A Framework of Composite Functional Gradient Methods for Generative Adversarial Models

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Abstract—Generative adversarial networks (GAN) are trained through a minimax game between a generator and a discriminator to generate data that mimics observations. While being widely used, GAN training is known to be empirically unstable. This paper presents a new theory for generative adversarial methods that does not rely on the traditional minimax formulation. Our theory shows that with a strong discriminator, a good generator can be obtained by composite functional gradient learning, so that several distance measures (including the KL divergence and the JS divergence) between the probability distributions of real data and generated data are simultaneously improved after each functional gradient step until converging to zero. This new point of view leads to stable procedures for training generative models. It also gives a new theoretical insight into the original GAN. Empirical results on image generation show the effectiveness of our new method.

Index Terms—Generative adversarial models, functional gradient learning, neural networks, image generation.

1 INTRODUCTION

Given examples of real data $x_1^n, \ldots, x_n^n \in \mathbb{R}^k$ from an unknown distribution $p_x$ on $\mathbb{R}^k$ and a random variable $Z$ with a known distribution $p_z$ (e.g., a Gaussian), we are interested in learning transformation $G$ of variable $Z$ so that the distribution of the transformed variable $G(Z)$ becomes close to the distribution of real data. This is the setting considered in generative adversarial networks (GAN) [10], and $G$ is often referred to as a generator.

While being widely used, GAN training is known to be difficult due to its instability. This fact has led to numerous studies, e.g., Wasserstein GAN (WGAN) and its extensions [2], [11], [30] to pursue a different minimax objective, regularization to tackle the issue of mode collapse and instability [5], [38], $f$-GAN [34], unrolled GAN [28], AdaGAN [44], MMD GAN [23], and so forth and references therein.

An important concept introduced by GAN is the idea of adversarial learner, denoted here by $d$, which tries to discriminate real data from generated data. GAN training can be described as the following minimax game between a discriminator $d$ and a generator $G$:

$$
\min_{G} \max_{d} \left[ \mathbb{E}_{x^* \sim p_x} \ln d(x^*) + \mathbb{E}_{z \sim p_z} \ln (1 - d(G(z))) \right]. \quad (1)
$$

It was shown in [10] that assuming the optimality of $d$, (1) is equivalent to minimizing the Jensen-Shannon (JS) divergence between the distribution of real data and that of generated data.

Parameterizing $G$ and $d$, the GAN training procedure (Algorithm 4 below) seeks to find the solution to the minimax formulation (1) by incrementally using a stochastic gradient method, where a gradient step is taken with respect to the model parameters of $d$ and $G$. As suggested by [10], however, minimization of $\ln (1 - d(G(z)))$ with respect to $G$ above is often replaced by maximization of $\ln (d(G(z)))$ with respect to $G$, called logd trick, in practice. GAN with the logd trick, though often more effective, can not directly be explained by the theory based on the minimax formulation (1).

This paper provides a new theory for generative adversarial methods which does not rely on the traditional minimax formulation. We show that a good generator can be learned where ‘goodness’ is measured by the divergence between the distributions of real data and generated data, by using functional gradient learning greedily, similar to gradient boosting [8]. However, unlike standard gradient boosting, which uses additive models, this paper considers functional compositions of the following form

$$
G_t(Z) = G_{t-1}(Z) + \eta_t g_t(G_{t-1}(Z)), \quad (t = 1, \ldots, T) \quad (2)
$$

to obtain $G(Z) = G_T(Z)$. Here $\eta_t$ is a small step size, and each $g_t$ is a function to be estimated from data. An initial generator $G_0(Z) \in \mathbb{R}^k$ is assumed to be given. We learn from data $g_t$ greedily from $t = 1$ to $t = T$ so that improvement in terms of the divergence between the two distributions is guaranteed.

The first part of the theory considers the limit where the step size $\eta_t$ approaches 0 and thus considers a generator that continuously evolves in time. We show that the algorithm suggested by our analysis simultaneously minimizes multiple distance measures such as the KL divergence and the JS divergence, and more generally, $f$-divergences with certain properties. The second part relaxes the condition on the step size and thus considers a generator that evolves in discrete steps.

Our theory leads to a new algorithm for learning generative adversarial models that is stable and effective. It also provides a new theoretical insight into the original GAN (either with or without the logd trick). The experiments show the effectiveness of our new method on image generation in comparison with GAN variants.
1.1 Preliminaries

Notation: Throughout the paper, we use $x$ to denote data in $\mathbb{R}^k$. The probability density function of real data is denoted by $p_x$. We use $\| \|_2$ to denote the vector 2-norm and the matrix spectral norm. Given a scalar function $h(x)$, we use $\nabla h(x)$ to denote the gradient with respect to $x$. Note that we have $\nabla h(x) \in \mathbb{R}^k$ as $x \in \mathbb{R}^k$. Given a vector function $g(x)$, we use $\nabla g(x)$ to denote its Jacobi matrix. Convergences are all pointwise.

Logistic regression: Our analysis will use the following known facts on logistic regression. Let $p_x$ and $p$ be the probability densities of real data and generated data, respectively, and define $\mathcal{D}(x)$ by

$$
\mathcal{D}(x) := \ln \frac{p_x(x)}{p(x)}.
$$

(3)

Then $\mathcal{D}$ is the analytical solution to a logistic regression problem for discriminating real data and generated data; i.e.,

$$
\mathcal{D} = \arg \min_{\mathcal{D}} \left[ \mathbb{E}_{x \sim p_x} \ln(1 + e^{-\mathcal{D}(x)}) + \mathbb{E}_{x \sim p} \ln(1 + e^\mathcal{D}(x)) \right].
$$

In practice, one can only approximate the theoretical optimum solution above by choosing some class of functions $\mathcal{C}$ using finite amounts of sample $S_x$ and $S$ to solve:

$$
\arg \min_{\mathcal{D} \in \mathcal{C}} \left[ \sum_{x \in S_x} \ln(1 + e^{-\mathcal{D}(x)}) \left| S_x \right| + \sum_{x \in S} \ln(1 + e^{\mathcal{D}(x)}) \left| S \right| \right].
$$

(4)

Statistical consistency of such approximation has been formally studied (e.g., [49]), but intuitively, approximation improves with larger sample and more universal $\mathcal{C}$.

2 CONTINUOUS THEORY

Our goal is to transform a random variable $Z \in \mathbb{R}^k$ with a known distribution by (2):

$$
G_t(Z) = G_{t-1}(Z) + \eta_t g_t(G_{t-1}(Z)), \quad (t = 1, \ldots, T),
$$

so that the probability density of the transformed variable $G_T(Z)$ is close to $p_x$, the density of real data. The sequence of transformation in (2) takes discrete steps from time $t = 1$ to time $t$, but in this section, let us instead take a small time step $\delta$ and set $\eta_t = \delta$ so that we have

$$
G_{t+\delta}(Z) = G_t(Z) + \delta g_t(G_t(Z)).
$$

(5)

By letting $\delta \to 0$, we can generate a generator that evolves continuously in time $t$ that satisfies an ordinary differential equation

$$
\frac{dG_t(Z)}{dt} = g_t(G_t(Z))
$$

(6)

In this section, we study this continuously evolving generator. In practice, we envision a learning process that starts with a given initial generator $G_0$ and proceeds with discretization by alternating (5) and $t \leftarrow t + \delta$ with a small $\delta$. Thus, having step-size $\delta \to 0$ is an idealization that simplifies the analysis and therefore helps to understand the problem. We will relax this condition in the next section.

2.1 Analysis

The goal is to learn $g_t : \mathbb{R}^k \to \mathbb{R}^k$ from data so that the probability density of $G_t(Z)$, which continuously evolves by (6), becomes close to the density $p_x$ of real data as $t$ continuously increases. To measure the 'closeness', we use a distance measure in the form of

$$
L(p) = \int \ell(p_x(x), p(x)) dx,
$$

(7)

where $\ell : \mathbb{R}^2 \to \mathbb{R}$ is a pre-defined function so that $L$ satisfies $L(p) = 0$ if and only if $p = p_x$ and $L(p) \geq 0$ for any probability density function $p$.

From the following theorem, we will derive the choice of $g_t(\cdot)$ that guarantees that transformation (5) with $\delta \to 0$ can always reduce/improve $L(\cdot)$.

Theorem 2.1. Using the definitions above, let $p_t$ be the probability density of random variable $G_t(Z)$. Let $\ell_2'(\rho, \rho) = \partial \ell(\rho, \rho)/\partial \rho$. Then we have

$$
\frac{dL(p_t)}{dt} = \int p_t(x) \nabla_x \ell_2'(p_t(x), p_t(x)) \cdot g_t(x) dx.
$$

(8)

The proof is given in Appendix A.

The theorem implies that for $\frac{dt(p_t)}{dt}$ to be negative so that the distance $L$ decreases/improves, we should choose $g_t(x)$ to be:

$$
g_t(x) = - s_t(x) \phi_0(\nabla_x \ell_2'(p_t(x), p_t(x))),
$$

(9)

where $s_t(x) > 0$ is an arbitrary scaling factor. $\phi_0(u)$ is a vector function such that $\phi(u) = u \cdot \phi_0(u)$ $\geq 0$ and that $\phi(u) = 0$ if and only if $u = 0$, e.g., $(\phi_0(u) = u, \phi(u) = \|u\|_2^2)$ or $(\phi_0(u) = \text{sign}(u), \phi(u) = \|u\|_1)$. With this choice of $g_t(x)$, we obtain

$$
\frac{dL(p_t)}{dt} = - \int s_t(x) p_t(x) \phi(\nabla_x \ell_2'(p_t(x), p_t(x))) dx \leq 0,
$$

(10)

that is, the distance $L$ is guaranteed to improve unless the equality holds. Moreover, this implies that we have

$$
lim_{t \to \infty} \int s_t(x) p_t(x) \phi(\nabla_x \ell_2'(p_t(x), p_t(x))) dx = 0.
$$

Otherwise, $L(p_t)$ would keep going down and become negative as $t$ increases, but $L(p_t) \geq 0$ by definition.) With a continuity condition (see Appendix B.5), this further implies

$$
limit_{t \to \infty} p_t(x) \nabla_x \ell_2'(p_t(x), p_t(x)) = 0.
$$

(11)

We show below the cases where (10) can further lead to

$$
limit_{t \to \infty} p_t(x) = p_x(x), \quad i.e., \quad \text{the distribution of generated data converges to that of real data provided that } g_t(x) \text{ is chosen as in (9)}.\n$$

2.2 $f$-divergences

Let us consider a case where the distance measure $L(\cdot)$ is an $f$-divergence. With a convex function $f : \mathbb{R}^+ \to \mathbb{R}$ such that $f(1) = 0$ and that $f$ is strictly convex at 1, $L(p_t)$ defined by

$$
L(p_t) = \int p_t(x) f(r_t(x)) dx \quad \text{where } r_t(x) = \frac{p_t(x)}{p_x(x)}
$$

(11)

is called $f$-divergence. Here we focus on a special case where $f$ is twice differentiable and strongly convex so that the second order derivative of $f$, denoted here by $f''$, is

1. The conventions are: $0f(0/0) = 0$, $f(0) = \lim_{x \to 0} f(x)$, $0f(a/0) = \lim_{x \to 0} f(ax/a)$; see e.g., [6].
For some divergences, this can be further rewritten as follows (see Table 1 for derivation):

- **KL divergence:** \( \lim_{t \to \infty} p_s(x) \nabla_x \ln(r_t(x)) = 0 \)
- **reverse KL divergence:** \( \lim_{t \to \infty} p_s(x) \nabla_x r_t(x) = 0 \)
- **JS divergence:** \( \lim_{t \to \infty} p_s(x) \frac{1}{1 + r_t(x)} \nabla_x r_t(x) = 0 \)
- **squared Hellinger distance:** \( \lim_{t \to \infty} p_s(x) \nabla_x \sqrt{r_t(x)} = 0 \)

Thus, with these divergences, if \( p_s \) has full support on \( \mathbb{R}^k \), then the pdf ratio \( r_t(x) \) goes to a constant for all \( x \), which implies that \( p_t \to p_s \) as \( t \to \infty \).

The convergence does not hold if \( p_s \) (or \( p_t \) as \( t \to \infty \)) does not have full support. Moreover, for \( x \) such that \( p_s(x) = 0 \) and \( p_t(x) > 0 \), \( r_t(x) \) goes to infinity, and \( r_t(x) \) is zero when \( p_s(x) = 0 \) and \( p_t(x) > 0 \), which pushes \( f''(\gamma) \) to infinity in some cases (see Table 1). Therefore, if \( p_s(x) \) or \( p_t(x) \) was zero in a substantial part of \( \mathbb{R}^k \), then \( f \)-divergences might not be suitable for the purpose. In that case, it would be rather sensible to either abandon \( f \)-divergences or work with approximations – by approximating such distributions with more manageable distributions that have full support. Essentially, the former argues for WGAN [2], and we take the latter approach. The practicality of the assumptions will be further discussed later in Section 4 after the whole picture is laid out.

### 2.2.1 Algorithms

To derive an algorithm from the results above, note that the suggested \( g_t(x) \) in (13) cannot be obtained from data in practice as it depends on unknown densities \( p_t \) and \( p_s \), but that it can be approximated using the discriminator. Let \( D(x) \) be the solution to the empirical logistic regression problem (4) for discriminating real data generated from data at time \( t \); for simplicity, we omit the subscript \( t \) from all variables in this section. Assuming that \( D(x) \approx D(x) = \ln \frac{p_s(x)}{p_t(x)} \) (3), let us define \( \bar{r}(x) \) so that

\[
\bar{r}(x) = \exp(-D(x)) \approx \frac{p_s(x)}{p_t(x)} = r(x)
\]

and replace \( r(x) \) in (13) with \( \bar{r}(x) \). Then, as \( \nabla \bar{r}(x) = -\bar{r}(x) \nabla D(x) \), we obtain

\[
g(x) = s(x)v(x)\nabla D(x),
\]

where \( v(x) = \bar{r}(x)f''(\bar{r}(x)) \). Since \( v(x) > 0 \) (because \( f''(\gamma) > 0 \) by assumption), \( v(x) \) can be absorbed into the data-dependent arbitrary scaling factor \( s(x) \). Thus, we obtain an algorithm that repeats the following:

- Update discriminator \( D \) to minimize logistic loss (4).
- Update generator \( G \) by \( G(z) \leftarrow G(z) + \delta g(G(z)) \) with \( g(x) = s(x)\nabla D(x) \).

This is essentially identical to the algorithm that we will derive from our discrete analysis in the next section (Algorithm 1), and so we will look into it in more detail there. Nevertheless, it is worth noting that the obtained algorithm can be regarded as simultaneously optimizing several distance measures (all the \( f \)-divergences with strongly convex \( f \) such as the KL divergence, JS divergence, and the Hellinger distance). That is, even if we simply fix \( s(x) \) to a constant (e.g., \( s(x) = 1 \)) instead of customizing it for each measure, the resulting algorithm optimizes several measures.

[34] extended GAN, which was shown to be associated with the JS divergence [10], to G-FAN for various \( f \)-divergences. One difference here is that our analysis indicates that a single algorithm (Algorithm 1) using a single optimization objective (i.e., minimization of the logistic loss) simultaneously optimizes multiple divergences. By contrast, the G-FAN study proposed different optimization objectives (leading to different computations) for minimizing different divergences.

**Least squares variant:** The pdf ratio can also be estimated by other optimization objectives such as least squares. Use of the least squares estimate also leads to the generator update procedure above, thus leading to the least squares variant that replaces the discriminator update using logistic regression with the least squares objective.

### 3 DISCRETE THEORY

Now we turn to our discrete theory on the generator \( G_T(Z) \) obtained by taking discrete steps (2):

\[
G_t(Z) = G_{t-1}(Z) + \eta_t g_t(G_{t-1}(Z)), \quad (t = 1, \ldots, T).
\]

Our analysis in this section will include the effect of the step size \( \eta_t \) and the deviation of the discriminator from the optimum. Before we start, let us first consider how the results of our continuous analysis apply towards this end.

**Corollary 3.1.** Let \( L(p) \) be the \( f \)-divergence \( L(p) = \int p_s(x)f(r(x))dx \) where \( r(x) = \frac{p_s(x)}{p_t(x)} \) with strongly convex \( f \) as in Section 2.2. Let \( p \) and \( p' \) be the densities...
Algorithm 1 CFG: Composite Functional Gradient Learning of GAN

Input: real data $x_1^*, \ldots, x_n^*$, initial generator $G_0$ with generated data $\{G_0(z_1), \ldots, G_0(z_m)\}$. Meta-parameter: $T$.

1: for $t = 1, 2, \ldots, T$ do
2: \hspace{1em} $D_t(x) \leftarrow \arg\min_D \left\{ \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \exp(-D(x^i_t))) + \frac{1}{m} \sum_{j=1}^{m} \ln(1 + \exp(D(G_{t-1}(z^j)))) \right\}$
3: \hspace{1em} $\theta_t(x) \leftarrow s_t(T) \nabla D_t(x)$ (s_t is for scaling, e.g., most simply s_t(x) = 1)
4: \hspace{1em} $G_t(z) \leftarrow G_{t-1}(z) + \eta_t \theta_t(G_{t-1}(z))$, for some $\eta_t > 0$
5: end for
6: return generator $G_T(z)$

of random variables $X$ and $X'$, respectively, such that $X' = X + \eta g(X)$. Let $D(x) = \ln \frac{p(x)}{p(x)}$. Then we have:

$$L(p') = L(p) - \eta \int p(x) v(x) \nabla D(x) \cdot g(x) dx + \cdot j(\eta)$$

where $v(x) = (r(x))^2 f''(r(x))$ and $j(\eta) = o(\eta)$ as $\eta \to 0$.

Proof

$$\frac{dL(p)}{dt} = \int p(x) f''(r(x)) \nabla r(x) \cdot g(x) dx$$

(15)

$$= - \int p(x) v(x) \nabla D(x) \cdot g(x) dx$$

(16)

(15) is from Theorem 2.1 and (12), and (16) uses $\nabla r(x) = -r(x) \nabla D(x)$ and $p(x) = r(x)p(x)$. The desired result is obtained by using (16) in the Taylor series of $L(p')$.

We have $v(x) \geq 0$ as $f$ is strongly convex, and so if $j(\eta)$ is small, ignoring the equality, this result would suggest that the reduction of the $f$-divergence is guaranteed with $g(x) = s(x)D(x)$ with any $s(x) > 0$. Although this is essentially true under appropriate conditions, making a formal statement has some complication. Since we no longer assume $\eta \to 0$, we need to bound $j(\eta)$ as $\eta$ increases. The regularity conditions for this purpose would be rather complex in the general $f$-divergence case. For this reason, we choose to prove a rigorous statement only for the KL divergence, which simplifies presentation. More details regarding this choice are given in Appendix B.4.

We start with stating the definitions and assumptions.

3.1 Definitions and assumptions

3.1.1 Definitions

As before, let $p_*$ and $p$ be the probability densities of real data and generated data, respectively. We continue to use $D(x) = \ln \frac{p_*(x)}{p(x)}$ from Section 1.1 to indicate the theoretical solution to the logistic regression problem, and let discriminator $D$ be the solution to the empirical logistic regression problem (4). We let $L$ be the KL divergence:

$$L(p) = \int p_*(x) \ln \frac{p_*(x)}{p(x)} dx.$$ 

3.1.2 Assumptions

Assumption 3.1 (Boundedness of the pdf ratio). $|D(x)|$ is bounded so that there exists a positive number $B < \infty$ such that $|D(x)| \leq B$.

As $D(x) = \ln \frac{p_*(x)}{p(x)}$, this assumption implies that both $p_*(x)$ and $p(x)$ are nonzero everywhere. (However, also note that we have in Appendix B an analysis with slightly more relaxed assumptions that allow $p$ without full support.)

Assumption 3.2 ($\epsilon$-approximation condition on the discriminator). Discriminator $D$ satisfies the following $\epsilon$-approximation condition for some $\epsilon$ such that $0 < \epsilon < \infty$:

$$\int q_*(x)|D(x) - D(x)| dx \leq \epsilon$$

$$q_*(x) = p_*(x) \max(1, |\nabla \ln p_*(x)|).$$

The optimal discriminator has been often assumed and we slightly relax it by quantifying the deviation from the optimal $D(x)$. Note that ‘smallness’ of $\epsilon$ (corresponding to a strong discriminator) is not required for proving our theorem below, but it is required for deriving the convergence.

Nonzero smooth light-tailed $p_*$. We assume that $p_*$, the density of real data, is nonzero and smooth with light tails; we use a constant $h_0 > 0$ that depends on the shape of $p_*$. Common exponential distributions such as Gaussians and Gaussian mixtures all satisfy the assumption. The precise statements are given in Appendix B.2.2.

Remark: To put it intuitively, we assume that any data point in $\mathbb{R}^k$ has some possibility (which changes smoothly) of being real as well as some possibility of being generated, and that $D(x)$ indicates which is more likely.

Our assumptions are traditional and so make a sharp contrast with the low dimensional manifold assumption of [1], which led to WGAN [2]. We will discuss the practicality of our assumptions later in Section 4 in the context of developing practical algorithms for image generation.

3.2 Analysis

The goal is to approximate the true density $p_*$ on $\mathbb{R}^k$ through $G_t(Z) = G_{t-1}(Z) + \eta_t g_t(G_{t-1}(Z)), (t = 1, \ldots, T)$. Our analysis here focuses on one step at time $t$, namely, random variable transformation of $G_{t-1}(Z)$ to $G_t(Z)$. To simplify notation, we assume that we are given a random variable $X$ with a probability density $p$ on $\mathbb{R}^k$. We are interested in finding a function $g : \mathbb{R}^k \to \mathbb{R}^k$, so that the transformed variable $X' = X + \eta g(X)$ for small $\eta > 0$ has a density closer to $p_*$, while closeness is measured by the KL divergence $L(\cdot)$.

The consequence of the following theorem shows that with an appropriately chosen $g(\cdot)$, the transformation $X \to X + \eta g(X)$ can always reduce the KL divergence $L(\cdot)$, and so transformation $X + \eta g(X)$ is an improvement from $X$.

Theorem 3.1. Under the assumptions in Section 3.1.2, let $g : \mathbb{R}^k \to \mathbb{R}^k$ be a continuously differentiable transformation such that $\|g(\cdot)\| \leq a$ and $\|\nabla g(\cdot)\| \leq b$. Let $p$ and $p'$ be the probability densities of random variables $X$ and $X'$, respectively, such that $X' = X + \eta g(X)$ where $0 < \eta < \infty$. 

min(1/b, h_0/a). Then there exists a positive constant c such that:
\[
L(p') \leq L(p) - \eta \int p_s(x) \nabla D(x) \cdot g(x) \, dx + c\eta^2 + c\epsilon.
\]
The proof is given in Appendix B.

If \( \epsilon \) is large, i.e., if the discriminator deviates from the optimal discriminator by a lot, then \( c\epsilon \) will dominate the right-hand side of the inequality and so whether or not \( L(p') < L(p) \) is unknown, which means that the generator may degrade. This is not surprising, \( \epsilon \) can become large, for example, when the sample is small or when the function class from which the discriminator is chosen is poor.

To examine the dependency on \( \eta \), let us assume that \( \epsilon \) is as small as \( \eta \) so that \( c\eta \) does not dominate. Then, the theorem implies that we should choose \( g(x) \) to be
\[
g(x) = s(x)\nabla D(x)
\]
where, as before, \( s(x) > 0 \) is an arbitrary scaling factor. With this choice of \( g \), and letting \( \epsilon = \eta \), we have
\[
L(p') \leq L(p) - \eta \int p_s(x)s(x) \| \nabla D(x) \|^2 \, dx + 2c\eta^2. \tag{17}
\]

This means that \( L \) will be reduced for a sufficiently small \( \eta \) unless the following functional gradient vanishes
\[
\int p_s(x)s(x) \| \nabla D(x) \|^2 \, dx.
\]

The vanishing condition implies that \( D(x) \) is a constant when \( p_s \) has full support on \( \mathbb{R}^k \). In this case, the discriminator is unable to distinguish the real data from the generated data. Thus, it is implied that letting \( g(x) = s(x)\nabla D(x) \) makes the probability density of generated data closer to that of real data until the discriminator becomes unable to distinguish the real data and generated data.

We note that taking \( g(x) = s(x)\nabla D(x) \) is analogous to taking a gradient descent step of \( L(p) \) in the function space, so that a step is taken to modify the function instead of the model parameters. Therefore, Theorem 3.1 presents a functional gradient view of variable transformation that can always improve the quality of the generator — when the quality is measured by the KL divergence between the real data and the generated data.

If we repeat the process described above, Algorithm 1 is obtained. We call it composite functional gradient learning of GAN (CFG-GAN), or simply CFG. CFG forms \( g_t \) using the functional gradient, as suggested by Theorem 3.1. Also note that the continuous theory with general \( f \)-divergences leads to the CFG algorithm too, as shown earlier.

By cascading (17) from \( t = 1 \) to \( t = T \), we obtain:
\[
L(p_{tr}) \leq L(p_0) - \eta \sum_{t=1}^{T} \int p_s(x)s_t(x)\| \nabla D_t(x) \|^2 \, dx + 2Tc\eta^2
\]
where \( p_{tr} \) is the probability density of generated data after updating the generator \( T \) times, and \( p_0 \) is the density of \( G_0(Z) \). With \( \eta = 1/\sqrt{T} \), this leads to
\[
\frac{1}{T} \sum_{t=1}^{T} \int p_s(x)s_t(x)\| \nabla D_t(x) \|^2 \, dx \tag{18}
\]
\[
\leq (L(p_0) - L(p_{tr}))/\sqrt{T} + 2c\eta
\]
\[
= (L(p_0) - L(p_{tr}))/\sqrt{T} + 2c/\sqrt{T} = O(1/\sqrt{T}) \tag{19}
\]

This implies \( \lim_{t \to \infty} \int p_s(x)s_t(x)\| \nabla D_t(x) \|^2 \, dx = 0 \). Otherwise, (18) would be no smaller than some positive constant, but (19) goes to 0 as \( T \) goes to infinity. With a continuity condition (see Appendix B.5), this further implies that as \( t \) increases, \( \nabla D_t(x) \to 0 \) and so \( D_t(x) \) approaches a constant if \( p_s \) has full support on \( \mathbb{R}^k \). That is, in the limit where \( T \to \infty \) and \( \eta = \epsilon = 1/\sqrt{T} \), the discriminator \( D_T(x) \) is unable to distinguish the real data from the generated data, and the algorithm converges.

4 ALGORITHMS

Starting from the CFG algorithm above, we empirically explored algorithms using image generation as an example task. This section describes variants of CFG that were found to be efficient and effective and discusses their relation to the original GAN.

Notation: The algorithms introduced below assume that parametric model definitions (e.g., neural network architectures) are given for use as a discriminator and others. We write \( \theta_D \) for the model parameters of \( D \) (or \( \theta_G \) for \( G \)).

4.1 Empirical behavior of CFG on image generation

In this section, we first describe empirical issues of CFG when applied to image generation. We then provide a theoretical interpretation of the issues and a solution to them.

CFG (Algorithm 1) optimizes a discriminator to convergence with a fixed generator in every iteration. This causes two empirical issues when applied to image generation. First, its computation is prohibitively expensive. Second, it is apparently harmful to excessively update the discriminator with a fixed generator; let us broadly call it overtraining. One example of overtraining we observed is as follows. We start with \( G_0 \) that generates high-quality images as a result of being trained elsewhere. As we keep updating discriminator \( D \) with the generator fixed to \( G_0 \), the discriminator starts assigning larger and larger values to real data and smaller values to generated data. But also it starts assigning large values (even larger than to real data) to garbled images that look like neither real data nor generated data. This pushes the generator in their directions in generator update as \( \nabla D(x) \) points to them, and degrades the generator.

Our theory above assumes that essentially, any data point in \( \mathbb{R}^k \) has some possibility of being real as well as some possibility of being generated, and that \( D(x) \approx D(x) \) indicates which is more likely. If it is reasonable to expect
that the pdf ratio \( D(x) = \ln \frac{p_D(x)}{p_G(x)} \approx 0 \) for the images that look like neither real nor generated, then having a large \( D(x) \) for such images means that the discriminator \( D \) deviates a lot from the optimal discriminator \( D^* \), i.e., \( \epsilon \) in the \( \epsilon \)-approximation condition is large. Thus, according to our theory, the degradation of the generator in the case above results from large \( \epsilon \).

Fortunately, we found that early stopping prevents overtraining. These problematic images belong to the low-density region where both \( p_D(x) \) and \( p_G(x) \) are small. From the viewpoint of classification learning, this is \( D^* \)'s failure of generalizing to unseen (and rarely occurring) data. If we regard it as a peculiar form of overfitting, it makes sense that early stopping, a common technique for preventing overfitting, can counteract it. Early stopping also solves the issue of expensive computation.

The harm of discriminator overtraining has been noted also in the training of GANs. In the analysis of GAN training by [1], which led to WGAN [2], it was shown that essentially, the optimal (as well as near-optimal) discriminator \( d_i(x) \in [0, 1] \) is harmful if real data and generated data are contained in respective low-dimensional manifolds (and so their distributions do not admit a density). With this assumption, the optimal \( d_i \) becomes a perfect classifier that achieves \( d_i(x) = 1 \) on the support of the real data distribution and \( d_i(x) = 0 \) on that of generated data. To see the relation between [1] and our analysis, note that as we use a logistic model \( d(x) = \frac{1}{1 + \exp(-D(x))} \), we have: \( d(x) = 1 \) iff \( D(x) = -\infty \), \( d(x) = 0 \) iff \( D(x) = +\infty \). This means that the optimal and yet harmful discriminator \( d_i \) of [1] is the kind of discriminator we also wish to avoid in modeling data, as expressed in our assumption \( |D(x)| < \infty \) (implied by \( |D(x)| < \infty \) and \( D(x) \approx D(x) \)). We found that such an extreme discriminator can also be avoided by early stopping.

Our assumptions do not hold if the supports of data distributions are indeed contained in respective low-dim manifolds. In that case, our approach should be viewed as approximating such hard and spiky distributions without a density by soft and smooth distributions with nonzero densities, which are much easier to work with. A discriminator can be encouraged to behave as assumed by, e.g., adding a small Gaussian noise to every observed data point [1]. Our empirical finding is, however, that noise addition is not needed for our algorithms; stable training with good performances can be achieved when we combine, as in the algorithms presented below, early stopping of discriminator training (like GANs) with functional gradient learning in generator update (unlike GANs). The latter ensures improvement of the generator, and we will later revisit this point.

### 4.2 ICFG: Incremental CFG

We therefore considered an incremental variant of CFG, \textit{incremental CFG of GAN (ICFG)}, shown in Algorithm 2. ICFG incrementally updates a discriminator little by little interleaved with the generator updates, so that the generator can keep providing new and more challenging examples to prevent the discriminator from going into an undesirable state. That is, similar to GANs, ICFG alternates between \( U \) updates of the discriminator using \( U \) minibatches (where \( U \) is a meta-parameter) and one update of the generator.

The switch to incremental update was for improving \( \epsilon \) (and efficiency); in that sense, our theory could still apply here. However, very small \( U \) (e.g., \( U = 1, 5, 10 \)) works well as shown later. In this case, it is unlikely that \( \epsilon \) (the deviation of \( D \) from the optimum) is always small, especially, at the beginning of training, and so an additional analysis is required to explain the situation. Informally, imagine smooth surrogate distributions, which are close to flat at the beginning and gradually approach to the true distributions as more and more data points are observed as training proceeds. We conjecture that when such surrogate distributions are considered in place of the true distributions, \( \epsilon \) could be small, and so improvement of the generator could be explained.

ICFG shares a nice property with CFG that there is no need to design a complex generator model. The generator model is automatically and implicitly derived from the discriminator, and it dynamically grows as training proceeds. Figure 1 illustrates a generator created by ICFG with \( T = 3 \) (i.e., 3 iterations). As is clear from the illustration, the generator forms a residual net [12], where each building block \( g_t \) is automatically derived from the discriminator at time \( t \).

A shortcoming of ICFG, however, is that the implicit generator network can become very large. At time \( t \), the size of the generator network is in \( O(t) \), and therefore, the cost for computing \( G_t(z) \) starting from scratch is in \( O(t) \). This means that the computational cost for performing \( T \) iterations of training could be in \( O(T^2) \). Therefore, on a task that requires many iterations (i.e., a large \( T \)), training would become quite expensive. We found that image generation requires a relatively large \( T \), e.g., \( T > 1000 \), and that \( T \) in this order is problematic, causing slow training, a large model that takes up a lot of space, and slow image generation.

### 4.3 xICFG: Approximate incremental CFG

As a solution to the issue of large generators, we propose \textit{Approximate Incremental CFG (xICFG, Algorithm 3)}. xICFG periodically compresses the generator obtained by ICFG, by training an approximator of a fixed size that approximates the behavior of the generator obtained by ICFG. That is, given a definition

---

2. We write “\( d_i \)” for “\( D_i \)” of the perfect discrimination theorems in [1].
of an approximator $\bar{G}$ and its initial state, xICFG repeatedly alternates the following:

- Using the approximator $\bar{G}$ as the initial generator, perform $T$ iterations of ICFG to obtain generator $G$.
- Update the approximator $\bar{G}$ to achieve $G(z) \approx \bar{G}(z)$.

The generator size is again in $O(T)$, but unlike ICFG, which requires $T$ to be large (e.g., $T > 1000$) for complex tasks such as image generation, $T$ for xICFG can be small (e.g., $T = 15$), and so xICFG is efficient. Optionally, one can perform input pooling for reducing computation, as was done in our short paper [19], but in this work we focus on xICFG without input pooling, which is simpler.

A small $N$ (the number of data points used for approximator update) and a small $T$ would reduce the runtime of one iteration of xICFG, but they would increase the number of required iterations, as they reduce the amount of the improvement achieved by one iteration of xICFG, and so a trade-off should be found empirically. In particular, one set of meta-parameters achieved stable training in all the tested settings across datasets and network architectures, as shown later.

Our theory does not apply to xICFG as a whole, but it applies to ICFG performed in each iteration of xICFG to the extent discussed above. Compression of the generator ($G$ grown by ICFG) by approximating its behavior with a smaller network (approximator $\bar{G}$) is related to distillation [14]. xICFG’s performance partly depends on the representation power of $\bar{G}$, which can become a bottleneck, and we will later report empirical results obtained by both high-capacity $G$ and low-capacity $\bar{G}$.

### 4.4 Relation to GAN

It is known that training of GANs can be hard due to its instability. In this section, we show that GAN training (Algorithm 4) can be regarded as a coarse approximation of ICFG, and in particular, it is closely related to a special case of xICFG that sets the meta-parameters to extreme values. This viewpoint leads to some insight into GAN’s instability.

We start with the fact that GANs with the logistic model (and so $d(x) = \frac{1}{1+\exp(-D(x))}$) and ICFG share the discriminator update procedure as both minimize the logistic loss. This fact becomes more obvious when we plug $d(x) = \frac{1}{1+\exp(-D(x))}$ into the GAN discriminator update step, Line 5 of Algorithm 4.

Next, we show that the generator update of GAN is equivalent to coarsely approximating a generator produced by ICFG; in more detail, it is equivalent to taking one step of gradient descent in order to approximate the generator produced by ICFG with $T = 1$. To see this, first note that GAN’s generator update (Line 8 of Algorithm 4) requires the gradient $\nabla_{G} \ln(1 - d(G(z)))$. Using $d(x) = \frac{1}{1+\exp(-D(x))}$ again, and writing $[v]_{i}$ for the $i$-th component of vector $v$, the $k$-th component of this gradient can be written in terms of $D$ as:

$$
\left[ \nabla_{\theta_{D}} \ln(1 - d(G(z))) \right]_{k} = \left[ \nabla_{\theta_{D}} \ln \left( \frac{\exp(-D(G(z)))}{1+\exp(-D(G(z)))} \right) \right]_{k}
= \left[ -s_{0}(G(z)) \right]_{k} \left[ \nabla D(G(z)) \right]_{k} \frac{\partial g(G(z))}{\partial \theta_{G}}_{k}
$$

where $s_{0}(x) = \frac{\exp(-D(x))}{1+\exp(-D(x))}$, a scalar resulting from differentiating $f(y) = -\ln \left( \frac{\exp(-y)}{1+\exp(-y)} \right)$ at $y = D(x)$.

Now suppose that we apply ICFG with $T = 1$ to a generator $G$ to obtain a new generator $G'$:

$$
G'(z) = G(z) + \eta s(G(z)) \nabla D(G(z))
$$

and then we update $G$ to approximate $G'$ so that

$$
\frac{1}{2} \left\| G'(z) - G(z) \right\|^{2}
$$

is minimized as in Line 5 of xICFG. To take one step of gradient descent for this approximation, we need the gradient of the square error above with respect to $\theta_{G}$. It is easy to verify that the $k$-th component of this gradient is:

$$
\left[ \nabla_{\theta_{G}} \frac{1}{2} \left\| G'(z) - G(z) \right\|^{2} \right]_{k} = \left[ -s_{0}(G(z)) \right]_{k} \left[ \nabla D(G(z)) \right]_{k} \frac{\partial g(G(z))}{\partial \theta_{G}}_{k}
$$

By setting the scaling factor $s(x) = s_{0}(x)/\eta$, this is exactly the same as (20), required for GAN’s generator update. (Recall that our theory and algorithms accommodate an arbitrary data-dependent scaling factor $s(x) > 0$.)

Thus, algorithmically GAN is closely related to a special case of xICFG that does the following:

- Let ICFG update the generator just once (i.e., $T = 1$).
- To update the approximator, take only one gradient descent step with only one mini-batch (i.e., small $N$)
instead of optimizing to the convergence with many examples. Therefore, the degree of approximation could be poor.

The same argument applies also to the log$d$-trick variant of GAN. The generator update with the log$d$ trick requires the same gradient as (20) except that $s_0$ becomes $s_1(x) = \frac{1}{1+\exp(-D(x))}$, note that the change from $s_0(x) = \frac{1}{1+\exp(-D(x))}$ is the sign in front of $D$. Thus, GAN with the log$d$ trick is also closely related to the special case of xICFG above.

To compare GANs with and without the log$d$ trick, consider the situation where generated data $x$ is very far from the real data and therefore $D(x) \ll 0$. In this situation, we have $s_0(x) \approx 0$ without the log$d$ trick, which would make the gradient (for updating $\theta_G$) vanish, as noted in [10], even though the generator is poor and so requires updating. In contrast, we have $s_1(x) \approx 1$ with the log$d$ trick in this poor generator situation, and when the generated data $x$ is close to the real data and therefore $D(x) \approx 0$, we have $s_1(x) \approx \frac{1}{2}$. Thus, with the log$d$ trick, the scaling factor of the gradient is likely to fall into $[\frac{1}{2}, 1]$, which is more sensible as well as more similar to our choice ($s(x) = 1$) for the xICFG experiments, compared with GANs without the trick.

xICFG vs. GANs: In spite of their connection, GANs are unstable, and xICFG with appropriate meta-parameters is stable (shown later). Thus, it is inferred that GAN’s instability derives from what is unique to GANs, the two bullets above – an extremely small $T$ and coarse approximation. Either can cause degradation of the generator, and when this happens, a GAN generator could fail to keep providing challenging examples to the discriminator, which would disrupt the balance of the progress of the discriminator and that of the generator, leading to instability.

ICFG vs. GANs: We have contrasted GANs and xICFG. Now we compare generator update of GANs and that of ICFG to consider the algorithmic merits of our functional gradient approach. The short-term goal of generator update can be regarded as the increase of the discriminator output on generated data, i.e., to have $D(G_{t+1}(z)) > D(G_t(z))$ for any $z \sim p_z$. ICFG updates the generator by $G_{t+1}(z) = G_t(z) + \eta \nabla D(G_t(z))$, and so with small $\eta$, $D(G_t(z))$ is guaranteed to increase for any $z$. This is because by definition $\nabla D(G_t(z))$ is the direction that increases the discriminator output for $z$, and it is precisely obtained on the fly for every $z$ at the time of generation.

By contrast, GAN training stochastically and approximately updates $\theta_G$ using a small sample (one mini-batch SGD step that backpropagates $\nabla D$), and so GAN’s update can be noisy, which can lead to instability through generator degradation. Noise in each mini-batch SGD step would not be an issue, for example, in standard classifier training because the noise could be collectively cancelled out after many steps are taken. The GAN setting is different in that each generator update is immediately followed by discriminator update where the generator is used to produce input, which makes it prone to cascading failure.

5 Experiments

We tested xICFG on the image generation task.

5.1 Experimental setup

5.1.1 Baseline methods

For comparison, we tested the original GANs without the log$d$ trick (‘GAN0’) and with the log$d$ trick (‘GAN1’), motivated by their relation to xICFG as analyzed above. As a representative of state-of-the-art methods, we tested WGAN with the gradient penalty [WGANpp] [11]. WGANpp has been shown to achieve stable training on a number of network architectures and datasets and rival or outperform a number of previous methods such as the original WGAN with weight clipping, Least Squares GAN [24], Boundary Equilibrium GAN [3], denoising feature matching [45], and Fisher GAN [30]. We also experimented with three of the more recent GAN training methods, which will be described later with their results.

5.1.2 Evaluation metrics

Making reliable likelihood estimates with generative adversarial models is known to be challenging [42], and we instead evaluated the visual quality of generated images by adopting the inception score [40] using datasets that come with labels for classification. The intuition behind this score is that high-quality images should lead to high confidence in classification. It is defined as $\exp(\mathbb{E}_{x \sim P}(\mathbb{E}_{y \sim P(y|x)} | p(y))$ where $p(y|x)$ is the label distribution conditioned on generated data $x$ and $p(y)$ is the label distribution over the generated data. Following previous work (e.g., [46], [5]), the probabilities were estimated by a classifier trained with the labels provided with the datasets (instead of the ImageNet-trained inception model used in [40]) so that the image classes of interest were well represented in the classifier. We, however, call this score the ‘inception score’, following custom. We note that the inception score is limited, e.g., it would not detect mode collapse or missing modes. Apart from that, we found that it generally corresponds well to human perception.

In addition, we used Fréchet inception distance (FID) of [13]. FID measures the distance between the distribution of $f(x^*)$ for real data $x^*$ and the distribution of $f(x)$ for generated data $x$, where function $f$ is set to convert an image to the internal representation of a classifier network to obtain function $f$ we used the same classifiers as used for the inception score evaluation. Let $P_1$ and $P_2$ be the two distributions of comparison, and let $\mu_1, \mu_2$ be their means and let $\Sigma_1, \Sigma_2$ be their covariance matrices. Then, the distance $d(P_1, P_2)$ we measure is defined by $d^2(P_1, P_2) = |\mu_1 - \mu_2|^2 + tr(\Sigma_1 + \Sigma_2 - 2\Sigma_1\Sigma_2)^{1/2}$. If $P_1$ and $P_2$ are multivariate normal distributions (which can be completely described by the mean and covariance), then $d(P_1, P_2)$ can be proved to be the Fréchet distance [7]. One advantage of this metric is that it would be high (poor) if mode collapse occurs, and a disadvantage is that its computation is relatively expensive.

In the results below, we call these two metrics the (inception) score and the (Fréchet) distance.

5.1.3 Data

We used MNIST, the Street View House Numbers dataset (SVHN) [32], and the large-scale scene understanding (LSUN) dataset [3]. These datasets are provided with class labels (digits

0’ – ‘9’ for MNIST and SVHN and 10 scene types for LSUN). A number of studies have used only one LSUN class (‘bedroom’) for image generation. However, since a single-class dataset would preclude evaluation using class labels described above, we instead generated a balanced two-class dataset using the same number of training images from the ‘bedroom’ class and the ‘living room’ class (LSUN BR+LR). Similarly, we generated a balanced dataset from ‘tower’ and ‘bridge’ (LSUN T+B). The number of the images used as the ‘bedroom’ class and the ‘living room’ class (LSUN BR+LR).

1.4 million (LSUN T+B). The number of held-out examples whose images are larger (64×64) was set to 10K (MNIST and SVHN), 32K (LSUN BR+LR), and 17K (LSUN T+B). The LSUN images were shrunk and cropped into 64×64 as in previous studies [37], [2]. The pixel values were scaled into [−1, 1].

5.1.4 Network architectures

The tests methods require as input a network architecture of a discriminator and that of an approximator or a generator. Among the numerous network architectures we could experiment with, we focused on two types with two distinct merits – good results and simplicity.

The first type (convolutional; stronger) aims at complexity appropriate for the dataset so that good results can be obtained. On MNIST and SVHN, we used an extension of DCGAN [37], adding 1×1 convolution layers. The DCGAN discriminator consists of convolution layers with stride 2 and batch normalization, and the generator is essentially the reverse of the discriminator, using transposed convolution layers with stride 2 and batch normalization. For LSUN, whose images are larger (64×64) and whose number of training examples is also larger, we used a residual net (ResNet) [12] of four residual blocks, which is a simplification from the WGANgp code release, for both the discriminator and the approximator/generator. Details are given in Appendix C.2.1.

These networks include batch normalization layers [18]. [11] states that WGANgp does not work well with a discriminator with batch normalization. Although it would be ideal to use exactly the same networks for all the methods, it would be rather unfair for the other methods if we always remove batch normalization. Therefore, we removed batch normalization from D (as suggested by [11]) for experimenting with WGANgp while we used the network definitions as they are for the rest; also, we tested cases without batch normalization anywhere for all the methods.

The second type (fully-connected G or G; weaker) uses a minimally simple approximator/generator, consisting of two 512-dim fully-connected layers with ReLU, followed by the output layer with tanh, which has a merit of simplicity, requiring less design effort. We combined it with a convolutional discriminator, the DCGAN extension above.

5.1.5 xICFG implementation details

To speed up training, we limited the number of epochs of the approximator training in xICFG to 10 while reducing the learning rate by multiplying by 0.1 whenever the training loss stops going down. The scaling function $s(x)$ in ICFG (Line 7 of Algorithm 2) was set to $s(x) = 1$. To initialize the approximator $\hat{G}$ for xICFG, we first created a simple generator $G_{\text{rand}}(z)$ consisting of a projection layer with random weights set by the Gaussian distribution with zero mean and standard deviation 0.01 to produce data points of the desired dimensionality, and then trained $\hat{G}$ to approximate the behavior of $G_{\text{rand}}$. The training time reported below includes the time spent for this initialization. Unlike our short paper [19], no input pooling was performed.

5.1.6 Other details

In all cases, the prior $p_r$ was set to generate 100-dimensional Gaussian vectors with zero mean and standard deviation 1. All the experiments were done using a single NVIDIA Tesla P100.

The meta-parameter values for xICFG were fixed to those in Table 2 unless otherwise specified. For GANs, we used the same mini-batch size as xICFG, and we set the discriminator update frequency $U$ to 1 as other values often led to poorer results. The SGD update was done with rmsprop [43] for xICFG and GANs. The learning rate for rmsprop was fixed for xICFG for both the discriminator update and the approximator training, but we tried several values for GANs as it turned out to be critical. Similarly, for xICFG, we found it important to set the step size $\eta$ for the generator update in ICFG to an appropriate value. The SGD update for WGANgp was done with Adam [21] with meta-parameters set to the values suggested by [11] except that we tried several values for the learning rate. Thus, the amount of tuning effort was about the same for all. Tuning was done based on the performances on the validation set of 10K input vectors (i.e., 10K 100-dim Gaussian vectors), and we report the results on the test set of 10K input vectors, disjoint from the validation set.

5.2 Results

5.2.1 On the quality of generated images

Inception score results: First, we report the inception score results. The scores of the real data (in the held-out sets) are 9.91 (MNIST), 9.13 (SVHN), 1.84 (LSUN BR+LR), and 1.90 (LSUN T+B), respectively, which roughly set the upper bounds that can be achieved by generated images. Fig. 2 and 3 show the score of generated images (in relation to training time) with the convolutional networks with and without batch normalization, respectively. As discussed in Section 4.3 a smaller $T$ has practical advantages of a smaller generator resulting in faster generation and smaller footprints while a larger $T$ stabilizes xICFG training by ensuring that training makes progress by overcoming the degradation caused by approximation. With convolutional networks, we tested $T=15$ in addition to $T=25$ (the value shown in Table 2 which worked well for all) and found that setting $T=15$ also achieves stable training. The results in Fig. 2–3 were obtained by setting $T=15$. xICFG generally performs well compared

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>$b$</td>
<td>mini-batch size</td>
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<tr>
<td>$U$</td>
<td>discriminator update frequency</td>
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<tr>
<td>$N$</td>
<td># of examples used for updating $G$</td>
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<tr>
<td>$T$</td>
<td>number of iterations in ICFG</td>
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**TABLE 2:** Meta-parameters for xICFG.
Fig. 2: Image quality measured by the inception score in relation to training time. Convolutional networks. The legends are roughly sorted from the best to the worst.

Fig. 3: Image quality measured by the inception score in relation to training time. Convolutional networks without batch normalization anywhere. The legends are roughly sorted from the best to the worst.

Fig. 4: Image quality measured by the inception score in relation to training time. Fully-connected approximators/generators.

Fig. 5: Fréchet distance in relation to training time (left) and the inception score (right) on the runs in Fig 2. The arrows in the right graphs show the direction of time flow. On both LSUN BR+LR (up) and T+B (down), GAN0 and GAN1 suffer from mode collapse or lack of diversity; their inception score fluctuates (Fig 2) and their Fréchet distance stays relatively high. xICFG (and WGANgp) shows no sign of mode collapse (Fig 13–14) and performs well in both metrics.

(a) Real images.  
(b) “Realistic” images (xICFG)  
(c) “Creative” images (xICFG)

Fig. 6: “Realistic” and “creative” images generated by xICFG. (a) Real Golden Gate Bridge images in the training set. (b) Images generated by xICFG that look like Golden Gate Bridge though not perfect. (c) Images generated by xICFG that look like modifications of Golden Gate Bridge.
with others. WGANgp also achieves stable training, but its score generally falls a little short of xICFG. On LSUN datasets, GAN1 occasionally exceeds xICFG, but inspection of generated images reveals that it suffers from severe mode collapse. The inception score results with the simple but weak fully-connected approximator/generator are shown in Fig. 4. xICFG achieved stable training. Among the baseline methods, only WGANgp succeeded in this setting, but its score fell behind xICFG. These results show that xICFG is effective and efficient.

Fréchet distance results: Table 3 shows the Fréchet distance results evaluated at the end of training runs shown in Fig. 2 and 4. xICFG generally performs well, followed by WGANgp except that with convolutional networks on MNIST and SVHN, WGANgp and xICFG produce similar values. We found that the Fréchet distance mostly correlates with the inception score, i.e., generally, when the score is good (large), the distance is also good (small). One prominent exception is when mode collapse occurs, and Fig. 5 shows examples of this on the LSUN datasets. That is, GAN0 and GAN1 both suffer from mode collapse or lack of diversity on these datasets (Fig. 5 right); while their inception score fluctuates, the Fréchet distance stays large, correctly indicating that the distribution of generated data differs from that of real data. By contrast, xICFG and WGANgp show no sign of severe mode collapse as shown later in Fig. 13–14, and their Fréchet distance improves (goes down) as their inception score improves (goes up), outperforming GAN0 and GAN1 in both metrics (Fig. 5).

Visual inspection of generated images: Examples of generated images are shown in Fig. 11–15. The MNIST and SVHN images in Fig. 11–12 were randomly chosen and sorted by the predicted classes. To use limited space effectively, we take a more focused approach for larger LSUN images and show the ‘best’ and ‘worst’ images, in terms of the confidence of a classifier. That is, in Fig. 13–15 we show images that were assigned (by the classifier used for evaluation) the highest probability of being, e.g., a “bedroom” or a “living room” on LSUN BR+LR and also show the images with the highest entropy values. They are the best and the worst contributors to the inception score, respectively, as well.

Note that small samples may not represent the population well due to variability. Even so, it is clear that the images in Fig. 11f, 12c, 12f, 13d, 14d, 15c, and 15f suffer from low quality and/or mode collapse or lack of diversity. These images were generated by either GAN0 or GAN1.

xICFG and the best-performing baseline (WGANgp) consistently produce visibly better images than the original GANs in all the settings. Overall, we feel that visual impressions of the images generated by xICFG are sometimes better than and at least as good as those of WGANgp, which is one of the state-of-the-art methods. More image examples are shown in Appendix C.1.

No memorization: When generated images look somewhat realistic, one may wonder if the generator is memorizing training images instead of capturing the essence of images. In Fig. 6, we show examples that indicate that xICFG does something more ‘creative’ than memorization. The LSUN T+B includes a number of pictures of Golden Gate Bridge. As seen in Fig. 6a, in reality, Golden Gate Bridge’s tower component (the reddish vertical object) has four grids above the horizontal part. xICFG generates images that look like Golden Gate Bridge (Fig. 6b) though they are not perfect (the towers look good, but the wires are wobbly and the ocean is missing from some). It also generates images that look like modifications of Golden Gate Bridge (Fig. 6c), making the tower component longer with more grids, placing it with objects that are not there in reality, and so forth.

5.2.2 Transition from GAN to ‘good’ xICFG

We have shown in Section 4.4 that the original GAN is closely related to the special (and extreme) case of xICFG that sets $T$ to the minimum ($T=1$) and makes the minimal effort for updating the approximator, going over only one mini-batch just once. We also presented an insight that since xICFG with appropriate meta-parameters is stable, GAN’s instability could be due to these differences – extremely small $T$ and poor approximation.

Fig. 7: xICFG. LSUN BR+LR. 4-block ResNets. The setting almost equivalent to GANs performs poorly, similar to GANs. The performance improves as we improve the setting of $T$ and the approximator update.

<table>
<thead>
<tr>
<th></th>
<th>MNIST</th>
<th>SVHN</th>
<th>BR+LR</th>
<th>T+B</th>
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<tbody>
<tr>
<td>Convolutional</td>
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<td>(Fig. 2)</td>
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<tr>
<td>xICFG</td>
<td>3.35</td>
<td>5.29</td>
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<td>2.92</td>
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<td>WGANgp</td>
<td>3.41</td>
<td>5.34</td>
<td>3.31</td>
<td>3.90</td>
</tr>
<tr>
<td>GAN0</td>
<td>4.55</td>
<td>10.60</td>
<td>10.21</td>
<td>6.50</td>
</tr>
<tr>
<td>GAN1</td>
<td>4.56</td>
<td>5.82</td>
<td>10.31</td>
<td>10.77</td>
</tr>
<tr>
<td>Fully-conn.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Fig. 4)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>xICFG</td>
<td>3.39</td>
<td>5.83</td>
<td>4.85</td>
<td>5.23</td>
</tr>
<tr>
<td>WGANgp</td>
<td>4.67</td>
<td>6.21</td>
<td>5.80</td>
<td>6.55</td>
</tr>
<tr>
<td>GAN0</td>
<td>5.59</td>
<td>18.25</td>
<td>14.86</td>
<td>32.49</td>
</tr>
<tr>
<td>GAN1</td>
<td>38.77</td>
<td>22.40</td>
<td>11.27</td>
<td>12.84</td>
</tr>
</tbody>
</table>

TABLE 3: Fréchet distance results. Evaluated at the maximum training time of the respective graphs.

The arrows in (c) indicate the direction of time flow.
To follow up on this, we experimented with xICFG with meta-parameter settings that transition from the poor setting corresponding to GAN towards the good setting used above. The results using the convolutional networks (used in Fig. 2) on LSUN BR+LR are shown in Fig. 7. The legends in this figure represent the following:

- “poor $T$”: $T=1$
- “good $T$”: $T=15$
- “poor approx”: Poor approximation iterating only once over only one mini batch ($N=b$) for updating the approximator.
- “good approx”: Good approximation iterating 10 times over 10 mini batches ($N=10b$) for updating the approximator, as was done in Fig. 2–5.

As predicted, “(poor $T$, poor approx)$\approx$ GAN” performs just like GANs – the inception score fluctuates a lot and the Fréchet distance stays large; manual inspection of images indicates severe mode collapse. When we improve either the value of $T$ (“(good $T$, poor approx)”) or approximation (“(poor $T$, good approx)”), training becomes more stable and the performance in both metrics improves as training proceeds; however, the performance improvement stops without catching up with “(good $T$, good approx)”. That is, in order to obtain the best results, we need to have both right – sufficiently large $T$ and good approximation. The results are consistent with our theoretical insight into GANs presented earlier and support our CFG approach.

### 5.2.3 On the discriminator output values

![Fig. 8: Relations between image quality and $|D(\text{real})-D(\text{gen})|$ ($=\Delta_D$).](image)

The arrows indicate the direction of time flow. A correlation is observed both when training is succeeding (blue solid arrows) and failing (red dotted arrows).

Successful training should make it harder and harder for the discriminator to distinguish real images and generated images, which would manifest as the discriminator output values for real images and generated images becoming closer and closer. We quantify this notion by the difference between discriminator output values for real images and generated images averaged over time intervals of a fixed length, obtained as a by-product of the forward propagation for updating the discriminator. We call it $'[D(\text{real})-D(\text{gen})]'$ or $\Delta_D$ in short.

Fig. 8 shows that, as expected, $\Delta_D$ generally correlates with the progress of training. When training is going well (indicated by blue solid arrows), $\Delta_D$ decreases and the inception score improves as training proceeds. When it is failing, $\Delta_D$ goes up rapidly and the inception score degrades rapidly; see the change from the state #3 to #4 in Fig 8c. Here, due to excessive training, the discriminator is overfitting little by little to relatively small MNIST training data (#2 to #3), increasing $\epsilon$ of the $\epsilon$-approximation. (Note that this is overfitting in the standard sense as it was confirmed that the average of $D(x)$ on the real data in the held-out set became smaller and smaller than that of the training set.) That slows down and eventually stops the progress of the generator, resulting in the rapid increase of $\Delta_D$ and rapid degradation of the generator (#3 to #4). In practice, training should be stopped before the rapid growth of $\Delta_D$ – early stopping. Thus, the decrease/increase of $\Delta_D$ values, which can be obtained at almost no cost during training, can be used as an indicator of the status of xICFG training.

Additionally, it might be worth mentioning that the $\Delta_D$ value is related to the sum of the KL divergence and the reverse KL divergence between the two distributions, which were shown to be optimized by the CFG algorithm (Section 2). Details are given in Appendix C.2.3.

### 5.2.4 On the values of $U$ and $N$

We have shown that $T$ can be reduced for practical advantages in some cases, and here we consider the effects of changing $U$ (discriminator update frequency) and $N$ (the number of examples used for updating the approximator) from their default values, $U=1$ and $N=10b$ where $b$ is the mini-batch size.

Essentially, a larger $U$ may make the discriminator closer to the optimum, but a very large $U$ would increase the risk of discriminator overtraining. A larger $N$ would make better approximation, but it may slow down training. If one takes the viewpoint that a discriminator should capture the essence of real data, and it should become better and better in doing so each time it is updated, then one can argue that a larger (but not too large) $U$ would increase the amount of discriminator improvement per each call of ICFG, and therefore, also increase the amount of xICFG generator improvement per xICFG iteration. This viewpoint suggests that to benefit from a larger $U$, we should also consider increasing $N$ so that the approximator $\hat{G}$ can keep up with the generator instead of becoming a bottleneck.

![Fig. 9: Larger values for $U$ and $N$ on MNIST. Convolutional.](image)

We tested $U=5$ and $U=10$ with convolutional networks used in Fig. 2 and found that stable training can be achieved also with these values while in some cases $N$ also needed to be increased as expected. On MNIST the increase of $U$ (and $N$) improved the Fréchet distance while producing similar inception scores (Fig. 9). On the other datasets, a larger $U$ and/or $N$ either exhibited similar performances (SVHN) or slowed down training (LSUN), and it was not clear whether doing so was advantageous.

We note that MNIST differs from the other tested datasets in that training data is much smaller (2–10% of the others)
and that the images are simpler (grayscale digits). These differences make MNIST somewhat uniquely prone to discriminator overfitting; indeed, if trained excessively long with the default meta-parameters, $\Delta_D$ starts going up (Fig 8c). On MNIST, a larger $U$ and $N$ makes training more stable (no increase of $\Delta_D$ after 30K seconds) and improves the Fréchet distance.

Thus, our finding is that the default values are a good starting point, and it depends on the datasets and possibly network architectures whether more careful meta-parameter tuning pays off.

5.2.5 Comparison with recent GAN variants

Finally, we compare xICFG with more recent GAN training methods that appeared around the first publication of this work: spectral normalization (hereafter GAN-sn) [29] and zero-centered gradient penalty regularization (GAN-gp) [26]. These methods stabilize GAN training by normalization/regularization of the discriminator. GAN-sn constrains the weight matrix of each layer to have the unit 2-norm. GAN-gp penalizes large gradients by a regularization term $\gamma \mathbb{E}_{z \sim q} \| \nabla D(x) \|^2$ where $q$ is the distribution of either real data or generated data (corresponding to $R_1$- or $R_2$- regularizer of [26]), and we tested both. Following the tuning protocol above, we made substantial efforts to obtain their best performances; details are given in Appendix C.2.4.

In this series of experiments, we performed 3 runs per method using 3 different random seeds in order to account for the variability caused by random factors such as weight initialization. For comparison, we also performed 3 runs of WGANgp and the original GANs.

Fig. 10 shows the scores ($x$-axis) and the Fréchet distances ($y$-axis) on (a) the convolutional networks and (b) the fully-connected approximators/generators, used in Fig. 2 and 4, respectively. Each method has three points in each graph, except that the original GAN results are shown only when they are as good as the rest and so they can fit in the same graph. Since higher scores and smaller distances are better, the points closer to the bottom right of each graph are better. The baseline methods are organized into two groups: ‘Original GANs’ (GAN0 and GAN1) and ‘Improved GANs’ (GAN-sn, GAN-gp of two types, and WGANgp);

Improved GANs indeed show clear and consistent improvements over the original GANs. In many cases, the performances of the original GANs are poor to the extent that they are out of range of the graphs. xICFG performs consistently well, irrespective of the random seeds, and it generally exceeds or rivals the improved GANs. It should also be noted again, however, that the generator model of xICFG is larger than the baseline methods; thus, footprints are larger and generation is slower, which may need consideration in practical applications.

6 Related Work

Analyzing and improving GANs: Improvements of GANs are often based on analyses of GAN training. As a result, they typically stay within the minimax optimization framework of the original GAN. In contrast, our framework is that of greedy learning of functional compositions, which puts our work in a relatively unique position. There are a large number of studies related to GANs, and here we focus on a small number of those perceived as most related.

One approach to improving GANs involves change of the training objective, e.g., WGAN [2], [1]. Least squares GAN [24], and f-GAN [34]. We have discussed f-GAN in Section 2.2.1 and the low-dim manifold view of [1] in Section 4.1. [11] regularizes the discriminator of WGAN with the gradient penalty term (WGANgp), adopted by many studies, and we compared it with xICFG in our experiments.

Another approach tries to do normalization or GANs. Spectral normalization constrains the weight matrix of each layer to have the unit 2-norm, proposed by [29] and adopted for class-conditional GANs [4], [47]. Regularization of the discriminator by penalizing large $\| \nabla D(x) \|$ was proposed in [38], [26]. Jacobian clamping [35] keeps the singular values of the input-output Jacobian of the generator in a pre-defined range. [31] regularizes the generator by penalizing large gradients with respect to model parameters of the discriminator. [27] penalizes large gradients with respect to model parameters both on the generator and the discriminator. We reported performance comparison with spectral normalization [29] and the gradient penalty regularization methods of [26].

While the theoretical motivations of these methods vary (e.g., approximating the effect of adding noise [38], [26], a local stability analysis near an equilibrium point [31], [26], a Jacobian analysis of the gradient vector field [27]), it appears that generally, these methods stabilize GAN training by preventing sudden large changes which could immediately push the minimax game into a vicious cycle. [4] and [27] have
Fig. 11: MNIST. Random samples sorted by the predicted classes. (a-c) Convolutional networks. (d-f) Fully-connected $\hat{G}$ or $G$.

Fig. 12: SVHN. Random samples sorted by the predicted classes. (a-c) Convolutional networks. (d-f) Fully-connected $\hat{G}$ or $G$.

Fig. 13: LSUN BR+LR (64×64). 4-block ResNets. These images are most likely bedrooms (1st row), most uncertain (2nd row), most likely living rooms (3rd row), among a random sample of 1000, according to a classifier.

Fig. 14: LSUN T+B (64×64). 4-block ResNets. These images are most likely towers (1st row), most uncertain (2nd row), most likely bridges (3rd row), among a random sample of 1000, according to a classifier.

Fig. 15: Weak $\hat{G}/G$ (fully-connected) on LSUN BR+LR (a-c) and T+B (d-f). 64×64. The images were chosen as in Fig. 13 and 14.
noted cases where regularization stabilizes GAN training but leads to a poor solution. Our xICFG is free of this potential problem since it does not involve regularization. On the other hand, many of these regularizationnormalization techniques (in particular, those which work on the discriminator) can be easily integrated into xICFG, and doing so may be useful in some situations.

Unrolled GANs [28] optimize the generator with respect to an unrolled optimization of the discriminator in order to make generator update closer to the state of using the optimal discriminator without actually updating the discriminator. There is a high-level similarity between unrolled GANs and xICFG as both involve multiple states of the discriminator.

[20] generated high-resolution images by incrementally adding layers for higher resolutions, using WGANgp as a base learner. We view xICFG as a component that, similar to WGANgp, can be used to build higher levels of architecture such as that of [20] and stacked GANs [15], [48].

[22] described a cascading process related to CFG, motivated by Langevin dynamics sampling, called introspective neural networks. Based on the theory of Langevin, their generation process requires repeated noise addition, and so our generation is simpler.

Functional gradient learning: Our approach can be regarded as functional gradient learning. Similar to gradient boosting, where more and more decision trees are added to the model as training proceeds, ICFG adds more and more components (layers if the discriminator is a neural network) to the generator, following the gradients in a function space.

Natural gradient descent [17], [16] has been applied to neural networks for deep learning, e.g., [41], [25], [36], [39]. It can be regarded as moving in a function space so that the change in the objective is maximized per a fixed amount of move in the function space, where moves are measured by the KL divergence. However, the function space explored by natural gradient descent corresponds to the one obtained by changing parameters of a fixed neural network structure. By contrast, CFG and its variants dynamically grows a generator, as illustrated in Fig. 1.

In parallel to our work, [33] proposed gradient layers for fine-tuning WGAN, which is similar to our ICFG. As noted above, ICFG suffers from the issue of large generators if used for image generation from scratch, and so does insertion of gradient layers. This issue was the motivation for xICFG, which periodically compresses the generator by approximation.

7 CONCLUSION
In the generative adversarial learning setting, we considered a generator that can be obtained using composite functional gradient learning. Our theoretical results led to the new stable algorithm xICFG. The experimental results showed that xICFG generated equally good or better images than GAN and WGAN variants in a stable manner.

REFERENCES


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