]} + c_1W_2(\bar{q}_{\mathrm{target}}, \mathcal{N}), \tag{31}$$

where the first inequality follows from (19), and the second inequality follows from (8) and the definition of q_{target} in (27).

Substituting (28), (30), and (31) into (26) completes the proof of (25). $\square$

Next, we shall convert the distribution-dependent surrogate on the right-hand side of (25) into a *PAC* lower bound using the standard *complexity* theory.

B.4 Proof of Theorem A.1

For the proof, we shall write q_{target} and $\bar{q}_{\text{target}}$ as $q^{\tilde{w}}_{\text{target}}$ and $\bar{q}^{\tilde{w}}_{\text{target}}$ respectively, to emphasize their dependencies on the normalized weight function $\tilde{w}$. Let us first recall from Proposition B.2 that the natural optimization objective $J_{\text{opt}}(\theta)$ can be bounded from below as:

$$J_{\text{opt}}(\theta) \geq \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(f(\mathbf{x}))f(\mathbf{x})\right] - c_0 K\sqrt{\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(f(\mathbf{x}))\ell^{\theta}_{\text{DSM}}(\mathbf{x})\right]} - c_1 K W_2(\bar{q}^{\tilde{w}}_{\text{target}}, \mathcal{N}). \tag{32}$$

To turn the right-hand side into a *PAC* lower bound on $J_{\text{opt}}(\theta)$, let us first *fix* a normalized weight function $\tilde{w} \in \tilde{\mathcal{W}}$.

Given $\tilde{w}$, let us first apply the standard Hoeffding's inequality to obtain a *concentration* lower bound on the expected utility $\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}[\tilde{w}(f(\mathbf{x}))f(\mathbf{x})]$. More specifically, by assumption we have $|f(\boldsymbol{x})| \leq F$ for any $\boldsymbol{x} \in \mathcal{X}$ and $0 \leq \tilde{w}(y) \leq B$ for any $y \in [-F, F]$. It follows that the *weighed* objective function $\tilde{w}(f(\boldsymbol{x}))f(\boldsymbol{x})$ satisfies $|\tilde{w}(f(\boldsymbol{x}))f(\boldsymbol{x})| \leq BF$ for any $\boldsymbol{x} \in \mathcal{X}$. By Hoeffding's inequality, with probability $\geq 1 - \delta'/2$ we have

$$\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(f(\mathbf{x}))f(\mathbf{x})\right] \geq \hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) - \sqrt{\frac{BF\log(2/\delta')}{m}}, \tag{33}$$

where $\hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^{m}\tilde{w}(f(\boldsymbol{x}_i))f(\boldsymbol{x}_i)$ is the empirical utility of $\tilde{w}$. Next by Lemma (B.1), with probability $\geq 1 - \delta'/2$ we have for *any* $\theta \in \Theta$

$$\begin{aligned}&\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(f(\mathbf{x}))\ell^{\theta}_{\text{DSM}}(\mathbf{x})\right]\\ &\leq \hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) + 2\Delta\sqrt{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} + 2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) + 3\sqrt{\frac{2B\Delta\log(4/\delta')}{m}}\end{aligned}$$

and hence

$$\begin{aligned}&\sqrt{\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\tilde{w}(f(\mathbf{x}))\ell^{\theta}_{DSM}(\mathbf{x})\right]}\\ &\leq \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) + 2\Delta\sqrt{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} + 2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) + 3\sqrt{\frac{2B\Delta\log(4/\delta')}{m}}}\\ &\leq \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})} + \sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} + \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} + \sqrt[4]{\frac{18B\Delta\log(4/\delta')}{m}},\end{aligned} \tag{34}$$

where $\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w}) = \frac{1}{m}\sum_{i=1}^{m}\tilde{w}(\boldsymbol{x}_i)\ell^{\theta}_{\text{DSM}}(\boldsymbol{x}_i)$ is the empirical weighted DSM loss of $\boldsymbol{s}^{\theta}_t$ over $\boldsymbol{x}_{[m]}$, $\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w}) = \frac{1}{m}\sum_{i=1}^{m}(\tilde{w}(\boldsymbol{x}_i) - 1)^2$ is the empirical variance of $\tilde{w}$ over $\boldsymbol{x}_{[m]}$, and $\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta) = \mathbb{E}_{\boldsymbol{\sigma}_{[m]}}\left[\sup_{\theta\in\Theta}\frac{1}{m}\sum_{i=1}^{m}\sigma_i\ell^{\theta}_{\text{DSM}}(\boldsymbol{x}_i)\right]$ is the empirical Rademacher complexity with respect to the parameter family Θ over $\boldsymbol{x}_{[m]}$. Substituting (33) and (34) into (32), with probability $\geq 1 - \delta'$ we have for *any* $\theta \in \Theta$

$$\begin{aligned}J_{\text{opt}}(\theta) \geq\ &\hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) - c_0 K\sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})} - c_0 K\sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} - c_1 K W_2(\bar{q}^{\tilde{w}}_{\text{target}}, \mathcal{N}) -\\ &c_0 K\sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - c_0 K\sqrt[4]{\frac{18B\Delta\log(4/\delta')}{m}} - \sqrt{\frac{BF\log(2/\delta')}{m}}.\end{aligned} \tag{35}$$

To remove the *conditioning* on $\tilde{w}$, let $\tilde{\mathcal{W}}_\epsilon$ be an ϵ-*cover* [47] of $\tilde{\mathcal{W}}$ under the L_∞ norm. By (35), for any *given* $\tilde{v} \in \tilde{\mathcal{W}}_\epsilon$, with probability $\geq 1 - \delta'$ we have for *any* $\theta \in \Theta$

$$\begin{aligned}J_{\text{opt}}(\theta) \geq\ &\hat{J}_{\boldsymbol{x}[m]}(\tilde{v}) - c_0 K\sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{v})} - c_0 K\sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{v})} - c_1 K W_2(\bar{q}^{\tilde{v}}_{\text{target}}, \mathcal{N}) -\\ &c_0 K\sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - c_0 K\sqrt[4]{\frac{18B\Delta\log(4/\delta')}{m}} - \sqrt{\frac{BF\log(2/\delta')}{m}}.\end{aligned}$$

By the *union* bound, with probability $\geq 1 - |\tilde{\mathcal{W}}_\epsilon|\delta'$ we have for *any* $\theta \in \Theta$ and *any* $\tilde{v} \in \tilde{\mathcal{W}}_\epsilon$

$$\begin{aligned}J_{\text{opt}}(\theta) \geq\ &\hat{J}_{\boldsymbol{x}[m]}(\tilde{v}) - c_0 K\sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{v})} - c_0 K\sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{v})} - c_1 K W_2(\bar{q}^{\tilde{v}}_{\text{target}}, \mathcal{N}) -\\ &c_0 K\sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - c_0 K\sqrt[4]{\frac{18B\Delta\log(4/\delta')}{m}} - \sqrt{\frac{BF\log(2/\delta')}{m}}.\end{aligned}$$

Choosing $\delta' = \delta/|\tilde{\mathcal{W}}_\epsilon|$, with probability $\geq 1-\delta$ we have for *any* $\theta \in \Theta$ and *any* $\tilde{v} \in \tilde{\mathcal{W}}_\epsilon$

$$J_{\text{opt}}(\theta) \geq \hat{J}_{\boldsymbol{x}[m]}(\tilde{v}) - c_0 K \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta,\tilde{v})} - c_0 K\sqrt{2\Delta}\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{v})} - c_1 K W_2(\bar{q}^{\tilde{v}}_{\text{target}}, \mathcal{N}) - \\ c_0 K \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - c_0 K \sqrt[4]{\frac{18B\Delta \log(4|\tilde{\mathcal{W}}_\epsilon|/\delta)}{m}} - \sqrt{\frac{BF\log(2|\tilde{\mathcal{W}}_\epsilon|/\delta)}{m}}. \tag{36}$$

By the definition of ϵ-cover, for any $\tilde{w} \in \tilde{\mathcal{W}}$, there exists an $\tilde{v} \in \tilde{\mathcal{W}}_\epsilon$ such that $|\tilde{w}(f(\boldsymbol{x})) - \tilde{v}(f(\boldsymbol{x}))| \leq \epsilon$ for any $\boldsymbol{x} \in \mathcal{X}$. Note that this immediately implies that:

$$\begin{aligned}\hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) - \hat{J}_{\boldsymbol{x}[m]}(\tilde{v}) &= \frac{1}{m}\sum_{i=1}^m (\tilde{w}(f(\boldsymbol{x}_i)) - \tilde{v}(f(\boldsymbol{x}_i)))\, f(\boldsymbol{x}_i) \\ &\leq \frac{1}{m}\sum_{i=1}^m |\tilde{w}(f(\boldsymbol{x}_i)) - \tilde{v}(f(\boldsymbol{x}_i))|\, |f(\boldsymbol{x}_i)| \leq F\epsilon, \end{aligned} \tag{37}$$

where the last inequality follows from the assumption that $|f(\boldsymbol{x})| \leq F$ for any $\boldsymbol{x} \in \mathcal{X}$;

$$\begin{aligned}\sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta,\tilde{v})} - \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta,\tilde{w})} &= \sqrt{\frac{1}{m}\sum_{i=1}^m \tilde{v}(f(\boldsymbol{x}_i))\ell^\theta_{\text{DSM}}(\boldsymbol{x}_i)} - \sqrt{\frac{1}{m}\sum_{i=1}^m \tilde{w}(f(\boldsymbol{x}_i))\ell^\theta_{\text{DSM}}(\boldsymbol{x}_i)} \\ &\leq \sqrt{\frac{1}{m}\sum_{i=1}^m |\tilde{v}(f(\boldsymbol{x}_i)) - \tilde{w}(f(\boldsymbol{x}_i))|\, \ell^\theta_{\text{DSM}}(\boldsymbol{x}_i)} \leq \sqrt{\Delta\epsilon}, \end{aligned} \tag{38}$$

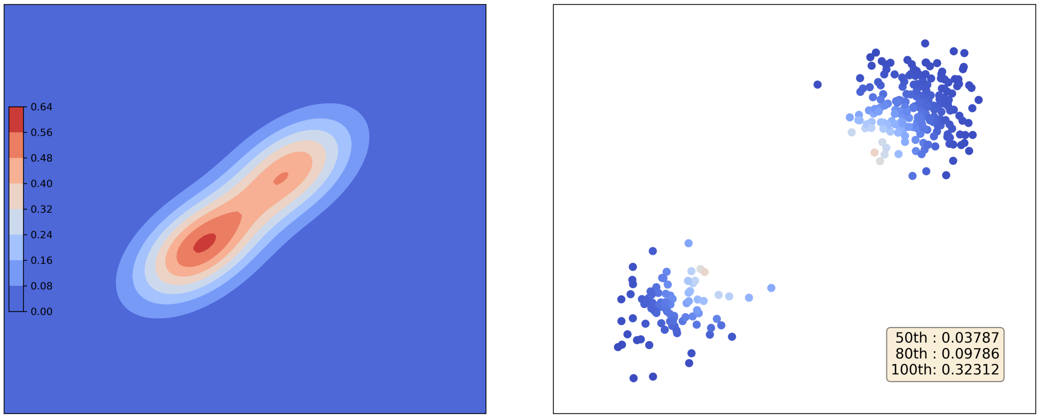
where the last inequality follows from the assumption that $0 \leq \ell^\theta_{\text{DSM}}(\boldsymbol{x}) \leq \Delta$ for any $\boldsymbol{x} \in \mathcal{X}$;

$$\begin{aligned}&\sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{v})} - \sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} \\ &= \sqrt[4]{\frac{1}{m}\sum_{i=1}^m (\tilde{v}(f(\boldsymbol{x}_i)) - 1)^2} - \sqrt[4]{\frac{1}{m}\sum_{i=1}^m (\tilde{w}(f(\boldsymbol{x}_i)) - 1)^2} \\ &= \sqrt[4]{\frac{1}{m}\sum_{i=1}^m (\tilde{v}(f(\boldsymbol{x}_i)) - \tilde{w}(f(\boldsymbol{x}_i)) + \tilde{w}(f(\boldsymbol{x}_i)) - 1)^2} - \sqrt[4]{\frac{1}{m}\sum_{i=1}^m (\tilde{w}(f(\boldsymbol{x}_i)) - 1)^2} \\ &\leq \sqrt[4]{\frac{1}{m}\sum_{i=1}^m (\tilde{v}(f(\boldsymbol{x}_i)) - \tilde{w}(f(\boldsymbol{x}_i)))^2} + \sqrt[4]{\frac{2}{m}\sum_{i=1}^m |\tilde{v}(f(\boldsymbol{x}_i)) - \tilde{w}(f(\boldsymbol{x}_i))|\, |\tilde{w}(f(\boldsymbol{x}_i)) - 1|} \\ &\leq \sqrt{\epsilon} + \sqrt[4]{2(B+1)\epsilon}, \end{aligned} \tag{39}$$

where the last inequality follows from the assumption that $0 \leq \tilde{w}(f(\boldsymbol{x})) \leq B$ for any $\boldsymbol{x} \in \mathcal{X}$; and

$$\begin{aligned}W_2(\bar{q}^{\tilde{v}}_{\text{target}}, \mathcal{N}) - W_2(\bar{q}^{\tilde{w}}_{\text{target}}, \mathcal{N}) &\leq W_2(\bar{q}^{\tilde{v}}_{\text{target}}, \bar{q}^{\tilde{w}}_{\text{target}}) \\ &\leq c_2 W_2(q^{\tilde{v}}_{\text{target}}, q^{\tilde{w}}_{\text{target}}) \\ &\leq c_2 d_2(\mathcal{X}) d_{\text{TV}}(q^{\tilde{v}}_{\text{target}}, q^{\tilde{w}}_{\text{target}}) \\ &= \frac{1}{2} c_2 d_2(\mathcal{X}) \int_{\mathcal{X}} |\tilde{v}(f(\boldsymbol{x})) - \tilde{w}(f(\boldsymbol{x}))| p_{\text{data}}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \\ &\leq \frac{1}{2} c_2 d_2(\mathcal{X})\epsilon, \end{aligned} \tag{40}$$

where c_2 is the *Wasserstein contraction constant* [9] of the forward process (3), $d_2(\mathcal{X}) := \max_{\boldsymbol{x},\boldsymbol{x}' \in \mathcal{X}} \|\boldsymbol{x} - \boldsymbol{x}'\|_2$ is the *diameter* of $\mathcal{X}$ with respect to the ℓ_2 norm, and $d_{\text{TV}}(q^{\tilde{v}}_{\text{target}}, q^{\tilde{w}}_{\text{target}})$ denotes the *total variation distance* between $q^{\tilde{v}}_{\text{target}}$ and $q^{\tilde{w}}_{\text{target}}$. Here, the first inequality follows from the fact that the 2-Wasserstein distance is a metric and hence follows the triangle inequality, the second inequality follows from the *Wasserstein contraction* property [9] of the forward process,



(a) Objective function (b) Offline examples

Figure 2: A toy example: Initial setting.

and the third inequality follows from the *total-variation* bound [20] on the 2-Wasserstein distance. Substituting (37)–(40) into (36), with probability $\geq 1-\delta$ we have for *any* $\theta \in \Theta$ and *any* $\tilde{w} \in \tilde{\mathcal{W}}$

$$\begin{aligned} J_{\text{opt}}(\theta) \quad \geq \quad & \hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) - c_0 K \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})} - c_0 K \sqrt{2\Delta} \sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} - c_1 K W_2(\bar{q}^{\tilde{w}}_{\text{target}}, \mathcal{N}) - \\ & c_0 K \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - c_0 K \sqrt[4]{\frac{18 B \Delta \log(4|\tilde{\mathcal{W}}_\epsilon|/\delta)}{m}} - \sqrt{\frac{BF \log(2|\tilde{\mathcal{W}}_\epsilon|/\delta)}{m}} - \\ & \left(F + \frac{1}{2} c_2 d_2(\mathcal{X})\right)\epsilon - \left(\sqrt{\Delta} + 1\right)\sqrt{\epsilon} - \sqrt[4]{2(B+1)\epsilon}. \end{aligned} \tag{41}$$

By assumption, any normalized weight function from $\tilde{\mathcal{W}}$ is L-Lipschitz and bounded by B. Therefore, the covering number $|\tilde{\mathcal{W}}_\epsilon|$ is of the order $O(\exp(1/\epsilon))$. Let $\epsilon = m^{-\gamma}$ for some $\gamma \in (0,1)$, and we have from (41)

$$\begin{aligned} J_{\text{opt}}(\theta) \quad \geq \quad & \hat{J}_{\boldsymbol{x}[m]}(\tilde{w}) - c_0 K \sqrt{\hat{\mathcal{L}}_{\boldsymbol{x}_{[m]}}(\theta, \tilde{w})} - c_0 K \sqrt{2\Delta} \sqrt[4]{\hat{V}_{\boldsymbol{x}_{[m]}}(\tilde{w})} - c_1 K W_2(\bar{q}^{\tilde{w}}_{\text{target}}, \mathcal{N}) - \\ & c_0 K \sqrt{2\hat{\mathfrak{R}}_{\boldsymbol{x}_{[m]}}(\Theta)} - O(m^{-(1-\gamma)/4}) - O(m^{-\gamma/4}). \end{aligned} \tag{42}$$

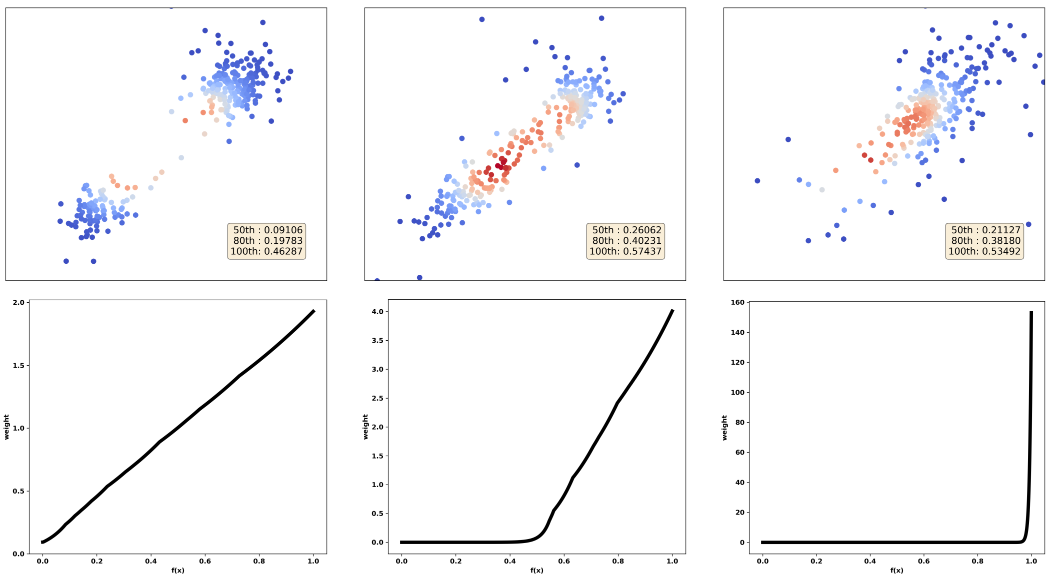
Choosing $\gamma = 1/2$ in (42) completes the proof of (1) and hence Theorem A.1.

C Additional Experiments and Details

C.1 A toy example

We first experimentally validate the proposed learning algorithm using a toy example in $\mathbb{R}^2$. In this example, the unknown objective function f is a mixture of two Gaussian density functions: $f(\boldsymbol{x}) = 2\sqrt{3}\pi\,[0.45 \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) + 0.55 \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma})]$, where $\boldsymbol{\mu}_1 = [1.5, 1.5]^t$, $\boldsymbol{\mu}_2 = [-1.5, -1.5]^t$, $\boldsymbol{\Sigma} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$, and the unknown data-generating distribution p_{data} is a mixture of two Gaussian distributions: $p_{\text{data}}(\boldsymbol{x}) = 0.3 \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_3, \boldsymbol{I}) + 0.7 \cdot \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_4, \boldsymbol{I})$, where $\boldsymbol{\mu}_3 = [-4, -4]^t$, $\boldsymbol{\mu}_4 = [4, 4]^t$, and $\boldsymbol{I}$ is the 2×2 identity matrix. The weight function w_ϕ and the score-function model $\boldsymbol{s}_t^\theta$ are jointly learned by maximizing the proposed objective (2).

The filled contour plot of the objective function f is shown in Figure 2a, with warmer colors representing higher objective values. Figure 2b shows 300 samples drawn from the data-generating distribution p_{data}, with the color of each sample rendered according to its ground-truth objective value. These 300 samples and their corresponding objective values are the offline examples from which the weight function w_ϕ and the score-function model $\boldsymbol{s}_\theta$ are trained. Figure 3 shows the optimized



(a) $\alpha = 1$ (b) $\alpha = 0.3$ (c) $\alpha = 0$

Figure 3: A toy example: Top: Optimized samples; bottom: Learned weight function.

samples and the learned weight function w_ϕ for several different values of the hyper-parameter α while fixing the hyper-parameter $\lambda = 0.1$.

The legitimacy of the proposed approach is demonstrated by the following observations. i) Even though the weight function is *not* constrained to be monotonic *a priori*, as shown in the bottom row of Figure 3, the learned weight functions are *monotone increasing* and hence put higher weights to samples with higher objective values. ii) When $\alpha = 1$, the learned weight function is relatively “flat" across its input domain. As a result, the learned generative model is very close to the data-generating distribution, and the optimized samples are very “similar" to the initial samples. As we decrease the value of α from 1 to 0.3, the learned weight function becomes much more skewed towards the higher input values. As a result, some of the optimized samples have been nudged along the direction of the gradient of the objective function and hence have much higher objective values than the initial samples. When we further decrease the value of α to 0, the learned weight function becomes extremely skewed. In this case, the hypothetical target distribution is *not* learnable. As a result, instead of the gradient direction, the optimized samples have been nudged along *all* directions. Therefore, the hyper-parameter α can effectively control the *utility–learnability tradeoff* for selecting a weight function w_ϕ. iii) Compared to the data-generating distribution, with an appropriate choice of the hyper-parameters α and λ, the learned generative model is substantially more *capable* of generating samples with higher objective values, as demonstrated by the differences of the 50th, 80th, and 100th percentiles between the samples drawn from these two distributions. More results on this toy example can be found in Appendix C.4.1.

C.2 Benchmark datasets

We conducted experiments on five standard offline optimization tasks:

- **Superconductor**, which aims to design a superconductor with 86 components to maximize the critical temperature;
- **TF (Transcription Factor) Bind 8**, which aims to find a DNA sequence of 8 base pairs to maximize its binding affinity to a particular transcription factor;
- **GFP (Green Fluorescent Protein)**, which aims to find a protein sequence of 238 amino acids to maximize the fluorescence;
- **UTR (Untranslated Region)**, which aims to find a human 5’ UTR DNA sequence of 50 base pairs to maximize the expression level of its corresponding gene;

Table 2: The benchmark datasets

	Supercond.	TFBind8	GFP	UTR	Fluores.
Type	continuous	discrete	discrete	discrete	discrete
Dimension	86	8	237	50	13
Category	N/A	4	20	4	2
# Train/Total	17014/21263	32898/65792	5000/56086	140k/280k	4096/8192
Min/Max	0.0/185.0	0.0/1.0	1.283/4.123	0.0/12.0	0.155/1.692
$\mathcal{D}_{\text{best}}$	74.0/0.4	0.439/0.439	3.525/0.789	7.123/0.594	0.900/0.485

- **Fluorescence**, which aims to identify a protein with high brightness. At each position, the selection of an amino acid is limited to those found in the sequences of the two parent fluorescent proteins. These parent proteins differ at precisely 13 positions in their sequences while being identical at all other positions.

For all previous tasks except for the Fluorescence, we utilized the Design-Bench package [46] to generate the training data, pre-process the data (including the conversion of categorical features to numerical values), and evaluate new designs. For the Fluorescence task, we collected raw data from Fannjiang et al. [18]. The objective value in this case is represented by the combined brightness. From a total of $2^{13} = 8192$ samples, we selected the worst 4096 examples as our training dataset. While the features in the Fluorescence dataset are binary, we simply treated them as continuous inputs to our algorithm.

The key attributes of the aforementioned benchmark datasets can be found in Table 2, which include:

- **Type**: The type of features represented in the dataset, which can be either continuous or discrete;
- **Dimension**: The feature dimension of the dataset;
- **Category**: The number of categories for each feature (only applicable to the discrete datasets);
- **# Train/Total**: The number of samples in the training and entire datasets. The entire dataset includes both the training dataset and additional data examples, which are used to help evaluate the new designs;
- **Min/Max**: The minimum and maximum objective values within the entire dataset;
- $\mathcal{D}_{\textbf{best}}$: The un-normalized and normalized maximum objective values within the training dataset.

C.3 Implementation details

Normalization. As we adopted DDPM as our generative model, we normalized each feature to the interval $[-1, 1]$. For the objective values, we mapped the original values in the training dataset to the range of $[0, 1]$. This step ensures consistency in the learning of the (un-normalized) weight function w_ϕ. For the GFP task, we employed a variational auto-encoder [31] to embed the high-dimensional features into a lower-dimensional space before normalizing them into the interval $[-1, 1]$.

Networks. In our implementation, we used neural networks to model both the (un-normalized) weight function w_ϕ and the score function $\boldsymbol{s}_t^\theta$. The weight function is a simple *scalar* function. In our implementation, we simply used a 4-layer multi-layer perceptron (MLP) with ReLU activation functions. In addition, we applied an *exponential* function to the output of the MLP to enforce the *non-negativity* of the weight function. The architecture for the score function model consists of a time-embedding layer and five blocks of "Dense-BatchNorm-ELU". Before each block, we injected time-embedding information by concatenating it with the input to the block.

Training. The noise scheduler for the DDPM was chosen as $\beta(t) = \beta_{\text{min}} + (\beta_{\text{max}} - \beta_{\text{min}})t$ for $t \in [0, 1]$, where $\beta_{\text{min}} = 0.1$ and $\beta_{\text{max}} = 20$. The detailed training procedure is described in Algorithm 1. The training scheme involves first identifying a suitable *initialization* of ϕ and θ and then followed by an *alternating* maximization over ϕ and θ. More specifically, to obtain a suitable initialization of ϕ and θ, we first note that the model θ *only* shows up in the second term of our learning objective (2). Maximizing the other two terms over ϕ gives us an initial estimate ϕ_0 (see Line 3 of Algorithm 1). In our implementation, this maximization was performed via full-batch gradient descent (GD), for which we used the Adam optimizer [30] with a constant leaning rate 10^{-3}. Once an initial estimate ϕ_0 has been obtained, we can obtain an initial estimate θ_0 by minimizing the second term over θ while setting $\phi = \phi_0$ (see Line 4 of Algorithm 1). To minimize the weighted denoising score matching loss, we considered a time range of $t \in [10^{-3}, 1]$ and used the Adam optimizer with a variable learning rate via stochastic gradient descent (SGD). The learning rate was gradually decreased from 10^{-3} to 10^{-4} during training. The alternating maximization of the learning objective (2) over the parameters ϕ and θ is described in Line 5–8 of Algorithm 1. Again the Adam optimizer was used, and the learning rates were set as $\eta_1 = \eta_2 = 10^{-4}$.

Sampling/Optimization. The sampling/optimization procedure is described in Algorithm 2. This procedure is identical to the probability-flow sampler in Song et al. [44].

C.4 Additional experimental results

C.4.1 Toy example

Additional choices of the hyper-parameter α. Previously in Section C.1, we described a toy example in $\mathbb{R}^2$ and used it to validate our proposed approach. In particular, in Figure 3 we reported the optimized samples and the learned weight function w_{ϕ^*} for several choices of the hyper-parameter α. Here in Figures 4 and 5 we report the optimized samples and the learned weight function w_{ϕ^*} for some additional choice of the hyper-parameter α. Note that when $\alpha = \infty$, the learned weight function w_{ϕ^*} is completely flat across its domain, and thus the hypothetical target distribution q_{target} is identical to the data-generating distribution p_{data}. It should become very clear from these reported results that the hyper-parameter α can effectively control the utility-learnability tradeoff for selecting a weight function.

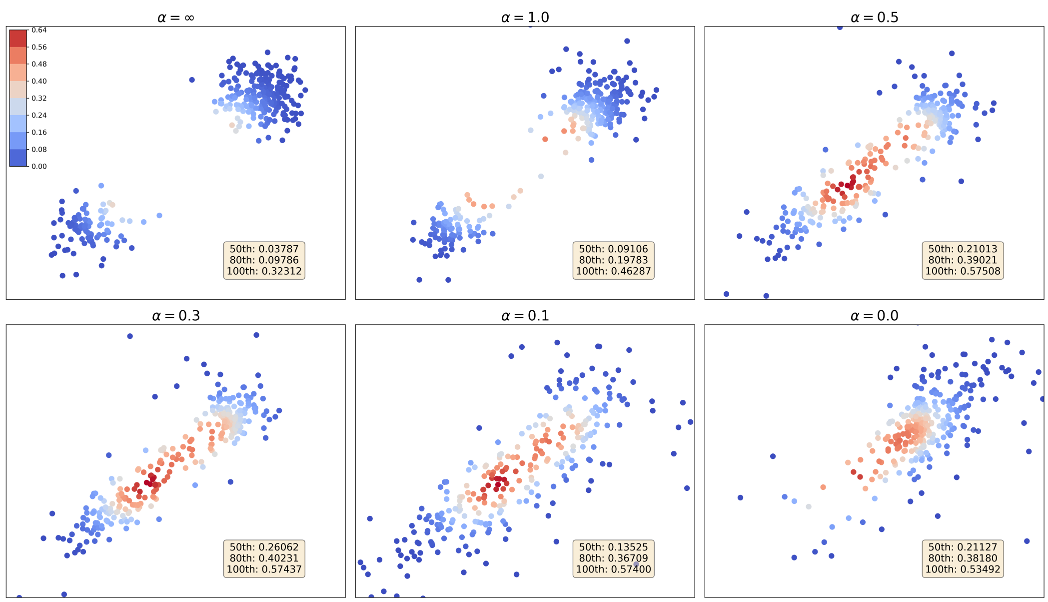


Figure 4: Optimized samples (with learnable weight function) for different choices of the hyper-parameter α.

Pre-selected weight function. Instead of considering a *learnable* weight function w_ϕ, we may also consider using a *pre-selected* weight function to train the generative model p_θ. Motivated by the learned weight functions w_{ϕ^*} from Figure 5, here we consider the simple *exponential* function $w_\psi(y) = \exp(\psi y)$, where ψ is a hyper-parameter. Note that when $\psi = 0$, the weight function w_ψ is completely flat across its domain, and as we increase the value of ψ, w_ψ becomes increasingly skewed towards the higher values in its domain. The optimized samples and the corresponding pre-selected weight functions are reported in Figures 6 and 7. Note here that we have purposely

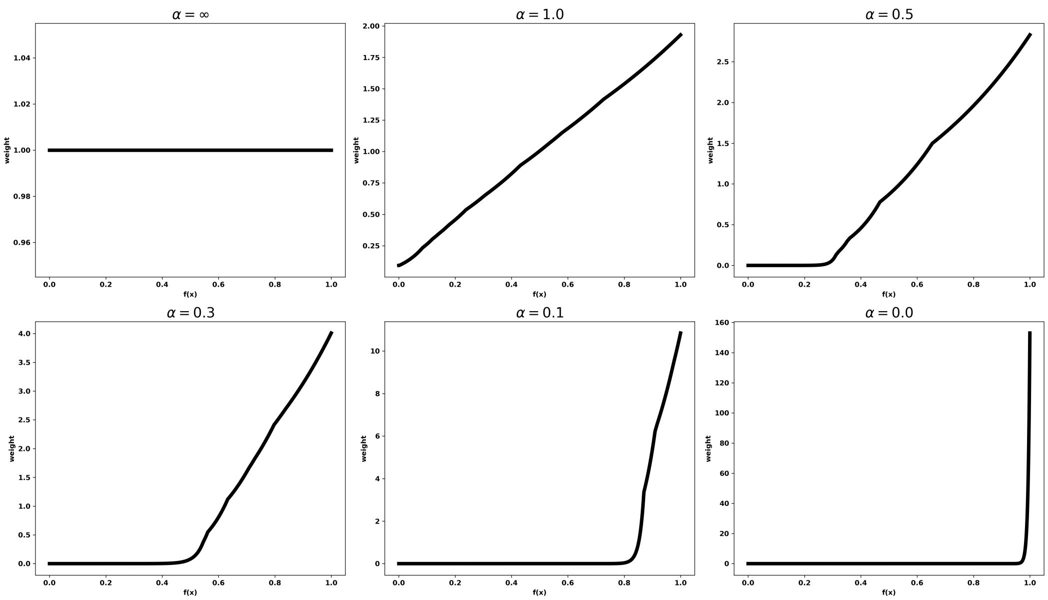


Figure 5: Learned Weight function w_{ϕ^*} for different choices of the hyper-parameter α.

chosen the values of the hyper-parameter ψ such that the pre-selected weight functions w_ψ in Figure 7 *mimic* the learned weight function w_{ϕ^*} in Figure 5. As a result, the optimized samples from Figures 6 have similar statistical profiles as those from Figures 4. Next, we shall use the benchmark datasets to illustrate that a learnable weight function can significantly outperform a pre-selected weight function in terms of generating samples with a consistent and superior statistical profile.

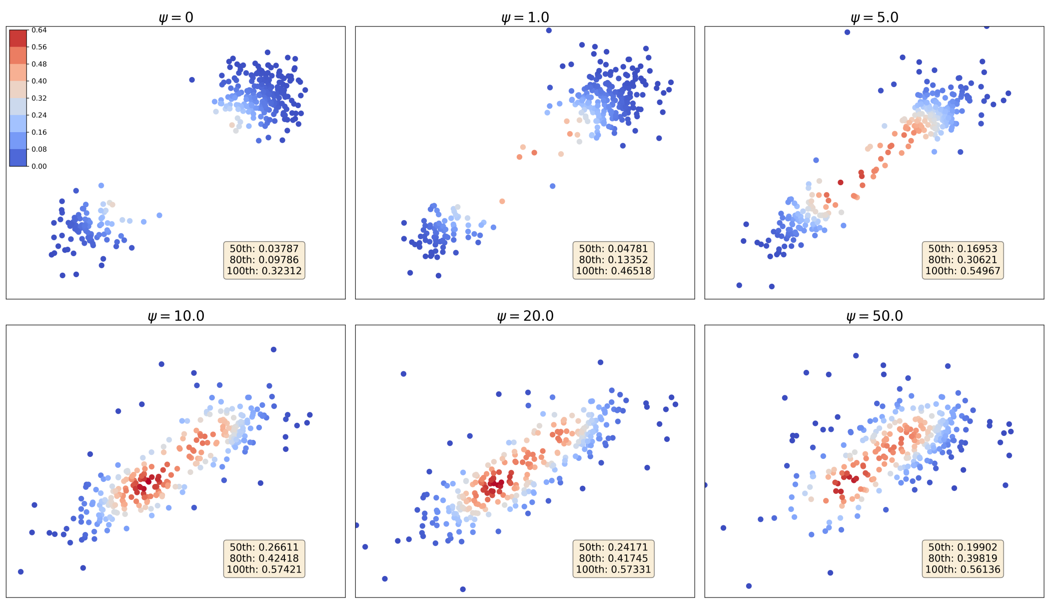


Figure 6: Optimized samples with pre-selected weight function for different choices of the hyper-parameter ψ.

C.4.2 Benchmark datasets

Here we report additional results on the benchmark datasets using both the learnable weight function w_ϕ and the pre-selected exponential weight function w_ψ. In our experiments, we fixed the value of the

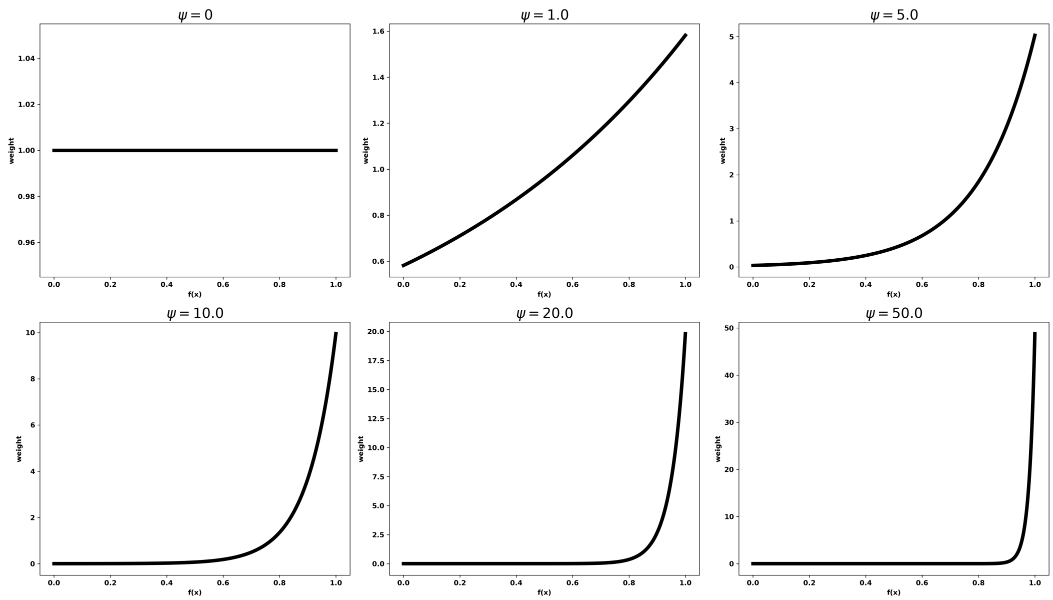


Figure 7: Pre-selected weight function w_ψ for different choices of the hyper-parameter ψ.

hyper-parameter $\lambda = 0.1$ and considered several different values for the hyper-parameter α (learnable weight function) and ψ (pre-selected weight function). The mean and standard deviation of the *best* generated samples for each benchmark dataset are reported in Table 3. The average improvements for different choices of the hyper-parameter α (learnable weight function) and ψ (pre-selected weight function) are also reported in Table 3. It is clear that the use of a learnable weight function with $\alpha = 0.25$ significantly outperform any pre-selected weight function considered here in terms of the average improvement. The learned weight functions w_{ϕ^*} that correspond to $\alpha = 0.25$ for each of the benchmark datasets are reported in Figure 8.

On the top row of Figure 8, the dashed lines represent pre-selected weight functions, while the solid line represents the learned weight function for each of the benchmark datasets. It is evident that the learned weight functions differ significantly from the pre-selected exponential weight functions. The label histograms of for each of the benchmark datasets are shown on the bottom row of Figure 8. Noticeably, labels of Superconductor and Fluorescence datasets are heavily skewed towards small objective values. Coincidentally, their learned weight functions tend to flatten when the objective values are large (roughly $0.8 - 1.0$). Given that the majority of data examples in these datasets have small objective values, assigning higher weights to large objective values would result in a smaller "effective sample size" in weighted learning. Therefore, it makes sense that these two datasets adopted a less steep slope in the learned weight function to maintain a reasonable effective sample size. This observation underscores that our learning objective (2) can adaptively choose an appropriate weight function to balance the utility-learnability tradeoff. Thus, to fully harness the potential of the proposed generative approach, it is crucial to make the weight function learnable as well.

In all the experiments involving a learnable weight function, we consistently set λ to 0.1. We also conducted additional experiments to investigate the impact of the hyper-parameter λ on the results. The findings, as depicted in Figure 9, reveal that λ proves to be a relatively insensitive hyper-parameter within our method. Across all datasets, variations in λ ranging from 0.01 to 1.0 only result in very minor differences in terms of the optimization performance.

D Further Discussions

To further elucidate the main contributions of this paper, we put the proposed *PAC-generative* approach to offline optimization in the context of several related works.

Modeling target distribution *vs*. modeling objective function. As mentioned previously in Section 1, the “standard" approach to offline optimization is to first learn a surrogate of the unknown

Table 3: Mean and standard deviation of the best generated samples for different choices of the hyper-parameter α (learnable weight function) and ψ (pre-selected weight function).

	Supercond.	TFBind8	GFP	UTR	Fluores.	Ave. Improv.
$\mathcal{D}_{\text{best}}$	0.399	0.439	0.789	0.593	0.485	
$\psi = 0.5$	0.493±0.033	0.892±0.054	0.865±0.000	0.669±0.009	0.881±0.036	0.462
$\psi = 1.0$	0.478±0.027	0.914±0.044	0.865±0.000	0.678±0.015	0.882±0.022	0.467
$\psi = 5.0$	0.496±0.026	0.917±0.022	0.865±0.000	0.689±0.009	0.859±0.052	0.472
$\psi = 20.0$	0.423±0.044	0.903±0.050	0.865±0.000	0.693±0.006	0.803±0.057	0.407
$\alpha = 0.15$	0.425±0.073	0.925±0.043	0.864±0.000	0.693±0.010	0.696±0.060	0.374
$\alpha = 0.2$	0.468±0.029	0.913±0.051	0.864±0.000	0.698±0.016	0.739±0.054	0.410
$\alpha = 0.25$	0.537±0.045	0.941±0.034	0.865±0.000	0.693±0.013	0.809±0.078	0.485
$\alpha = 0.3$	0.502±0.054	0.924±0.029	0.865±0.000	0.697±0.008	0.798±0.045	0.456

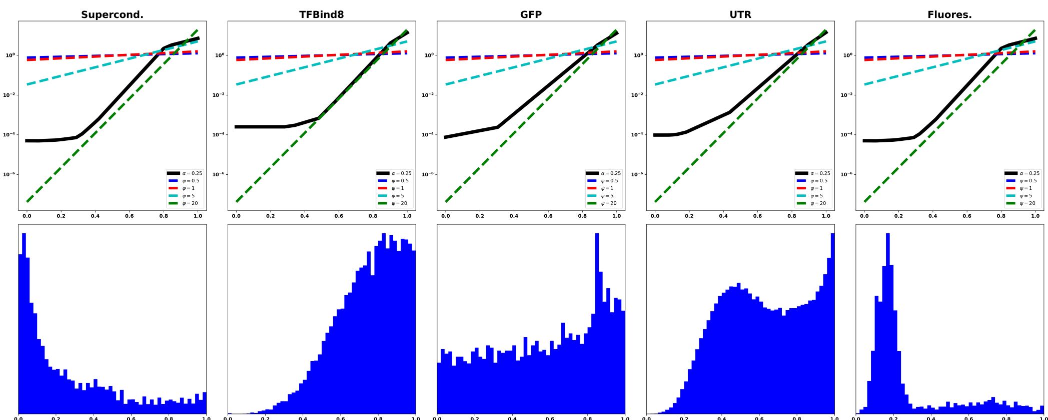


Figure 8: Top: Learned weight functions w_{ϕ^*} (solid, black line) for the benchmark datasets; bottom: histograms of offline training labels.

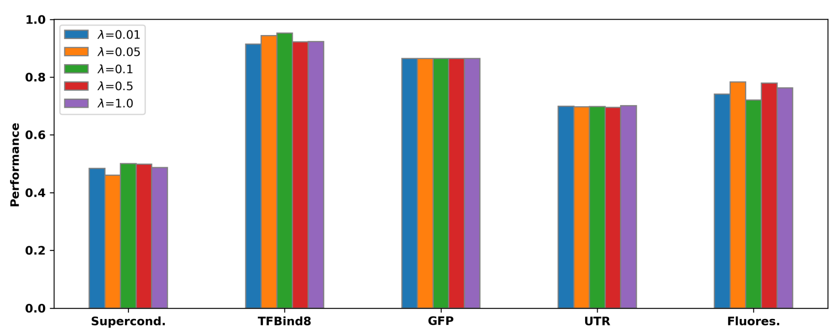


Figure 9: Investigation of λ when $\alpha = 0.2$.

objective function and then apply existing optimization algorithms. The main challenge for modeling the objective function is the so-called *distributional shift*. That is, when the optimization algorithm explores regions *away* from the offline observations, the learned surrogate tends to become less accurate. It is thus crucial to understand how far the optimization algorithm can explore away from the offline observations and how to maintain the accuracy of the learned surrogate throughout the exploration process. Notable efforts in the literature include Qi et al. [41] and Trabucco et al. [45], which considered regularized surrogate models in favor of invariance and conservatism; Fannjiang and Listgarten [17] and Chen et al. [13], which considered surrogate models learned via importance sampling and contrastive learning; and Fannjiang et al. [18], which used conformal prediction to quantify the uncertainty of the learned surrogate.

Despite these efforts, however, it remains unclear how to align the objective of learning a surrogate of the unknown objective function with the objective of optimization. This is evidenced by the very recent work Beckham and Pal [7], which discussed how one may interpret the conservative approach proposed in Trabucco et al. [45], and Beckham et al. [8], which suggested that an alternative evaluation metric is potentially better than simply choosing the best candidates using the learned surrogate. In contrast, the PAC-generative approach proposed in this paper is based on modeling a target distribution (as opposed to the objective function). As we have shown, under this generative view, it is possible to tune the objective of the learner according to a natural optimization objective.

Weighted learning *vs*. conditional/guided generation. Recent years have seen remarkable success in conditional/guided image generation [15, 23]. Conditional/guided generation can be easily adapted to offline optimization. Specifically, one can simultaneously learn a *standard* score-based generative model and a surrogate of the objective function and then use the *gradient* of the learned surrogate to guide the generation of the optimized samples [40]. Alternatively, one may also model the target distribution q_{target} as the *conditional* distribution p_{data} given $f(\mathbf{x}) \geq y_0$ for some *threshold* y_0 and train a generative model that approximates this conditional distribution [11, 22]. However, learning the conditional distribution may also require a surrogate of the objective function. In contrast, in our approach we model the target distribution q_{target} using a weight function. As discussed in Section 2.1, in our *weighted-learning* model, the score of q_{target} is *intrinsically* aligned with the gradient of the objective function. Hence we directly train a generative model from the offline data examples to learn the score of q_{target}, and there is *no* need to learn a surrogate of the objective function separately.

Offline optimization *vs*. offline reinforcement learning (RL). While the focus of this paper is offline optimization, recent years have also seen a substantial amount of interest in *offline RL* [36, 49, 27, 50]. Even though these two problems face some similar challenges, in our evaluation offline RL is the considerably more challenging setting. It is thus of interest to see whether the proposed PAC-generative approach can lead to any success in offline RL as well.

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