MONOFLOW: A UNIFIED GENERATIVE MODELING FRAMEWORK FOR GAN VARIANTS

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ABSTRACT

Generative adversarial networks (GANs) play a minmax two-player game via adversarial training. The conventional understanding of adversarial training is that the discriminator is trained to estimate a divergence and the generator learns to minimize this divergence. We argue that despite the fact that many variants of GANs are developed following this paradigm, the existing theoretical understanding of GANs and the practical algorithms are inconsistent. In order to gain deeper theoretical insights and algorithmic inspiration for these GAN variants, we leverage Wasserstein gradient flows which characterize the evolution of particles in the sample space. Based on this, we introduce a unified generative modeling framework – MonoFlow: the particle evolution is rescaled via an arbitrary monotonically increasing mapping. Under our framework, adversarial training can be viewed as a procedure first obtaining MonoFlow's vector field via the discriminator and then the generator learns to parameterize the flow defined by the corresponding vector field. We also reveal the fundamental difference between variational divergence minimization and adversarial training. These analysis help us to identify what types of generator loss functions can lead to the successful training of GANs and suggest that GANs may have more loss designs beyond those developed in the literature, e.g., non-saturated loss, as long as they realize MonoFlow. Consistent empirical studies are also included to validate the effectiveness of our framework.

1 INTRODUCTION

Generative adversarial nets (GANs) (Goodfellow et al., 2014; Jabbar et al., 2021) are a powerful generative modeling framework that has gained tremendous attention in recent years. GANs have achieved significant successes in applications, especially in high-dimensional image processing such as high-fidelity image generation (Brock et al., 201; Karras et al., 2019), super-resolution (Ledig et al., 2017) and domain adaption (Zhang et al., 2017).

In the GAN framework, a discriminator d and a generator g play a minmax game. The discriminator is trained to distinguish real and fake samples and the generator is trained to generate fake samples to fool the discriminator. The equilibrium of the vanilla GAN is defined by[1]

$$\min_{g} \max_{d} V(g,d) = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\big\{\log \sigma[d(\mathbf{x})]\big\} + \mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\big\{\log\big(1-\sigma[d(g(\mathbf{z}))]\big)\big\} \tag{1}$$

The elementary optimization approach to solve the minmax game is adversarial training. Previous perspectives explained it as first estimating Jensen-Shannon divergence then the generator learns to minimize this divergence. Several variants of GANs have been developed based on this point of view for other probability divergences, e.g., χ^2 divergence (Mao et al., 2017), Kullback-Leibler (KL) divergence (Arbel et al., 2021) and general f-divergences (Nowozin et al., 2016; Uehara et al., 2016), while others are developed with Integral Probability Metrics (Arjovsky et al., 2017; Dziugaite et al., 2015; Mroueh et al., 2018b). However, we emphasize that the traditional understanding over GANs is incomplete and here we present three non-negligible facts which are commonly associated with adversarial training, making it different from the standard variational divergence minimization (VDM) problem (Blei et al., 2017):

[1]We use a slightly different notation: $d(\mathbf{x})$ is the logit output of the classifier and $\sigma(\cdot)$ is the Sigmoid activation.

1. The generator typically minimizes a divergence with a missing term, e.g., the vanilla GAN only minimizes the second term of Jensen-Shannon divergence $\mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left\{\log\left(1-\sigma[d(g(\mathbf{z}))]\right)\right\}$ where $\log\left(1-\sigma[d(g(\mathbf{z}))]\right)$ is a monotonically increasing function of $d(g(\mathbf{z}))$.
2. The estimated divergence is computed from the discriminator $d(\mathbf{x})$. It is a function only depending on samples $\mathbf{x}$ and does not include any density information from the generator's distribution p_g. However, the original proof of GAN (Proposition 1 by Goodfellow et al. (2014)) requires knowing the density of p_g, i.e., p_g as a functional variable.
3. Practical algorithms are inconsistent with theory, a heuristic trick "non-saturated loss" is commonly adopted to mitigate the gradient vanishing problem, but it still lacks a rigorous mathematical understanding.

To gain a deeper understanding of adversarial training of GANs, we study the Wasserstein gradient flow of the KL divergence which characterizes a deterministic evolution of particles described by an ordinary differential equation (ODE). This ODE is a Euclidean gradient flow of a time-dependent logarithm density ratio. Based on this ODE, we propose the **MonoFlow** framework – transforming the log density ratio by a monotonically increasing mapping such that the vector field of the gradient flow is rescaled along the same direction. Consequently, approximating and learning to parameterize MonoFlow is synonymous to adversarial training. Under our framework, we gain a comprehensive understanding of adversarial training over GANs: the discriminator obtains a bijection of the log density ratio that suggests the vector field and the generator learns to parameterize the particles of MonoFlow. All variants of divergence GANs are a subclass of our framework. Finally, we reveal that the discriminator and generator loss do not need to follow the same objective. The discriminator maximizes the lower bound of a probability divergence to obtain a bijection of the log density ratio. The generator loss can be any monotonically increasing mapping of this log density ratio. Our contributions are summarized as follows:

- A novel generative modeling framework unifies divergence GANs, providing a new theoretically and practically consistent understanding of the underlying mechanism of adversarial training over GANs.
- We reveal the fundamental difference between VDM and adversarial training, which indicates that the previous analysis of GANs based on the perspective of VDM might not provide benefits and insteand we should treat GANs as a gradient flow method.
- An analysis of what types of generator loss functions can lead to the success of training GAN. Our framework explains why and how non-saturated loss works.
- An algorithmic inspiration where GANs may have more variants of loss designs than we have already known.

2 Wasserstein Gradient Flows

In this section, we review the definition of gradient flows in Wasserstein space $(\mathcal{P}(\mathbb{R}^n), W_2)$, the space of Borel probability measures $\mathcal{P}(\mathbb{R}^n)$ defined on $\mathbb{R}^n$ with finite second moments and equipped with the Wasserstein-2 metric. An absolutely continuous curve of probability measures $\{q_t\}_{t\geq 0} \in \mathcal{P}(\mathbb{R}^n)$ is a Wasserstein gradient flow if it satisfies the following continuity equation (Ambrosio et al., 2008),

$$\frac{\partial q_t}{\partial t} = \operatorname{div}\big(q_t \nabla_{W_2}\mathcal{F}(q_t)\big), \tag{2}$$

where $\nabla_{W_2}\mathcal{F}(q_t)$ is called the Wasserstein gradient of the functional $\mathcal{F}:\mathcal{P}(\mathbb{R}^n)\to\mathbb{R}$. The Wasserstein gradient is defined as $\nabla_{\mathbf{x}}\frac{\delta\mathcal{F}}{\delta q_t}$, i.e. the Euclidean gradient of the functional's first variation $\frac{\delta\mathcal{F}(q_t)}{\delta q_t}$. Specifically, for the functional $\mathcal{F}(q_t) = \int \log\frac{q_t}{p}dq_t$ as the KL divergence [2] where p is a fixed target probability measure, we have $\frac{\delta\mathcal{F}(q_t)}{\delta q_t} = \log\frac{q_t}{p}+1$. Hence, the Wasserstein gradient flow of the KL divergence reads the Fokker-Planck equation,

$$\frac{\partial q_t}{\partial t} = \operatorname{div}\big(q_t(\nabla_{\mathbf{x}}\log q_t - \nabla_{\mathbf{x}}\log p)\big). \tag{3}$$

[2] We abuse 'KL divergence' here. It refers to 'reverse KL divergence' or 'exclusive KL divergence' in some literature.

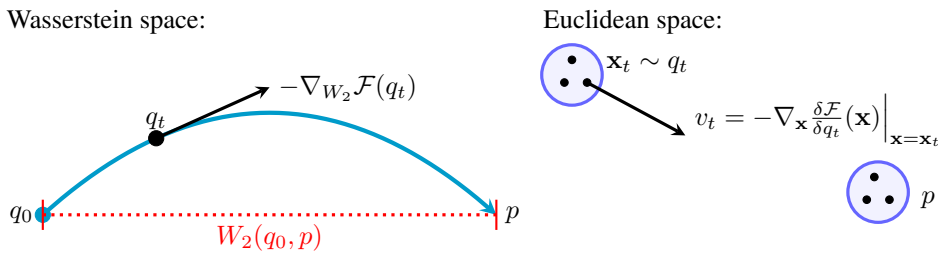


Figure 1: The illustration of a Wasserstein gradient flow and its particle evolution. In Wasserstein space, the blue curve is a gradient flow and the red dotted line is a geodesic. q_t evolves along a curve whose tangent vector is given by $-\nabla_{W_2}\mathcal{F}(q_t)$ such that the functional is always decreasing with time. Correspondingly, particles evolve in Euclidean space towards the target measure p with the vector field $-\nabla_{\mathbf{x}} \frac{\delta \mathcal{F}}{\delta q_t}(\mathbf{x})$. Note that directly minimizing the Wasserstein-2 metric $W_2(q_t, p)$ instead yields a path $\{q_t\}_{t\geq 0}$ along the geodesic connecting q_0 and p over Wasserstein space.

As $t \to \infty$, the stationary probability measure of q_t is the target p. Denote the Euclidean path of random variables as $\{\mathbf{x}_t\}_{t\geq 0} \in \mathbb{R}^n$ with the initial condition $\mathbf{x}_0 \sim q_0$, we can define an ordinary differential equation (ODE) which describes the evolution of particles in $\mathbb{R}^n$,

$$d\mathbf{x}_t = \big(\nabla_{\mathbf{x}} \log p(\mathbf{x}_t) - \nabla_{\mathbf{x}} \log q_t(\mathbf{x}_t)\big)dt := v_t(\mathbf{x}_t)dt, \quad \mathbf{x}_0 \sim q_0, \tag{4}$$

where the vector field v_t of these particles is the negative Euclidean gradient of the functional's first variation. As shown in Figure 1, Wasserstein gradient flows establish a connection between the probability evolution in Wasserstein space and its associated particle evolution in Euclidean space.

Applying Itô integral to Langevin dynamics $d\mathbf{x}_t = \nabla_{\mathbf{x}} \log p(\mathbf{x}_t)dt + \sqrt{2}d\mathbf{w}$ where $d\mathbf{w}$ is a Wiener process, we get the same Fokker-Planck equation in Eq (3). This indicates the deterministic particle evolution by the ODE can be approximated via a stochastic differential equation (SDE). Langevin dynamics admits the same marginal probability measure q_t as Eq (4), this relation of SDE and its corresponding ODE were also studied in score-based diffusion models (Song et al., 2021). Langevin dynamics was first interpreted as the Wasserstein gradient flow of the KL divergence by Jordan et al. (1998); Otto (2001). It plays an important role in generative modeling as a sampling scheme. In order to transform noises into the target data distribution by Langevin dynamics, an essential step is to fit the data distribution using energy-based models (Song & Kingma, 2021) or to directly estimate its scores with score-matching techniques (Hyvärinen & Dayan, 2005; Vincent, 2011; Song & Ermon, 2019).

3 MonoFlow: A Unified Generative Modeling Framework

This section presents our main contribution that connects gradient flows and divergence GANs into a unified framework. We first introduce MonoFlow where the ODE evolution is rescaled via a monotonically increasing function. Consequentially, learning to parameterize the rescaled flow by a neural network recovers the bi-level optimization dynamics of training GANs. This gives us a novel understanding of the hidden mechanism of adversarial training.

3.1 MonoFlow

We consider the ODE in Eq (4) with a fixed target measure p, e.g., a data distribution in a generative modeling scenario. Assume that we have a time-dependent log density ratio function as $\log r_t(\mathbf{x}) = \log \frac{p(\mathbf{x})}{q_t(\mathbf{x})}$, the ODE can be rewritten as

$$d\mathbf{x}_t = \nabla_{\mathbf{x}} \log r_t(\mathbf{x}_t)dt, \quad \mathbf{x}_0 \sim q_0. \tag{5}$$

This is a gradient flow in Euclidean space where its vector field is the gradient of the log density ratio. With a monotonically increasing mapping $h : \mathbb{R} \to \mathbb{R}$ where h is first-order differentiable, we can define another ODE:

$$d\mathbf{x}_t = \nabla_{\mathbf{x}} h\big(\log r_t(\mathbf{x}_t)\big)dt = h'\big(\log r_t(\mathbf{x}_t)\big)\nabla_{\mathbf{x}} \log r_t(\mathbf{x}_t)dt, \quad \mathbf{x}_0 \sim q_0 \tag{6}$$

By transforming the time-dependent log density ratio under the mapping h, its first-order derivative rescales the vector field of the original gradient flows defined in Eq (5). We call Eq (6) as **MonoFlow**.

MonoFlow defines a different family of vector fields $\{v_t\}_{t\geq 0}$ for the particle evolution where $v_t(\mathbf{x}_t) = h'\big(\log r_t(\mathbf{x}_t)\big)\nabla_{\mathbf{x}} \log r_t(\mathbf{x}_t)$. Conversely, the vector fields $\{v_t\}_{t\geq 0}$ also determine an absolutely continuous curve $\{q_t\}_{t\geq 0}$ in Wasserstein space by the continuity equation (see Theorem 4.6 in (Ambrosio et al., 2008))

$$\frac{\partial q_t}{\partial t} = -\text{div}(q_t v_t), \tag{7}$$

under mild regularity conditions. Hence the probability evolution of MonoFlow is described by

$$\frac{\partial q_t}{\partial t} = \text{div}\big(D_t \nabla_{\mathbf{x}} q_t\big) - \text{div}\big(\zeta_t^{-1} q_t \nabla_{\mathbf{x}} \log p\big), \tag{8}$$

where $D_t = \zeta_t^{-1} = h'(\log r_t)$. Eq (8) is a special case of convection–diffusion equations where D_t is called the diffusion coefficient and ζ_t^{-1} is called mobility. MonoFlow defines a positive diffusion coefficient. This has a physical interpretation that particles diffuse to spread probability mass over the target measure other than concentrate. Next, we study the properties of MonoFlow.

Theorem 3.1. *If h is monotonically increasing, i.e., $h'(\cdot) > 0$, the dissipation rate $\frac{\partial \mathcal{F}(q_t)}{\partial t}$ for the KL divergence $\mathcal{F}(q_t) = \int \log \frac{q_t}{p} dq_t$ satisfies*

$$\frac{\partial \mathcal{F}(q_t)}{\partial t} \leq 0, \tag{9}$$

the equality is achieved if and only if $q_t = p$ and the marginal probability q_t of MonoFlow evolves to p as $t \to \infty$.

Theorem 3.1 shows that MonoFlow does not disturb the equilibrium of Eq (3), and the convergence to the target probability measure p is guaranteed. The negative dissipation rate ensures that the gradient flow curve $\{q_t\}_{t\geq}$ of MonoFlow always decreases the KL divergence with time.

MonoFlow is obtained by transforming the log density ratio which arises from the Wasserstein gradient flow of KL divergence. We can also obtain other forms of deterministic particle evolution by considering Wasserstein gradient flows of the general f-divergences,

$$\mathcal{D}_f(p||q) = \int f\left(\frac{p}{q}\right) dq, \tag{10}$$

where $f : \mathbb{R}^+ \to \mathbb{R}$ is a convex function and $f(1) = 0$.

Theorem 3.2. *The Wasserstein gradient flow of a f-divergence characterizes the evolution of particles in $\mathbb{R}^n$ by*

$$d\mathbf{x}_t = r(\mathbf{x}_t)^2 f''\big(r(\mathbf{x}_t)\big)\nabla_{\mathbf{x}} \log r_t(\mathbf{x}_t)dt, \quad \mathbf{x}_0 \sim q_0 \tag{11}$$

A similar result can also be derived with the reversed f-divergence $\mathcal{D}_f(q||p)$ used by (Gao et al., 2019; Ansari et al., 2021). Theorem 3.2 shows that the particle evolution of the Wasserstein gradient flow of f-divergences is a special instance of MonoFlow where $h'(\log r) = r^2 f''(r) > 0$ because f is a convex function. It indicates once a curve $\{q_t\}_{t\geq 0}$ evolves with the time t in Wasserstein space to decrease a f-divergence, it simultaneously decreases the KL divergence as well since the dissipation rate of MonoFlow is negative.

3.2 Practical Approximations of Density Ratios

We first discretize the ODE in eq (6) by the forward Euler method such that we obtain standard gradient ascent iterations with step size β and the index of the discretized time step k [3]:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \beta \nabla_{\mathbf{x}} h\big(\log r_k(\mathbf{x}_k)\big), \quad t_{k+1} = t_k + \alpha. \tag{12}$$

Therefore, we can sample initial particles $\mathbf{x}_0 \sim q_0$ and perform gradient ascend iterations by estimating the density ratio $r_k(\mathbf{x}) = \frac{p(\mathbf{x})}{q_k(\mathbf{x})}$ using samples from q_k and p. In order to enable a practical algorithm to obtain the time-dependent density ratio, we introduce a general framework that solves the following optimization problem, similar to Moustakides & Basioti (2019),

$$\max_d \big\{\mathbb{E}_{\mathbf{x}\sim p}\left[\phi\big(d(\mathbf{x})\big)\right] + \mathbb{E}_{\mathbf{x}\sim q_k}\left[\psi\big(d(\mathbf{x})\big)\right]\big\}, \tag{13}$$

where $d : \mathbb{R}^n \to \mathbb{R}$ is a decision function (also called discriminator in adversarial training), e.g., it can be a neural network, ϕ and ψ are scalar functions upon design later.

[3] For the sake of simplicity, we briefly replace t_k by its index k, though it is not rigorous.

Lemma 3.3. *Solving Eq (13), the optimal decision d^* satisfies*

$$d^*(\mathbf{x}) = \mathcal{T}^{-1}(r(\mathbf{x})), \quad r(\mathbf{x}) = \frac{p(\mathbf{x})}{q_k(\mathbf{x})}, \tag{14}$$

with $r(\mathbf{x}) = -\frac{\psi'(d^*(\mathbf{x}))}{\phi'(d^*(\mathbf{x}))} := \mathcal{T}(d^*(\mathbf{x}))$. Note that the resulting $\mathcal{T}$ must be a bijection such that the inverse exists.

Remark. Note that two-sample density ratio estimation will lost density information from q_k. The functions $d(\mathbf{x})$ and $r(\mathbf{x})$ only depend on $\mathbf{x}$.

To this end, we can train d to solve the optimization problem in Eq (13) and the density ratio is approximated by $\mathcal{T}(d(\mathbf{x}))$. For example, in the standard binary classification problem where we can design $\phi(d) = \log \sigma(d)$ and $\psi(d) = \log(1 - \sigma(d))$, we have $d^*(\mathbf{x}) = \log r(\mathbf{x})$. The log density ratio estimator is approximately the logit output of a well-trained classifier (Sugiyama et al., 2012). Other types of density ratio estimation can be found in Table 1 as they have been already used in GAN variants where q_k refers to the generator's distribution p_g. In practice, since the change of $\mathbf{x}_k$ is sufficiently small at every step k, we can use a single decision function $d(\mathbf{x})$ and perform a one-step gradient update to solve Eq (13) per iteration k to approximate the time-dependent density ratio $r_k(\mathbf{x})$, which is identical to adversarial training.

Table 1: Different types of divergence GANs. f is a convex function and $\tilde{f}$ is the convex conjugate by $\tilde{f}(d) = \sup_{r \in \mathrm{dom} f}\{rd - f(r)\}$.

	$\phi(d)$	$\psi(d)$	$d^*(\mathbf{x})$	$h_{\mathcal{T}}(d)$
Vanilla GAN	$\log \sigma(d)$	$\log(1 - \sigma(d))$	$\log r(\mathbf{x})$	$-\log(1 - \sigma(d))$
Non-saturated GAN	$\log \sigma(d)$	$\log(1 - \sigma(d))$	$\log r(\mathbf{x})$	$\log \sigma(d)$
f-GAN	d	$-\tilde{f}(d)$	$f'(r(\mathbf{x}))$	d
b-GAN	$f'(d)$	$f(d) - df'(d)$	$r(\mathbf{x})$	$df'(d) - f(d)$
Least-square GAN	$(d-1)^2$	d^2	$\frac{r(\mathbf{x})}{1+r(\mathbf{x})}$	$-(d-1)^2$
Generalized EBM	$-(d+\lambda)$	$-\exp(-d-\lambda)$	$-\log r(\mathbf{x}) - \lambda$	$\exp(-d-\lambda)$

3.3 Parameterization of the Discretized MonoFlow

The previous method directly pushes particles in the Euclidean space towards the target distribution. We can use a neural network generator to mimic the distribution of these particles, i.e., the generator learns to draw samples. If we parameterize particles with a neural network generator g_θ that takes as input random noises $\mathbf{z} \sim p_{\mathbf{z}}$ and output particles $\mathbf{x}_{(\theta,\mathbf{z})} = g_\theta(\mathbf{z})$, the infinitesimal change of parameters of the generator is

$$\frac{d\theta_t}{dt} = \int \frac{\partial g_{\theta_t}(\mathbf{z})}{\partial \theta_t} \nabla_{\mathbf{x}} h\big(\log r_t(\mathbf{x}_t)\big) p_{\mathbf{z}}(\mathbf{z}) d\mathbf{z}, \quad \text{where } \mathbf{x}_t = g_{\theta_t}(\mathbf{z}), \tag{15}$$

where $\frac{\partial g_{\theta_t}(\mathbf{z})}{\partial \theta_t}$ is the Jacobian of the neural network generator. Apply the forward Euler method with the step size β, we have

$$\theta_{k+1} = \theta_k + \beta \nabla_\theta \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}} \big[h\big(\log r_k(g_{\theta_k}(\mathbf{z}))\big) \big]. \tag{16}$$

Eq (15) can be regarded as amortizing particles of the gradient flow into a neural network generator by approximately solving $\theta_{k+1} = \arg\min_\theta \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}} ||g_\theta(\mathbf{z}) - \mathbf{x}_{k+1}||^2$ where $\mathbf{x}_{k+1} = g_{\theta_k}(\mathbf{z}) + \nabla_{\mathbf{x}} h\big(\log r_k(g_{\theta_k}(\mathbf{z}))\big)$ with a one-step gradient descent (Wang & Liu, 2017).

Consequently, by the chain rule we have $d\mathbf{x}_t = \frac{\partial g_{\theta_t}(\mathbf{z})}{\partial \theta_t} d\theta_t$, replace $d\theta_t$ with Eq(15),

$$d\mathbf{x}_t = \mathbb{E}_{\mathbf{z}' \sim p_{\mathbf{z}}} \left[K_g^t(\mathbf{z}, \mathbf{z}') \nabla_{\mathbf{x}} h\big(\log r_t(\mathbf{x}_t)\big) \right] dt \tag{17}$$

where $K_g^t(\mathbf{z}, \mathbf{z}') = \langle \frac{\partial g_{\theta_t}(\mathbf{z})}{\partial \theta_t}, \frac{\partial g_{\theta_t}(\mathbf{z}')}{\partial \theta_t} \rangle$ is the neural tangent kernel (NTK) (Jacot et al., 2018) defined by the generator. Note that Eq(17) realizes Stein Variational Gradient Descent (Liu & Wang, 2016; Franceschi et al., 2022) if h is an identity mapping.

3.4 A Unified Formulation of Generative Adversarial Nets

Based on the above derivation, we propose a general formulation for GAN variants. We clarify that GANs can be treated with different objective functions for training discriminator and generator. All of these variants are algorithmic instantiations of the parameterized MonoFlow. The unified framework is summarized as: given a discriminator d and a generator g, the discriminator d learns to maximize

$$\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\phi\big(d(\mathbf{x})\big)\right] + \mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[\psi\big(d(g(\mathbf{z}))\big)\right], \tag{18}$$

where p_{data} refers to the data distribution. Next, we train the generator g to minimize

$$\mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[-h_{\mathcal{T}}\big(d(g(\mathbf{z}))\big)\right]. \tag{19}$$

where $h_{\mathcal{T}}(d) = h(\log \mathcal{T}(d))$ and h can be any monotonically increasing function. We summarize some typical GAN variants in Table 1. We view adversarial training as maximizing Eq (18) to obtain the density ratio which suggests the vector field for MonoFlow and minimizing Eq (19) as learning to parameterize MonoFlow corresponding to Eq (16). Especially, we find that Bregman-divergence GAN (b-GAN) realizes parameterized Wasserstein gradient flows of f-divergences since its generator loss is aligned with Theorem 3.2 for the design of h. .

4 Understanding Adversarial Training via MonoFlow

The dominating understanding of adversarial training over GANs is that the generator learns to minimize the divergence estimated by the discriminator. However, as pointed out in Section 1, the theoretical explanation over GAN and its practical algorithm is inconsistent since the generator only minimizes the second term of JS-divergence or alternative non-saturated loss. In this section, through the lens of MonoFlow, we will explain why this inconsistency of adversarial training still can lead to convergence to the target distribution and how it differs from variational divergence minimization (VDM) (Blei et al., 2017) for generative modeling.

4.1 Why Adversarial Training Works?

In adversarial training, the discriminator is trained to maximize the lower bound of f-divergences. This lower bound can be derived via the dual representation of the f-divergence (Nguyen et al., 2010) between p_{data} and p_g,

$$\mathcal{D}_f(p_{\text{data}}||p_g) = \max_{d\in\mathcal{H}} \{ \underbrace{\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\big[d(\mathbf{x})\big] - \mathbb{E}_{\mathbf{x}\sim p_g}\big[\tilde{f}\big(d(\mathbf{x})\big)\big]}_{\text{lower bound}} \}, \quad r(\mathbf{x}) = \frac{p_{\text{data}}(\mathbf{x})}{p_g(\mathbf{x})}, \tag{20}$$

where $\tilde{f}(d) = \sup_{r\in \text{dom}_f}\{rd - f(r)\}$ is the convex conjugate of $f(r)$ and $\mathcal{H}$ is a function class of d. Since the first term of the lower bound in Eq (20) is irrelevant to p_g, thus in adversarial training, the generator actually only learns to minimize the second term,

$$\min_g -\mathbb{E}_{\mathbf{x}\sim p_g}\left[\tilde{f}\big(d(\mathbf{x})\big)\right] \tag{21}$$

This is known as the vanilla generator loss in GAN. Meanwhile, the generator can also alternatively minimizes the heuristic non-saturated loss $-\mathbb{E}_{\mathbf{x}\sim p_g}\big[d(\mathbf{x})\big]$, which has been proven to work well in practice (Goodfellow et al., 2014). By the Fenchel duality, the optimal d is given by $d^* = f'(r)$ with the equality $\tilde{f}(d^*) = rf'(r) - f(r)$. Fortunately, $f'(r)$ and $rf'(r) - f(r)$ are both monotonically increasing functions of the density ratio (as well as log density ratio). Hence, adversarial training falls into the framework of MonoFlow which has convergence guarantees. We should notice that the first variation of f-divergence is given by $f(r) - rf'(r) = \tilde{f}(d^*)$, see Eq (30). The negative Euclidean gradient of the first variation is the vector field of a Wasserstein gradient flow of f-divergence. This suggests that adversarial training is naturally aligned with gradient flows.

4.2 Difference between Adversarial Training and Variational Divergence Minimization

VDM differs from adversarial training because it requires density information from the generator, as elaborated in the following. In variational divergence minimization, the generator g_θ usually defines

Table 2: Comparisons the convergence when using different f and h on three density ratio models: "✓" means the generator converges to the data distribution and "✗" means not converges. For $r(\mathbf{x}, \theta)$ and $r(\mathbf{x}, \theta_{\text{de}})$, the convergences means the generator parameter (μ, σ) can converge to the true value. For $r_{\text{GAN}}(\mathbf{x})$, convergence means the parameter can closely approximate the true value. Visualization results are included in Appendix B.1.

	if f convex	if h mono increase	$r(\mathbf{x}, \theta)$	$r(\mathbf{x}, \theta_{\text{de}})$	$r_{\text{GAN}}(\mathbf{x})$
KL	Yes	Yes	✓	✓	✓
Forward KL	Yes	No	✓	✗	✗
Chi-Square	Yes	No	✓	✗	✗
Hellinger	Yes	No	✓	✗	✗
Jensen-Shannon	Yes	No	✓	✗	✗
Exp	No	Yes	✗	✓	✓

a distribution via an explicit density function $p_g(\mathbf{x}; \theta)$. For example, $\mathbf{x}$ can be reparameterized as a Gaussian random variable where θ is its mean and variance. We are interested in minimizing an f-divergence $\mathcal{D}_f(p_{\text{data}}||p_g) = \mathbb{E}_{\mathbf{x}\sim p_g}\left[f\big(r(\mathbf{x}, \theta)\big)\right]$ where the density ratio $r(\mathbf{x}, \theta) = \frac{p_{\text{data}}(\mathbf{x})}{p_g(\mathbf{x};\theta)}$ is a function of $\mathbf{x}$ as well as θ to include the density information of p_g. Under reparameterization tricks (Kingma & Welling, 2014; Rezende et al., 2014), the gradient of the f-divergence with respect to the generator's parameter θ is

$$\nabla_\theta \mathcal{D}_f(p_{\text{data}}||p_g) = \mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[\nabla_\theta f\left(r(\mathbf{x}_{(\theta,\mathbf{z})}, \theta)\right)\right] \tag{22}$$

By Fenchel-duality, we can rewrite f-divergences as $\mathcal{D}_f(p_{\text{data}}||p_g) = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[d^*(\mathbf{x}, \theta)\right] - \mathbb{E}_{\mathbf{x}\sim p_g}\left[\tilde{f}\big(d^*(\mathbf{x}, \theta)\big)\right]$ where $d^*(\mathbf{x}, \theta) = f'(r(\mathbf{x}, \theta))$, the gradient estimation is

$$\nabla_\theta \mathcal{D}_f(p_{\text{data}}||p_g) = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\nabla_\theta d^*(\mathbf{x}, \theta)\right] - \mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[\nabla_\theta \tilde{f}\big(d^*(\mathbf{x}_{(\theta,\mathbf{z})}, \theta)\big)\right] \tag{23}$$

Eq (23) is different from Eq (20), where the gradient of VDM depends on the first term of the dual representation of f-divergences. However, in an adversarial training scenario, the density ratio $r(\mathbf{x})$ is a irrelevant of p_g and only depends on $\mathbf{x}$ because it is a bijection from the output of the discriminator $d(\mathbf{x})$ of Eq (13). Plugging $r(\mathbf{x})$ into f-divergence to replace $r(\mathbf{x}, \theta)$, we can recover an approximated f-divergence but minimizing it w.r.t. θ would never obtain a correct gradient estimation in Eq (22) or(23).

4.3 Empirical Study of Gaussians

This part highlights the differences between density ratio models in terms of the convergence of generators. We start from the simplest form of a generator $p_{g_\theta} : \mathbf{x} = \mu + \sigma\mathbf{z}$, where $\mathbf{z} \sim N(0, I)$ and $\theta = (\mu, \sigma)$, where μ is the mean and σ is a scale matrix. Let the data distribution be $p_{\text{data}} = N(\mu_0, \sigma_0^T\sigma_0)$. We can define three density ratio models assuming the generator and data distributions are Gaussians. The first model is $r(\mathbf{x}, \theta) = \frac{p_{\text{data}}(\mathbf{x})}{p_g(\mathbf{x};\theta)}$, where the density ratio function depends on $\mathbf{x}$ and θ simultaneously. The second model is $r(\mathbf{x}, \theta_{\text{de}}) = \frac{p_{\text{data}}(\mathbf{x})}{p_g(\mathbf{x};\theta_{\text{de}})}$, where θ_{de} means we detach the gradient of θ such that the second model is only a function of $\mathbf{x}$ but has the same output as the first model. The third model is $r_{\text{GAN}}(\mathbf{x})$ where the density ratio is approximated by performing a single gradient update for the classifier using samples in standard adversarial training. We solve the following optimization problem with the above three density ratio models respectively (for $r_{\text{GAN}}(\mathbf{x})$, we use the standard adversarial training),

$$\min_\theta \mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[f(r)\right] \text{ or equivalently } \min_\theta -\mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[h(\log r)\right] \tag{24}$$

Given $f(r)$ we can rewrite it as a function of log density ratio $h(\log r) = -f(r)$. Similarly, given $h(\log r)$, we can write it as a function of density ratio $f(r) = -h(\log r)$. In this experiment, we consider five types of f-divergences (expressions summarized in Appendix B.1). In addition, we also study a monotonically increasing function given by $h(\log r) = \exp\big(1.5 \log r\big)$ where its $f(r) = -\exp\big(1.5 \log r\big)$ is concave. The results are summarized in Table 2, which verifies our analysis that the objective of VDM should be a convex function of the density ratio, whereas MonoFlow only requires it to be a monotonically increasing function of the log density ratio. $r(\mathbf{x}, \theta_{\text{de}})$ can recover the true f-divergence, but minimizing this f-divergence has no effects except for KL divergence.

Remark: Minimizing the KL divergence using the detached model $r(\mathbf{x}, \theta_{\text{de}})$ also leads to convergence. This mechanism is called 'Variational Inference via Wasserstein Gradient Flows' (Lambert et al., 2022) and it also have a lower variance (Roeder et al., 2017).

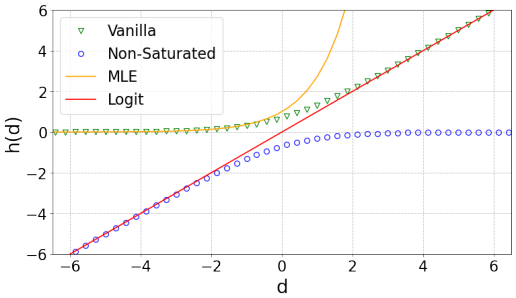


Figure 2: The plot of different generator losses as a function of d.

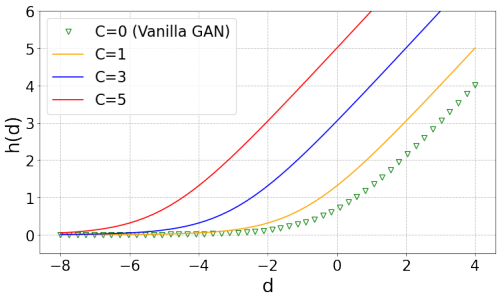


Figure 3: The plots of the vanilla losses by adding different Cs.

5 Algorithimic Insights: Alternatives of Generator Loss

5.1 Analyzing Practical Effectiveness of Generator Loss

In this part, we explain what types of generator loss functions can lead to the successful training of GANs via the lens of MonoFlow. We provide a study for the vanilla GAN since the logit output of the binary classifier is the log density ratio where we have $d(\mathbf{x}) = \log r(\mathbf{x})$ [4] (see Table 1). We consider four generator losses which are monotonically increasing functions of the log density ratio: **1). Vainilla loss**: $h(d) = -\log(1 - \sigma(d))$; **2). Non-saturated (NS) loss**: $h(d) = \log(\sigma(d))$. **3). Maximum likelihood loss**: $h(d) = \exp(d)$. **4). Logit loss**: $h(d) = d$. Notably, the non-saturated loss (proposed as a heuristic in the previous works) has a theoretic guarantee of convergence under our framework MonoFlow because it is simply a monotonically increasing function.

The plot of these functions is shown in Figure 2. The vanilla loss and the MLE loss do not work well in practice (Goodfellow, 2016), since at initial training steps, the generator is weak and $d(\mathbf{x}) = \log \frac{p_{\text{data}}(\mathbf{x})}{p_g(\mathbf{x})} \ll 0$, for $\mathbf{x} \sim p_g(\mathbf{x})$. We may observe in Figure 2, the curves of the vanilla loss and the MLE loss are fairly flat on the left side, which means the derivative $h'(\cdot)$ is nearly zero. According to Eq (6), such a rescaling scheme gives a bad path of gradient flow such that the generator can be trapped at the initial steps as the infinitesimal change of particles $d\mathbf{x}_t \approx 0$. The NS and logit loss both have non-zero derivatives when $d(\mathbf{x}) < 0$ despite that the NS loss is flat on the right side. This is not a problem since $d(\mathbf{x})$ gradually increases from a negative value during the training and when $d(\mathbf{x}) = 0$, it means $p_g = p_{\text{data}}$ such that the generator converges.

5.2 An Embarrassingly Simple Trick to Fix Vanilla GAN

We have justified that GANs can work with any generator loss as long as it is a monotonically increasing mapping of the log density ratio and its derivative deviates from zero when the $\log r(\mathbf{x}) \ll 0$. We show the effects of shifting the generator loss of the vanilla GAN left by adding a constant C to the sigmoid function,

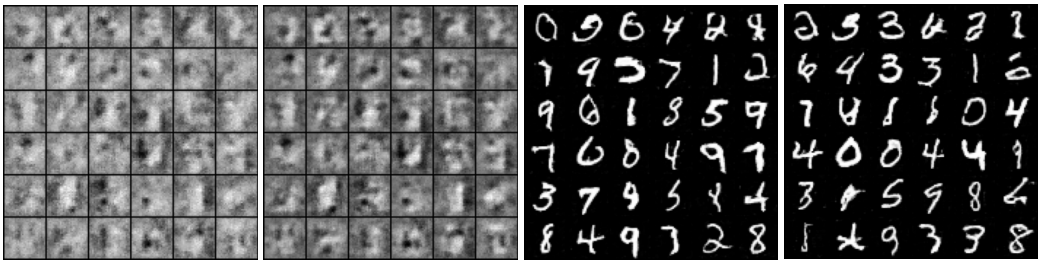
$$h(d) = -\log(1 - \sigma(d + C)) \tag{25}$$

By adding a constant, we can obtain a better monotonically increasing function whose derivative deviates from zero significantly, see Figure 3. The neural network architecture used here is DCGAN (Radford et al., 2015) and we follow the vanilla GAN framework where the log density ratio is obtained by logit output from the binary classifier and the model is trained with 15 epochs. The generated samples are shown in Figure 4. We observe that when $C = 3$ and $C = 5$, the generator loss in Eq (25) begin to work, i.e., generators output plausible fake images.

6 Related Works

Gradient Flow: Another particle transportation method is based on JKO scheme (Jordan et al., 1998) which relates to the backward Euler discretizations of gradient flows. Mokrov et al. (2021)

[4] This can be simply done with PyTorch via removing the final sigmoid layer of the discriminator and using the criteria function 'nn.BCEWithLogitsLoss'



(a) $C = 0$ (b) $C = 1$ (c) $C = 3$ (d) $C = 5$

Figure 4: Generated samples with different Cs.

studied the JKO scheme with input convex neural networks (Amos et al., 2017). The deterministic particle evolution ODE is hard to simulate since it has an intractable term which is the log density of particles. Given the known target distribution with a density function, Maoutsa et al. (2020) studied this ODE by directly estimating the log density of particles. Thereafter (Boffi & Vanden-Eijnden, 2022) used a time-dependent score network (Song & Ermon, 2019) to instead estimate the gradient of this log density such that their method applies to higher dimensional problems. Stein variational gradient descent (SVGD) (Liu & Wang, 2016) is a particle approximation method that can also be viewed as a gradient flow of KL divergence but associated with a different metric space with Stein geometry (Duncan et al., 2019). Wasserstein gradient flows of reversed f-divergences $\mathcal{D}_f(q||p)$ have been previously studied in deep generative modeling as a refinement approach to improve sample quality (Ansari et al., 2021). A close work to ours is (Gao et al., 2019) where the authors proposed to use gradient flows to refine fake samples output by the generator and the generator learns to minimize the squared distance between the refined samples and the original fake samples. **IPM GANs**: Our framework unifies divergence GANs since estimating a probability divergence is naturally related to density ratio estimation (Sugiyama et al., 2012). However, some variants of GANs are developed with Integral Probability Metric (IPM) (Sriperumbudur et al., 2009). For example, WGANs (Arjovsky et al., 2017; Gulrajani et al., 2017) estimate the Wasserstein-1 metric and then minimize this metric. While MonoFlow is associated with Wasserstein-2 metric, minimizing a functional in $\mathcal{P}(\mathbb{R}^d)$ naturally decreases Wasserstein-2 metric as well. Other types of IPM GANs are MMD GAN (Dziugaite et al., 2015) and Sobolev GAN (Mroueh et al., 2018b). Both of them have been interpreted as gradient flow approaches (Mroueh & Nguyen, 2021; Mroueh et al., 2018a) but associated with different vector fields. **Diffussion Models**: diffusion models (Ho et al., 2020; Song et al., 2021; Luo, 2022) are another line of generative modeling framework. This framework first perturbs data by adding noises with different scales to create a path $\{q_t\}_{t\geq 0}$ interpolating the data distribution and the noise distribution. Subsequently, the generative modeling is to reverse $\{q_t\}_{t\geq 0}$ as denoising. The similarity of MonoFlow and diffusion models is that they both involves particle evolution associated with different paths of marginal probabilities. The difference is as follows: the vector field of MonoFlow is obtained with the log denisty ratio and the log denisty ratio must be corrected per iteration by gradient update; diffusion models directly estimate vector fields by time-dependent neural networks and they are straightforward particle methods.

7 Conclusions

We introduce a unified framework for GAN variants. Our framework provides a comprehensive understanding to help us get insights into why and how adversarial training works. The mechanism of adversarial training is not as adversarial as we used to think. It instead approximates a gradient flow in the Wasserstein space, the bi-level step of adversarial can be regarded as it first estimates the vector field of the gradient flow and next the generator is updated to learn to draw particles guided by the vector field, aka we call it as parameterizing the gradient flow. Therefore, all GAN variants discussed in this paper are equal at the methodology level. They all are different methods estimating the bijection of the log density ratio then mapping the log density ratio by different monotonically increasing functions. Compared to previous studies of GANs, our framework is highly theoretically and practically consistent. The limitation of this paper is that our framework does not cover the variants of IPM GANs since these variants give a vector field that is different from the gradient of log density ratios. We will leave it as a future work.

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A PROOFS

A.1 PROOF OF THEOREM 3.1 (INFORMAL)

Proof. Eq(6) defines the vector field $v_t = h'\big(\log r_t\big)\big(\nabla_{\mathbf{x}} \log p - \nabla_{\mathbf{x}} \log q_t\big)$ such that

$$\begin{aligned}\frac{\partial q_t}{\partial t} &= \text{div}\left(q_t h'\left(\log r_t\right)\left(\nabla_{\mathbf{x}} \log q_t - \nabla_{\mathbf{x}} \log p\right)\right) \\ &= \text{div}\left(h'\left(\log r_t\right)\nabla_{\mathbf{x}} q_t\right) - \text{div}\left(h'\left(\log r_t\right) q_t \nabla_{\mathbf{x}} \log p\right)\end{aligned} \tag{26}$$

The equilibrium (stationary) distribution is achieved if the probability current $q_t h'\left(\log r_t\right)\left(\nabla_{\mathbf{x}} \log q_t - \nabla_{\mathbf{x}} \log p\right) = 0$. Since $h'\left(\log r_t\right) > 0$, we directly get $q_t\left(\nabla_{\mathbf{x}} \log q_t - \nabla_{\mathbf{x}} \log p\right) = 0$. Hence $q_t \to p$, which is the same as the standard Fokker Planck equation of Eq (3).

For any curve $\{q_t\}_{t\geq 0}$ evolving according to the vector field $\{v_t\}_{t\geq 0}$ in Wasserstein space, the dissipation rate of the functional $\frac{\partial \mathcal{F}(q_t)}{\partial t} = \mathbb{E}_{q_t}\langle \nabla_{W_2}\mathcal{F}(q_t), v_t\rangle$, where the Wasserstein gradient of KL divergence is $\nabla_{W_2}\mathcal{F}(q_t) = \nabla_{\mathbf{x}} \log \frac{q_t}{p}$

Therefore, the dissipation rate of the reverse KL divergence under MonoFlow is

$$\frac{\partial \mathcal{F}(q_t)}{\partial t} = \mathbb{E}_{q_t}\left[-h'\big(\log r_t\big)\left\|\nabla_{\mathbf{x}} \log \frac{q_t}{p}\right\|^2\right] \leq 0 \tag{27}$$

Hence, MonoFlow always decreases the reverse KL divergence with the time. □

A.2 PROOF OF THEOREM 3.2 (INFORMAL)

Define the functional $\mathcal{F}(q)$ as

$$\mathcal{F}(q) = \mathcal{D}_f(p||q) = \int f\left(\frac{p}{q}\right)(x) q(x) dx \tag{28}$$

Let the test function be $\phi(\mathbf{x})$,

$$\begin{aligned}\int \frac{\delta \mathcal{F}}{\delta q}(\mathbf{x})\phi(\mathbf{x}) d\mathbf{x} &= \lim_{\epsilon\to 0} \frac{\mathcal{F}(q+\epsilon\phi) - \mathcal{F}(q)}{\epsilon} \\ &= \frac{d}{d\epsilon}\mathcal{F}(q+\epsilon\phi)\Big|_{\epsilon=0} \\ &= \frac{d}{d\epsilon}\int f\left(\frac{p}{q+\epsilon\phi}\right)(\mathbf{x})\big(q(\mathbf{x}) + \epsilon\phi(\mathbf{x})\big) d\mathbf{x}\Big|_{\epsilon=0} \\ &= \int \left\{f\left(\frac{p}{q+\epsilon\phi}\right)(\mathbf{x})\phi(\mathbf{x}) - f'\left(\frac{p}{q+\epsilon\phi}\right)(\mathbf{x})\frac{p(\mathbf{x})\phi(\mathbf{x})}{q(\mathbf{x}) + \epsilon\phi(\mathbf{x})}\right\} d\mathbf{x}\Big|_{\epsilon=0} \\ &= \int \left\{f\left(\frac{p}{q}\right) - f'\left(\frac{p}{q}\right)\frac{p}{q}\right\}(\mathbf{x})\phi(\mathbf{x}) d\mathbf{x}\end{aligned} \tag{29}$$

Thus

$$\frac{\delta \mathcal{F}}{\delta q} = f(r) - r f'(r), \quad \text{where} \quad r = \frac{p}{q} \tag{30}$$

The Wasserstein gradient of $\mathcal{F}(q)$ is

$$\nabla_{W_2}\mathcal{F}(q) = \nabla_{\mathbf{x}}\frac{\delta \mathcal{F}}{\delta q} = -r f''(r)\nabla_{\mathbf{x}} r. \tag{31}$$

The corresponding vector field is

$$v(\mathbf{x}) = r(\mathbf{x}) f''(r(\mathbf{x}))\nabla_{\mathbf{x}} r(\mathbf{x}) = r(\mathbf{x})^2 f''(r(\mathbf{x}))\nabla_{\mathbf{x}} \log r(\mathbf{x}). \tag{32}$$

We have $h'(\log r) = r^2 f''(r) > 0$, concluding the proof.

A.3 PROOF OF LEMMA 3.3

Given the optimization problem

$$\max_{d} \ \mathbb{E}_{\mathbf{x}\sim p}\left[\phi\big(d(\mathbf{x})\big)\right] + \mathbb{E}_{\mathbf{x}\sim q}\left[\psi\big(d(\mathbf{x})\big)\right] \tag{33}$$

We rewrite it as

$$\max_{d} \ \mathbb{E}_{\mathbf{x}\sim q}\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}\phi\big(d(\mathbf{x})\big) + \psi\big(d(\mathbf{x})\big)\right] \tag{34}$$

Let the derivative $\frac{\partial}{\partial d}\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}\phi\big(d(\mathbf{x})\big) + \psi\big(d(\mathbf{x})\big)\right] = 0$, we obtain

$$r(\mathbf{x})\phi'\big(d(\mathbf{x})\big) + \psi'\big(d(\mathbf{x})\big) = 0, \quad r(\mathbf{x}) = \frac{p(\mathbf{x})}{q(\mathbf{x})} \tag{35}$$

From Eq(35), the optimal decision function d^* satisfies $r(\mathbf{x}) = -\frac{\psi'(d^*(\mathbf{x}))}{\phi'(d^*(\mathbf{x}))} := \mathcal{T}(d^*(\mathbf{x}))$. To ensure d^* is a global optimizer for every $\mathbf{x}$, $\mathcal{T}$ must be a bijection.

- For binary classification, $\phi(\cdot) = \log\sigma(\cdot)$ and $\psi(\cdot) = \log(1-\sigma(\cdot))$, $r(\mathbf{x}) = \exp(d^*(\mathbf{x}))$.
- Fenchel-duality, $\phi(\cdot) = (\cdot)$, $\psi(\cdot) = -\tilde{f}(\cdot)$, $r(\mathbf{x}) = \tilde{f}'\big(d^*(\mathbf{x})\big)$ where the convex conjugate is $\tilde{f}(d) = \sup_{r\in \mathrm{dom} f}\{rd - f(r)\}$
- For least-square GAN, $\phi(\cdot) = ((\cdot)-1)^2, \psi(\cdot) = (\cdot)^2$, $r(\mathbf{x}) = \frac{d^*(\mathbf{x})}{1-d^*(\mathbf{x})}$

B EXPERIMENTS

B.1 DETAILS FOR 4.3

Table 3: Explicit forms of f and h

	$f(r)$	$h(u), u = \log r$
KL	$-\log r$	u
Forward KL	$r\log r$	$-u\exp(u)$
Chi-Square	$(r-1)^2$	$-(\exp(u)-1)^2$
Hellinger	$(\sqrt{r}-1)^2$	$-(\sqrt{\exp(u)}-1)^2$
Jensen-Shannon (GAN)	$r\log\frac{2r}{1+r} + \log\frac{2}{1+r}$	$-\exp(u)\log\frac{2\exp(u)}{1+\exp(u)} - \log\frac{2}{1+\exp(u)}$
Exp	$-\exp(1.5\log r)$	$\exp(1.5u)$

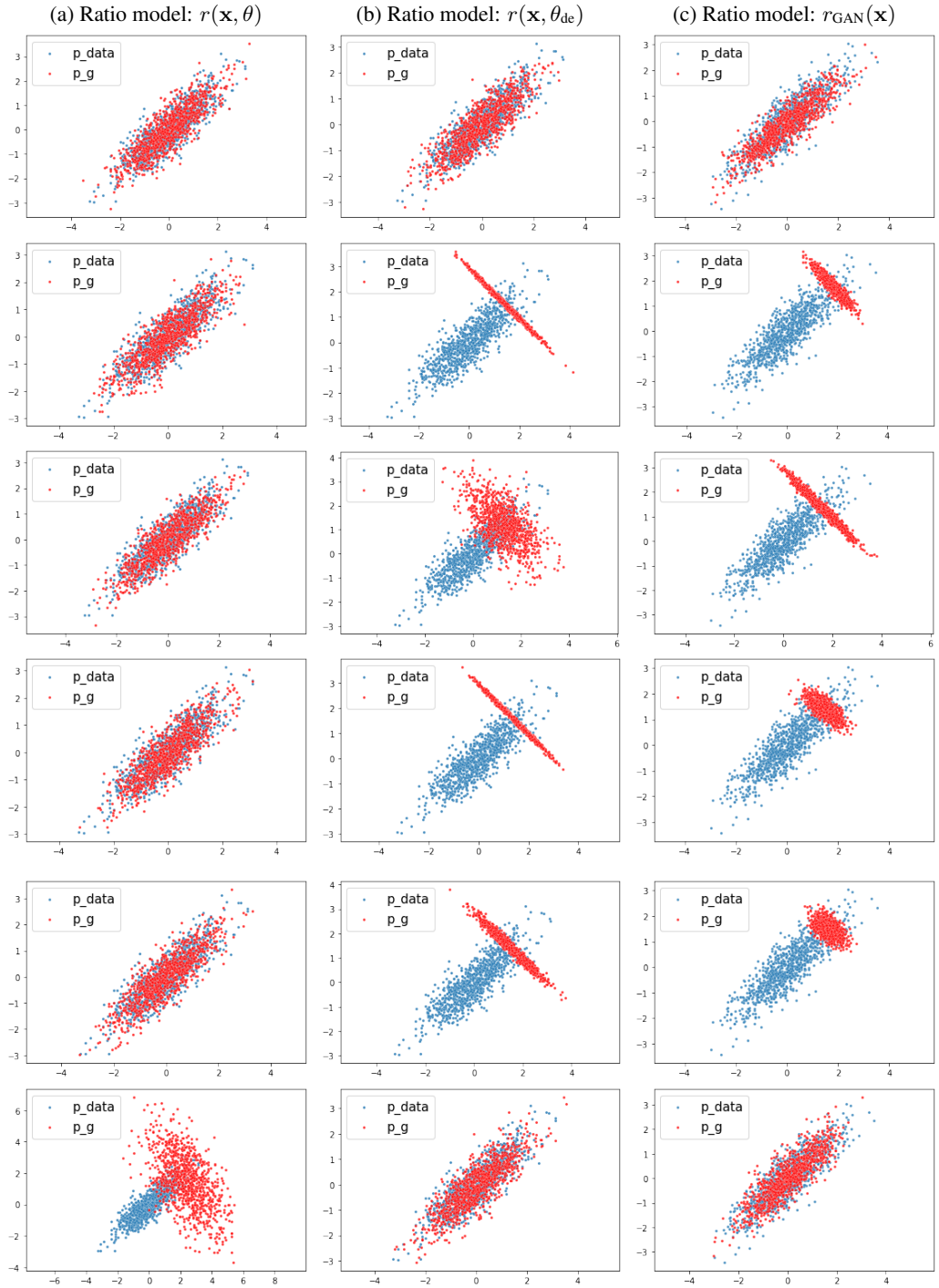
The generator is initialized at:

$$N\left[\begin{pmatrix}1.0\\1.0\end{pmatrix}, \begin{pmatrix}1.00 & 0.00\\0.00 & 1.00\end{pmatrix}\right]$$

and the target distribution is

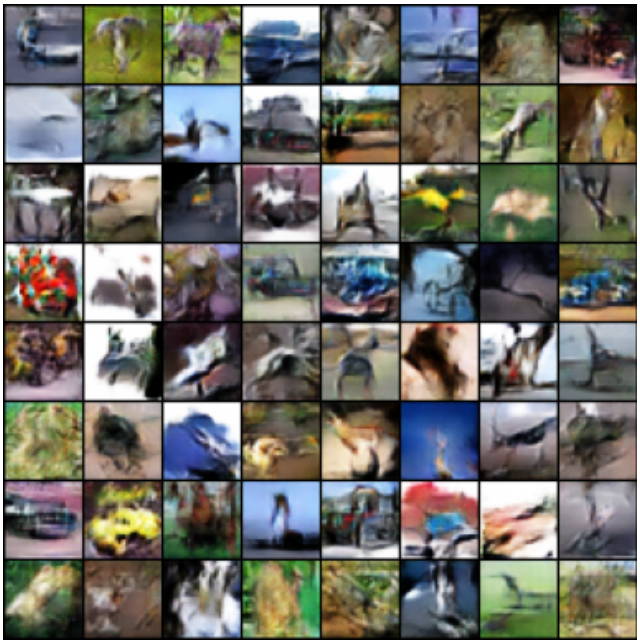
$$N\left[\begin{pmatrix}0.0\\.0\end{pmatrix}, \begin{pmatrix}1.00 & 0.80\\0.80 & 0.89\end{pmatrix}\right]$$

The visulation results follow the order: KL, Forward KL, Chi-Square, Hellinger, Jensen-Shannon (GAN), Exp. $r_{\text{GAN}}(\mathbf{x})$ uses a simple 2-layer discriminator with Leaky ReLU activation that has logit output as the the log density ratio.



B.2 Experiment on Vanilla GAN with An Arbitrary Increasing Function

We change the generator loss to: $-\mathbb{E}_{\mathbf{z}\sim p_{\mathbf{z}}}\left[\operatorname{arc\,sinh}\left(\left(d(g(\mathbf{z}))-3\right)^3\right)\right]$. This has no meaning for reconstructing any probability divergences, but GAN still works. We did an experiment on Cifar10 and Celeb-A using DCGAN architecture (Radford et al., 2015). The generated samples are shown in Figure 6.



(a) Generated images of Cifar10

(b) Generated images of Celeb-A

Figure 6: Generated samples via an arbitrary increasing function.