D.4 CONVERGENCE OF DISCRIMINATOR-GUIDED LANGEVIN DIFFUSION

We provide a preliminary analysis of the convergnce of the closed-form discriminator guided Langevin diffusion in a fashion similar to (Kim et al., 2023). For consistency with the literature, we fall back to the some of the notation of (Kim et al., 2023). Before we proceed, as a preliminary, we recall the Girsanov Theorem. Consider two diffusion process,

$$\begin{aligned} \mathrm{d}\boldsymbol{X}_t &= \mu_1(\boldsymbol{X}_t)\mathrm{d}t + \sigma(t)\mathrm{d}\boldsymbol{W}_t, \text{ and} \\ \mathrm{d}\boldsymbol{Y}_t &= \mu_2(\boldsymbol{Y}_t)\mathrm{d}t + \sigma(t)\mathrm{d}\boldsymbol{W}_t, \end{aligned}$$

with identical diffusion terms, and associated densities p_1 and p_2. Then, the Girsanov theorem states that the Radon-Nikodym derivative (the ratio of probability densities) between these processes is given by:

$$\frac{\mathrm{d}p_1}{\mathrm{d}p_2} = \exp\left\{\int \left(\frac{\mu_1 - \mu_2}{\sigma(t)}\right)\mathrm{d}\boldsymbol{W}_t + \frac{1}{2}\int \left(\frac{\mu_1 - \mu_2}{\sigma(t)}\right)^2 \mathrm{d}t\right\}. \tag{13}$$

Then, we have:

$$\begin{aligned} \mathcal{D}_{KL}(p_1 \| p_2) &= \mathbb{E}_{p_1}\left[\ln\left(\frac{\mathrm{d}p_1}{\mathrm{d}p_2}\right)\right] \\ &= \mathbb{E}_{p_1}\left[\int \left(\frac{\mu_1 - \mu_2}{\sigma(t)}\right)\mathrm{d}\boldsymbol{W}_t\right] + \frac{1}{2}\mathbb{E}_{p_1}\left[\int \left(\frac{\mu_1 - \mu_2}{\sigma(t)}\right)^2 \mathrm{d}t\right] \\ &= \frac{1}{2}\mathbb{E}_{p_1}\left[\int \left(\frac{\mu_1 - \mu_2}{\sigma(t)}\right)^2 \mathrm{d}t\right], \end{aligned}$$

where the last equality is due to the martingale property of the $\boldsymbol{W}_t$. In the context of the proposed discriminator guidance, we have the following two diffusion processes:

$$\mathrm{d}\boldsymbol{X}_t = \left(f(t) + g^2(t)\nabla_{\boldsymbol{X}} \ln p_t^*(\boldsymbol{X}_t)\right)\mathrm{d}t + g(t)\mathrm{d}\boldsymbol{W}_t, \text{ and} \tag{14}$$

$$\mathrm{d}\boldsymbol{Y}_t = \left(f(t) + g^2(t)\left(\epsilon_\theta(\boldsymbol{Y}_t) + h(t)\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{Y}_t)\right)\right)\mathrm{d}t + g(t)\mathrm{d}\boldsymbol{W}_t, \tag{15}$$

associated with the target reverse process, and the discriminator guided score-based reverse process, respectively, where $h(t)$ models the weight associated with the discriminator guidance term. The following Lemma gives us a convergence result on the discriminator guidance:

Lemma 5. *Consider the reverse diffusion processes associated with the base score-based approach, and the proposed closed-form discriminator guidance model. Let the probability densities associated with these two processes be p_t^* and p_t, with $p_T^* = p_T = \mathcal{N}(\mathbf{0}, \mathbb{I})$, the standard Gaussian distribution and $p_0^* = p_d$ and $p_0 = p_m$, denoting the data distribution and the modeled data distribution, respectively. The, we have:*

$$\mathcal{D}_{KL,\mathrm{DG}^*}(p_d \| p_m) \leq \mathcal{D}_{KL}(p_T^* \| \pi) + \varepsilon_{D^*},$$

where

$$\varepsilon_{D^*} = \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\left\| E_{S^*} - h(t)\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)\right\|^2 \mathrm{d}t\right] \tag{16}$$

$$= \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\left\| \nabla D_{SGAN,t}^*(\boldsymbol{X}_t) - \nabla D_t^*(\boldsymbol{X}_t)\right\|^2 \mathrm{d}t\right], \tag{17}$$

where in turn, $E_{S^*} = \ln p_t^*(\boldsymbol{X}_t) - \epsilon_\theta(\boldsymbol{X}_t)$, which is the error present in the standard score-based Langevin sampler, and $D_{SGAN,t}^*(\boldsymbol{X}_t) = \ln \frac{p_t^*}{p_t}$ is the optimal SGAN discriminator.

Proof. Let the probability densities associated with these two processes be p_t^* and p_t, with $p_T^* = p_T = \mathcal{N}(\mathbf{0}, \mathbb{I})$, the standard Gaussian distribution and $p_0^* = p_d$ and $p_0 = p_m$, denoting the data distribution and the *modeled* data distribution, respectively. Following the procedure presented by Kim et al. (2023), we apply the Girsanov theorem to obtain:

$$\mathcal{D}_{KL}(p_d \| p_m) \leq \mathcal{D}_{KL}(p_T^* \| \pi) + \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\Big\| \underbrace{\nabla \ln p_t^*(\boldsymbol{X}_t) - \left(\epsilon_\theta(\boldsymbol{X}_t) + h(t)\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)\right)}_{E_{D^*}}\Big\|^2 \mathrm{d}t\right].$$

Similarly, for the standard score-based sampler (without DG*), we have:

$$\mathrm{d}\boldsymbol{X}_t = \left(f(t) + g^2(t)\nabla_{\boldsymbol{X}} \ln p_t^*(\boldsymbol{X}_t)\right)\mathrm{d}t + g(t)\mathrm{d}\boldsymbol{W}_t, \text{ and}$$
$$\mathrm{d}\boldsymbol{Y}_t = \left(f(t) + g^2(t)\epsilon_\theta(\boldsymbol{Y}_t)\right)\mathrm{d}t + g(t)\mathrm{d}\boldsymbol{W}_t.$$

Applying the Girsanov theorem to the above setting, we get:

$$\mathcal{D}_{KL}(p_d \| p_m) \le \mathcal{D}_{KL}(p_T^* \| \pi) + \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\Big\| \underbrace{\ln p_t^*(\boldsymbol{X}_t) - \epsilon_\theta(\boldsymbol{X}_t)}_{E_{S^*}} \Big\|^2 \mathrm{d}t\right].$$

In order to analyze the gains obtained by introducing the closed-form discriminator guidance, we analyze the behavior of $E_{D^*} - E_S$, and note that, when $E_{D^*} - E_S$ is positive, the proposed discriminator-guided Langevin diffusion improves convergence, as the associated KL-divergence between p_d and its model p_m, improved (reduced). Consider:

$$\begin{aligned} E_{D^*} &= \ln p_t^*(\boldsymbol{X}_t) - \epsilon_\theta(\boldsymbol{X}_t) - h(t)\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t) \\ \Rightarrow E_{D^*} &= E_{S^*} - h(t)\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t). \end{aligned} \tag{18}$$

As we can see, the gain obtained by the discriminator guidance depends on (a) The sign, and (b) The magnitude of $\nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)$. To quantify this gain, first in the setting considered in Section 4, consider the expression for the discriminator gradient:

$$\begin{aligned} \nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t) &= \mathfrak{C}_\kappa \nabla_{\boldsymbol{X}}((p_{t-1} - p_d) * \kappa)(\boldsymbol{X}_t) \\ &= \mathfrak{C}_\kappa \int_{\boldsymbol{y}} \left(p_{t-1}(\boldsymbol{y}) - p_d(\boldsymbol{y})\right) \nabla_{\boldsymbol{X}} \kappa(\boldsymbol{X} - \boldsymbol{y}) \Big|_{\boldsymbol{X}=\boldsymbol{X}_t} \mathrm{d}\boldsymbol{y} \\ &= \mathfrak{C}_\kappa \int_{\boldsymbol{y}} \nabla_{\boldsymbol{X}} \left(p_{t-1}(\boldsymbol{X} - \boldsymbol{y}) - \nabla_{\boldsymbol{X}} p_d(\boldsymbol{X} - \boldsymbol{y})\right) \Big|_{\boldsymbol{X}=\boldsymbol{X}_t} \kappa(\boldsymbol{y})\mathrm{d}\boldsymbol{y} \end{aligned}$$

where $\mathfrak{C}_\kappa$ is a kernel-dependent positive-valued constant. To analyze the above for $0 \le t \le T$, noting that $p_0 = p_m \approx p_d$ and $p_T = \mathcal{N}(\mathbf{0}, \mathbb{I})$, we make the following observations

- **Gradient of $\boldsymbol{\kappa}$**: The kernel $kappa$ are derived as solutions to Fokker-Plank equations that govern the optimality of GAN discriminator, and as shown in Table 3, are all radially symmetric functions. Consequently the gradients of the kernel are anti-symmetric in nature.
- **Magnitude of $\boldsymbol{\kappa}$**: Considering either the popular n-dimensional Gaussian kernel, or the polyharmonic family of kernels for order $m \le \frac{n}{2}$, we observe that the kernels peak at the origin (or alternatively, $\kappa(\cdot - \boldsymbol{X}_t$ peaks at $\boldsymbol{X}_t$), and decay rapidly.
- **Sign and Magnitude of** $(p_{t-1}(\boldsymbol{y}) - p_d(\boldsymbol{y}) * \kappa))$. Given that p_d is the data distribution, which is known to be drawn from a low-dimensional manifold in a high-dimensional space, and that p_{t-1} is *closer* to Gaussian noise (or noise-convolved version of p_d in early iterations, the density difference ($p_{t-1} - p_d$ These results are also in alignment with the observations made by (Asokan & Seelamantula, 2023b; de Deijn et al., 2024), in the context of the signed Inception distance, which leveraged the kernel-based discriminator to evaluate GANs.

From the above argument, we see that the gain in KL-divergence, when $\boldsymbol{X}_t simp_t$ far from p_d, the discriminator improves the performance of the standard score-based sampler.

For the special case where $h(t) = 1$, and adding and subtracting $\nabla D_{SGAN,t}^*$ to Equation 16, ε_{D^*} can be simplified as:

$$\frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\Big\|\nabla \ln p_t^*(\boldsymbol{X}_t) - \epsilon_\theta(\boldsymbol{X}_t) - \nabla D_{SGAN,t}^*(\boldsymbol{X}_t) + \nabla D_{SGAN,t}^*(\boldsymbol{X}_t) - \nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)\Big\|^2 \mathrm{d}t\right]$$
$$= \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\Big\|\nabla \ln p_t^*(\boldsymbol{X}_t) - \nabla \ln p_t(\boldsymbol{X}_t) - \nabla \ln \frac{p_t^*(\boldsymbol{X}_t)}{p_t(\boldsymbol{X}_t)} + \nabla D_{SGAN,t}^*(\boldsymbol{X}_t) - \nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)\Big\|^2 \mathrm{d}t\right]$$
$$= \frac{1}{2}\mathbb{E}_{p_t^*}\left[\int g^2(t)\Big\|\nabla D_{SGAN,t}^*(\boldsymbol{X}_t) - \nabla_{\boldsymbol{X}} D_t^*(\boldsymbol{X}_t)\Big\|^2 \mathrm{d}t\right]$$

□

The above result suggests that, in moving from the standard score-based sampler to the closed-form discriminator-guided sampler, the bound on the KL divergence between the true and learnt distributions is transformed from the error in estimating the score, to the error between the optimal SGAN and IPM-GAN discriminators.

However, we remark that this analysis in not entirely aligned with the derived optimal discriminator, as DG* is optimal in the sense of the Wasserstein-2 metric, and the convergence of score-based diffusion is in the f-divergence sense, and in particular, the KL divergence. A more in-depth analysis of the proposed SDE, in terms of the Wasserstein metric, is a promising direction for future research.

E ADDITIONAL EXPERIMENTAL RESULTS ON DISCRIMINATOR-GUIDED LANGEVIN SAMPLING

We present additional experimental results on generating 2-D shapes, and images using the discriminator-guided Langevin sampler.

E.1 ADDITIONAL RESULTS ON SYNTHETIC DATA LEARNING

On the 2-D learning task, we present additional combinations on the *shape morphing experiment*.

Training Parameters: All samplers are implemented using TensorFlow (Abadi et al., 2016) library. The discriminator gradient is built as a custom radial basis function network, whose weights and centers are assigned at each iteration. At $t = 0$, the centers $\boldsymbol{g}^j \sim p_{t-1}$ are sampled from the unit Gaussian, *i.e.,* $p_{-1} = \mathcal{N}(\mathbf{0}, \mathbb{I})$. In subsequent iterations, the batch of samples from time instant $t-1$ serve as the centers for D_t^*. Based on experiments presented in Appendix E.2, we set $\gamma_t = 0$ and $\alpha_t = 1 \ \forall\, t$. The input and target distributions are created following the approach presented by (Mroueh & Rigotti, 2020). Figure 5 shows the supports of the input/output distributions (black denotes the support). For grayscale images, the support corresponds to regions with pixel intensities below the threshold of 128.

Experimental Results: We consider the *Heart* and *Cat* shapes as the target, while considering various input shapes, corresponding to varying levels of difficulty in matching the target distribution. In the case of learning the *Heart* shape, for input shapes that do not contain *gaps/holes*, the convergence is relatively fast, and shape matching occurs in about 100 to 250 iterations. For more challenging input shapes, such as the *Cat* logo, the discriminator-guided Langevin sampler converges in about 500 iterations. This is superior to the reported 800 iterations in the Unbalanced Sobolev descent formulation. The results are similar in the case where the *Cat* image is the target (cf. Figure 7).

E.2 ADDITIONAL RESULTS ON IMAGE LEARNING

We present ablation experiments on generating images with the discriminator-guided Langevin sampler to determine the choice of α_t and γ_t in the update regime. We also provide additional images pertaining to the experiments presented in the *Main Manuscript*.

Choice of coefficients α_t and γ_t: For the ablation experiments, we consider MNIST, SVHN, and 64-dimensional CelebA images. Based on the analysis presented in Asokan & Seelamantula (2023a), we consider the kernel-based discriminator with the polyharmonic spline kernel in all subsequent experiments. Recall the update scheme:

$$\boldsymbol{x}_t = \boldsymbol{x}_{t-1} - \alpha_t \nabla_{\boldsymbol{x}} D_t^*(\boldsymbol{x}_t; p_{t-1}, p_d) + \gamma_t \boldsymbol{z}_t, \quad \text{where} \quad \boldsymbol{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbb{I}).$$

Based on the observations made by Karras et al. (2022), to ascertain the optimal choice of the coefficients, we consider the following scenarios:

- **The ordinary differential equation (ODE) formulation**, wherein the noise perturbations are ignored, giving rise to an ODE that the samples are evolved through. Here $\gamma_t = 0, \ \forall\, t$.
- **The stochastic differential equation (SDE) formulation**, wherein we retain the noise perturbations. Based on the links between score-based approaches and the GANs, we consider the approach presented in noise-conditioned score networks (NCSNv1) (Song & Ermon, 2019), with $\gamma_t = \sqrt{2\alpha_t}$.