A DIFFUSIVE CLASSIFICATION LOSS FOR LEARNING ENERGY-BASED GENERATIVE MODELS

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Paper under double-blind review

ABSTRACT

Score-based generative models have recently achieved remarkable success. While they are usually parameterized by the score, an alternative way is to use a series of time-dependent energy-based models (EBMs), where the score is obtained from the negative input-gradient of the energy. Crucially, EBMs can be leveraged not only for generation, but also for tasks such as compositional sampling or model recalibration via Monte Carlo methods. However, training EBMs remains challenging. Direct maximum likelihood is computationally prohibitive due to the need for nested sampling, while score matching, though efficient, suffers from mode blindness. To address these issues, we introduce the Diffusive Classification (DiffCLF) objective, a simple method that avoids blindness while remaining computationally efficient. DiffCLF reframes EBM learning as a supervised classification problem across noise levels, and can be seamlessly combined with standard score-based objectives. We validate the effectiveness of DiffCLF by comparing the estimated energies against ground truth in analytical Gaussian mixture cases, and by applying the trained models to tasks such as model composition and recalibration. Our results show that DiffCLF enables EBMs with higher fidelity and broader applicability than existing approaches.

1 Introduction

Probabilistic modeling is a cornerstone of modern machine learning, providing a principled framework to capture complex data distributions and to generate realistic samples. A classical approach is density estimation, often carried out by explicitly modeling it using Energy-Based Models (EBMs), where the density is parametrized as the exponential of the negation of a learnable function, referred to as the energy (LeCun et al., 2006; Kim & Bengio, 2016; Nijkamp et al., 2019; Du & Mordatch, 2019; Grathwohl et al., 2020; Che et al., 2020; Song & Kingma, 2021). While conceptually appealing, EBMs are notoriously hard to train due to the intractable normalizing constant that prevents maximum likelihood estimation, forcing reliance on costly sampling procedures. Despite advances in amortized and efficient sampling (Du & Mordatch, 2019; Du et al., 2021; Grathwohl et al., 2021; Carbone et al., 2023; Senetaire et al., 2025), training EBMs remains computationally challenging.

A popular alternative avoids the difficulty of modeling energies directly by targeting their negative gradient, the score function. Score matching methods (Hyvärinen, 2005) leverage the fact that the intractable normalizing constant disappears upon differentiation, making the score easier to estimate. This approach became especially prominent with the advent of score-based generative models such as Diffusion Models (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song et al., 2021b) and Stochastic Interpolants (Albergo & Vanden-Eijnden, 2023; Albergo et al., 2023), where a forward noising process gradually transforms data into pure noise (or another tractable distribution), and sampling is achieved by reversing this process through a denoising dynamic. Crucially, these denoising dynamics depend on the score of the perturbed data distribution, which can be efficiently learned using Denoising Score Matching (Sohl-Dickstein et al., 2015; Song et al., 2021b).

Beyond generating samples, estimating the underlying energy function, rather than only the score, enables a range of downstream applications. Examples include recalibrating generative models via Monte Carlo methods (Phillips et al., 2024; Zhang et al., 2025a) and composing multiple models (Du et al., 2023; Skreta et al., 2025b;a; Thornton et al., 2025; He et al., 2025), both of which fundamentally require access to energies. While prior works (Skreta et al., 2025b;a; Zhang et al., 2025a;

He et al., 2025) focus on estimating marginal density ratios using only scores, they typically rely on assumptions such as perfectly learned scores or approximations of transition kernels in small time steps. In contrast, direct access to the energy often leads to improved performance.

While several works (Salimans & Ho, 2021; Phillips et al., 2024; Thornton et al., 2025) have explored training energy-based generative models through score-based objectives, yielding approximations of the energies, these methods face significant limitations. Chief among them is mode blindness, where the relative proportions of disjoint high-density regions are misrepresented (Wenliang & Kanagawa, 2021; Zhang et al., 2022; Shi et al., 2024). Recent efforts aim to recover energies of diffusion models directly, but they often demand heavy computation or fragile hyperparameter tuning (Gao et al., 2021; Zhang et al., 2023; Schröder et al., 2023; Zhu et al., 2024).

Our contributions. We address the problem of training energy-based generative models in a way that enables direct downstream use of energies. Our main contributions are:

- We introduce the Diffusive Classification (DiffCLF) objective, which reframes log-density estimation as a supervised classification problem. DiffCLF is lightweight, flexible, and can be seamlessly combined with classical score-matching objectives.
- We prove that DiffCLF consistently recovers the ground-truth distribution at optimality and, unlike score-based methods, is *not mode-blind*.
- We establish connections between DiffCLF and prior approaches that exploit temporal correlations in stochastic processes to learn energy-based models.
- We demonstrate the effectiveness of DiffCLF across different generative processes and for a range of downstream tasks, including model recalibration and compositional generation.

2 Preliminary

2.1 GENERAL FRAMEWORK

This work considers stochastic processes on \mathbb{R}^d for $t \in [0,T]$ of the form

$$Y_t = X_t + \gamma(t)Z , \qquad (1)$$

where $\gamma \in C^2([0,T])$, T denotes the terminal time which may be infinite, $(X_t)_t$ is a stochastic process from which samples can be drawn at any time t, and Z is a standard Gaussian noise independent of $(X_t)_t$. Let q_t denote the marginal density of X_t and p_t the marginal density of Y_t . This framework serves as a generic setting, with concrete instances and applications provided later. The objective is to estimate the densities $(p_t)_t$ up to a normalizing constant, given access only to samples from X_t . To achieve this, a parametric family of energy-based models is introduced

$$p_t^{\theta}(y_t) = \exp(-\mathbf{U}_t^{\theta}(y_t))/\mathcal{Z}_t^{\theta}, \quad \mathcal{Z}_t^{\theta} = \exp(\mathbf{F}_t^{\theta}) = \int \exp(-\mathbf{U}_t^{\theta}(y_t)) dy_t , \qquad (2)$$

where $U^{\theta}:[0,T]\times\mathbb{R}^{d}\to\mathbb{R}$ is the energy function, parameterized by $\theta\in\Theta$ (for instance, neural networks), and \mathcal{Z}^{θ}_{t} is the associated normalizing constant, which is intractable in general. A natural approach to estimating this model is *Maximum Likelihood* (ML) which writes as

$$\mathcal{L}_{\mathrm{ML}}(\theta) = \mathbb{E}_t \left[\mathcal{L}_{\mathrm{ML}}(\theta; t) \right], \quad \mathcal{L}_{\mathrm{ML}}(\theta; t) = -\mathbb{E}_{p_t} [\log p_t^{\theta}(Y_t)] = \mathbb{E}_{p_t} [\mathrm{U}_t^{\theta}(Y_t)] + \log \mathcal{Z}_t^{\theta}. \tag{3}$$

Given $t \in [0, T]$, taking gradients of $\mathcal{L}_{ML}(\cdot; t)$ with respect to θ yields

$$\nabla_{\theta} \mathcal{L}^{\mathrm{ML}}(\theta; t) = \mathbb{E}_{p_t} [\nabla_{\theta} \mathbf{U}_t^{\theta}(Y_t)] - \mathbb{E}_{p_t^{\theta}} [\nabla_{\theta} \mathbf{U}_t^{\theta}(Y_t)] . \tag{4}$$

The difficulty of this approach lies in the second term, which requires sampling from p_t^{θ} . Since this distribution can be as complex as the original data distribution q_t , sampling typically demands expensive Monte Carlo methods, making ML estimation impractical.

An alternative is to exploit the structure of Equation (1) and apply *Denoising Score Matching* (DSM) (Sohl-Dickstein et al., 2015; Song et al., 2021b) which aims at learning the gradient of the log-density (the score) to recover the energy up to an additive constant as a by-product. Let $p_t(\cdot|x_t)$ be the density of Y_t conditional on $X_t = x_t$. By construction, for all $t \in [0,T]$ and $x_t, y_t \in \mathbb{R}^d$

$$p_t(y_t|x_t) = \mathcal{N}(y_t; x_t, \gamma^2(t)I_d) . \tag{5}$$

Using that $p_t(y_t) = \int p_t(y_t|x_t)q_t(x_t)dx_t$, the score ¹ can then be expressed as

$$\nabla \log p_t(y_t) = \mathbb{E}\left[\nabla_{y_t} \log p_t(y_t|X_t) \mid Y_t = y_t\right] = \mathbb{E}\left[-\frac{y_t - X_t}{\gamma^2(t)} \middle| Y_t = y_t\right] . \tag{6}$$

Equation (6) is often referred to as the Tweedie's formula (Efron, 2011). This characterization shows that the score is a conditional expectation over the posterior distribution of X_t given Y_t . Building on this, DSM defines the following loss

$$\mathcal{L}_{\text{DSM}}(\theta) = \mathbb{E}_t \left[\mathcal{L}_{\text{DSM}}(\theta; t) \right], \quad \mathcal{L}_{\text{DSM}}(\theta; t) = \mathbb{E} \left[\left\| \nabla \log p_t^{\theta}(Y_t) - \nabla_{y_t} \log p_t(Y_t | X_t) \right\|^2 \right], \quad (7)$$

where $X_t \sim q_t$ and $Y_t \sim p_t(\cdot|X_t)$. Note that various heuristics exist for designing the time distribution see for instance (Song et al., 2021b; Karras et al., 2022; Kingma & Gao, 2023). The DSM objective doesn't require to compute the normalizing constant or to sample from the model.

The framework introduced in Equation (1) underlies many widely used generative models. The core idea is to generate new samples via a Markov process, typically formulated as a *Stochastic Differential Equation* (SDE), whose marginals coincide with those of Y_t . Crucially, constructing such processes relies on access to the score function $\nabla \log p_t$. Below, two concrete and widely used instances of this framework are presented.

Example 1: Diffusion Models In Diffusion Models (DMs) (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song et al., 2021b), the process $(X_t)_t$ is defined as $X_t = S(t)X_0$ with $X_0 \sim \pi$ and S(0) = 1, where π is a distribution with an available dataset of samples, from which new samples are generated. The noise schedule γ factorizes as $\gamma(t) = S(t)\sigma(t)$ with $\sigma(0) = 0$, chosen such that $Y_0 \sim \pi$ and $Y_T \sim p_T$ where p_T is a simple known distribution. This construction induces a noising (forward) SDE, and, under mild conditions on π (Anderson, 1982), one can derive the corresponding denoising (backward) SDE satisfied by $(Y_t)_t$

$$dY_t = \left[f(t)Y_t - g^2(t)\nabla \log p_t(Y_t) \right] dt + g(t)dW_t, \quad Y_T \sim p_T ,$$
 (8)

where $f(t) = \dot{S}(t)/S(t)$, $g(t) = S(t)\sqrt{2\dot{\sigma}(t)\sigma(t)}$ and $(W_t)_t$ is a standard Brownian motion. Estimating the score function $\nabla \log p_t$ via DSM (7) allows approximating this SDE which can be solved backward in time to new samples from π .

Example 2 : Stochastic Interpolants Stochastic Interpolants (SIs) (Albergo & Vanden-Eijnden, 2023; Albergo et al., 2023) generalize diffusion models by constructing generative processes that interpolate between any two distributions, not necessarily with a Gaussian endpoint. In this setting, $X_t = I_t(X_0, X_1)$ with $X_0 \sim q_0$, $X_1 \sim q_1$, where datasets are available for both q_0 and q_1 . The interpolation function I is chosen so that X_0 and X_1 are recovered at times t=0 and t=1, while $\gamma(0) = \gamma(1) = 0$ ensures that $Y_0 \sim q_0$ and $Y_1 \sim q_1$. Under mild assumptions, the dynamics of $(Y_t)_t$ are given by the SDE

$$dY_t = \left[v_t(Y_t) - \left(\dot{\gamma}(t)\gamma(t) + \frac{g(t)^2}{2} \right) \nabla \log p_t(Y_t) \right] dt + g(t)dW_t , \qquad (9)$$

where $(W_t)_t$ is a standard Brownian motion, g is any positive function and v_t is defined via a conditional expectation as $v_t(y_t) = \mathbb{E}[\partial_t I_t(X_0, X_1) \mid Y_t = y_t]$. As in DSM, v_t and the score can be learned via simple regression objectives, and once approximated, the SDE can be integrated to generate new samples from q_1 ². Notably, DMs appear as a special case of this framework.

2.2 Why modeling energies ?

As illustrated by DMs and SIs, the most natural quantity to model is often the score $\nabla \log p_t$. However, directly learning the energies themselves brings several important advantages, with only a few highlighted below.

¹For clarity, we write $\nabla \log p_t(y)$ as shorthand for $\nabla_y \log p_t(y)$ whenever no ambiguity arises.

²The transport from q_1 to q_0 can be obtained by changing the sign of the diffusion coefficient in front of the score in SDE (9), i.e. $g(t)^2/2 \to -g(t)^2/2$, and integrating from t=1 to t=0 with $Y_1 \sim p_1$.

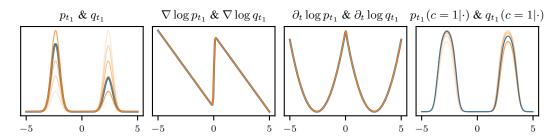


Figure 1: Densities, scores, time-scores, and classification posterior probabilities of Gaussian mixtures with varying weights. From left to right: (1) Reference mixture (blue, weights 2/3-1/3) and perturbed mixtures (orange, left mode weight ranging in [0.2, 0.8], with transparency proportional to the value) at $t_1 = 0.1$ under variance-preserving noising (Song et al., 2021b). (2) Scores remain nearly identical across mixtures, (3) Time-scores show the same limitation, while (4) 3-class classification posterior probabilities (10) (with $t_2 = 0.5$, $t_3 = 0.7$) vary with the mixture weights.

Recalibration of generative models. Energy estimation enables recalibration of trained generative models such as DMs or SIs. The goal is to compute expectations under a target distribution π with known energy (up to a constant), leveraging both a dataset of samples and density information. When only the energy is available, classical Monte Carlo approaches (e.g., importance sampling, MCMC) or annealed techniques such as AIS (Jarzynski, 1997; Neal, 2001), SMC (Doucet et al., 2001; Del Moral et al., 2006), and RE (Swendsen & Wang, 1986; Geyer et al., 1991; Hukushima & Nemoto, 1996) rely on intermediate distributions bridging a base law and π . Recent works construct these bridges using trained energy-based generative models, often diffusion-based: AIS-based methods (Zhang et al., 2024; 2025a) require only scores, while SMC (Phillips et al., 2024) and RE (Zhang et al., 2025b) achieve lower-variance estimates by also exploiting energies.

Compositionality. Accurate energy estimation also enables training-free compositional operations between generative models. Recent work shows that multiple diffusion models trained on different targets can be combined to form new models of their mixtures or products. Such constructions can be sampled using score-only methods like AIS (Skreta et al., 2025a;b), or more powerful schemes that exploit both scores and energies, including annealed Langevin dynamics (Du et al., 2023; Lee et al., 2023; Zhu et al., 2024) and SMC (Thornton et al., 2025; He et al., 2025).

2.3 On the limitation of score-matching methods

While score-based methods learn energies via their gradients, they suffer from fundamental limitations. Perhaps the most critical is the the "blindness" of score matching (Wenliang & Kanagawa, 2021; Zhang et al., 2022; Shi et al., 2024): divergences that rely solely on scores, such as the Fisher divergence, the Stein discrepancy or any SM-based objective, are not valid when distributions have disjoint supports, since a zero distance does not guarantee equality (Zhang et al., 2022, Theorem 2). Intuitively, the score of a multi-modal distribution captures only local information within each mode, ignoring other high-probability regions. Consequently, distributions with identical modes but different mixture weights produce nearly identical scores. Figure 1 illustrates this: Gaussian mixtures with differing weights (1^{st} panel) yield almost identical scores (2^{nd} panel). This limitation prevents SM objectives from reliably recovering the correct weighting across disconnected regions.

3 LEARNING ENERGIES VIA CLASSIFICATION

In this work, the energy is modeled by jointly learning the time-dependent energy function U_t^{θ} and the log-normalizing constant $F_t^{\theta} = -\log \mathcal{Z}_t^{\theta}$, rather than focusing on the score.

³Note that F_t^{θ} is not the true negative log-normalizing constant, but only a learnable parameter.

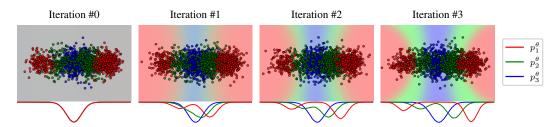


Figure 2: Classification posterior probabilities and associated EBM during training. Red, green, and blue dots are samples from $p_{t_1}, p_{t_2}, p_{t_3}$, with learned densities shown as curves of the same colors. The background encodes posterior probabilities from the classifier (11) (RGB channels). The target distribution is a mixture of $\mathcal{N}((-1,0),0.02I_2)$ with weight 0.3 and $\mathcal{N}((+1,0),0.02I_2)$ with weight 0.7, and the intermediate distributions are obtained via a variance-preserving noising scheme. As optimization progresses, class separation improves in the background, enabling accurate recovery of the underlying densities.

Our approach is based on minimizing the following Diffusive Classification (DiffCLF) objective

$$\mathcal{L}_{\text{clf}}(\theta; N) = \mathbb{E}_{t_{1:N}}[\mathcal{L}_{\text{clf}}(\theta; t_{1:N})], \quad \mathcal{L}_{\text{clf}}(\theta; t_{1:N}) = -\frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{p_{t_i}} \left[\log \frac{p_{t_i}^{\theta}(Y_i)}{\sum_{j=1}^{N} p_{t_j}^{\theta}(Y_i)} \right] , \quad (10)$$

where $p_{t_i}^{\theta}(y) = \exp(-\mathrm{U}_{t_i}^{\theta}(y) + \mathrm{F}_{t_i}^{\theta})$ and t_i are sampled independently and uniformly from [0,T]. The objective (10) reformulates the task of estimating the EBM as a multi-class classification problem. Consider a sample y associated with a label c. If c=i, this indicates that y was generated from the marginal distribution at time t_i . In multinomial logistic regression, the goal is to estimate the posterior distribution over classes given the data y. Here, the class-conditional probability $p(\cdot|c=i)$ is modeled by $p_{t_i}^{\theta}$. If we further assume that all N labels are equally likely, i.e., p(c=i) = 1/N, then the posterior probabilities take the following form

$$p^{\theta}(c=i \mid y) = p_{t_i}^{\theta}(y) / \sum_{j=1}^{N} p_{t_j}^{\theta}(y) .$$
(11)

The categorical cross-entropy of this classifier corresponds exactly to Equation (10). Figure 2 illustrates this in the 3-level setting: given samples from three distinct time steps, the objective solves the classification problem to progressively separate them, as visualized by the posterior probabilities in the background. Because the classifier is constructed as a softmax over the EBMs (shown along the bottom edge of the figure), optimizing this objective also directly learns the marginal distribution of each sample group. As shown in the rightmost panel of Figure 1, the posterior probabilities (11) reflect changes in the mixture weights, unlike the score. This highlights that, in contrast to DSM, the classification objective doesn't suffer from mode blindness.

Furthermore, Proposition 1 guarantees that the true marginals $(p_t)_t$ are recovered at optimality.

Proposition 1. The minimizer of objective (10) is given by $p_t^{\theta^*} = p_t$, for every $t \in [0, T]$.

In the simplest case of two times $t, t' \in [0, T]$, the objective reduces to binary classification, yielding

$$\mathcal{L}_{clf}(\theta; (t, t')) = -\frac{1}{2} \mathbb{E}_{p_t} \left[\log \frac{p_t^{\theta}(X_t)}{p_t^{\theta}(X_t) + p_{t'}^{\theta}(X_t)} \right] - \frac{1}{2} \mathbb{E}_{p_{t'}} \left[\log \frac{p_{t'}^{\theta}(X_{t'})}{p_t^{\theta}(X_{t'}) + p_{t'}^{\theta}(X_{t'})} \right] \\
= -\frac{1}{2} \mathbb{E}_{p_t} \left[\log \frac{1}{1 + \exp(-U_{t'}^{\theta}(X_t) + F_{t'}^{\theta} + U_{t'}^{\theta}(X_t) - F_{t'}^{\theta})} \right] \\
- \frac{1}{2} \mathbb{E}_{p_{t'}} \left[\log \frac{1}{1 + \exp(-U_{t}^{\theta}(X_{t'}) + F_{t}^{\theta} + U_{t'}^{\theta}(X_{t'}) - F_{t'}^{\theta})} \right] . \tag{12}$$

Computational cost. While the DSM objective (7) requires exactly two neural network evaluations per time sampled⁴, the multi-class classification objective (10) requires N.

⁴One for the forward pass and one for the backward pass to compute the score with auto-differentiation.

Consequently, minimizing both \mathcal{L}_{DSM} and \mathcal{L}_{clf} simultaneously requires only N+1 evaluations per time (N-1) more evaluations than DSM). In the binary case, this amounts to just one additional evaluation compared to DSM, making the computational budgets highly comparable.

Beyond Euclidean spaces. It is noticeable that DiffCLF remains valid on different processes and manifolds, since it only requires $(p_t^{\theta})_t$ to compute the loss. We discuss the case for applying DiffCLF on continuous-time Markov chains (CMTCs) for discrete diffusion in Appendix E.

4 Connection to other works

This section discusses connections between the proposed approach and existing methods. It first focuses on approaches that constrain higher-order derivatives of the log-density (Section 4.1), and then considers works that directly operate on the log-density itself (Section 4.2). All the losses introduced, including DiffCLF, operate on the log-densities, without imposing a hard constraint to ensure the learned energies are normalized.

4.1 Constraining other derivatives of the log-density

As highlighted in Section 2.3, regressing solely against the score is insufficient to recover the full energy landscape. Our approach tackles this challenge by using a loss that depends directly on the energy values, while alternative methods attempt to mitigate the same limitations through additional constraints on the model's higher-order derivatives.

4.1.1 Connection to regressing time derivatives of log-densities.

Time Score Matching. An intuitive direction is to exploit the temporal structure of the process. This leads to optimizing EBMs so that their time-derivative aligns with that of the true marginals. We refer to this objective as *Time Score Matching (tSM)*.

$$\mathcal{L}_{tSM}(\theta) = \mathbb{E}_t[\mathcal{L}_{tSM}(\theta;t)] \quad \text{with } \mathcal{L}_{tSM}(\theta;t) = \mathbb{E}_{p_t} \left[\left(\partial_t \log p_t^{\theta}(Y_t) - \partial_t \log p_t(Y_t) \right)^2 \right] . \tag{13}$$

Figure 1 shows that, similar to the score, the time-score $\partial_t \log p_t$ also exhibits blindness of mode-weights. A theoretical justification is provided in Appendix C. Moreover, Proposition 2 establishes that the binary classification loss (12) converges to the tSM objective (13) in the continuous-time limit (see Appendix D.2 for the proof).

Proposition 2. Let $t \in [0,T)$ and $\delta > 0$, we have

$$\lim_{\delta \to 0^+} \frac{8}{\delta^2} \left(\mathcal{L}_{\text{clf}}(\theta; t, t + \delta) - \log 2 \right) = \mathcal{L}_{tSM}(\theta; t) + C , \qquad (14)$$

where $C = \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t(Y_t) \right)^2 \right]$ is a constant with respect to θ .

DRE-∞. However, as with the score, directly regressing the time-score is generally infeasible because it is intractable in most cases. (Choi et al., 2022, Proposition 4) extends Proposition 2 by showing that the optimal binary classifier associated with objective (12) (using a general classifier) can be used to approximate the time-score. In contrast, the proposed approach embeds the parameterized marginals directly into the classification problem, bypassing the need to approximate the time-score altogether.

Conditional Time Score Matching. In parallel, (Yu et al., 2025; Guth et al., 2025) propose an alternative objective, termed Conditional Time Score Matching (CtSM), which leverages the tractable conditional time score and enjoys the same gradients as the original formulation. For instance, in the DMs case where $X_t = S(t)X_0$, the time score can be expressed as $\partial \log p_t(y_t) = \mathbb{E}[\partial_t \log p_t(y_t|X_t)|Y_t = y_t]$ where the conditional time-score is

$$\partial_t \log p_t(Y_t | X_t) = -d \frac{\dot{\gamma}(t)}{\gamma(t)} - \frac{\partial_t X_t^{\top} (Y_t - X_t)}{\gamma(t)^2} + \frac{\|Y_t - X_t\|^2}{\gamma(t)^2} \frac{\dot{\gamma}(t)}{\gamma(t)},$$
 (15)

which leads to the following mean square regression problem

$$\mathcal{L}_{\text{CtSM}}(\theta) = \mathbb{E}_t[\mathcal{L}_{\text{CtSM}}(\theta; t)], \quad \mathcal{L}_{\text{CtSM}}(\theta; t) = \mathbb{E}\left[\left(\partial_t \log p_t^{\theta}(Y_t) - \partial_t \log p_t(Y_t | X_t)\right)^2\right], \quad (16)$$

with $X_t \sim q_t$ and $Y_t \sim p_t(\cdot|X_t)$. This derivation closely parallels that of DSM (see Section 2.1). Similar to our approach, Choi et al. (2022) and Yu et al. (2025) suggest combining this loss with DSM (7) to enhance model learning. Further, the conditional time score for SIs follows exactly the form in Equation (15); however, it remains intractable for general $(X_t)_t$ (see Appendix A for the proof and additional details).

4.1.2 Learning Log-densities with Self-Consistency.

Another strategy for estimating log-densities is to enforce *self-consistency* relations implied by the dynamics of $(Y_t)_t$. Two main approaches have been explored: one derived from the *Fokker–Planck* equation (FPE) and another from *Bayes' rule*. These methods typically require stronger assumptions on the process and are best understood in structured settings such as DMs or SIs. The detailed introduction and discussion are provided in appendix A.3.

Consistency via Fokker-Planck. When $(Y_t)_t$ admits an SDE representation, its marginals follow the FPE, a partial differential equation governing the log-densities $(\log p_t)_t$. Several works (Sun et al., 2024; Shi et al., 2024) exploit this by penalizing deviations from the log-density FPE. While conceptually appealing, this requires backpropagating through time-derivatives, scores, and Laplacians, leading to high computational cost. Variants mitigate these issues by approximating derivatives with finite differences (Plainer et al., 2025). Moreover, Appendix C shows that such objectives remain subject to mode blindness, despite claims to the contrary.

Consistency via Bayes' Rule. An alternative derives from the relation between marginals at two times s and t, $p_t(y_t) p_{s|t}(y_s|y_t) = p_s(y_s) p_{t|s}(y_t|y_s)$ for all $y_s, y_t \in \mathbb{R}^d$, where $p_{t|s}$ (resp. $p_{s|t}$) is the conditional distribution of Y_t given $Y_s = y_s$ (resp. Y_s given $Y_t = y_t$). Using approximations of the conditional distributions given by Euler–Maruyama integration of SDEs (8) or (9) (which depend on the score), one can regularize $(\log p_t^\theta)_t$ by enforcing approximate Bayes consistency (He et al., 2025). However, this method remains valid only when the approximations are sufficiently accurate, which occurs for s,t close together, precisely the regime where the objective is prone to mode blindness. In fact, Proposition 3 in Appendix A.3 shows that the Bayes and FPE regularizations coincide asymptotically, inheriting the same limitations.

4.2 Connection to other training methods

Maximum likelihood approaches. While direct ML on a single distribution (3) is notoriously difficult, leveraging temporal correlations in $(Y_t)_t$ can help alleviate those limitations. Noble et al. (2025) leverage annealed sampling where $(p_t^\theta)_t$ defines the annealing path, while Zhang et al. (2023) model the joint time–state distribution and use Gibbs transitions across levels. In the DMs case, Gao et al. (2021); Zhu et al. (2024) exploit tractable conditionals $p_{t|s}$ to model posteriors as EBM with $p_{s|t}^\theta \propto p_{t|s} \times p_t^\theta$, enabling more efficient ML when $t-s \to 0$. Despite their advantages, these methods still depend on costly sampling loops.

Noise contrastive estimation. The binary objective (12) closely resembles the well-known *Noise Contrastive Estimation* (NCE) framework (Gutmann & Hyvärinen, 2010), with the multi-class extension (10) being related to the generalization considered in Matsuda & Hyvärinen (2019). Intuitively, our formulation can be interpreted as using the marginal at time t as the "noise distribution" when learning the density at t', and vice versa, but in a fully parametric setting. This connection highlights an additional flexibility of our approach: whenever some marginal densities p_t are known exactly (for example, p_T in diffusion models, or p_0 and p_1 in stochastic interpolants) these can be seamlessly incorporated into the learning framework, potentially improving accuracy.

Table 1: Comparison on synthetic 40-mode Gaussian mixtures. A DM with variance preserving noising scheme was trained on MOG-40 using the different objectives. We explore different values of the number of levels $N \in \{2,4,8,16\}$ and ensure equal computational comparison between methods. We report the classification loss (10), Fisher divergence (FD), and Maximum Mean Discrepancy (MMD) (\times 100) from the denoising SDE. The classification approach matches DSM in Fisher divergence and MMD, while yielding markedly better consistency in classification loss.

| | $\mathcal{L}_{	ext{clf}}$ | $+\mathcal{L}_{\mathrm{DSM}}$ (o | urs) | L | $\mathcal{L}_{	ext{CtSM}} + \mathcal{L}_{	ext{DSI}}$ | М | $\mathcal{L}_{	extsf{DSM}}$ | | |
|-----|---------------------------|----------------------------------|-----------------------------|---------------------------|--|------------------------------|-----------------------------|-----------------------------|-----------------------------|
| Dim | $\mathcal{L}_{	ext{clf}}$ | FD | MMD | $\mathcal{L}_{	ext{clf}}$ | FD | MMD | $\mathcal{L}_{	ext{clf}}$ | FD | MMD |
| 8 | 4.41±0.12 | $2.00{\pm}1.48$ | 0.69 ± 0.59 | 6.80±0.86 | 5.74 ± 2.21 | 19.41 ± 0.77 | 9.19±0.33 | 4.09 ± 3.89 | 0.99 ± 0.64 |
| 16 | 4.19 ± 0.14 | $2.81{\scriptstyle\pm1.38}$ | $0.91{\scriptstyle\pm0.32}$ | $8.33{\pm}2.36$ | $7.96{\scriptstyle\pm2.11}$ | $22.62{\scriptstyle\pm0.45}$ | 22.36 ± 0.76 | $5.49{\scriptstyle\pm5.23}$ | $1.28{\pm0.56}$ |
| 32 | 4.04 ± 0.23 | $3.68{\scriptstyle\pm1.47}$ | $1.20{\scriptstyle\pm0.44}$ | 6.13 ± 1.45 | $10.30{\scriptstyle\pm1.95}$ | $18.18{\scriptstyle\pm1.51}$ | 85.07 ± 9.53 | 3.88 ± 3.49 | $1.20{\scriptstyle\pm0.42}$ |
| 64 | 4.01 ± 0.46 | $4.87{\scriptstyle\pm1.95}$ | $2.18{\scriptstyle\pm1.02}$ | 7.78 ± 1.64 | $9.96{\scriptstyle\pm1.84}$ | $12.67{\pm}3.66$ | 149.45 ± 33.76 | $3.93{\pm}3.48$ | $1.51{\scriptstyle\pm0.15}$ |
| 128 | 4.40 ± 1.00 | $6.91{\scriptstyle\pm2.47}$ | $3.54{\scriptstyle\pm1.34}$ | 20.86 ± 4.93 | $9.42{\scriptstyle\pm1.82}$ | $5.20{\scriptstyle\pm0.34}$ | 383.53 ± 35.99 | $6.78{\scriptstyle\pm5.94}$ | 1.99 ± 0.35 |

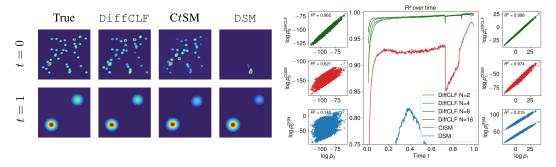


Figure 3: Learned EBMs with SI between a bi-modal and a 40-mode 2D Gaussian mixture. We use \mathcal{L}_{DSM} , $\mathcal{L}_{\text{DSM}} + \mathcal{L}_{\text{CtSM}}$, and $\mathcal{L}_{\text{DSM}} + \mathcal{L}_{\text{clf}}$ (DiffCLF, ours). (Left): Learned densities at t=0 (top row) and t=1 (bottom row) for the different methods, showing that DiffCLF best captures the target distributions. (Right): Comparison of learned log-densities $\log p_t^\theta$ versus the exact $\log p_t$ on exact samples from $(Y_t)_t$ across time in terms of scatter plots and R^2 statistic. Plots at the left and right edges correspond to t=0 and t=1, respectively; the middle shows the coefficient of determination R^2 over $t\in(0,1)$, indicating that only DiffCLF achieves consistently high agreement with the true log-densities.

5 Numerical experiments

We begin our numerical study by comparing DiffCLF with DSM and CtSM ⁵ on controlled high-dimensional Gaussian mixtures, before turning to the practical applications outlined in Section 2.2.

DMs and SIs on MOGs. In the mixture of Gaussian (MOG) setting, the closed-form expression of p_t is available (see Appendix F.1), allowing us to quantitatively assess approximation errors of different training objectives. In Table 1, we train diffusion models on the 40-mode mixture (MOG-40) across increasing dimensions. We evaluate the trained models using three metrics: the classification loss (10), which the optimal model should minimize, the Fisher Divergence (FD), measuring accuracy of the learned score and the Maximum Mean Discrepancy (MMD) (Gretton et al., 2012), reflecting the quality of generated samples. While all objectives achieve comparable FD and MMD, our method is the only one that consistently achieves low values of the classification loss, thereby satisfying the self-consistency condition that other approaches fail to capture. In Figure 3, SIs are trained to bridge MOG-40 and a 2-mode mixture (MOG-2) in 2D. The figure demonstrates that DiffCLF learns significantly more accurate energies than the baselines. Additional results and experimental details are provided in Appendix F.2.

⁵For clarity, DiffCLF refers to $\mathcal{L}_{DSM} + \mathcal{L}_{clf}$ training and CtSM refers $\mathcal{L}_{DSM} + \mathcal{L}_{CtSM}$ training.

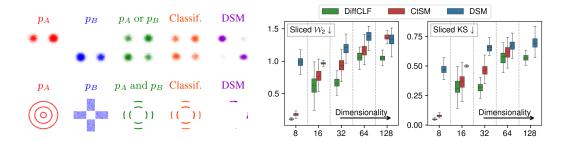


Figure 4: (Left) OR and AND model composition. *Top*: OR composition, *Bottom*: AND composition. Red/Blue: input distributions, Green: ground truth, Orange: DiffCLF, Purple: DSM. Results obtained via 512-step SMC on the product of learned marginals. (Right) SMC-Recalibration metrics. Box plots of Sliced Wasserstein (W_2) and Kolmogorov-Smirnov (KS) distances for a 512-step SMC on the SI between MOG-40 and MOG-2. Optimal scores and velocities are used for kernels, with learned EBMs for marginals. DiffCLF consistently outperforms other methods.

Composition. Following Du et al. (2023); Thornton et al. (2025), we evaluate <code>DiffCLF</code> against DSM on two toy composition tasks shown on the left of Figure 4: an "OR" between two Gaussian mixtures with different weights (top row) and an "AND" between a mixture of rings and uniform rectangles (bottom row). We perform composition using standard SMC (Doucet et al., 2001; Del Moral et al., 2006) with a Metropolized Langevin (MALA) (Roberts & Tweedie, 1996) kernel applied to either the mixture or the product of the learned densities. In this toy setting, this strategy consistently outperformed the annealed Langevin approach of Du et al. (2023) and the diffusion—SMC approach of Thornton et al. (2025). As seen in the two right-most columns, models trained with <code>DiffCLF</code> produce substantially better results than DSM, particularly in preserving the correct proportions of each region, a direct consequence of avoiding mode blindness. Experimental details are provided in Appendix F.3.

Recalibration. To demonstrate the potential of using trained EBMs for recalibration, we consider recalibrate the energy-based SI between MOG-40 and MOG-2 by embedding the learned energy into the SMC framework of Phillips et al. (2024), which exploits integration of the SDE (9) to enhance transitions between levels. Specifically, the algorithm is provided with learned energies from either DiffCLF, CtSM, or DSM, with the last marginal constrained post-training to match the true distribution. To focus the comparison solely on the energies, we use the analytical velocity and score (see Appendix F.1) to calculate the densities of transitions. As shown in the right part of Figure 4, DiffCLF yields substantially more accurate samples than DSM and CtSM in all dimensions, highlighting its advantage for recalibration tasks.

6 CONCLUSION

Energy-based generative models provide a compelling perspective on score-based methods, extending their utility well beyond pure sample generation to a wide range of downstream applications. Despite this promise, the existing literature on energy-based training remains limited, with available methods often being computationally demanding, hyperparameter-sensitive, or biased. This work introduced the *Diffusive Classification* (DiffCLF) objective, a simple, efficient, and unbiased training principle. The method is broadly applicable across different stochastic processes and integrates seamlessly with existing approaches such as DSM, offering both theoretical clarity and practical flexibility. Empirical results demonstrate clear advantages of DiffCLF, resulting in more accurate and consistent energy estimates, which in turn improves model composition and recalibration. Nonetheless, our experiments are limited in scale. Exploring applications to large-scale tasks such as image modeling, where SMC-based composition has already shown promise (Thornton et al., 2025), constitutes an exciting direction for future work. Another promising extension lies in the discrete domain: since DiffCLF remains valid for general stochastic processes, including Continous-Time Markov Chain, applying it to textual modeling appears especially compelling in light of recent advances at the intersection of EBMs and DMs (Xu et al., 2025).

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A ADDITIONAL BACKGROUND

A.1 BACKGROUND AND FOUNDATIONS FOR ITÔ SDES

In this section, we will introduce the Itô SDEs, its time reversal, and the Fokker Planck Equation.

Forward and Backward Processes of Itô SDEs. Given $f:[0,T]\times\mathbb{R}^d\to\mathbb{R}^d$ and $g:[0,T]\times\mathbb{R}^d\to\mathbb{R}^d$ with regularity, the Itô SDE is defined as

$$dX_t = f(t, X_t)dt + g(t, X_t)dW_t, \quad t \in [0, T],$$
(17)

where $(W_t)_{t \in [0,T]}$ is the standard Wiener process. With additional regularity on f and g (see Anderson (1982)), its *time reversal* is given as

$$dX_t = \left[f(t, X_t) - g(t, X_t) g(t, X_t)^\top \nabla \log p_t(X_t) \right] dt + g(t, X_t) d\tilde{W}_t , \qquad (18)$$

where $(\tilde{W}_t)_{t\in[0,T]}$ is the time-reversed Wiener process. We denote $(p_t)_{t\in[0,T]}$ as the marginal distributions admitted by the SDE, starting either from $(t=0,X_0\sim p_0)$ or $(t=T,X_T\sim p_T)$. For

simplicity, in the rest of context, we consider the Additive-noise Itô SDEs, i.e. with g(t, x) = g(t), which gives

(forward SDE)
$$dX_t = f(t, X_t)dt + g(t)dW_t$$
, (19)

(backward SDE)
$$dX_t = \left[f(t, X_t) - g(t)^2 \nabla \log p_t(X_t) \right] dt + g(t) d\tilde{W}_t.$$
 (20)

Fokker Planck Equation. The *Fokker Planck Equation* (FPE), which is also known as the *Forward Kolmogorov Equation*, describes the density change along the forward SDE as follows

$$\partial_t p_t(x) = -\nabla \cdot (f(t, x)p_t(x)) + \frac{g(t)^2}{2} \Delta \cdot p_t(x) , \qquad (21)$$

where ∇ is the divergence operator and Δ is the Laplacian operator both with respect to the variable x. Its log-density version, *i.e.* log-density FPE is given by

$$\partial_t \log p_t(x) = -\nabla \cdot f(x,t) - f(x,t)^\top \nabla \log p_t(x) + \frac{g(t)^2}{2} \left[\nabla \cdot \nabla \log p_t(x) + \|\nabla \log p_t(x)\|^2 \right]. \tag{22}$$

A.2 CONDITIONAL TIME SCORE

This section recaps and extends the analyses of Guth et al. (2025) and Yu et al. (2025), providing a unified presentation of the conditional time score framework. Using the stochastic process introduced in Equation (1), the log-density evolution can be written as

$$\partial_{t} \log p_{t}(y) = \partial_{t} \log \int q_{t}(x) p_{t}(y|x) dx$$

$$= \frac{1}{p_{t}(y)} \left(\int p_{t}(y|x) \partial_{t} q_{t}(x) + q_{t}(x) \partial p_{t}(y|x) dx \right)$$

$$= \int \frac{q_{t}(x) p_{t}(y|x)}{p_{t}(y)} (\partial_{t} \log q_{t}(x) + \partial_{t} \log p_{t}(y|x)) dx$$

$$= \mathbb{E} \left[\partial_{t} \log q_{t}(X_{t}) + \partial_{t} \log p_{t}(Y_{t}|X_{t}) | Y_{t} = y \right] ,$$

$$(23)$$

where

$$\begin{split} \partial_t \log p_t(y|x) &= \partial_t \log \mathcal{N}(y; x, \gamma(t)^2 I) \\ &= \partial_t \left(-\frac{d}{2} \log 2\pi - d \log \gamma(t) - \frac{\|y - x\|^2}{2\gamma(t)^2} \right) \\ &= -d \frac{\dot{\gamma}(t)}{\gamma(t)} + \frac{\|y - x\|^2}{\gamma(t)^2} \frac{\dot{\gamma}(t)}{\gamma(t)} \;, \end{split}$$

while $\partial_t \log q_t(X_t)$ doesn't have a general form and therefore should be treated case-by-case.

In this work, we mainly discuss special cases of Equation (1), where $(X_t)_{t\in[0,T]}$ is deterministic once the source(s), *i.e.* X_0 for DMs and (X_0,X_1) for SIs, are given. For simplicity, we define $\xi\sim\mu$ as the source and $X_t=T_t(\xi)$ is obtained by a deterministic map T_t (see examples bellow). In such case, the marginal of X_t can be defined by a Dirac delta

$$q_t(x) = \int \mu(\xi)\delta(x - T_t(\xi))d\xi \Rightarrow p_t(y) = \int \mu(\xi)p_t(y|T_t(\xi))d\xi$$
.

Therefore, Equation (23) can be written as

$$\begin{split} \partial_t \log p_t(y) &= \partial_t \log \int \mu(\xi) p_t(y|T_t(\xi)) \mathrm{d}\xi \\ &= \frac{1}{p_t(y)} \int \mu(\xi) p_t(y|T_t(\xi)) \partial_t \log p_t(y|T_t(\xi)) \mathrm{d}\xi \\ &= \int p(\xi|y) \partial_t \log \mathcal{N}(y; T_t(\xi), \gamma(t)^2 I) \mathrm{d}\xi \\ &= \mathbb{E} \left[-d \frac{\dot{\gamma}(t)}{\gamma(t)} - \frac{(Y_t - T_t(\xi))^\top \partial_t T_t(\xi)}{\gamma(t)^2} + \frac{\|Y_t - T_t(\xi)\|^2}{\gamma(t)^2} \frac{\dot{\gamma}(t)}{\gamma(t)} \Big| Y_t = y \right] \;. \end{split}$$

Example 1: Diffusion Models As introduced in Section 2.1, $(X_t)_{t \in [0,T]}$ in DMs are defined as $X_t = S(t)X_0$ with $X_0 \sim \pi$ and $S : \mathbb{R} \to \mathbb{R}$. Therefore, $\xi = X_0$, $\mu = \pi$, and $T_t(\xi) = S(t)\xi$:

$$\partial_t \log p_t(y) = \mathbb{E} \left[-d \frac{\dot{\gamma}(t)}{\gamma(t)} - \frac{\dot{S}(t) X_0^\top (y - S(t) X_0)}{\gamma(t)^2} + \frac{\|y - S(t) X_0\|^2}{\gamma(t)^2} \frac{\dot{\gamma}(t)}{\gamma(t)} \right]. \tag{24}$$

Example 2: Stochastic Interpolants As introduced in Section 2.1, SIs are defined by two ends, *i.e.* $X_t = I_t(X_0, X_1)$ given (X_0, X_1) . Therefore, $\xi = (X_0, X_1)$, μ any coupling of p_0, p_1 with marginals p_0, p_1 , and $T_t(\xi_0, \xi_1) = I_t(\xi_0, \xi_1)$.

$$\partial_t \log p_t(y) = \mathbb{E}\left[-d\frac{\dot{\gamma}(t)}{\gamma(t)} - \frac{\partial_t I_t(X_0, X_1)^\top (y - I_t(X_0, X_1))}{\gamma(t)^2} + \frac{\|y - I_t(X_0, X_1)\|^2}{\gamma(t)^2} \frac{\dot{\gamma}(t)}{\gamma(t)}\right]. \tag{25}$$

A.3 LEARNING LOG-DENSITIES WITH SELF-CONSISTENCY

In this section, we will introduce two strategies to learn log-densities via enforcing their self-consistency relations: the Fokker-Planck regularization (Sun et al., 2024; Shi et al., 2024; Plainer et al., 2025) and the Bayes (or RNE) regularization He et al. (2025). Such relations naturally arise from the underlying dynamics of the process and can be exploited to design training objectives. These methods typically rely on stronger assumptions about the generative process Y_t , which is why we primarily focus on the well-structured settings of DMs and SIs.

A.3.1 Consistency from Fokker-Planck Equation

Assume that the dynamic of the process $(Y_t)_t$ can be described by an (additive-noise) Itô SDE

$$dY_t = \alpha_t(Y_t)dt + \beta_t dW_t, \tag{26}$$

where $\alpha_t: [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ and $\beta_t: [0,T] \to \mathbb{R}_+$. Then the evolution of densities induced by this process is governed by the *Fokker-Planck Equation* (FPE), (see Appendix A.1 for more details) given by

$$\partial_t p_t + \nabla \cdot (\alpha_t p_t) - \frac{\beta_t^2}{2} \Delta p_t = 0 , \qquad (27)$$

where $\nabla \cdot$ is the divergence operator and Δ is the Laplacian operator both with respect to y. This formulation arises when the stochastic process admits an SDE representation. For example, in Diffusion Models we have $\alpha_t(y) = f(t)y$ and $\beta_t = g(t)$, while in Stochastic Interpolants $\alpha_t(y) = \mathbb{E}[\partial_t I_t(Y_0, Y_1) + \dot{\gamma}(t)Z|Y_t = y] + \frac{1}{2}\beta_t^2\nabla \log p_t(y)$ and $\beta_t = g(t)^6$. Although the Fokker–Planck equation (27) is formulated in terms of the density p_t , it can equivalently be rewritten in terms of the log-density $\log p_t$ as

$$\partial_t \log p_t - \mathcal{F}_t(p_t) = 0, \quad \mathcal{F}_t(p_t) = \frac{\beta_t^2}{2} \left[\Delta \log p_t(y) + \|\nabla p_t(y)\|^2 \right] - \alpha_t \cdot \nabla \log p_t - \nabla \cdot \alpha_t .$$

To enhance the accuracy of $(p_t^{\theta})_t$, recent works (Sun et al., 2024; Shi et al., 2024; Plainer et al., 2025) propose enforcing its self-consistency by optimizing the following objective

$$\mathcal{L}_{\text{FPE}}(\theta) = \mathbb{E}_t[\mathcal{L}_{\text{FPE}}(\theta;t)], \quad \mathcal{L}_{\text{FPE}}(\theta;t) = \mathbb{E}_{p_t}\left[\left(\partial_t \log p_t^{\theta}(Y_t) - \mathcal{F}_t(p_t^{\theta})(Y_t)\right)^2\right].$$
 (28)

Although Shi et al. (2024) claim that this approach overcomes the blindness of score matching, we demonstrate in Appendix C that it remains susceptible to the same issue. The objective can also be combined with DSM, and a pretrained score estimator may be directly incorporated into \mathcal{F} without further optimization. However, the method is computationally demanding, as training requires backpropagating through high-order derivatives of U^{θ} (specifically, the time derivative, the score, and the Laplacian) resulting in a substantial increase in cost. To mitigate this, Plainer et al. (2025) propose approximating the time-score using finite differences and estimating the residual term \mathcal{F}_t with an unbiased estimator.

⁶Note that $\alpha_t = v_t$ and $\beta_t = \sqrt{2\dot{\gamma}(t)\gamma(t)}$ is also a valid choice but we keep the previous decomposition to make the following proofs easier.

A.3.2 Consistency from Bayes Rule

A complementary perspective arises by considering the correlation between the distribution at two consecutive times 0 < s < t < T. In this case, the marginal densities of Y_s and Y_t are connected through Bayes' rule

$$p_t(y_t)p_{s|t}(y_s|y_t) = p_s(y_s)p_{t|s}(y_t|y_s), \quad \text{for all } y_s, y_t \in \mathbb{R}^d,$$
 (29)

where $p_{t|s}$ and $p_{s|t}$ denote the conditional distributions of Y_t given Y_s and Y_s given Y_t , respectively. Although these conditional distributions are generally intractable, they admit tractable approximations when $(Y_t)_t$ is defined as the solution of an SDE, as in DMs or SIs. We should first note that the time-reversal, which generally exists for DMs or SIs, of Equation (26) is written as

$$dY_t = \left[\alpha_t(Y_t) - \beta_t^2 \nabla \log p_t(Y_t)\right] dt + \beta_t d\tilde{W}_t, \qquad (30)$$

where $(\tilde{W}_t)_t$ is a standard Brownian motion in reversed time. By letting $\delta = t - s$, one can approximate the transition kernels via an Euler–Maruyama (EM) discretization of the corresponding SDEs (8) and (9), yielding

$$p_{t|s}(\cdot|y_s) \approx \mathcal{N}\left(y_s + \delta\alpha_s(y_s), \ \delta\beta_s^2 \mathbf{I}_d\right) ,$$
 (31)

$$p_{s|t}(\cdot|y_t) \approx \mathcal{N}\left(y_t - \delta\left[\alpha_t(y_t) - \beta_t^2 \nabla \log p_t(y_t)\right], \ \delta\beta_t^2 \mathbf{I}_d\right). \tag{32}$$

In He et al. (2025), the authors propose to regularize the sequence $(\log p_t^{\theta})_t$ by minimizing the squared discrepancy between the logarithm of the two sides of the Bayes rule (29)

$$\mathcal{L}_{\text{Bayes}}(\theta) = \mathbb{E}_{s,t}[\mathcal{L}_{\text{Bayes}}(\theta; s, t)],$$

with

$$\mathcal{L}_{\text{Bayes}}(\theta; s, t) = \mathbb{E}_{p_s, p_t} \left[\left(\log p_s^{\theta}(Y_s) - \log p_t^{\theta}(Y_t) + \log p_{t|s}^{\theta}(Y_t|Y_s) - \log p_{s|t}^{\theta}(Y_s|Y_t) \right)^2 \right],$$

where $p_{t|s}^{\theta}$ and $p_{s|t}^{\theta}$ denote approximations of $p_{t|s}$ (31) and $p_{s|t}$ (32), obtained by replacing $\nabla \log p_t$ with its approximation $\nabla \log p_t^{\theta}$. As highlighted in He et al. (2025), for DMs, the specific choices of f and g allow a closed-form expression for the forward-time kernel $p_{t|s}$. This yields a more accurate approximation of the time-forward kernel than the EM scheme (31) and avoids reliance on intractable quantities such as the score. However, even in this favorable case, the time-backward kernel (32) remains approximate, introducing bias that breaks self-consistency. Exact self-consistency is only recovered in the small-step limit ($\delta \to 0$), where the EM scheme becomes accurate.

A.3.3 BAYES AND FOKKER-PLANK REGULARIZATIONS: DISCRETE V.S. CONTINUOUS

Now, we are going to show that $\mathcal{L}_{\mathrm{Bayes}}$ and $\mathcal{L}_{\mathrm{FPE}}$ are asymptotically related as follows:

Proposition 3. Let $\delta > 0$. In the small step-size regime, the Bayes objective $\mathcal{L}_{\text{Bayes}}$ recovers the Fokker-Planck regularization \mathcal{L}_{FPE} , i.e.,

$$\lim_{\delta \to 0} \frac{1}{\delta} \mathcal{L}_{\text{Bayes}}(\theta; t, t + \delta) = \mathcal{L}_{\text{FPE}}(\theta; t) . \tag{33}$$

The proof is provided at appendix D.3. This result is also closely related to the derivations in (Skreta et al., 2025b, Appendix D.2). Building on this observation, Proposition 3 implies that $\mathcal{L}_{\mathrm{Bayes}}$ is either in the small step-size regime, where it remains mode blind, or in the non-small step-size regime, where it becomes biased.

B ADDITIONAL CONNECTION TO RELATED WORKS

B.1 CONNECTION TO RELATED WORKS IN TRAINING ENERGY-BASED GENERATIVE MODELS

Figure 5 illustrates the connections between DiffCLF and other existing methods that train energy-based generative models (usually diffusion models), while Table 2 summurizes the computational overhead, assumptions/requirements, and mode-blindness issue for those methods.

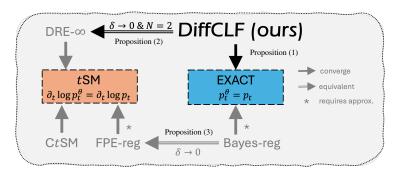


Figure 5: Connections between DiffCLF (ours) and other related works.

Table 2: Comparison of properties between DiffCLF (ours) and related methods. For *Number of Function Evaluation* (NFE), we report the actual evaluations when jointly training with \mathcal{L}_{DSM} , where we treat auto-differentiation costing roughly twice a network forward pass. For DRE- ∞ , though Choi et al. (2022) proposes to directly parameterize the score, we choose to treat it a way for energy-based training and therefore report the NFE for energy-parameterization, which doubles the original calculation. For FPE-reg, we follow the approximations made in Plainer et al. (2025) and count their NFE.

| Method | NFE | No approx. | Prior knowledge of $(p_t)_t$ | mode-weight aware |
|---|-----|------------|------------------------------|-------------------|
| DRE-∞ (Choi et al., 2022) | 4 | Х | _ | X |
| CtSM (Yu et al., 2025; Guth et al., 2025) | 2 | ✓ | $\partial_t X_t$ | X |
| FPE-reg (Plainer et al., 2025) | 14 | × | Induced from known FPE | X |
| Bayes-reg (He et al., 2025) | 3 | X | $p_{t s} \ \& \ p_{s t}$ | X |
| N-DiffCLF (ours) | N+1 | ✓ | _ | ✓ |

DRE- ∞ (Choi et al., 2022), CtSM (Yu et al., 2025; Guth et al., 2025), and FPE-reg (Plainer et al., 2025) train models such that their time derivatives match the ground-truth ones, which is termed Time Score Matching (tSM) (Choi et al., 2022). Jointly training with DSM, the optimality yields $\nabla \log p_t^{\theta} = \nabla \log p_t$ and $\partial_t \log p_t^{\theta} = \partial_t \log p_t$. However, it is not sufficient to reach the optimality of log density, i.e. $\log p_t^{\theta} = \log p_t$, especially when the modes are disconnected (see Appendix C for more discussions).

Bayes-reg (He et al., 2025) leverages the transition kernels for energy-based training, which is guaranteed to reach optimal $(p_t^{\theta})_t$ if training with arbitrary time pairs (t,t'). However, in practical cases such as DMs or SIs, the transition kernels can only be approximated when t and t' close enough, through a Euler-Maruyama discretization of the dynamic's SDE. Proposition 3 shows that when t and t' are close enough, Bayes-reg recovers FPE-reg, and therefore, it shares the same issues in tSM.

DiffCLF treats the energy training as classification tasks, which, in the 2-class case, recovers tSM in the continuous-time limit (see Proposition 2). In fact, when (t, t') in Equation (12) are close enough, one could approximate

$$\log p_{t'}^{\theta}(x) = \log p_t^{\theta}(x) + \partial_t \log p_t^{\theta}(x)(t - t') + \mathcal{O}(|t - t'|^2) .$$

Therefore, the first term in Equation (12) can be approximated as ⁷

$$\mathbb{E}_{p_t} \left[\log \frac{p_t^{\theta}(X)}{p_t^{\theta}(X) + p_{t'}^{\theta}(X)} \right] = \mathbb{E}_{p_t} \left[\log \frac{1}{1 + \exp(\partial_t \log p_t^{\theta}(X)(t - t') + \mathcal{O}(|t - t'|^2))} \right] , \quad (34)$$

$$\approx \mathbb{E}_{p_t} \left[\log \left(\frac{1}{2} + \frac{1}{4} \partial_t \log p_t^{\theta}(X)(t - t') \right) \right] . \quad (35)$$

⁷This is induced by the first order approximation of the log sigmoid function, i.e. $\log \frac{1}{1+e^{-z}} = -\log 2 + \frac{z}{2} + \mathcal{O}(z^2)$.

Analogously, the second term in Equation (12) can be approximated as

$$\mathbb{E}_{p_{t'}}\left[\log \frac{p_{t'}^{\theta}(X)}{p_t^{\theta}(X) + p_{t'}^{\theta}(X)}\right] \approx \mathbb{E}_{p_{t'}}\left[\log \left(\frac{1}{2} - \frac{1}{4}\partial_t \log p_t^{\theta}(X)(t - t')\right)\right]. \tag{36}$$

DRE- ∞ (Choi et al., 2022) proposes to parameterize a time-score network s_{θ} and optimize Equation (12) with approximations given by Equations (35) and (36):

$$\mathcal{L}_{DRE-\infty}(\theta) = \mathbb{E}_t[\mathcal{L}_{DRE-\infty}(\theta; t, \delta)]$$
(37)

with
$$\mathcal{L}_{DRE-\infty}(\theta; t, \delta) = -\frac{1}{2} \mathbb{E}_{p_t}[\log(1 - h_{\theta}(Y, t, \delta))] - \frac{1}{2} \mathbb{E}_{p_{t+\delta}}[\log h_{\theta}(Y, t, \delta)],$$
 (38)

$$h_{\theta}(Y,t,\delta) = \frac{1}{2} + \frac{1}{4} s_{\theta}(x,t)\delta. \tag{39}$$

B.2 CONNECTION TO MBAR

Computing free-energy differences, differences in log-normalizing constants between two potentials, is a central task in statistical physics and molecular dynamics (Lelièvre et al., 2010). In this section, we first introduce the free-energy estimation problem and the golden standard method MBAR (Shirts & Chodera, 2008) and build connection between with <code>DiffCLF</code>, which shows that their difference is the choice of model-parameterization.

Free-energy estimation and MBAR. Given a distribution

$$p(y) = \frac{1}{\mathcal{Z}} \exp(-\mathrm{U}(y)), \text{ with } \mathcal{Z} = \int_{\Omega} \exp(-\mathrm{U}(y)) \mathrm{d}y,$$

where $\Omega \subseteq \mathbb{R}^d$ is the support and $U : \Omega \to \mathbb{R}$ is the energy function, the *free energy* is defined as the negative log-partition function, i.e.

$$F = -\log \mathcal{Z} = \int_{\Omega} \exp(-U(y)) dy$$
.

While direct estimation of F is difficult, one typically estimates the *free-energy difference* between two states A and B with supports Ω_A , Ω_B and energy functions U_A , U_B respectively,

$$\Delta F_{AB} = F_A - F_B = \log \frac{Z_B}{Z_A}.$$

The golden-standard method for estimating this free-energy difference is *Multi-state Bennett Acceptance Ratio* (MBAR) (Shirts & Chodera, 2008), which generalizes *Bennett Acceptance Ratio* (BAR) (Bennett, 1976) to multi-states by introducing (i) a sequence of intermediate distributions with tractable energy functions bridging the two states $\{U_i\}_{n=1}^N$ and (ii) associated samples with these distributions $\{y_n^{(k)}\}_{n=1,k=1}^{N,K_n}$ such that

$$\mathbf{U}_0 = \mathbf{U}_A, \quad \mathbf{U}_N = \mathbf{U}_B, \quad p_n(y) = \frac{\exp(-\mathbf{U}_n(y))}{\mathcal{Z}_n}, \quad y_n^k \sim p_n ,$$

where $Z=\mathcal{Z}_n=\int_{\Omega_n}\exp(-\mathrm{U}_n(y))\mathrm{d}y$. Let $\mathrm{F}_n=-\log\mathcal{Z}_n$, by defining

$$p(c=n|y) = \frac{\exp(-\mathbf{U}_n(y) + \mathbf{F}_n)}{\sum_{m=1}^N \exp(-\mathbf{U}_m(y) + \mathbf{F}_m)} \quad \text{ and } \quad p(y|n) = p_n(y) \;.$$

MBAR treats the free energy estimation problem as a multiclass classification problem with maximum likelihood

$$F_{1:N}^{*} = \arg \max_{F_{1:N}} \mathbb{E}_{p(n)} \mathbb{E}_{p_{n}} [\log p(c = n|y)]$$

$$= \arg \max_{F_{1:N}} \mathbb{E}_{p(n)} \mathbb{E}_{p_{n}} \left[\frac{\exp(-U_{n}(y) + F_{n})}{\sum_{m=1}^{N} \exp(-U_{m}(y) + F_{m})} \right]$$

$$\approx \arg \max_{F_{1:N}} \frac{1}{N} \sum_{n=1}^{N} \frac{1}{K_{n}} \sum_{k=1}^{K_{n}} \log \frac{\exp(-U_{n}(y_{n}^{(k)}) + F_{n})}{\sum_{m=1}^{N} \exp(-U_{m}(y_{n}^{(k)}) + F_{m})},$$
(40)

which solved using a fixed point iteration (see (Shirts & Chodera, 2008, Equation 3)) or using the Newton-Raphson algorithm (see (Shirts & Chodera, 2008, Equation 6)). Although the optimization problem is easy to solve, it requires equilibrium samples $\{y_n^{(k)}\}_k$ from each intermediate distribution p_n , where the intermediate energy functions are usually defined by tempering e.g.

$$U_n(y) = (1 - \beta_n)U_A(y) + \beta_n U_B(y) \quad \text{, with } \beta_1 = 0 \text{ and } \beta_N = 1.$$
 (41)

To get equilibrium samples from each intermediate distributions, one typically used annealed Markov Chain Monte Carlo samplers which are expensive.

Connection between MBAR and DiffCLF. By comparison with the DiffCLF objective (40) and the MBAR objective (10), one could observe that the difference between MBAR and DiffCLF is the *model-parameterization*.

• In MBAR, the energy functions $(U_t)_t$ 8 are assumed known and the learnable objects are only the free energies $(F_t)_t$, i.e.

$$p_t^{\theta}(y) = \exp(-U_t(y) + \mathcal{F}_t^{\theta})$$
.

• In DiffCLF, the EBMs are fully parameterized (see Equation (2)).

Besides, the accuracy of MBAR critically depends on the choice of the path, e.g. the anealling temperatures. Similarly to the recalibration case, learned energies could directly provides a data-driven approach to construct more effective paths, potentially surpassing hand-crafted designs.

C BLINDNESS OF SCORE MATCHING AND TIME SCORE MATCHING

In this section, we revisit the blindness of score matching, first analyzed in Wenliang & Kanagawa (2021); Zhang et al. (2022), and show that the problem persists even when matching higher-order derivatives or the time derivative of the trajectory $(\log p_t)_t$.

Let a set of time-dependent distributions with differentiable densities $\{g_t^1,\ldots,g_t^K\}$ having mutual disjoint (disconnected) support sets $\{\mathcal{X}_t^1,\ldots,\mathcal{X}_t^K\}$, where $\mathcal{X}_t^i\cap\mathcal{X}_t^j=\emptyset$ for any $i\neq j$ For all $t\in[0,T]$, we define two mixture distributions $p_t=\sum_{k=1}^K\alpha_t^kg_t^k$ and $q_t=\sum_{k=1}^K\beta_t^kg_t^k$, where $\sum_{k=1}^K\alpha_t^k=1$ and $\sum_{k=1}^K\beta_t^k=1$.

Score Matching is blind. Score Matching is minimizing the *Fisher Divergence* (FD) between p_t and q_t . Let $t \in [0, T]$, following the (Zhang et al., 2022, Proposition 1) we have that

$$FD(p_t, q_t) := \mathbb{E}_{p_t} \left[\|\nabla \log p_t(X_t) - \nabla \log q_t(X_t)\|^2 \right],$$

$$= \sum_{k=1}^K \int_{\mathcal{X}_t^k} \left\| \frac{\nabla \left(\sum_{j=1}^K \alpha_t^j g_t^j(x)\right)}{p_t(x)} - \frac{\nabla \left(\sum_{j=1}^K \beta_t^j g_t^j(x)\right)}{q_t(x)} \right\|^2 \alpha_t^k g_t^k(x) dx,$$

$$= \sum_{k=1}^K \int_{\mathcal{X}_t^k} \left\| \frac{\varphi_t^k \nabla g_t^k(x)}{\varphi_t^k g_t^k(x)} - \frac{\beta_t^k \nabla g_t^k(x)}{\beta_t^k g_t^k(x)} \right\|^2 \alpha_t^k g_t^k(x) dx = 0,$$

using $g_t^i(x_j) = 0$ and $\nabla g_t^i(x_j) = 0$ for $\forall x_j \in \mathcal{X}_j$ when $i \neq j$. Therefore, SM (or FD) is ill-defined on disconnected sets and has the blindness problem.

Remark 4. The marginal p_t needs not be supported on disjoint sets for all $t \in [0, T]$. For example, in DMs the terminal distribution p_T is typically Gaussian and thus fully connected. In such cases, mixture proportions may be correctly estimated. However, at intermediate times where the support is disconnected, the proportions can be misestimated. Since the objective averages losses across time, the blindness issue may persist overall.

⁸For clarity, we change the index of n to a set of discretized time t as in DiffCLF.

 $^{^{9}}$ Note that multi-modality could be modified depending on t by simply setting two components and respective weights equal.

Higher-order Score Matching is blind. As suggested in Lu et al. (2022), one could minimize the divergence between the Hessian or Laplacian of log-densities, i.e.

$$\mathbb{E}_{p_t} \left[\left\| \nabla^2 \log p_t(X_t) - \nabla^2 \log q_t(X_t) \right\|_F^2 \right] \quad \text{or} \quad \mathbb{E}_{p_t} \left[\left(\Delta \log p_t(X_t) - \Delta \log q_t(X_t) \right)^2 \right] ,$$

where $\|\cdot\|_F$ is the Frobenius norm. Similarly as the previous paragraph, for all $t \in [0,T]$ and $x \in \mathcal{X}_t^k$,

$$\begin{split} \nabla^2 \log p_t(x) &= \frac{p_t(x) \sum_{j=1}^K \alpha_t^j \nabla^2 g_t^j(x) - \left(\sum_{j=1}^K \alpha_t^j \nabla g_t^j(x)\right) \nabla p_t(x)^\top}{p_t(x)^2} \;, \\ &= \frac{\cancel{p_t^{k'}} g_t^k(x) \cancel{p_t^{k'}} \nabla^2 g_t^k(x) - \cancel{p_t^{k'}} \nabla g_t^k(x) \cancel{p_t^{k'}} \nabla g_t^k(x)^\top}{(\cancel{p_t^{k'}} g_t^k(x))^2} \;, \end{split}$$

which doesn't depend on the weights α . The cases for Laplacian or other higher-order (w.r.t. x) regression are analogous.

Time Score Matching can be blind. The Time Score Matching (see Appendix A.2 for details) objective can be written for any $t \in [0, T]$ as

$$\mathbb{E}_{p_t} \left[\left(\partial_t \log p_t(X_t) - \partial_t \log q_t(X_t) \right)^2 \right] = \sum_{k=1}^K \int_{\mathcal{X}_t^k} \left(\frac{\partial_t \left(\sum_{j=1}^K \alpha_t^j g_t^j(x) \right)}{p_t(x)} - \frac{\partial_t \left(\sum_{j=1}^K \beta_t^j g_t^j(x) \right)}{q_t(x)} \right)^2 \alpha_t^k g_t^k(x) dx , \quad (42)$$

where $\partial_t(\sum_{j=1}^K \alpha_t^j g_t^j(x))$ can be expanded by leveraging $g_t^i(x_j) = 0$ for any $x_j \in \mathcal{X}_j$ and $i \neq j$

$$\partial_t \left(\sum_{j=1}^K \alpha_t^j g_t^j(x) \right) = (\partial_t \alpha_t^k) g_t^k(x) + \sum_{j=1}^K \alpha_t^j \partial_t g_t^j(x), \quad \forall x \in \mathcal{X}_t^k ,$$
 (43)

hence,

$$\mathbb{E}_{p_t} \left[\left(\partial_t \log p_t(X_t) - \partial_t \log q_t(X_t) \right)^2 \right]$$

$$= \sum_{k=1}^K \int_{\mathcal{X}_t^k} \left(\frac{(\partial_t \alpha_t^k) g_t^k(x) + \sum_{j=1}^K \alpha_t^j \partial_t g_t^j(x)}{\alpha_t^k g_t^k(x)} - \frac{(\partial_t \beta_t^k) g_t^k(x) + \sum_{j=1}^K \beta_t^j \partial_t g_t^j(x)}{\beta_t^k g_t^k(x)} \right)^2 \alpha_t^k g_t^k(x) dx ,$$

$$= \sum_{k=1}^K \int_{\mathcal{X}_t^k} \left(\frac{\partial_t \alpha_t^k}{\alpha_t^k} - \frac{\partial_t \beta_t^k}{\beta_t^k} + \frac{\sum_{j \neq k} \alpha_t^j \partial_t g_t^j(x)}{\alpha_t^k g_t^k(x)} - \frac{\sum_{j \neq k} \beta_t^j \partial_t g_t^j(x)}{\beta_t^k g_t^k(x)} \right)^2 \alpha_t^k g_t^k(x) dx \ge 0 ,$$

which can be 0 in some cases. For example, if the mixture weights α , β are time-independent (as in DMs) and the supports of g_t vary only slowly over time (also typical in DMs), then the loss becomes mode-blind.

The Fokker-Planck regularization is mode blind. When p_t, q_t are generated from the same Itô SDE, say $dX_t = f(t, X_t) dt + g(t, X_t) dW_t$, starting from p_0, q_0 respectively, the Fokker-Planck Equation (see Appendix A.1) tells us

$$\partial_t \log p_t(x) = -\nabla \cdot f(t, x) - f(t, x)^\top \nabla \log p_t(x) + \frac{1}{2} g(t, x)^\top g(t, x) \left(\Delta \log p_t(x) + \|\nabla \log p_t\|^2 \right) ,$$

$$\partial_t \log q_t(x) = -\nabla \cdot f(t, x) - f(t, x)^\top \nabla \log q_t(x) + \frac{1}{2} g(t, x)^\top g(t, x) \left(\Delta \log q_t(x) + \|\nabla \log q_t\|^2 \right) .$$

Therefore, the FPE regularization is equivalent to regressing a combination of (i) the score and its squared norm, and (ii) the Laplacian, which are all mode-blind. Therefore, FPE regularization in such cases is blind in this case.

Alleviating the blindness of score matching. Several approaches have been proposed to address mode blindness. Zhang et al. (2022) introduce an auxiliary noise distribution m and minimize the Fisher divergence between mixtures of (π, m) and (p^{θ}, m) , which indirectly enforces proximity between π and p^{θ} . Similarly, Schröder et al. (2023) propose the energy discrepancy, a contrastive objective between π and its noisy counterpart that provably avoids blindness (see (Schröder et al., 2023, Figure 1)). However, both methods hinge on the careful design and tuning of the auxiliary noise distribution or kernel, limiting their scalability in practice.

D PROOFS OF PROPOSITIONS 1, 2, AND 3

D.1 PROOF OF PROPOSITION 1

 Proposition 5. Let $N \in \mathbb{N}^*$ and $t_{1:N} \in [0,T]^N$. The energy classification loss is defined as

$$\mathcal{L}_{\text{clf}}(\theta; t_{1:N}) = -\frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{p_{t_i}} \left[\log \frac{p_{t_i}^{\theta}(Y_i)}{\sum_{j=1}^{N} p_{t_j}^{\theta}(Y_i)} \right] ,$$

where $p_t^{\theta}(y_t) = \exp(-U_t^{\theta}(y_t) + F_t^{\theta})$. The minimizer of $\mathcal{L}_{clf}(\theta; t_{1:N})$ is given by $p_t^{\theta^*} = p_t$ for all $t \in \{t_1, \dots, t_N\}$.

Proof. For clarity, we denote for all $i \in [1, N]$, we denote $p_i = p_{t_i}$ and $p_i^{\theta} = p_{t_i}^{\theta}$. Assume the supports of $\{p_i\}_{i \in [1, N]}$ are the same, denoted as Ω , one could have

$$\sum_{i=1}^{N} \mathbb{E}_{p_i} \left[\log \frac{p_i^{\theta}(Y_{t_i})}{\sum_{j=1}^{N} p_j^{\theta}(Y_{t_i})} \right] = \int_{\Omega} \sum_{i=1}^{N} p_i(y) \log \frac{p_i^{\theta}(y)}{\sum_{j=1}^{K} p_j^{\theta}(y)} dy.$$
 (44)

One could easily show that $\hat{p}_i = p_i$ is the unique maximizer of a constraint optimization problem

$$\max_{\hat{p}_{1:N}} \sum_{i=1}^{N} p_i \log \frac{\hat{p}_i}{\sum_{j=1}^{N} \hat{p}_j} \quad \text{s.t. } \sum_{i=1}^{N} \hat{p}_j = 1 .$$

Let $\mathcal{L}(\hat{p}_{1:N}, \lambda) = \sum_{i=1}^{N} p_i \log \left[\hat{p}_i / \sum_{j=1}^{N} \hat{p}_j \right] + \lambda (\sum_{i=1}^{N} \hat{p}_i - 1)$. For all $i \in [1, N]$,

$$\frac{\partial \mathcal{L}}{\partial \hat{p}_i} = 0 \iff \frac{p_i}{\hat{p}_i} - \sum_{k=1}^{N} \frac{p_k}{\sum_{i=1}^{N} \hat{p}_i} - \lambda = 0 \iff \frac{p_i}{\hat{p}_i} - 1 - \lambda = 0,$$

which leads to $p_i/\hat{p}_i = 1 + \lambda$. Since $\sum_{i=1}^N \hat{p}_i = 1$, we have $\hat{p}_i = p_i$. Therefore

$$\sum_{i=1}^{N} \mathbb{E}_{p_i} \left[\log \frac{p_i^{\theta}(Y_i)}{\sum_{j=1}^{N} p_j^{\theta}(Y_i)} \right] \le \int_{\Omega} \sum_{i=1}^{N} p_i(y) \log \frac{p_i(y)}{\sum_{j=1}^{N} p_j(y)} dy ,$$

where the equality holds when $p_t^{\theta^*}(y) = p_t(y)$, for $\forall t \in \{t_k\}_{k=1}^K$ and $y \in \Omega$.

D.2 Proof of Proposition 2

Lemma 6 (Kolmogorov semigroup expansion). Let X_t solves the Itô SDE $dX_t = f(t, X_t)dt + g(t, X_t)dW_t$ and $\phi \in \mathbb{C}^4_b$. Then with a small time increment δ ,

$$\mathbb{E}[\phi(X_{t+\delta})|X_t = x] = \phi(x) + \delta \mathcal{L}_t \phi(x) + \frac{\delta^2}{2} \mathcal{L}_t^2 \phi(x) + \mathcal{O}(\delta^2) , \qquad (45)$$

or equivalently

$$\mathbb{E}_{p_{t+\delta}}[\phi(X)] = \mathbb{E}_{p_t}[\phi(X)] + \delta \mathbb{E}_{p_t}[\mathcal{L}_t\phi(X)] + \frac{\delta^2}{2} \mathbb{E}_{p_t}[\mathcal{L}_t^2\phi(X)] + \mathcal{O}(\delta^2) , \qquad (46)$$

where $\mathcal{L}_t \phi := f(t,\cdot)^\top \nabla \phi + \frac{1}{2} g(t,\cdot) g(t,\cdot)^\top \Delta \phi$ is the time-dependent backward generator.

Lemma 7 (Generator-Adjoint Identity). Given the Itô SDE, ϕ , and \mathcal{L}_t defined in lemma 6, we have

$$\mathbb{E}_{p_t}[\mathcal{L}_t \phi(X)] = \mathbb{E}_{p_t} \left[\phi(X) \frac{\partial}{\partial t} \log p_t(X) \right] . \tag{47}$$

Proposition 8. Let $t \in [0,T)$ and $\delta > 0$, we have

$$\lim_{\delta \to 0^{+}} \frac{8}{\delta^{2}} \left(\mathcal{L}_{\text{clf}}(\theta; t, t + \delta) - \log 2 \right) = \mathcal{L}_{tSM}(\theta; t) + C , \tag{48}$$

where $C = \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t(Y_t) \right)^2 \right]$ is a constant with respect to θ .

Proof. In the binary case, we first rewrite the classification loss as follows

$$\mathcal{L}_{\text{clf}}(\theta; t, t + \delta) = -\frac{1}{2} \left\{ \mathbb{E}_{p_t} \left[\log \frac{p_t^{\theta}(x)}{p_t^{\theta}(x) + p_{t+\delta}^{\theta}(x)} \right] + \mathbb{E}_{p_{t+\delta}} \left[\log \frac{p_{t+\delta}^{\theta}(x)}{p_t^{\theta}(x) + p_{t+\delta}^{\theta}(x)} \right] \right\}$$

$$= -\frac{1}{2} \left\{ \underbrace{\mathbb{E}_{p_t} \left[\log \sigma(\log p_t^{\theta}(x) - \log p_{t+\delta}^{\theta}(x)) \right]}_{A} + \underbrace{\mathbb{E}_{p_{t+\delta}} \left[\log \sigma(\log p_{t+\delta}^{\theta}(x) - \log p_{t}^{\theta}(x)) \right]}_{B} \right\},$$

where $\sigma(z) = 1/(1 + e^{-z})$ is the sigmoid function. By Taylor expansion,

$$\log p_t^{\theta}(x) - \log p_{t+\delta}^{\theta}(x) = -\delta \frac{\partial}{\partial t} \log p_t^{\theta}(x) + \mathcal{O}(\delta^2),$$
$$\log \sigma(z) = -\log 2 + \frac{z}{2} - \frac{z^2}{8} + \mathcal{O}(z^4).$$

Therefore, A and B can be simplified as

$$\begin{split} A &= -\log 2 + \mathbb{E}_{p_t} \left[-\frac{\delta}{2} \frac{\partial}{\partial t} \log p_t^{\theta}(x) - \frac{\delta^2}{8} \left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] + \mathcal{O}(\delta^3), \\ B &= -\log 2 + \mathbb{E}_{p_{t+\delta}} \left[\frac{\delta}{2} \frac{\partial}{\partial t} \log p_t^{\theta}(x) - \frac{\delta^2}{8} \left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] + \mathcal{O}(\delta^3). \end{split}$$

Next, we use Lemma 6 with $\phi_1(x) = \frac{\partial}{\partial t} \log p_t^{\theta}(x)$ and $\phi_2(x) = \left(\frac{\partial}{\partial t} \log p_t^{\theta}(x)\right)^2$ as follows

$$\mathbb{E}_{p_{t+\delta}} \left[\phi_1(x) \right] = \mathbb{E}_{p_t} \left[\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right] + \delta \mathbb{E}_{p_t} \left[\mathcal{L}_t \frac{\partial}{\partial t} \log p_t^{\theta}(x) \right] + \mathcal{O}(\delta^2),$$

$$\mathbb{E}_{p_{t+\delta}} \left[\phi_2(x) \right] = \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] + \mathcal{O}(\delta).$$

Plugging $\mathbb{E}_{p_{t+\delta}}\left[\phi_1(x)\right]$ and $\mathbb{E}_{p_{t+\delta}}\left[\phi_2(x)\right]$, B can be written as

$$B = -\log 2 + \frac{\delta}{2} \mathbb{E}_{p_t} \left[\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right]$$

$$+ \frac{\delta^2}{2} \mathbb{E}_{p_t} \left[\mathcal{L}_t \frac{\partial}{\partial t} \log p_t^{\theta}(x) \right] - \frac{\delta^2}{8} \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] + \mathcal{O}(\delta^3).$$
 (49)

Therefore,

$$A + B = -2\log 2 + \frac{\delta^2}{2} \mathbb{E}_{p_t} \left[\mathcal{L}_t \frac{\partial}{\partial t} \log p_t^{\theta}(x) \right] - \frac{\delta^2}{4} \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] + \mathcal{O}(\delta^3).$$

By lemma 7, the $\mathbb{E}_{p_t} \left[\mathcal{L}_t \frac{\partial}{\partial t} \log p_t^{\theta}(x) \right]$ term could be written as

$$\mathbb{E}_{p_t} \left[\mathcal{L}_t \frac{\partial}{\partial t} \log p_t^{\theta}(x) \right] = \mathbb{E}_{p_t} \left[\frac{\partial}{\partial t} \log p_t^{\theta}(x) \frac{\partial}{\partial t} \log p_t(x) \right], \tag{50}$$

which results in

$$\begin{split} &A + B + 2\log 2 \\ &= -\frac{\delta^2}{4} \left(\mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) \right)^2 \right] - 2\mathbb{E}_{p_t} \left[\frac{\partial}{\partial t} \log p_t^{\theta}(x) \frac{\partial}{\partial t} \log p_t(x) \right] \right) + \mathcal{O}(\delta^3) \\ &= -\frac{\delta^2}{4} \left(\mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t^{\theta}(x) - \frac{\partial}{\partial t} \log p_t(x) \right)^2 \right] + \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t(x) \right)^2 \right] \right) + \mathcal{O}(\delta^3). \end{split}$$

Therefore, given a small time-increment δ , the binary-classification loss can be written as

$$\mathcal{L}_{\text{clf}}(\theta; t, t + \delta) = \frac{\delta^{2}}{8} \mathbb{E}_{p_{t}} \left[\left(\frac{\partial}{\partial t} \log p_{t}^{\theta}(x) - \frac{\partial}{\partial t} \log p_{t}(x) \right)^{2} \right] + \frac{\delta^{2}}{8} \mathbb{E}_{p_{t}} \left[\left(\frac{\partial}{\partial t} \log p_{t}(x) \right)^{2} \right] + \log 2 + \mathcal{O}(\delta^{3}). \quad (51)$$

Since $C = \frac{\delta^2}{8} \mathbb{E}_{p_t} \left[\left(\frac{\partial}{\partial t} \log p_t(x) \right)^2 \right] + \log 2$ is constant w.r.t. θ , it recovers the tSM regularization.

D.3 Proof of Proposition 3

Proposition 9. Let $\delta > 0$. In the small step-size regime, the Bayes objective $\mathcal{L}_{\text{Bayes}}$ recovers the Fokker–Planck regularization \mathcal{L}_{FPE} , i.e.,

$$\lim_{\delta \to 0} \frac{1}{\delta} \mathcal{L}_{\text{Bayes}}(\theta; t, t + \delta) = \mathcal{L}_{\text{FPE}}(\theta; t) . \tag{52}$$

Proof of Proposition 3. From Equation (28), we write the full learning objective of the FPE regularization for reference:

$$\mathcal{L}_{\text{FPE}}(\theta) = \int_{0}^{1} \mathbb{E}_{p_{t}} \left[\left(\partial_{t} \log p_{t}^{\theta}(y) + \nabla \cdot \alpha_{t}(y) + \alpha_{t}(y)^{\top} \nabla \log p_{t}^{\theta}(y) - \frac{1}{2} \beta_{t}^{2} \|\nabla \log p_{t}^{\theta}(y)\|^{2} \right)^{2} \right] dt . \quad (53)$$

Now, let's look at the Bayes regularization. Given the EM discretizations for both the forward (31) and backward (32) kernels and assume that the $(y_{t-\delta},y_t)$ are sampled forwardly, *i.e.* $y_t=y_{t-\delta}+\alpha_{t-\delta}(y_{t-\delta})\delta+\beta_{t-\delta}\sqrt{\delta}z$, where $z\sim\mathcal{N}(0,I)$ and $\delta>0$. In this case, the forward kernel should be corrected for the volume change induced by the drift α , *i.e.*

$$p_{t|t-\delta}(y_t|y_{t-\delta}) \approx \frac{1}{1 + \delta \nabla \cdot \alpha_{t-\delta}(y_{t-\delta})} \mathcal{N}(y_t; y_{t-\delta} + \alpha_{t-\delta}(y_{t-\delta})\delta, \beta_{t-\delta}^2 \delta I).$$
 (54)

Let $b_t(y) = \alpha_t(y) - \beta_t^2 \nabla \log p_t(y)$, then the log forward and backward kernels can be further approximated using Taylor expansion around (t, y_t) as follows

$$\log p_{t|t-\delta}(y_t|y_{t-\delta}) \approx C - \frac{1}{2} \|z\|^2 - \log(1 + \delta \nabla \cdot \alpha_{t-\delta}(y_{t-\delta}))$$

$$\approx C - \frac{1}{2} \|z\|^2 - \delta \nabla \cdot \alpha_t(y) + \mathcal{O}(\delta) , \qquad (55)$$

$$\log p_{t-\delta|t}(y_{t-\delta}|x_t) \approx C - \frac{1}{2\beta_t^2 \delta} \|\alpha_{t-\delta}(y_{t-\delta})\delta + \beta_{t-\delta} \sqrt{\delta} z - b_t(y_t)\delta\|^2$$

$$= C - \frac{1}{2\beta_t^2 \delta} \|\alpha_t(y_t)\delta + \beta_t \sqrt{\delta} z - b_t(y_t)\delta + \mathcal{O}(\delta)\|^2$$

$$= C - \frac{1}{2} \|z\|^2 - \frac{\delta}{2\beta_t^2} \|\alpha_t(y_t) - b_t(y_t)\|^2 - \frac{\sqrt{\delta}}{\beta_t} z^{\top} (\alpha_t(y_t) - b_t(y_t)) + \mathcal{O}(\delta) , \qquad (56)$$

where $C=-\frac{d}{2}\log 2\pi-d\log g(t)$. Plugging back $b_t(y)=\alpha_t(y)-\beta_t^2\nabla\log p_t(y)$, the log Radon–Nikodym derivative can be approximated as

$$\log \frac{p_{t|t-\delta}(y_t|y_{t-\delta})}{p_{t-\delta|t}(y_{t-\delta}|x_t)} \approx \frac{\beta_t^2 \delta}{2} \|\nabla \log p_t(y_t)\|^2 + \beta_t \sqrt{\delta} z^\top \nabla \log p_t(y_t) - \delta \nabla \cdot \alpha_t(y_t) + \mathcal{O}(\delta) . \quad (57)$$

In meanwhile, one could Taylor expand the log marginal density $\log p_{t-\delta}(y_{t-\delta})$ around (t,y_t)

$$\log p_{t-\delta}(y_{t-\delta}) \approx \log p_t(y_t) - \frac{\partial}{\partial t} \log p_t(y_t) \delta + \nabla \log p_t(y_t)^\top (y_{t-\delta} - y_t) + \frac{1}{2} (y_{t-\delta} - y_t)^\top \nabla^2 \log p_t(y_t) (y_{t-\delta} - y_t) + \mathcal{O}(\delta^{3/2}) . \quad (58)$$

By plugging $y_t - y_{t-\delta} \approx \alpha_t(y_t)\delta + \beta_t \sqrt{\delta}z + \mathcal{O}(\delta^{3/2})$, we have

$$\log p_{t-\delta}(y_{t-\delta}) \approx \log p_t(y_t) - \frac{\partial}{\partial t} \log p_t(y_t) \delta - \nabla \log p_t(y_t)^{\top} \alpha_t(y_t) \delta$$
$$-\beta_t \sqrt{\delta} z^{\top} \nabla \log p_t(y_t) + \frac{\beta_t^2 \delta}{2} z^{\top} \nabla^2 \log p_t(y_t) z + \mathcal{O}(\delta^{3/2}) . \quad (59)$$

Now, we could plug all the approximations together, and take the expectation

$$\frac{1}{\delta} \mathbb{E}_{z} \left[\log p_{t-\delta}(y_{t-\delta}) - \log p_{t}(y_{t}) + \log \frac{p_{t|t-\delta}(y_{t}|y_{t-\delta})}{p_{t-\delta|t}(y_{t-\delta}|x_{t})} \right] \\
= \left(-\frac{\partial}{\partial t} \log p_{t}(y_{t}) - \nabla \cdot \alpha_{t}(y_{t}) - \nabla \log p_{t}(y_{t})^{\top} f(t, x_{t}) + \frac{\beta_{t}^{2}}{2} (\operatorname{tr}(\nabla^{2} \log p_{t}(y_{t})) + \|\nabla \log p_{t}(y_{t})\|^{2}) \right), \tag{60}$$

which recovers the Fokker Plank residual when $\delta \to \infty$, and therefore RNE regularization recovers the Fokker Plank regularization in the limit.

E EXTENSION TO DISCRETE DIFFUSIONS

Recent works Campbell et al. (2022); Meng et al. (2023); Lou et al. (2023); Campbell et al. (2024); Gat et al. (2024); Shaul et al. (2025) extend diffusion models to discrete state spaces $\mathbb Y$ by formulating the forward noising process as a continuous-time Markov chain (CTMC). A CTMC is specified by a family of (possibly time-dependent) transition rate matrices $(Q_t)_t$, a.k.a. *generators*, where for each t: (i) $Q_t = (Q_t(y,y'))_{y,y' \in \mathbb Y}$, (ii) $Q_t(y,y) = -\sum_{y' \neq y} Q_t(y,y')$ for any $y \in \mathbb Y$, and (iii) $Q_t(y,y') \geq 0$ for all $y \neq y' \in \mathbb Y$. We write

$$Y_t \sim \text{CTMC}(Q_t)$$
.

to mean that $Y_0 \sim p_0$ followed by infinitesimal transitions governed by Q_t . As a stochastic process starting from a target distribution p_0 , $(Q_t)_t$ induces a sequence of intermediate marginals $(p_t)_t$, which satisfy the *Kolmogorov forward equation* (also called the master equation):

$$\frac{\partial}{\partial t} p_t(y) = \sum_{y'} p_t(y') Q_t(y', y) \iff \partial_t p_t = Q_t^{\mathsf{T}} p_t . \tag{61}$$

Analogous to the Stein score in continuous spaces, one can define the *concrete score* in discrete spaces as the vector of marginal density ratios

$$S_t(y)_{y'} := \frac{p_t(y')}{p_t(y)}$$
.

In terms of this score, the log-density dynamics admit the compact form

$$\frac{\partial}{\partial t} \log p_t(y) = \frac{1}{p_t(y)} \sum_{y'} p_t(y') Q_t(y', y) = \sum_{y'} S_t(y)_{y'} Q_t(y', y) . \tag{62}$$

 Finally, under mild regularity conditions, the *time-reversed process* $(Y_t)_t$ is again a CTMC with generator $(\tilde{Q}_t)_t$ (Kelly, 2011) given by

$$Y_t \sim \text{CTMC}(\tilde{Q}_t), \quad \text{where} \quad \tilde{Q}_t(y, y') = \begin{cases} Q_t(y', y) \frac{p_t(y')}{p_t(y)}, & y \neq y', \\ -\sum_{y' \neq y} \tilde{Q}_t(y, y'), & y = y'. \end{cases}$$
(63)

Though the marginals $(p_t)_t$ are intractable, one could train time-dependent neural networks $s_t^{\theta}(y)$ to minimize the following *Score Entropy* (SE) loss

$$\mathcal{L}_{SE}(\theta;t) = \mathbb{E}_{p_t} \left[\sum_{y \neq Y_t \in \mathbb{Y}} Q_t(Y_t, y) \left(S_t(Y_t)_y \log \frac{S_t(Y_t)_y}{s_t^{\theta}(Y_t)_y} - S_t(Y_t)_y + s_t^{\theta}(Y_t)_y \right) \right], \tag{64}$$

by optimizing the following Conditional Score Entropy loss analogous to DSM

$$\mathcal{L}_{\text{CSE}}(\theta;t) = \mathbb{E}_{p_0} \mathbb{E}_{p_{t|0}} \left[\sum_{y \neq Y_t \in \mathbb{Y}} Q_t(Y_t, y) \left(-S_t(Y_t|Y_0)_y \log s_t^{\theta}(Y_t)_y + s_t^{\theta}(Y_t)_y \right) \right], \tag{66}$$

where $S_t(Y_t|Y_0)$ is the conditional concrete score, $\nabla_{\theta} \mathcal{L}_{CSE}(\theta;t) = \nabla_{\theta} \mathcal{L}_{SE}(\theta;t)$, and $p_{t|0}$ is the conditional distribution obtained by solving the following ODE

$$\frac{\partial}{\partial t} p_{t|0}(y|y_0) = \sum_{y'} p_{t|0}(y'|y_0) Q_t(y',y) \quad \text{with } p_{0|0}(y|y_0) = \delta_{y_0}(y). \tag{67}$$

Energy-based training. Similar to eq. (2), one could define a family of EBMs on \mathbb{Y} as follows

$$p_t^{\theta}(y_t) = \exp(-\mathbf{U}_t^{\theta}(y_t))/\mathcal{Z}_t^{\theta}, \quad \mathcal{Z}_t^{\theta} = \exp(\mathbf{F}_t^{\theta}) = \sum_{y_t \in \mathbb{Y}} \exp(-\mathbf{U}_t^{\theta}(y_t)). \tag{68}$$

Simply plugging p_t^{θ} into eq. (66) we have

$$\mathcal{L}_{CSE}(\theta;t) = \mathbb{E}_{p_0} \mathbb{E}_{p_{t|0}} \left[\sum_{y \neq Y_t \in \mathbb{Y}} Q_t(Y_t, y) \left(-S_t(Y_t)_y \log \frac{p_t^{\theta}(y)}{p_t^{\theta}(Y_t)} + \frac{p_t^{\theta}(y)}{p_t^{\theta}(Y_t)} \right) \right]$$

$$= \mathbb{E}_{p_0} \mathbb{E}_{p_{t|0}} \left[\sum_{y \neq Y_t \in \mathbb{Y}} Q_t(Y_t, y) \left\{ S_t(Y_t)_y (\mathbb{U}_t^{\theta}(y) - \mathbb{U}_t^{\theta}(Y_t)) + \exp(\mathbb{U}_t^{\theta}(Y_t) - \mathbb{U}_t^{\theta}(y)) \right\} \right]$$
(69)

Combined with classification loss. Therefore, it is straightforward to combine the classification loss 10 with Equation (66) to train an energy-based discrete Diffusion model.

F EXPERIMENTAL DETAILS

F.1 GAUSSIAN MIXTURES AND CLOSED FORM EXPRESSIONS FOR DMS AND SIS

Mixture of Gaussians (MOG) is distribution having the following density

$$\pi(x) = \sum_{n=1}^{N} w_n \mathcal{N}(x; \mu_n, \Sigma_n) .$$

Diffusion Models case. In DMs, we require the exact marginal density, which is a convolution of the noising kernel and the target distribution. Assume the noising kernel is $p_{t|0}(y_t|y_0) = \mathcal{N}(y_t; S(t)y_0, \gamma(t)^2 \mathbf{I}_d)$, we have

$$p_t(y_t) = \int p_0(y_0) p_{t|0}(y_t|y_0) dy_0 = \sum_{n=1}^{N} w_n \mathcal{N}(y_t; S(t)\mu_n, S(t)^2 \Sigma_n + \gamma(t)^2 \mathbf{I}_d) , \qquad (71)$$

again a MOG. Therefore the marginal density and score are tractable.

Stochastic Interpolant case. In SIs, we consider $p_0(y) = \sum_{n=1}^N w_n \mathcal{N}(y; \mu_n, \Sigma_n)$ and $p_1(y) = \sum_{m=1}^M \tilde{w}_m \mathcal{N}(y; \tilde{\mu}_m, \Sigma_m)$ are both MOGs with independent coupling and a linear interpolation $I_t(y_0, y_1) = (1 - t)y_0 + ty_1$, therefore

$$p_t(y_t) = \iint p_0(y_0) p_1(y_1) \mathcal{N}(y_t; I_t(y_0, y_1), \gamma(t)^2 \mathbf{I}_d) dy_0 dy_1$$
(72)

$$= \sum_{n} \sum_{m} w_{n} \tilde{w}_{m} \mathcal{N}(y_{t}; (1-t)\mu_{n} + t\tilde{\mu}_{m}, (1-t)^{2} \Sigma_{n} + t^{2} \tilde{\Sigma}_{m} + \gamma(t)^{2} I_{d}), \qquad (73)$$

allowing exact marginal density and score calculation. Moreover, we require the velocity in SIs, which is $\mathbb{E}[\partial_t I_t(Y_0,Y_1)|Y_t=y_t]=\mathbb{E}[Y_1-Y_0|Y_t=y_t]$. To get the analytical velocity, notice that

$$p(y_0, y_1 \mid y_t) = \sum_{n=1}^{N} \sum_{m=1}^{M} \pi_{n,m}(y_t) \,\mathcal{N}\left(\begin{bmatrix} y_0 \\ y_1 \end{bmatrix}; \begin{bmatrix} \mu_{0|t}^{(n,m)} \\ \mu_{1|t}^{(n,m)} \end{bmatrix}, \, \Sigma_{|t}^{(n,m)} \right) , \quad (74)$$

$$\pi_{n,m}(y_t) = \frac{w_n \tilde{w}_m \, \mathcal{N}(y_t; \bar{\mu}_{n,m}, S_{n,m})}{\sum\limits_{n'=1}^{N} \sum\limits_{m'=1}^{M} w_{n'} \tilde{w}_{m'} \, \mathcal{N}(y_t; \bar{\mu}_{n',m'}, S_{n',m'})},$$
(75)

with

$$\bar{\mu}_{n,m} = (1-t)\mu_n + t\tilde{\mu}_m , \qquad (76)$$

$$S_{n,m} = (1 - t)^2 \Sigma_n + t^2 \tilde{\Sigma}_m + \gamma(t)^2 I_d , \qquad (77)$$

$$\mu_{0|t}^{(n,m)} = \mu_n + (1-t)\Sigma_n S_{n,m}^{-1}(y_t - \bar{\mu}_{n,m}) , \qquad (78)$$

$$\mu_{1|t}^{(n,m)} = \tilde{\mu}_m + t\tilde{\Sigma}_m S_{n,m}^{-1} (y_t - \bar{\mu}_{n,m}) . \tag{79}$$

Therefore, the exact velocity in this case is given by

$$v_t(y_t) = \mathbb{E}[Y_1 - Y_0 \mid Y_t = y_t] = \sum_{n=1}^{N} \sum_{m=1}^{M} \pi_{n,m}(y_t) \left(\mu_{1|t}^{(n,m)} - \mu_{0|t}^{(n,m)} \right) . \tag{80}$$

F.2 ANALYTICAL COMPARISON WITH DSM ON MOG

In this section, we provide the experimental setup for Gaussian mixture experiments along with additional results.

F.2.1 GAUSSIAN MIXTURE DESIGN

We study two types of Gaussian mixtures. The first, introduced in Midgley et al. (2023), is a widely used benchmark consisting of 40 Gaussians with uniform weights (MOG-40). The means are sampled from $U([-40,40]^d)$, and all components share the same covariance $\log(1+e)\mathrm{I}_d$. The second, taken from Grenioux et al. (2024); Noble et al. (2025), is a two-component mixture with modes at $-5 \times \mathbf{1}_d$ and $+5 \times \mathbf{1}_d$ (where $\mathbf{1}_d$ denotes the d-dimensional vector of ones), covariance 5×10^{-2} , I_d , and imbalanced weights 2/3 and 1/3. For training, we standardize these distributions (subtracting the mean and dividing by the standard deviation).

F.2.2 ARCHITECTURE, TRAINING AND EVALUATION DETAILS

We train log-densities using three settings: (i) \mathcal{L}_{DSM} alone, (ii) a convex combination of \mathcal{L}_{DSM} with either \mathcal{L}_{clf} or \mathcal{L}_{CtSM} . In the latter case, simply summing the two losses generally worked best.

Diffusion Model. For DMs, we adopt the Variance Preserving (VP) schedule Song et al. (2021b) with a linear β -schedule ending at $\beta_{\rm max}=20$. Time is discretized linearly into 512 steps between 10^{-4} and $1-10^{-4}$. We follow the energy parameterization of Thornton et al. (2025), use the DSM weighting from Karras et al. (2022), and implement a 4-layer MLP of width 128 with sinusoidal time embeddings Song et al. (2021b). The conditional t-SM loss is reweighted by $\gamma^2/\dot{\gamma}^2$ as recommended

Table 3: Comparison of classification and score matching on synthetic Gaussian mixtures. Mixtures with two modes are trained using the same architecture under DSM as well as conditional time-score matching and our classification objective, averaged over seeds and number of classification levels $N \in {2,4,8,16}$ (DSM uses the same number of score evaluations for every N). We report the classification loss (10), Fisher divergence, and MMD (×100) from the denoising SDE (all on 512 time-steps). The classification approach matches DSM in Fisher divergence and MMD, while yielding markedly better consistency in classification loss.

| | $\mathcal{L}_{	ext{clf}} + \mathcal{L}_{	ext{DSM}}$ | | | \mathcal{L}_{0} | $\mathcal{L}_{\text{DSM}} + \mathcal{L}_{\text{DSM}}$ | | $\mathcal{L}_{	ext{DSM}}$ | | | |
|-----|---|-----------------------------|------------------------------|---------------------------|---|------------------------------|---------------------------|-----------------|-----------------------------|--|
| Dim | $\mathcal{L}_{	ext{clf}}$ | FD | MMD | $\mathcal{L}_{	ext{clf}}$ | FD | MMD | $\mathcal{L}_{	ext{clf}}$ | FD | MMD | |
| 8 | 4.14 ± 0.02 | 2.48 ± 2.34 | 6.94 ± 0.59 | $5.55{\pm}1.27$ | 6.78 ± 3.29 | 20.45 ± 8.43 | 17.88 ± 4.13 | 1.21 ± 1.14 | 5.91 ± 0.68 | |
| 16 | 3.95 ± 0.04 | $3.47{\pm}3.15$ | $8.57{\pm}1.83$ | 17.97 ± 9.77 | 9.15 ± 2.82 | $22.50{\pm}6.13$ | 191.78 ± 51.04 | 0.83 ± 0.74 | 7.13 ± 0.83 | |
| 32 | 3.84 ± 0.15 | $4.86{\scriptstyle\pm3.87}$ | $11.91{\scriptstyle\pm1.00}$ | 27.05 ± 13.99 | 10.54 ± 2.99 | $28.59{\scriptstyle\pm2.31}$ | 194.54 ± 23.85 | 1.04 ± 0.89 | $8.62{\scriptstyle\pm1.15}$ | |
| 64 | 3.83 ± 0.52 | $4.39{\scriptstyle\pm1.77}$ | $15.30{\scriptstyle\pm2.08}$ | 47.65 ± 22.47 | 11.57 ± 3.48 | 27.49 ± 1.93 | 208.32 ± 14.77 | 1.16 ± 0.89 | 10.73 ± 1.04 | |
| 128 | 3.85 ± 0.51 | $6.86{\scriptstyle\pm2.26}$ | 17.61 ± 2.09 | 151.48 ± 51.21 | 17.25 ± 9.12 | 30.69 ± 3.09 | 1521.54 ± 538.48 | 3.01 ± 2.30 | 15.48 ± 0.57 | |

by Yu et al. (2025). Models are trained on 60k samples for 500 epochs with DSM only, followed by 500 epochs with the chosen loss combination. We use a batch size of 2048, Adam optimizer with learning rate 10^{-3} . We average results over two random training seeds. Metrics for sample quality and log-density estimation are computed on 4096 samples. The Fisher devergence and the classification objective are computed on the full time-grid. Sampling is performed using the DDIM denoising kernel Song et al. (2021a).

Stochastic Interpolant. For SIs, we use the linear interpolant $I_t(x_0, x_1) = (1 - t)x_0 + tx_1$ and $\gamma : t \mapsto \sqrt{t(1-t)}$ bridging the 40-mode and 2-mode Gaussian mixtures described earlier. Time is discretized into 512 steps between 10^{-3} and $1 - 10^{-3}$. The potential is parameterized as

$$U_{(\theta_1,\theta_2)}(t,x) = x^{\top} NN^{\theta_1}(t,x) + NN^{\theta_2}(t,x) ,$$

where $\mathrm{NN}^{\theta_1}:[0,T]\times\mathbb{R}^d\to\mathbb{R}^d$ and $\mathrm{NN}^{\theta_2}:[0,T]\times\mathbb{R}^d\to\mathbb{R}$ are MLPs with depth 4 and width 64 (if $d\leq 32$) or 256 otherwise. Time embeddings follow Song et al. (2021b). Training proceeds for 10k steps with DSM only, then 50k steps with the chosen objective. We use a batch size of 1024 and a learning rate of 5×10^{-4} , sampling endpoint distributions at each step. To reduce variance in $\mathcal{L}_{\mathrm{DSM}}$ and $\mathcal{L}_{\mathrm{CtSM}}$, we apply the antithetic trick (Albergo et al., 2023, Appendix 6.1). Results are averaged over two seeds, and evaluation metrics are computed on 4096 samples. The Fisher devergence and the classification objective are computed on the full time-grid.

F.2.3 ADDITIONAL RESULTS

In this section, we complete the results of Section 5 with additional metrics and problems.

Diffusion Model While Table 3 provides the same comparison as Table 1 but for the bi-modal case, Tables 4 and 6 examine how the number of classification levels affects log-density estimation, whereas Tables 5 and 7 focus on generation quality.

Stochastic Interpolant Like Figure 3, Figures 6a to 6d we visualize the determination coefficient \mathbb{R}^2 between learned log-densities and the ground truth ones across time for each modal, as well as the log-density log-density scatter plots at two ends which should be a perfect diagonal line in optimality. In Tables 9 and 8, we report the quality of the estimated log-densities using the stochastic interpolant model.

F.3 COMPOSITION

In this section, we give the experimental details for the toy composition example from Section 5.

F.3.1 DISTRIBUTIONS DETAILS

Table 4: Log-density estimation on synthetic 40-mode Gaussian mixtures. We report classification loss, Fisher divergence, and average Effective Sample Size (ESS). The ESS is computed between the learned and exact log-densities using exact samples, averaged across time levels. Unlike Table 1, this table shows results for varying numbers of classification levels N. For fairness, each setting of N uses the same total number of score evaluations as \mathcal{L}_{DSM} .

| | | | $\mathcal{L}_{	ext{clf}} + \mathcal{L}_{	ext{DSM}}$ | | | $\mathcal{L}_{\text{CtSM}} + \mathcal{L}_{\text{DSM}}$ | | | $\mathcal{L}_{	ext{DSM}}$ | |
|-----|----|-----------------------------|---|-----------------------------|---------------------------|--|------------------------------|--------------------------------|---------------------------|-----------------------------|
| Dim | N | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD |
| 8 | 2 | 4.61 ± 0.04 | $89.9\% \pm 0.9\%$ | 3.61 ± 0.25 | 5.14 ± 0.08 | 88.2%±0.4% | 5.27 ± 0.08 | 8.80 ± 0.13 | 90.1%±1.2% | 5.45 ± 0.83 |
| 8 | 4 | $4.40{\scriptstyle\pm0.03}$ | $93.2\% \pm 0.6\%$ | 2.50 ± 0.00 | 5.48 ± 0.19 | $90.6\% \pm 0.4\%$ | 4.69 ± 0.01 | 9.06 ± 0.05 | $90.4\% \pm 0.1\%$ | 4.18 ± 0.20 |
| 8 | 8 | $4.32{\scriptstyle\pm0.00}$ | $94.2\% \pm 0.3\%$ | $1.20{\scriptstyle\pm0.03}$ | 6.77 ± 0.48 | $91.9\% \pm 0.4\%$ | 4.09 ± 0.00 | 9.20 ± 0.05 | $91.6\% \pm 1.1\%$ | 3.94 ± 0.11 |
| 8 | 16 | $4.31{\scriptstyle\pm0.00}$ | $96.2\% \pm 0.3\%$ | $0.69{\scriptstyle\pm0.01}$ | 7.83 ± 0.16 | $92.8\% \pm 0.2\%$ | 3.92 ± 0.04 | 9.68 ± 0.08 | $91.5\% \pm 0.1\%$ | 2.78 ± 0.08 |
| 16 | 2 | $4.40{\scriptstyle\pm0.05}$ | $85.8\% \pm 0.7\%$ | $4.15{\scriptstyle\pm0.11}$ | 5.17 ± 0.42 | $77.7\% \pm 0.4\%$ | 8.77 ± 0.26 | 22.36 ± 0.55 | $84.7\% \pm 1.1\%$ | 6.83 ± 0.71 |
| 16 | 4 | $4.22{\scriptstyle\pm0.04}$ | $86.8\%{\pm}1.6\%$ | $3.37{\pm0.04}$ | 11.40 ± 2.85 | $78.4\% \pm 0.4\%$ | $8.33{\pm}0.17$ | 21.45 ± 0.36 | $85.8\% \pm 0.3\%$ | $7.13{\scriptstyle\pm1.34}$ |
| 16 | 8 | 4.09 ± 0.00 | $88.8\% \pm 0.1\%$ | $2.26{\scriptstyle\pm0.12}$ | 10.04 ± 1.60 | $80.8\% \pm 0.6\%$ | 7.52 ± 0.29 | 22.93 ± 0.46 | $87.7\% \pm 0.9\%$ | 4.64 ± 0.89 |
| 16 | 16 | $4.05{\scriptstyle\pm0.00}$ | $91.5\% \pm 0.4\%$ | $1.48{\scriptstyle\pm0.01}$ | 5.48 ± 0.18 | $81.6\% \pm 0.7\%$ | 7.11 ± 0.03 | 22.69 ± 0.61 | $88.9\% \pm 0.0\%$ | 3.38 ± 0.14 |
| 32 | 2 | $4.41{\scriptstyle\pm0.04}$ | $76.8\%{\pm}1.1\%$ | $4.70{\scriptstyle\pm0.11}$ | 5.66 ± 0.11 | $67.8\% \pm 0.1\%$ | 10.19 ± 0.10 | 73.34 ± 0.94 | $76.4\% \pm 0.4\%$ | 4.88 ± 0.38 |
| 32 | 4 | 4.03 ± 0.07 | $77.1\% \pm 0.4\%$ | $4.04{\scriptstyle\pm0.03}$ | 6.63 ± 0.38 | $70.7\% \pm 0.1\%$ | 9.46 ± 0.35 | 81.87 ± 3.99 | $81.9\% \pm 0.3\%$ | 4.43 ± 0.10 |
| 32 | 8 | 3.89 ± 0.00 | $79.7\% \pm 0.4\%$ | $3.33{\scriptstyle\pm0.06}$ | 6.46 ± 0.26 | $71.4\% \pm 0.4\%$ | 9.64 ± 0.43 | 86.24 ± 2.31 | $80.4\% \pm 1.3\%$ | $3.49{\scriptstyle\pm0.24}$ |
| 32 | 16 | $3.83{\scriptstyle\pm0.01}$ | $84.7\% \pm 0.9\%$ | $2.65{\scriptstyle\pm0.03}$ | 13.92 ± 2.81 | $72.7\% \pm 0.4\%$ | 9.32 ± 0.06 | 98.82 ± 1.74 | $82.9\% \pm 0.4\%$ | $2.72{\scriptstyle\pm0.01}$ |
| 64 | 2 | $4.68{\scriptstyle\pm0.34}$ | $66.0\% \pm 2.9\%$ | $5.88{\scriptstyle\pm0.13}$ | 21.25 ± 2.64 | $55.9\% \pm 1.2\%$ | 10.10 ± 0.23 | 121.14 ± 12.99 | $69.5\% \pm 2.2\%$ | 4.86 ± 0.68 |
| 64 | 4 | 4.04 ± 0.10 | $69.0\% \pm 0.5\%$ | $5.16{\scriptstyle\pm0.03}$ | 62.11 ± 47.56 | $55.8\% \pm 0.1\%$ | $10.42{\scriptstyle\pm0.02}$ | 121.76 ± 3.21 | $71.3\% \pm 1.1\%$ | 4.00 ± 0.09 |
| 64 | 8 | 3.70 ± 0.04 | $72.8\% \pm 0.1\%$ | $4.42{\scriptstyle\pm0.10}$ | 34.83 ± 5.43 | $56.5\% \pm 0.1\%$ | 10.17 ± 0.03 | 152.74 ± 1.00 | $72.6\% \pm 0.6\%$ | 3.57 ± 0.03 |
| 64 | 16 | $3.61{\scriptstyle\pm0.01}$ | $72.3\% \pm 0.4\%$ | $4.05{\scriptstyle\pm0.03}$ | 85.59 ± 68.72 | $57.8\% \pm 1.4\%$ | $10.47{\scriptstyle\pm0.27}$ | 202.18 ± 4.46 | $75.1\% \pm 1.7\%$ | 3.28 ± 0.18 |
| 128 | 2 | 5.98 ± 0.05 | $54.1\% \pm 0.1\%$ | $7.30{\scriptstyle\pm0.06}$ | 11.80 ± 2.10 | $44.7\% \pm 0.0\%$ | 9.33 ± 0.00 | $427.77{\pm}12.04$ | $60.0\% \pm 0.3\%$ | 8.34 ± 0.43 |
| 128 | 4 | $4.52{\scriptstyle\pm0.11}$ | $54.6\% \pm 0.4\%$ | $7.39{\scriptstyle\pm0.04}$ | 17.12 ± 1.23 | $44.8\% \pm 0.0\%$ | 9.33 ± 0.01 | $383.60{\pm}15.45$ | $62.6\% {\pm} 0.2\%$ | 6.88 ± 0.13 |
| 128 | 8 | 3.63 ± 0.07 | $55.8\% \pm 0.3\%$ | $6.79{\scriptstyle\pm0.01}$ | 54.49 ± 28.78 | $45.0\% {\pm} 0.1\%$ | 9.40 ± 0.01 | 356.38 ± 39.38 | $61.9\% \pm 0.7\%$ | 5.83 ± 0.33 |
| 128 | 16 | $3.47{\scriptstyle\pm0.01}$ | $55.0\% \pm 0.1\%$ | $6.17{\scriptstyle\pm0.01}$ | 24.84 ± 9.45 | $45.1\% {\pm} 0.1\%$ | $9.51{\scriptstyle\pm0.10}$ | $366.36{\scriptstyle\pm16.04}$ | $62.6\% {\pm} 0.4\%$ | $6.09{\scriptstyle\pm0.05}$ |

Table 5: **Generation quality on 40-mode Gaussian mixtures.** We report Maximum Mean Discrepancy (MMD) Gretton et al. (2012) (\times 100), sliced 2-Wasserstein distance (\times 100), and total variation (TV) distance between mode-weight histograms (as in Noble et al. (2025)). Results are reported for varying classification levels N.

| | | | <i>C</i> + <i>C</i> | | | 2 | | | <i>C</i> | |
|-----|----|-----------------|---|-----------------------------|------------------|--|-----------------------------|-----------------|-----------------------------|-----------------------------|
| | | | $\mathcal{L}_{\text{clf}} + \mathcal{L}_{\text{DSM}}$ | | | $\mathcal{L}_{\text{CtSM}} + \mathcal{L}_{\text{DSM}}$ | | | $\mathcal{L}_{	ext{DSM}}$ | |
| Dim | N | MMD | Sliced W_2 | TV | MMD | Sliced W_2 | TV | MMD | Sliced W_2 | TV |
| 8 | 2 | 1.34 ± 0.37 | 6.32 ± 0.28 | 0.09 ± 0.00 | 1.65 ± 0.28 | $7.55{\pm0.61}$ | 0.15 ± 0.01 | 1.75 ± 0.07 | 7.74 ± 0.42 | 0.13 ± 0.00 |
| 8 | 4 | 0.56 ± 0.56 | 5.88 ± 0.36 | $0.12{\pm0.00}$ | 1.41 ± 1.09 | $7.12{\scriptstyle\pm0.94}$ | $0.12{\scriptstyle\pm0.02}$ | 0.54 ± 0.54 | $5.70{\scriptstyle\pm0.81}$ | 0.11 ± 0.01 |
| 8 | 8 | 0.87 ± 0.05 | 5.28 ± 0.19 | $0.09{\scriptstyle\pm0.02}$ | 1.07±0.03 | 6.14 ± 0.03 | $0.12{\scriptstyle\pm0.01}$ | 0.46 ± 0.46 | 5.49 ± 0.37 | 0.10 ± 0.01 |
| 8 | 16 | 0.00 ± 0.00 | 4.77 ± 0.68 | $0.09{\scriptstyle\pm0.01}$ | 1.49 ± 0.13 | 6.82 ± 0.54 | 0.11 ± 0.01 | 1.21 ± 0.06 | $6.34{\scriptstyle\pm0.02}$ | 0.11 ± 0.01 |
| 16 | 2 | 0.81 ± 0.31 | $6.15{\scriptstyle\pm0.03}$ | 0.11 ± 0.00 | 2.40 ± 0.21 | 10.74 ± 0.55 | $0.22{\scriptstyle\pm0.01}$ | 1.81±0.18 | $7.50{\scriptstyle\pm0.35}$ | 0.13 ± 0.00 |
| 16 | 4 | 1.15±0.03 | 5.86 ± 0.19 | 0.10 ± 0.01 | 3.18 ± 0.31 | 11.78 ± 0.81 | $0.23{\scriptstyle\pm0.02}$ | 1.33 ± 0.58 | $6.86{\scriptstyle\pm0.44}$ | 0.12 ± 0.00 |
| 16 | 8 | 1.00 ± 0.17 | $5.96{\scriptstyle\pm0.41}$ | 0.10 ± 0.00 | 1.82 ± 0.47 | $8.85{\pm}1.12$ | $0.21{\scriptstyle\pm0.01}$ | 0.80 ± 0.39 | $5.90{\scriptstyle\pm0.68}$ | 0.12 ± 0.01 |
| 16 | 16 | 0.68 ± 0.41 | 5.93 ± 0.27 | $0.09{\scriptstyle\pm0.01}$ | 2.40 ± 0.36 | 9.39 ± 0.48 | $0.19{\scriptstyle\pm0.02}$ | 1.19 ± 0.49 | $6.30{\scriptstyle\pm0.37}$ | 0.11 ± 0.01 |
| 32 | 2 | 1.67 ± 0.50 | $7.51{\scriptstyle\pm0.53}$ | $0.12{\scriptstyle\pm0.01}$ | 3.11 ± 0.37 | 12.96 ± 0.85 | $0.21{\scriptstyle\pm0.05}$ | 1.66 ± 0.28 | $7.47{\pm0.50}$ | $0.14{\scriptstyle\pm0.01}$ |
| 32 | 4 | 1.21 ± 0.12 | $6.69{\scriptstyle\pm0.29}$ | 0.11 ± 0.01 | 2.32 ± 0.02 | 10.92 ± 0.18 | $0.17{\pm0.03}$ | 1.40 ± 0.04 | 6.91 ± 0.09 | $0.12{\scriptstyle\pm0.01}$ |
| 32 | 8 | 0.94 ± 0.22 | 6.41 ± 0.06 | 0.10 ± 0.01 | 2.40 ± 0.04 | 10.90 ± 0.42 | $0.18{\scriptstyle\pm0.01}$ | 1.09 ± 0.22 | $6.22{\scriptstyle\pm0.82}$ | 0.09 ± 0.00 |
| 32 | 16 | 0.97 ± 0.38 | $6.22{\scriptstyle\pm0.61}$ | $0.09{\scriptstyle\pm0.01}$ | 1.86 ± 0.20 | 9.76 ± 0.36 | $0.15{\scriptstyle\pm0.01}$ | 0.67 ± 0.16 | 5.84 ± 0.09 | $0.10{\scriptstyle\pm0.01}$ |
| 64 | 2 | 3.68 ± 0.80 | $10.41{\scriptstyle\pm1.11}$ | $0.15{\pm}0.02$ | 12.25 ± 5.58 | $30.15{\scriptstyle\pm10.58}$ | $0.52{\scriptstyle\pm0.19}$ | 1.52 ± 0.24 | 7.40 ± 0.09 | $0.14{\scriptstyle\pm0.01}$ |
| 64 | 4 | 2.13 ± 0.18 | 7.88 ± 0.39 | $0.13{\scriptstyle\pm0.01}$ | 10.80±0.89 | $26.86{\scriptstyle\pm1.25}$ | $0.48{\scriptstyle\pm0.00}$ | 1.65 ± 0.02 | 8.11 ± 0.45 | $0.16{\scriptstyle\pm0.01}$ |
| 64 | 8 | 1.69 ± 0.11 | $7.66{\scriptstyle\pm0.27}$ | $0.12{\scriptstyle\pm0.01}$ | 9.12 ± 0.93 | $21.78{\scriptstyle\pm1.74}$ | $0.43{\scriptstyle\pm0.04}$ | 1.41 ± 0.02 | $7.18{\scriptstyle\pm0.09}$ | $0.12{\pm0.00}$ |
| 64 | 16 | 1.22 ± 0.25 | 6.67 ± 0.38 | 0.10 ± 0.00 | 7.60 ± 2.05 | 18.46 ± 2.06 | 0.34 ± 0.09 | 1.46 ± 0.08 | $6.78{\scriptstyle\pm0.59}$ | 0.13 ± 0.01 |
| 128 | 2 | 5.34 ± 0.27 | $15.18{\scriptstyle\pm1.27}$ | $0.16{\scriptstyle\pm0.02}$ | 5.23 ± 0.47 | $22.31{\scriptstyle\pm1.14}$ | $0.61{\scriptstyle\pm0.01}$ | 2.37 ± 0.19 | 9.41 ± 0.26 | 0.18 ± 0.01 |
| 128 | 4 | 4.27 ± 0.15 | $13.29{\scriptstyle\pm0.34}$ | $0.15{\scriptstyle\pm0.01}$ | 14.73 ± 0.26 | $32.63{\scriptstyle\pm0.32}$ | $0.80{\scriptstyle\pm0.05}$ | 2.02 ± 0.13 | $8.20{\scriptstyle\pm0.60}$ | $0.15{\scriptstyle\pm0.00}$ |
| 128 | 8 | 2.42 ± 0.20 | $10.51{\scriptstyle\pm0.07}$ | $0.12{\scriptstyle\pm0.01}$ | 22.79 ± 1.63 | 47.99 ± 4.90 | $1.11{\pm}0.03$ | 1.95 ± 0.37 | $7.61{\scriptstyle\pm0.72}$ | $0.14{\scriptstyle\pm0.00}$ |
| 128 | 16 | 2.12 ± 0.25 | $9.72{\scriptstyle\pm0.55}$ | $0.13{\scriptstyle\pm0.01}$ | $22.97{\pm}6.80$ | $42.97{\scriptstyle\pm11.55}$ | $1.02{\scriptstyle\pm0.30}$ | 1.61 ± 0.01 | $7.25{\scriptstyle\pm0.24}$ | $0.12{\scriptstyle\pm0.02}$ |

Gaussian mixtures The Gaussian mixtures p_A and p_B in the left part of Figure 4 (top row) are both bi-modal. For p_A , the modes are centered at $\mu_1=(-a,+a)$ and $\mu_2=(+a,+a)$ with weights 0.3 and 0.7, respectively. For p_B , the modes are at $\mu_1=(-a,-a)$ and $\mu_2=(+a,-a)$ with weights 0.7 and 0.3. We chose a=0.5. Both mixtures share identical covariances $\Sigma_1=\Sigma_2=0.01\times I_2$.

Table 6: **Log-density estimation on synthetic 2-mode Gaussian mixtures.** We report classification loss, Fisher divergence, and average Effective Sample Size (ESS). The ESS is computed between the learned and exact log-densities using exact samples, averaged across time levels. Unlike Table 1, this table shows results for varying numbers of classification levels N. For fairness, each setting of N uses the same total number of score evaluations as \mathcal{L}_{DSM} .

| | | | $\mathcal{L}_{	ext{clf}} + \mathcal{L}_{	ext{DSM}}$ | | | $\mathcal{L}_{\text{CtSM}} + \mathcal{L}_{	ext{DSM}}$ | | | $\mathcal{L}_{	ext{DSM}}$ | |
|-----|----|-----------------------------|---|-----------------------------|---------------------------|---|-------------------------------|---------------------------|---------------------------|-----------------------------|
| Dim | N | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD |
| 8 | 2 | 4.18 ± 0.01 | $95.7\% \pm 2.3\%$ | 2.83 ± 0.19 | 5.05 ± 0.67 | $91.8\% \pm 0.1\%$ | 5.02 ± 0.38 | 14.70±1.88 | $91.6\% \pm 0.9\%$ | 2.20 ± 0.73 |
| 8 | 4 | $4.13{\scriptstyle\pm0.00}$ | $96.5\% \pm 0.4\%$ | $3.70{\scriptstyle\pm0.34}$ | 4.72 ± 0.49 | $83.3\% \pm 1.5\%$ | $7.25{\scriptstyle\pm0.15}$ | 14.58 ± 1.91 | $90.9\% \pm 1.5\%$ | 1.29 ± 0.34 |
| 8 | 8 | $4.12{\scriptstyle\pm0.00}$ | $98.2\% \pm 0.0\%$ | $2.22{\scriptstyle\pm0.18}$ | 6.02 ± 0.43 | $88.0\% \pm 8.3\%$ | 5.36 ± 1.63 | 18.21 ± 1.49 | $92.6\% \pm 1.2\%$ | 0.91 ± 0.30 |
| 8 | 16 | $4.12{\scriptstyle\pm0.00}$ | $97.5\% \pm 0.1\%$ | $1.17{\scriptstyle\pm0.17}$ | $6.39{\pm}1.93$ | $85.9\% \pm 1.8\%$ | 9.50 ± 2.75 | 24.02 ± 0.36 | $92.6\% \pm 1.0\%$ | 0.44 ± 0.00 |
| 16 | 2 | 4.00 ± 0.01 | $90.8\% \pm 4.0\%$ | 2.93 ± 0.61 | 14.16 ± 7.75 | $66.5\% \pm 2.3\%$ | 9.32 ± 0.11 | 157.79 ± 0.87 | $81.3\% \pm 0.3\%$ | 1.19 ± 0.21 |
| 16 | 4 | $3.94{\scriptstyle\pm0.03}$ | $95.3\% \pm 0.5\%$ | $4.49{\scriptstyle\pm1.22}$ | 12.38 ± 3.86 | $76.9\% \pm 3.6\%$ | 8.53 ± 0.46 | 278.78 ± 1.52 | $82.2\% \pm 1.5\%$ | 1.08 ± 0.03 |
| 16 | 8 | 3.94 ± 0.03 | $92.7\% \pm 1.3\%$ | 3.99 ± 0.75 | 27.12 ± 5.10 | $73.3\% \pm 9.8\%$ | 8.74 ± 1.83 | 156.97 ± 1.03 | $82.5\% \pm 0.5\%$ | 0.68 ± 0.08 |
| 16 | 16 | $3.91{\scriptstyle\pm0.04}$ | $97.9\% \pm 0.4\%$ | $2.44{\scriptstyle\pm0.13}$ | 18.21 ± 12.30 | $59.5\% \pm 1.5\%$ | 10.02 ± 0.01 | 173.58 ± 12.17 | $83.7\% \pm 0.3\%$ | 0.37 ± 0.06 |
| 32 | 2 | 3.99 ± 0.17 | $83.8\% \pm 3.9\%$ | 2.77 ± 0.45 | 45.50 ± 9.22 | $55.3\%{\pm}6.1\%$ | 10.49 ± 0.74 | 164.35 ± 12.67 | $74.4\% \pm 0.9\%$ | 1.81 ± 0.55 |
| 32 | 4 | 3.87 ± 0.06 | $87.2\% \pm 6.5\%$ | $4.26{\scriptstyle\pm1.03}$ | 27.16 ± 10.23 | $48.8\% \pm 0.5\%$ | 10.84 ± 0.00 | 220.25 ± 11.54 | $75.2\% \pm 0.2\%$ | 0.98 ± 0.14 |
| 32 | 8 | 3.70 ± 0.05 | $90.0\% \pm 1.2\%$ | 5.10 ± 0.59 | 16.21 ± 3.15 | $53.1\% \pm 4.5\%$ | 10.75 ± 0.63 | 185.16 ± 8.36 | $76.3\% \pm 0.1\%$ | 0.81 ± 0.05 |
| 32 | 16 | $3.81{\scriptstyle\pm0.08}$ | $87.3\% \pm 0.8\%$ | $7.30{\scriptstyle\pm0.60}$ | 19.32 ± 8.11 | $50.5\% \pm 2.0\%$ | 10.06 ± 0.60 | 208.39 ± 7.67 | $76.9\% \pm 0.8\%$ | 0.54 ± 0.10 |
| 64 | 2 | $3.72{\scriptstyle\pm0.12}$ | $78.8\%{\pm}1.2\%$ | $4.53{\scriptstyle\pm0.54}$ | 29.66 ± 11.12 | $43.7\% \pm 0.4\%$ | 11.07 ± 0.04 | 214.31 ± 8.38 | $67.1\% \pm 0.5\%$ | 1.96 ± 0.31 |
| 64 | 4 | $4.29{\scriptstyle\pm0.84}$ | $81.3\% \pm 0.0\%$ | 3.83 ± 0.66 | $62.44{\pm}6.10$ | $45.0\% \pm 0.9\%$ | 12.10 ± 0.42 | 210.10 ± 3.03 | $68.2\% \pm 0.4\%$ | 1.14 ± 0.05 |
| 64 | 8 | $3.73{\scriptstyle\pm0.21}$ | $80.9\% \pm 6.9\%$ | $5.65{\pm}2.41$ | 43.24 ± 2.78 | $43.7\% \pm 1.7\%$ | 11.22 ± 0.33 | 206.46 ± 25.51 | $69.2\% \pm 0.4\%$ | 0.84 ± 0.08 |
| 64 | 16 | $3.57{\scriptstyle\pm0.15}$ | $75.6\% \pm 7.0\%$ | $3.54 {\pm} 0.76$ | 55.28 ± 35.08 | $44.2\% \pm 0.2\%$ | 11.87 ± 0.93 | $202.40{\pm}8.05$ | $70.3\% \pm 0.6\%$ | 0.69 ± 0.02 |
| 128 | 2 | $3.79{\scriptstyle\pm0.13}$ | $56.5\% {\pm 0.7\%}$ | $6.99{\scriptstyle\pm1.01}$ | 93.67 ± 7.28 | $37.5\% \pm 0.1\%$ | 11.27 ± 0.25 | 2192.68±397.10 | $56.3\% \pm 0.3\%$ | 4.27 ± 0.34 |
| 128 | 4 | $4.66{\scriptstyle\pm0.14}$ | $61.5\% \pm 0.7\%$ | 5.89 ± 0.50 | 141.52 ± 40.48 | $36.8\% \pm 0.1\%$ | $28.36{\scriptstyle\pm13.03}$ | 1637.77±155.21 | $56.5\% \pm 0.3\%$ | 3.15 ± 0.71 |
| 128 | 8 | $3.66{\scriptstyle\pm0.14}$ | $57.7\% \pm 1.6\%$ | $8.87{\pm0.54}$ | 195.62 ± 16.22 | $39.6\% \pm 2.9\%$ | 14.67 ± 1.39 | 1401.30±161.64 | $56.8\% \pm 0.1\%$ | 1.95 ± 0.06 |
| 128 | 16 | $3.30{\scriptstyle\pm0.03}$ | $62.4\% {\pm} 0.6\%$ | $5.71{\scriptstyle\pm0.41}$ | 175.09 ± 50.85 | $37.0\% \pm 0.7\%$ | $14.69{\scriptstyle\pm1.52}$ | 854.42±168.79 | $56.8\% \pm 0.3\%$ | $2.66{\scriptstyle\pm0.30}$ |

Table 7: **Generation quality on 2-mode Gaussian mixtures.** We report Maximum Mean Discrepancy (MMD) Gretton et al. (2012) (\times 100), sliced 2-Wasserstein distance (\times 100), and total variation (TV) distance between mode-weight histograms (as in Noble et al. (2025)). Results are reported for varying classification levels N.

| | | | $\mathcal{L}_{	ext{clf}} + \mathcal{L}_{	ext{DSM}}$ | | L | $\mathcal{L}_{\text{CtSM}} + \mathcal{L}_{	ext{DSM}}$ | | | $\mathcal{L}_{	ext{DSM}}$ | |
|-----|----|------------------------------|---|-----------------------------|------------------|---|-----------------------------|------------------|-------------------------------|-----------------------------|
| Dim | N | MMD | Sliced W_2 | TV | MMD | Sliced W_2 | TV | MMD | Sliced W_2 | TV |
| 8 | 2 | 7.42 ± 0.31 | 20.82 ± 1.74 | 0.01 ± 0.01 | 13.79 ± 0.24 | 15.87 ± 1.78 | 0.03 ± 0.01 | 6.32 ± 0.78 | 21.37 ± 1.77 | 0.01 ± 0.00 |
| 8 | 4 | 7.05 ± 0.29 | 14.28 ± 5.52 | 0.03 ± 0.00 | 21.67 ± 5.75 | 47.94 ± 22.18 | $0.11{\scriptstyle\pm0.10}$ | 6.28 ± 0.42 | 19.70 ± 3.09 | 0.02 ± 0.01 |
| 8 | 8 | 6.31 ± 0.60 | $19.07{\scriptstyle\pm2.13}$ | 0.01 ± 0.00 | 22.03 ± 11.45 | $48.37{\pm}30.22$ | $0.19{\scriptstyle\pm0.18}$ | 5.84 ± 0.49 | $25.29{\pm}6.98$ | 0.02 ± 0.02 |
| 8 | 16 | 6.96 ± 0.47 | 13.43 ± 2.67 | $0.02{\scriptstyle\pm0.01}$ | 24.33 ± 7.51 | 59.01 ± 25.17 | $0.19{\scriptstyle\pm0.13}$ | 5.18 ± 0.01 | 13.89 ± 0.77 | $0.01{\scriptstyle\pm0.01}$ |
| 16 | 2 | 9.93 ± 2.64 | 15.48 ± 1.49 | $0.02{\pm}0.00$ | 21.18 ± 7.41 | $68.65{\pm}16.57$ | $0.18{\scriptstyle\pm0.06}$ | 7.63 ± 0.78 | 11.31 ± 7.99 | 0.00 ± 0.00 |
| 16 | 4 | $8.56{\pm}1.09$ | 22.40 ± 0.20 | $0.02{\scriptstyle\pm0.01}$ | $22.40{\pm}5.68$ | 46.29 ± 5.80 | 0.08 ± 0.03 | 7.69 ± 0.43 | 22.83 ± 6.96 | 0.04 ± 0.01 |
| 16 | 8 | $8.56{\scriptstyle\pm1.22}$ | 10.92 ± 0.28 | $0.01{\scriptstyle\pm0.01}$ | 19.38 ± 1.92 | 48.88 ± 25.33 | 0.06 ± 0.00 | 6.70 ± 0.89 | 22.80 ± 9.18 | 0.04 ± 0.02 |
| 16 | 16 | $7.25{\scriptstyle\pm0.26}$ | $13.33{\pm}6.27$ | 0.01 ± 0.00 | 27.06±5.19 | $115.65{\pm}38.93$ | $0.31{\scriptstyle\pm0.15}$ | 6.50 ± 0.09 | 17.29 ± 4.43 | 0.03 ± 0.01 |
| 32 | 2 | 11.98 ± 0.45 | $18.86{\scriptstyle\pm4.51}$ | $0.02{\scriptstyle\pm0.01}$ | 26.50 ± 1.32 | 76.92 ± 6.78 | $0.37{\scriptstyle\pm0.01}$ | 9.99 ± 0.06 | 28.01 ± 0.00 | 0.03 ± 0.01 |
| 32 | 4 | $12.27{\scriptstyle\pm1.72}$ | 18.98 ± 5.11 | 0.03 ± 0.00 | 30.14 ± 0.64 | 85.84 ± 0.70 | $0.57{\pm0.03}$ | 9.50 ± 0.17 | 14.84 ± 2.00 | 0.01 ± 0.00 |
| 32 | 8 | 11.19 ± 0.07 | 11.49 ± 3.99 | $0.03{\scriptstyle\pm0.01}$ | 28.07±3.31 | 76.61 ± 3.20 | $0.54{\scriptstyle\pm0.09}$ | 7.29 ± 0.05 | 10.69 ± 3.76 | 0.00 ± 0.00 |
| 32 | 16 | 12.22 ± 0.30 | 9.63 ± 3.58 | 0.01 ± 0.00 | 29.68 ± 0.20 | 85.34 ± 2.66 | 0.63 ± 0.03 | 7.71 ± 0.15 | $26.74{\scriptstyle\pm4.60}$ | 0.05 ± 0.02 |
| 64 | 2 | $15.68{\scriptstyle\pm1.39}$ | 20.10 ± 3.14 | 0.01 ± 0.00 | 27.41±2.15 | 87.37 ± 3.11 | $0.64{\scriptstyle\pm0.01}$ | 11.62 ± 1.10 | 19.19 ± 9.18 | 0.03 ± 0.00 |
| 64 | 4 | $15.06{\scriptstyle\pm1.70}$ | $22.11{\scriptstyle\pm12.00}$ | 0.03 ± 0.03 | 27.12 ± 1.68 | 86.51 ± 1.15 | $0.51{\scriptstyle\pm0.03}$ | 11.21 ± 0.29 | 18.76 ± 5.50 | 0.00 ± 0.00 |
| 64 | 8 | $15.39{\scriptstyle\pm2.67}$ | 21.27 ± 3.64 | $0.02{\scriptstyle\pm0.01}$ | 27.09 ± 2.34 | 91.65 ± 4.87 | $0.67{\pm0.00}$ | 10.44 ± 0.86 | 18.83 ± 0.14 | 0.02 ± 0.01 |
| 64 | 16 | $15.07{\scriptstyle\pm2.26}$ | $23.33{\pm}8.53$ | $0.03{\scriptstyle\pm0.02}$ | 28.35 ± 0.95 | 83.80 ± 2.62 | $0.55{\scriptstyle\pm0.12}$ | 9.63 ± 0.06 | 19.02 ± 8.67 | $0.02{\scriptstyle\pm0.01}$ |
| 128 | 2 | $17.21{\scriptstyle\pm0.47}$ | 31.28 ± 8.20 | 0.01 ± 0.00 | 29.11 ± 0.04 | 82.95 ± 0.86 | $0.67{\pm0.00}$ | 15.72 ± 0.52 | 34.61 ± 6.61 | 0.04 ± 0.02 |
| 128 | 4 | $16.78{\scriptstyle\pm0.69}$ | 32.77 ± 0.65 | 0.06 ± 0.01 | 31.45 ± 0.19 | $82.31{\pm}6.71$ | $0.66{\scriptstyle\pm0.01}$ | 15.84 ± 0.57 | $15.26{\scriptstyle\pm2.56}$ | $0.02{\scriptstyle\pm0.01}$ |
| 128 | 8 | 19.74 ± 3.16 | $49.72{\scriptstyle\pm10.95}$ | $0.07{\pm}0.03$ | 32.18 ± 5.65 | $92.22{\scriptstyle\pm1.62}$ | 0.66 ± 0.00 | 14.99 ± 0.25 | $31.94{\scriptstyle\pm13.94}$ | $0.01{\scriptstyle\pm0.01}$ |
| 128 | 16 | $16.69{\scriptstyle\pm0.72}$ | 39.50 ± 0.44 | 0.05 ± 0.01 | 30.01±0.74 | 88.74 ± 7.63 | 0.64 ± 0.02 | 15.38 ± 0.42 | $22.36{\pm}7.18$ | 0.02 ± 0.02 |

Rings mixture The ring distribution is constructed as the product of a uniform distribution on $[0,2\pi]$ and a Gaussian distribution on the radius with mean r and variance $\sigma^2=10^{-2}$ (with $r\gg\sigma$). Applying the polar transformation maps this distribution on $[0,2\pi]\times\mathbb{R}^+$ into a ring shape in \mathbb{R}^2 . In the left part of Figure 4 (bottom row), p_A is defined as a mixture of four such rings with radii $r\in\{1,3,5\}$, where each ring is assigned a weight proportional to its radius. This weighting makes the rings appear visually balanced in the mixture.

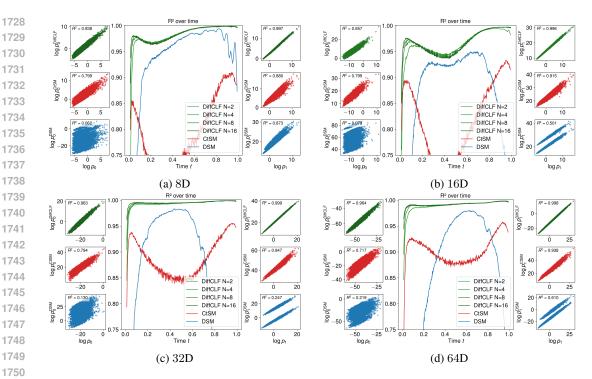


Figure 6: R^2 of learned versus exact log-densities for SIs between MoG-40 and MoG-2 across different dimensions. Complementing Figure 3, which shows detailed 2D scatter plots, this figure demonstrates that DiffCLF maintains consistently higher R^2 as dimensionality increases.

Table 8: Log-density focused metrics for stochastic interpolants. We report classification loss, time-average ESS, and Fisher divergence for a SI model learned between MOG-40 and MOG-2. The results present different values of N but the computational budgets remain equal across methods.

| | | | $\mathcal{L}_{	ext{clf}} + \mathcal{L}_{	ext{DSM}}$ | | , | $\mathcal{L}_{\mathrm{C}t\mathrm{SM}} + \mathcal{L}_{\mathrm{DSM}}$ | | | $\mathcal{L}_{	ext{DSM}}$ | |
|-----|----|---------------------------|---|-----------------------------|---------------------------|---|-----------------------------|---------------------------|---------------------------|-----------------------------|
| Dim | N | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD | $\mathcal{L}_{	ext{clf}}$ | ESS | FD |
| 8 | 2 | 5.26 ± 0.00 | $91.45\% \pm 0.02\%$ | 0.16 ± 0.00 | - | - | - | - | - | - |
| 8 | 4 | 5.24 ± 0.00 | $91.78\% \pm 0.08\%$ | 0.16 ± 0.00 | - | - | - | - | - | - |
| 8 | 8 | 5.23 ± 0.00 | $91.83\% \pm 0.07\%$ | 0.16 ± 0.00 | - | - | - | - | - | - |
| 8 | 16 | 5.23 ± 0.00 | $91.96\% \pm 0.20\%$ | $0.16{\scriptstyle\pm0.00}$ | 6.54 ± 0.01 | $5.10\% \pm 0.11\%$ | 0.96 ± 0.00 | 6.85 ± 0.01 | $76.91\% \pm 0.07\%$ | $0.39{\scriptstyle\pm0.00}$ |
| 16 | 2 | 4.87 ± 0.00 | $68.08\% \pm 0.14\%$ | $0.22{\scriptstyle\pm0.00}$ | - | - | - | - | - | - |
| 16 | 4 | 4.86 ± 0.00 | $70.26\% \pm 0.10\%$ | $0.23{\scriptstyle\pm0.00}$ | - | - | - | - | - | - |
| 16 | 8 | 4.85 ± 0.00 | $69.73\% \pm 0.14\%$ | $0.23{\scriptstyle\pm0.00}$ | - | - | - | - | - | - |
| 16 | 16 | 4.85 ± 0.00 | $69.44\% \pm 0.13\%$ | $0.23{\scriptstyle\pm0.00}$ | 8.97 ± 0.01 | $2.74\% \pm 0.01\%$ | $1.04{\pm}0.00$ | 7.33 ± 0.00 | $46.93\% {\pm} 0.01\%$ | $0.46{\scriptstyle\pm0.00}$ |
| 32 | 2 | 4.47 ± 0.00 | $88.76\% \pm 0.02\%$ | 0.06 ± 0.00 | - | - | - | - | - | - |
| 32 | 4 | 4.46 ± 0.00 | $90.52\% \pm 0.12\%$ | $0.05{\pm}0.00$ | - | - | - | - | - | - |
| 32 | 8 | 4.46 ± 0.00 | $91.36\% \pm 0.08\%$ | $0.05{\pm}0.00$ | - | - | - | - | - | - |
| 32 | 16 | 4.46 ± 0.00 | $91.87\% \pm 0.01\%$ | $0.05{\pm}0.00$ | 11.62 ± 0.02 | $1.35\% \pm 0.16\%$ | 0.61 ± 0.00 | 5.75 ± 0.00 | $48.72\% \pm 0.10\%$ | $0.30{\scriptstyle\pm0.00}$ |
| 64 | 2 | 4.12 ± 0.00 | $71.00\% \pm 0.04\%$ | $0.08{\pm}0.00$ | - | - | - | - | - | - |
| 64 | 4 | 4.12 ± 0.00 | $75.26\% \pm 0.26\%$ | 0.07 ± 0.00 | - | - | - | - | - | - |
| 64 | 8 | 4.12 ± 0.00 | $74.01\% \pm 0.06\%$ | 0.07 ± 0.00 | - | - | - | - | - | - |
| 64 | 16 | 4.12 ± 0.00 | $74.42\% \pm 0.34\%$ | 0.07 ± 0.00 | 16.52 ± 0.05 | $0.76\% \pm 0.03\%$ | $0.43{\scriptstyle\pm0.00}$ | 5.67 ± 0.02 | $28.38\% \pm 0.14\%$ | $0.31{\scriptstyle\pm0.00}$ |
| 128 | 2 | 3.81 ± 0.00 | $54.51\% \pm 0.09\%$ | $0.08{\pm}0.00$ | - | - | - | - | - | - |
| 128 | 4 | 3.79 ± 0.00 | $47.37\% {\pm} 0.02\%$ | $0.07{\pm0.00}$ | - | - | - | - | - | - |
| 128 | 8 | 3.78 ± 0.00 | $50.34\% \pm 0.07\%$ | $0.07{\pm0.00}$ | - | - | - | - | - | - |
| 128 | 16 | 3.78 ± 0.00 | $52.65\% {\pm 0.22\%}$ | 0.06 ± 0.00 | 21.33 ± 0.00 | $0.23\% \pm 0.00\%$ | $0.38{\scriptstyle\pm0.00}$ | 67.03±0.12 | $12.35\% \pm 0.07\%$ | $0.32{\scriptstyle\pm0.00}$ |

Uniforms mixture The distribution used as p_B in the bottom row of Figure 4 is an equilibrated mixture of 4 uniform distributions : $\mathcal{U}([-6.0, -1.6] \times [-1.4, 1.4])$, $\mathcal{U}([-1.4, 1.4] \times [1.6, 6.0])$, $\mathcal{U}([1.6, 6.0] \times [-1.4, 1.4])$ and $\mathcal{U}([-1.4, 1.4] \times [-6.0, -1.6])$.

Table 9: **Averaged log-density metrics for stochastic interpolants.** We report classification loss and Fisher divergence across different dimensions. The different computation budgets of Table 8 are here averaged.

| | $\mathcal{L}_{	ext{clf}}$ $+$ | $\mathcal{L}_{	ext{DSM}}$ | $\mathcal{L}_{	ext{C}t	ext{SM}}$ - | $+ \mathcal{L}_{	ext{DSM}}$ | \mathcal{L}_{DSM} | | |
|-----|-------------------------------|---------------------------|------------------------------------|-----------------------------|---------------------|-------------------|--|
| Dim | Classif | Fisher | Classif | Fisher | Classif | Fisher | |
| 8 | $5.35{\pm}0.07$ | 4.38 ± 0.77 | 8.59 ± 0.16 | 40.69 ± 1.88 | 8.03 ± 0.44 | 0.37 ± 0.06 | |
| 16 | 4.88 ± 0.02 | 5.21 ± 0.93 | 16.10 ± 0.46 | 42.04 ± 2.17 | 10.15 ± 0.82 | 0.52 ± 0.09 | |
| 32 | $4.67{\scriptstyle\pm0.10}$ | 5.63 ± 0.97 | 30.88 ± 2.49 | 40.60 ± 2.58 | 17.69 ± 2.56 | $0.53 {\pm} 0.08$ | |
| 64 | 4.17 ± 0.02 | 2.71 ± 0.51 | 56.54 ± 2.91 | 35.63 ± 2.57 | 9.36 ± 2.82 | 0.23 ± 0.04 | |
| 128 | 3.84 ± 0.03 | 2.66 ± 0.44 | 128.28 ± 8.23 | 279.37 ± 3.91 | 4.54 ± 0.28 | 0.24 ± 0.04 | |

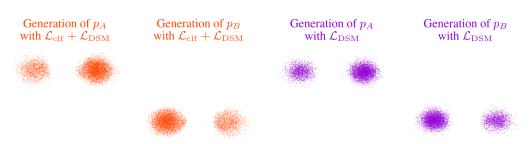


Figure 7: Samples generated by the models trained on the p_A and p_B distribution for the "OR" composition task. 8192 samples are displayed obtained by discretization of the denoising SDE (8) using the exponential integrator for 512 steps.

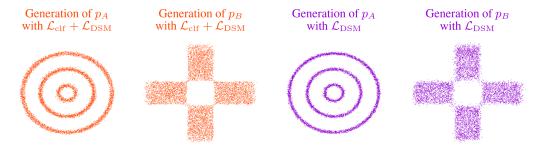


Figure 8: Samples generated by the models trained on the p_A and p_B distribution for the "AND" composition task. 8192 samples are displayed obtained by discretization of the denoising SDE (8) using the exponential integrator for 512 steps.

F.3.2 MODELS TRAINING

The models follow the energy parameterization of Thornton et al. (2025), implemented with a 3-layer MLP of width 128 and trained under the variance-preserving noising scheme. The DSM baseline was trained for 500 epochs with a batch size of 4096, while DiffCLF was trained for the same number of epochs using the N=4 version of the objective (10) with a batch size of 1024. Both models used a learning rate of 10^{-4} and were trained on a dataset of 100k samples. Figures 7 and 8 show samples generated via their respective denoising SDEs, demonstrating that both approaches successfully capture all target distributions.

F.3.3 COMPOSITION ALGORITHM DETAILS

A variety of training-free strategies have been proposed to compose diffusion models. Here, we focus on the "AND" operator, defined as the product distribution $p_{A,B} = p_A \times p_B$. The "OR" operator covered in Section 5 is given by $p_{A,B} = (1/2)p_A + (1/2)p_B$. As emphasized in Du et al. (2023), if $p_A(t,\cdot)$ and $p_B(t,\cdot)$ denote the time-dependent marginals obtained by noising p_A and p_B , then their product $p_A(t,\cdot) \times p_B(t,\cdot)$ is not equal to the marginal of the noised operator $p_{A,B}$.

Thus, we do not obtain the correct sequence of marginals "for free". Nevertheless, this construction defines a valid interpolation: it recovers $p_{A,B}$ at t=0 and approaches a Gaussian at t=T.

Based on this observation, Du et al. (2023) proposed annealed Langevin sampling over this sequence, i.e., running an MCMC chain at each noise level, with improved performance when denoising steps (via the discretized SDE equation 8 using $\nabla \log p_A(t,\cdot) + \nabla \log p_B(t,\cdot)$) are inserted between MCMC transitions. Building on this, Thornton et al. (2025) suggested using the discretized denoising dynamics, (Ithough formally incorrect, as noted above) as a proposal distribution within a Sequential Monte Carlo (SMC) (Doucet et al., 2001; Del Moral et al., 2006) framework.

In this work, we combine the strengths of both approaches: we apply standard SMC to the sequence $p_A(t,\cdot) \times p_B(t,\cdot)$, using the Metropolis-adjusted Langevin algorithm (MALA) (Roberts & Tweedie, 1996) as the transition kernel. This strategy retains the theoretical guarantees of SMC without depending on the incorrect denoising kernel, which we found prone to divergence. Concretely, we run 64 MALA steps at each level, tuning the step size to maintain a 75% acceptance rate, and perform adaptive resampling with a threshold of 30% (Chopin & Papaspiliopoulos, 2020).

F.4 RECALIBRATION

In this section, we describe how diffusion models or stochastic interpolants can be integrated into annealed sampling methods to build unbiased estimators. Let ρ denote a simple base distribution (e.g., a Gaussian), and π the target distribution, known up to a normalizing constant. Our goal is to compute expectations $\mathbb{E}_{\pi}[\phi(X)]$ for a π -measurable test function ϕ .

Importance Sampling (IS). A natural approach is *Importance Sampling (IS)*. Provided $\operatorname{supp}(\rho) \subseteq \operatorname{supp}(\pi)$,

$$\mathbb{E}_{\pi}[\phi(X)] = \int \phi(x)\pi(x)\mathrm{d}x = \mathbb{E}_{\rho}[w(X)\phi(X)] \quad w = \pi/\rho \ . \tag{81}$$

This yields the Monte Carlo estimator

$$\mathbb{E}_{\pi}[\phi(X)] \approx \frac{1}{N} \sum_{i=1}^{N} W_i \phi(X_i), \quad X_i \sim \rho ,$$

where $\{X_i\}_{i=1}^N$ are called particles. When π is unnormalized, we use normalized weights $\tilde{W}_i = W_i / \sum_j W_j$, leading to a biased but consistent estimator. The main drawback of IS is variance explosion when ρ poorly overlaps with π , particularly in high dimensions (Agapiou et al., 2017).

Annealed Importance Sampling (AIS). To alleviate mismatch between ρ and π , Neal (2001) introduced Annealed Importance Sampling (AIS). AIS extends the problem to a sequence of distributions and defines an augmented target–proposal pair

$$\bar{\pi}(x_{0:K}) = \pi(x_0) \prod_{k=0}^{K-1} q_{k+1|k}(x_{k+1}|x_k), \quad \bar{\rho}(x_{0:K}) = \rho(x_K) \prod_{k=0}^{K-1} q_{k|k+1}(x_k|x_{k+1}), \quad (82)$$

where $\{q_{k+1|k}\}_{k=0}^{K-1}$ and $\{q_{k|k+1}\}_{k=0}^{K-1}$ are forward and backward Markov kernels, often chosen as reversible MCMC kernels (see Neal (2001)). Expectations under π can then be expressed as expectations under $\bar{\pi}$ and estimated via IS with proposal $\bar{\rho}$

$$\mathbb{E}_{\pi}[\phi(X)] = \int \phi(x_0)\bar{\pi}(x_{0:K}) dx_{0:K}.$$
 (83)

AIS thus interpolates between ρ and π by gradually refining proposals through intermediate distributions.

Sequential Monte Carlo (SMC). A challenge in AIS is weight degeneracy: as k increases, particles sampled from $\bar{\rho}$ may diverge from the marginals of $\bar{\pi}$, especially in high dimensions. Sequential Monte Carlo (SMC) (Doucet et al., 2001; Del Moral et al., 2006) addresses this by introducing a sequence of intermediate distributions p_k with tractable unnormalized densities which aim to approximate the marginals of $\bar{\pi}$ (i.e., $p_k(x_k) \approx \int \bar{\pi}(x_{0:K}) \mathrm{d}x_{0:k-1} \mathrm{d}x_{k:K}$). SMC proceeds by:

1. running AIS between ρ and p_k ,

- 2. resampling particles to match p_k using the previous AIS approximation, and
- 3. running AIS between p_k and π .

This resampling step prevents degeneracy and improves stability. While early methods performed resampling at every step, modern implementations use adaptive criteria to trigger resampling only when needed (Chopin & Papaspiliopoulos, 2020).

SMC in DMs and SIs. When dealing with a stochastic process such as Equation (1), a natural construction for annealed methods is to take the conditional distributions of $Y_{t_{k+1}}|Y_{t_k}$ as forward kernels, $Y_{t_k}|Y_{t_{k+1}}$ as backward kernels, and the marginals of Y_{t_k} as intermediate distributions p_k , with $Y_{t_0} \sim \pi$ and $Y_{t_K} \sim \rho$. DMs and SIs provide this setup by design, as their dynamics satisfy the endpoint conditions. In the case of DMs, Zhang et al. (2025a) propose using the exact noising kernel as forward kernel and the discretized denoising SDE (8) as the backward kernel in AIS, requiring only the score. Extending this principle to SMC, Phillips et al. (2024) additionally incorporate approximations of the marginals, precisely the focus of this work. In our experiments (Section 5), we apply the same idea to SIs: the forward and backward kernels are discretizations of SDE (9), both depending only on the score, while the marginal approximations required by SMC are learned either via DSM (7) or DiffCLF (10) (with N=2 levels). We run SMC with 8192 particles and adaptive resampling.