Bidirectional Generative Modeling Using Adversarial Gradient Estimation

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Abstract
This paper considers the general $f$-divergence formulation of bidirectional generative modeling, which includes VAE and BiGAN as special cases. We present a new optimization method for this formulation, where the gradient is computed using an adversarially learned discriminator. In our framework, we show that different divergences induce similar algorithms in terms of gradient evaluation, except with different scaling. Therefore this paper gives a general recipe for a class of principled $f$-divergence based generative modeling methods. Theoretical justifications and extensive empirical studies are provided to demonstrate the advantage of our approach over existing methods.

1 Introduction

Deep generative modeling has aroused a lot of interest as a method for data generation and representation learning. Consider the observed real data $X$ from an unknown distribution $p_r$ on $\mathcal{X} \subseteq \mathbb{R}^d$ and the latent variable $Z$ with a known prior $p_z$ on $\mathcal{Z} \subseteq \mathbb{R}^k$. In unidirectional data generation, we are interested in learning a transformation $G: Z \times E \rightarrow \mathcal{X}$ so that the distribution of the transformed variable $G(Z, \epsilon)$ becomes close to $p_r$, where $\epsilon \in E$ is the source of randomness with a specified distribution $p_\epsilon$ and $G$ is referred to as a generator. In many applications, bidirectional generative modeling is favored due to the ability to learn representations, where we additionally learn a transformation $E: \mathcal{X} \times E \rightarrow Z$, known as an encoder. The principled formulation of bidirectional generation is to match the distributions of two data-latent pairs $(X, E(X, \epsilon))$ and $(G(Z, \epsilon), Z)$.

Classical methods including Variational Autoencoder (VAE) [1] and Bidirectional Generative Adversarial Networks (BiGAN) [2,3] turn out to handle this task using one specific distance measure as the objective. In this paper, we generally consider the $f$-divergence which is a natural and broad class of distance measures. We discuss the advantages of this general formulation in several concerned issues including unidirectional generation, mode coverage and cycle consistency, especially for the Kullback-Leibler (KL) divergence which is our main choice.

For optimization, both VAE and BiGAN are limited to specific divergences and assumptions for the encoder and generator distributions, and hence do not apply in our general formulation. $f$-GAN [4] extends GAN [5] to $f$-divergence and can be applied in the formulation here. Like GAN, $f$-GAN introduces a discriminator to distinguish between two data-latent pairs. However, we find that limited by the minimax formulation, the discriminator loss of $f$-GAN tends to behave poorly in both statistical efficiency and training stability.

This paper proposes a new optimization method for this formulation. We present a theorem to evaluate the gradient of the divergence with respect to the generator and encoder parameters, which generally applies to various divergences and unifies the treatment of $f$-divergence GAN. Then we propose an efficient gradient estimator using a discriminator learned with Logistic regression. Based on the theory and estimation, we obtain a family of algorithms, and hence gives a general recipe for a class of principled $f$-divergence based generative modeling methods. We further propose an applicable technique and obtain an algorithm which locally minimizes several divergences simultaneously with a lower variance and stable gradients. The approach differs from existing ones that use a discriminator to estimate the objective [6-9], which is further discussed in Section 6.2.
Based on the proposed formulation with the optimization approach, we present a unifying view of VAEs and GANs. We evaluate our method extensively on synthetic datasets, Stacked MNIST, CelebA and ImageNet to demonstrate: (i) the effectiveness of the proposed optimization method for $f$-divergence minimization, and (ii) the advantages of our learned bidirectional generative models in mode coverage, realistic generation and high-level semantic representation.

**Notation** Throughout the paper, all distributions are assumed to be absolutely continuous with respect to Lebesgue measure unless indicated otherwise. Let $p_g(x|z)$ and $p_e(z|x)$ be the conditional distributions induced by $G$ and $E$. For a scalar function $h(x, y)$, let $\nabla_x h(x, y)$ denote its gradient with respect to $x$. For a vector function $g(x, y)$, let $\nabla_x g(x, y)$ denote its Jacobian matrix with respect to $x$.

## 2 Bidirectional generative modeling

### 2.1 General formulation

The goal of bidirectional generative modeling is to match the two joint distributions

$$
\min_{G, E} \mathcal{L}(p_e(x, z), p_g(x, z)),
$$

(1)

where $\mathcal{L}$ is any chosen distance measure between two probability distributions, $p_e(x, z) = p_e(x)p_e(z|x)$ is the encoder joint distribution and $p_g(x, z) = p_g(z)p_g(x|z)$ is the generator joint distribution. Let us consider a case where $\mathcal{L}$ is an $f$-divergence. Formally, given two density functions $p_e(x, z)$ and $p_g(x, z)$, abbreviated as $p_e$ and $p_g$ for simplicity, the $f$-divergence is defined by

$$
D_f(p_e, p_g) = \mathbb{E}_{p_e(x, z)}[f(r(x, z))] = \mathbb{E}_{p_e(x, z)}\left[\frac{1}{r(x, z)}\right]
$$

(2)

where $f : \mathbb{R}_+ \to \mathbb{R}$ is a convex, lower-semicontinuous function satisfying $f(1) = 0$, $\hat{f}(r) = rf(1/r)$ is a notation for convenience, and $r(x, z) = p_e(x, z)/p_g(x, z)$. Here we focus on a special case where $f$ is twice continuously differentiable and strongly convex so that the second order derivative of $f$, denoted by $f''$, is always positive. The commonly used special cases are listed in Table 1.

We parametrize the two transformations using deep neural networks and write $G\phi(z, \epsilon)$ and $E\phi(x, \epsilon)$. Examples of transformations include additive Gaussian $E(x, \epsilon) = E_\phi(x) + \phi_1 \cdot \epsilon$ where $\epsilon$ follows a Gaussian distribution, or a black-box transformation $G\phi(z, \epsilon)$ where $\epsilon$ is fed into the input or intermediate layers of the network $G$, leading to an implicit conditional distribution $p_g(x|z)$. A detailed discussion on the choice of transformations is given in Appendix. Finally our goal is to minimize the objective

$$
L(\theta, \phi) = D_f(p_e, p_g) = \int \ell(p_e, p_g) dx dz,
$$

(3)

with respect to the parameters $\theta$ and $\phi$, where $\ell(p_e, p_g)$ denotes the integrands in (2).

| Name | $f(r)$ | $r f''(r)$ | $\hat{f}(r)$ | $r \hat{f}''(r)$ |
|------|--------|------------|-------------|-----------------|
| KL   | $r \log r$ | 1          | $- \log r$ | 1               |
| RevKL | $- \log r$ | $1/r$      | $r \log r$ | 1               |
| 2JS  | $-(r + 1) \log \frac{1 + r}{2} + r \log r$ | $\frac{1}{1+r}$ | $\frac{1}{1+r}$ | 1               |
| $H^2$ | $(\sqrt{r} - 1)^2$ | $\frac{1}{2\sqrt{r}}$ | $\frac{1}{2\sqrt{r}}$ | 1               |

Table 1: List of $f$-divergences: KL, reverse KL divergence, Jensen-Shannon divergence×2, and squared Hellinger distance. When the divergence is symmetric, $\hat{f} = \hat{f}$, e.g., JS and $H^2$. 

2
2.2 Advantages

In this section, we discuss the advantages of the above formulation that minimizes the bidirectional $f$-divergence, especially the KL divergence which is the main choice in this paper. Our justifications cover three aspects of interest.

Unidirectional generation Decompose the joint KL as

$$D_{KL}(p_e, p_g) = D_{KL}(p_r(x), p_g(x)) + \mathbb{E}_{x \sim p_r(x)}[D_{KL}(p_e(z|x), p_g(z|x))],$$

where we have marginal densities $p_g(x) = \mathbb{E}_{z \sim p_e}[p_g(x|z)]$, $p_r(x) = \mathbb{E}_{z \sim p_e}(p_r(z|x))$, and the posterior $p_g(z|x) = p_g(x,z)/p_g(x)$. We prove the equivalence in Appendix A.1. Because KL is always non-negative, we know that by minimizing $D_{KL}(p_e, p_g)$, we minimize an upper bound of $D_{KL}(p_r(x), p_g(x))$, which is a standard objective for unidirectional generative modeling equivalent to maximum likelihood. By symmetry, same results also hold for $D_{KL}(p_z(z), p_r(z))$. Therefore, this bidirectional formulation can approximately achieve the goal of unidirectional generation, while the performance depends on how well the bidirectional model can match the two conditional distributions $p_e(z|x)$ and $p_g(z|x)$, or ensure the consistency between the two transformations.

Mode collapse Write the joint KL as

$$D_{KL}(p_e(x, z), p_g(x, z)) = \mathbb{E}_{p_r(x, z)} \left[ \log \frac{p_r(x)p_e(z|x)}{p_g(x)p_g(z|x)} \right].$$

We see that it imposes a heavy penalty when $p_g(x) \approx 0$ while $p_r(x) > 0$, which is a case of mode dropping. In contrast, other divergences like JS, reverse KL divergence or Square Hellinger distance do not have this property. This is consistent with the commonly known conjecture in unidirectional generation that KL has an advantage in diminishing mode collapse. However this was not well verified in practice [4], partially due to lack of effective optimization. In this work equipped with the proposed optimization approach introduced in Section 3, we are able to provide more convincing evidence on this.

Cycle consistency Another important issue in bidirectional generative modeling is the cycle consistency, roughly meaning that the inferred latent variable $E(x)$ from data $x$ can generate a data $G(E(x))$ that is very close to $x$. When using stochastic transformations, we define the cycle consistency from a probabilistic view:

$$\mathbb{E}_{x \sim p_r(x)}[\mathbb{E}_{z \sim p_e(z|x)}[\log p_g(x|z)]] = 0.$$ (5)

We would like to maximize the above quantity, that is, to reconstruct $x$ with a high probability, in order to ensure cycle consistency. Previous methods ensure cycle consistency using an explicit reconstruction error term, i.e., $\|G(E(x)) - x\|$, and commonly used norms include $L_1$ and $L_2$ [10, 11] which can be regarded as special cases of (5) with the generator being a Laplace or a Gaussian distribution. Write the joint KL equivalently as

$$D_{KL}(p_e, p_g) = -\mathbb{E}_{x \sim p_r}[\mathbb{E}_{z \sim p_e(z|x)}[\log p_g(x|z)]] - \mathbb{E}_{x \sim p_r}[D_{KL}(p_e(z|x), p_g(z))] + \mathbb{E}_{x \sim p_r}[\log p_r(x)],$$ (6)

which is proved in Appendix A.1. Note that the third term on the right-hand side of (6) is free of parameters. Hence our formulation equivalently minimizes an upper bound of the negation of (5) and hence ensures cycle consistency.

3 $f$-divergence minimization

3.1 Adversarial gradient estimation

We formally propose an optimization approach for the above formulation, leading to a general recipe for principled $f$-divergence based generative modeling. From the following theorem, we can evaluate the gradients of the $f$-divergence in objective (3) with respect to the parameters. The proof can be found in Appendix A.2.

1 For simplicity we omit the randomness $\epsilon$ in the notations of encoder $E$ and generator $G$.
Theorem 1. Let \( D(x, z) = \log(p_e(x, z)/p_g(x, z)) \). Then we have

\[
\begin{align*}
\nabla_{\theta} L &= -\mathbb{E}_{x \sim p_x, \epsilon \sim p_\epsilon} \left[ s_\theta(x, z) \nabla_x D(x, z) \right] \bigg|_{G_{\theta}(z, \epsilon)} \nabla_{\theta} G_{\theta}(z, \epsilon), \\
\nabla_{\phi} L &= \mathbb{E}_{x \sim p_x, \epsilon \sim p_\epsilon} \left[ s_\phi(x, z) \nabla_z D(x, z) \right] \bigg|_{E_{\phi}(x, \epsilon)} \nabla_{\phi} E_{\phi}(x, \epsilon),
\end{align*}
\]

(7)

where \( s_\theta(x, z) = \hat{f}''(r(x, z))/r(x, z) \) and \( s_\phi(x, z) = f''(r(x, z))r(x, z) \) are scaling factors.

This theorem presents a general formula to evaluate gradients that applies to various divergences with the only difference being the scaling, which unifies the treatment of \( f \)-divergence based generative modeling.

Notice that the gradients in (7) depend on the unknown densities \( p_e \) and \( p_g \) and thus cannot be obtained from data. We use a discriminator to estimate them. Let \( D(x, z) \) be the solution to the empirical Logistic regression problem that distinguishes between the data-latent pairs from \( p_e \) and \( p_g \):

\[
\min_{D''} \left[ \sum_{i \in S_e} \log(1 + e^{-D'(x_i, z_i)}) + \sum_{i \in S_g} \log(1 + e^{D'(x_i, z_i)}) \right]
\]

where \( S_e \) and \( S_g \) are finite samples from \( p_e(x, z) \) and \( p_g(x, z) \) respectively. When the number of samples is sufficiently large, the statistical consistency theory of Logistic regression \([12]\) indicates that \( D(x, z) \approx D(x, z) \).

Replacing \( D \) and \( r \) in the gradients (7) with \( D \) and \( \hat{r} = \exp(D) \), we obtain the maximum likelihood estimator (MLE) for the gradients. We then optimize the objective using stochastic gradient descent (SGD) and end up with a practical implementation. The convergence of the procedure follows naturally from the consistency of the estimation and the convergence results of SGD. Since the proposed approach involves an adversarially learned discriminator, we call it adversarial gradient estimation (AGE). We adopt early stopping in training \( D \) to avoid overtrained extreme discriminators. We summarize the procedure of bidirectional generative modeling using AGE in Algorithm 1.

The technique introduced in Theorem 1 can be generally applied to other tasks involving \( f \)-divergence minimization such as unidirectional generative modeling or \( f \)-divergence as a regularization term. In Appendix B we present the gradient formula and estimation in unidirectional generation.

**Algorithm 1: Bidirectional Generative Modeling using AGE**

**Input:** training set, initial parameters \( \theta, \phi, \psi \), batch-size \( n \)

1. **while not convergence do**
2. 2. **for multiple steps do**
3. 3. Sample \( \{x_1, \ldots, x_n\} \) from the training set
4. 4. Sample \( \{z_1, \ldots, z_n\} \) from the prior \( p_z(z) \)
5. 5. Sample \( \{\epsilon_1, \ldots, \epsilon_n\} \) and \( \{\epsilon'_1, \ldots, \epsilon'_n\} \) from \( p_e \) and \( p_{e'} \)
6. 6. Update \( \psi \) by descending the stochastic gradient:
7. \[
\frac{1}{n} \sum_{i=1}^{n} \nabla_{\psi} \left[ \log(1 + e^{-D_e(x_i, E_{\psi}(x_i, \epsilon_i))}) + \log(1 + e^{D_{e'}(G_{\psi}(z_i, \epsilon_i), z_i)}) \right]
\]
8. Sample \( \{x_1, \ldots, x_n\}, \{\epsilon_1, \ldots, \epsilon_n\}, \{z_1, \ldots, z_n\}, \{\epsilon'_1, \ldots, \epsilon'_n\} \) as above
9. Compute \( \theta \)-gradient: \[
\frac{1}{n} \sum_{i=1}^{n} s_\theta(G_{\theta}(z_i, \epsilon'_i), z_i) \nabla_{\theta} D_{\psi}(G_{\theta}(z_i, \epsilon'_i), z_i)
\]
10. Compute \( \phi \)-gradient: \[
\frac{1}{n} \sum_{i=1}^{n} s_\phi(x_i, E_{\phi}(x_i, \epsilon_i)) \nabla_{\phi} D_{\psi}(x_i, E_{\phi}(x_i, \epsilon_i))
\]
11. **end for**
12. **Update parameters \( \theta, \phi \) using the gradients**

13. **Return: \( \theta, \phi \)**

### 3.2 Scaling clipping

In this section, we introduce a technique to reduce the variance and stabilize training of AGE algorithms for various divergences, and further obtain a modified algorithm that is more applicable on real datasets. From Table 1 we know that for all commonly used \( f \)-divergences, one or both of the scaling factors in (7) are unbounded above or can infinitely approach 0, which may lead to the exploding or vanishing gradient
problem especially on real datasets. To address this, we propose to clip the scaling factors of each divergence into a bounded positive range.

From the definition \( f(r) = rf(1/r) \) we know \( s_\theta(x, z) = s_\phi(x, z)r(x, z) \). Consider the nearly optimal case where the two joint distributions \( p_x(x, z) \) and \( p_y(x, z) \) approximately match, and hence \( r(x, z) \approx 1 \). Because \( f'' \) and \( f''' \) are positive and continuous, we have \( s_\theta(x, z) \approx s_\phi(x, z) \approx f''(1) \) which is a positive constant. Therefore we propose to clip the density ratio \( r \) into a bounded range containing its optimal value 1. Then the consequent scaling factors globally fall into a bounded positive range containing \( f''(1) \). We call this technique scaling clipping (SC). In this way the corresponding gradient estimator has a smaller variance and we obtain a modified family of algorithms for different divergences with stable gradients.

Motivated by the local property that \( s_\phi(x, z) \approx s_\phi(x, z) \approx constant \), we consider the extreme case of scaling clipping where we set \( s_\theta = s_\phi = 1 \). By this means we obtain an algorithm which is locally equivalent to simultaneously minimizing several divergences, i.e., all the \( f \)-divergences with strongly convex \( f \). We hence call it AGE-ALL. As scaling clipping, AGE-ALL is globally bounded and thus has a smaller variance and does not suffer from the vanishing or exploding gradient problem.

3.3 Comparison with \( f \)-GAN

\( f \)-GAN [4] extends GAN to general \( f \)-divergences and makes use of their variational representation for optimization. One can also derive a bidirectional version of \( f \)-GAN solves the following minimax optimization problem:

\[
\min_{G,E} \max_D \left\{ \mathbb{E}_{p_\theta}[a_f(D(x, z))] + \mathbb{E}_{p_y}[f^*(a_f(D(x, z)))] \right\}
\]

where \( f^*(t) = \sup_{r \in \text{dom} f} \{rt - f(r)\} \) is the conjugate function of \( f \) and \( a_f \) is an output activation function specific to the \( f \)-divergence used. However, \( f \)-GAN generally obtains different training objectives from AGE given the same distance measure, especially the loss of the discriminator.

For instance, Table 2 lists the training objectives of \( f \)-GAN and AGE for KL. Note that for comparison we present AGE in the “GAN form” where we separately write the objectives for the three agents – discriminator \( D \), encoder \( E \) and generator \( G \), and in each objective we should ignore the dependence of it on the other two agents according to Theorem 1. We notice that using KL as the objective, AGE differs from \( f \)-GAN only in the \( D \) loss. Viewing the role of \( D \) as the density ratio estimator, we know that AGE obtains the MLE with higher efficiency than \( f \)-GAN. Moreover, the exponential in the \( D \) loss given by \( f \)-GAN may cause instability during training. We conduct experiments to verify the advantage of AGE against \( f \)-GAN.

We summarize the main differences between \( f \)-GAN and AGE for \( f \)-divergence minimization as follows:

- Based on Theorem 1 our framework provides a more unifying treatment of various divergences than \( f \)-GAN.
- For estimating the density ratio (or its function), AGE always applies Logistic regression which owns the highest statistical efficiency, while \( f \)-GAN, limited by the minimax formulation, uses other losses except for JS divergence and hence is not as efficient.

| Method | Objectives |
|--------|------------|
| AGE    | \( D: \mathbb{E}_{p_\theta}[\log(1 + e^{-D(x, z)})] + \mathbb{E}_{p_y}[\log(1 + e^{D(x, z)})] \) |
|        | \( E: \mathbb{E}_{p_x}[D(x, z)] \) |
|        | \( G: -\mathbb{E}_{p_y}[e^{D(x, z)}] \) |
| \( f \)-GAN | \( D: -\mathbb{E}_{p_\theta}[D(x, z)] + \mathbb{E}_{p_y}[e^{D(x, z)} - 1] \) |
|        | \( E: \mathbb{E}_{p_x}[D(x, z)] \) |
|        | \( G: -\mathbb{E}_{p_y}[e^{D(x, z)} - 1] \) |
• We obtain a single algorithm to approximately minimize several distance measures simultaneously, while f-GAN uses different objectives specific to each divergence.
• For practical considerations, our scaling clipping technique addresses the unstable gradient issue via clear justification on the globally bounded scaling, while f-GAN is heuristically motivated following GAN.

4 Unifying VAEs and GANs

In this section we establish a unifying view of VAEs and GANs. We regard BiGAN as the full version of GAN and point out that both VAEs and GANs are special cases of the general bidirectional formulation optimized using AGE, with different divergences and distribution assumptions.

4.1 Variational Autoencoders

VAEs [1] learn the encoder \( p_e(z|x) \) and the generator \( p_g(x|z) \) by minimizing the negative variational lower bound or evidence lower bound (ELBO)

\[
L_{\text{VAE}} = -\mathbb{E}_{x \sim p_r} [\mathbb{E}_{z \sim p_{e}(z|x)} [\log p_g(x|z)] - D_{KL}(p_e(z|x), p_z(z))].
\]

According to [6], we have the following relationship between \( L_{\text{VAE}} \) and our objective in [8] with \( D_f \) being KL:

\[
L_{\text{VAE}} = D_{KL}(p_e(x, z), p_g(x, z)) - \mathbb{E}_{p_r(z)} [\log p_r(x)].
\]

Because the second term on the right-hand side is free of any learnable parameters, minimizing \( L_{\text{VAE}} \) is equivalent to minimizing [8]. In the original VAE, both the encoder and generator distributions are set as factorized Gaussian distributions, leading to an analytic form of \( L_{\text{VAE}} \) that can be easily optimized. Therefore VAE is a special case of our general formulation optimized with AGE when \( L \) is KL and gradients can be evaluated analytically.

However, the Gaussian assumption in the original VAE may not be expressive enough [13][14]. Adversarial Variational Bayes (AVB) [6] extends the Gaussian encoder in VAE to an implicit distributions. Then the bound or evidence lower bound (ELBO)

\[
\log p_g(x, z) = \mathbb{E}_{z \sim p_z(z)} [\log p_{g}(x|z)]
\]

is KL and gradients \( \nabla \phi \mathbb{E}_{x \sim p_r} [D_{KL} (p_e(z|x), p_z(z))] = \mathbb{E}_{x \sim p_r, \epsilon \sim p_\epsilon} \left[ \nabla_x D'(x, z) \right] \nabla \phi \mathbb{E}_\phi (x, \epsilon)
\]

which can be derived according to Theorem 1 by noting that \( f''(r) = 1 \) for KL. Notice the relationship between \( D' \) and \( D \) defined in Theorem 1 as \( D'(x, z) = D(x, z) + \log p_g(x|z) - \log p_r(x|z) \) that has an analytic form since AVB uses a Gaussian generator. Therefore, AVB can also be regarded as a special case of our formulation involving partial gradient estimation.

4.2 Bidirectional Generative Adversarial Networks

BiGAN [2][3] directly adopts the original GAN in bidirectional generative modeling. With an additional encoder, it formulates the problem as a minimax game:

\[
\min_{G} \max_{E, D} \left\{ -\mathbb{E}_{p_r} [\log (1 + e^{-D(x, z)}))] - \mathbb{E}_{p_g} [\log (1 + e^{D(x, z))}]) \right\}
\]

When we choose \( D_f \) in [3] as JS, applying the formula in Theorem 1 we obtain the gradients as follows:

\[
\nabla_{\theta} L = -\mathbb{E}_{z \sim p_z, \epsilon \sim p_\epsilon} [\nabla_{\theta} \log (1 + e^{D(G(\theta, z), z))})]
\]

\[
\nabla_{\phi} L = -\mathbb{E}_{x \sim p_r, \epsilon \sim p_\epsilon} [\nabla_{\phi} \log (1 + e^{-D(x, E_\phi (x, \epsilon))})]
\]

where the dependence of \( D \) on parameters \( \theta \) and \( \phi \) is ignored when taking the gradients. Comparing them with the above minimax problem, we know that BiGAN is again a special case of our bidirectional formulation with AGE.
5 Experiments

We evaluate our method in three aspects. First we investigate the performance of the proposed algorithm in divergence optimization, to verify that AGE can indeed minimize the divergence effectively. Second we explore the influence of different divergences and bidirectional formulations on the issue of mode collapse. Lastly we apply the bidirectional generative model learned with AGE on real datasets and test the performance in both generation and representation, which further shows the effectiveness of our method.

5.1 Divergence optimization

In order to make a fair comparison, we consider the scenario where the original VAE applies and use the same objective function and model settings for different methods. Specifically, we choose $\mathcal{L}$ as the KL divergence and set both encoder $p_e(z|x)$ and generator $p_g(x|z)$ as factorized Gaussians. As a result, problem (1) is equivalent to minimizing $L_{VAE}$ which has an analytic form so that we can compute the exact objective values for comparison.

To make the model assumptions suitable for data, we synthesize a toy dataset from a 2D mixture of Gaussians (MoG) with 9 components laid out on a grid. We assume imbalanced class probabilities with 4 minority classes and 5 majority classes, which makes it a decently hard task.

We compare three algorithms for optimization. The first one is VAE where we analytically minimize $L_{VAE}$ using SGD. The second one is the proposed AGE with $\mathcal{L}$ being the KL divergence, which we call AGE-KL. The third one is the bidirectional f-GAN with KL, abbreviated as f-GAN-KL. Note that the solution obtained from VAE is regarded as the “ideal” solution, since it makes use of the analytic form of the objective while the other two use estimated gradients and minimax approximation respectively.

We use three metrics to evaluate the performance. The first one is the value of objective function $L_{VAE}$ which directly indicates the optimization performance. The second is the negation of (5) to measure the cycle consistency. The last one is the marginal negative log-likelihood $-\mathbb{E}_{p_r(x)}[\log p_g(x)]$ to validate the performance in unidirectional generation. We estimate the first two metrics with samples and the third one using the annealed importance sampling (AIS) with 1000 intermediate distributions and 30 parallel chains on 10,000 test examples.

As reported in Table 3, AGE is comparable to VAE in all three metrics, indicating that our proposed method can minimize the KL objective almost as effective as optimizing the closed-form objective when available. In contrast, f-GAN performs far worse due to the low statistical efficiency of the discriminator. Moreover, f-GAN is highly unstable with a large variability between multiple repetitions, which is also observed in [4]. This experiment directly suggests that AGE outperforms f-GAN in both effective optimization and training stability.

| Method     | Objective | CC     | Uni-gen |
|------------|-----------|--------|---------|
| VAE        | 2.739 (0.02) | 0.025 (0.07) | 0.753 (0.01) |
| AGE-KL     | 2.784 (0.06) | -0.018 (0.16) | 0.737 (0.02) |
| f-GAN-KL   | 3.786 (1.05) | 1.173 (1.04) | 1.401 (1.24) |

5.2 Mode coverage

In this section we focus on the influence of the choice of divergence on mode collapse. Note that orthogonal to methods that target on alleviating mode collapse [7, 16, 17], our discussion here only considers the factor of divergence.

Datasets We consider two scenarios. One is a synthesis MoG dataset like above while we add the number of components to 25 with 12 minority classes. In this case, the 25 modes have imbalanced probabilities and the

\footnote{The code is available at \url{https://github.com/xwshen51/AGE}}
Table 4: Two measures of mode collapse on the imbalanced MoG dataset. All results are averaged over 10 trials shown with the standard error.

| Method    | Modes  | KL       |
|-----------|--------|----------|
| AGE-KL    | 24.9 (0.36) | 0.0284 (0.0035) |
| f-GAN-KL  | 24.1 (1.33) | 0.0477 (0.0418) |
| AGE-$H^2$ | 24.5 (0.94) | 0.0439 (0.0102) |
| AGE-RevKL | 21.8 (3.21) | 0.2498 (0.2120) |
| GAN (JS)  | 24.1 (1.23) | 0.0462 (0.0159) |
| AGE-ALL   | 23.2 (1.33) | 0.1133 (0.0273) |
| logD-GAN  | 20.0 (3.14) | 0.3437 (0.1723) |
| Hinge     | 20.9 (0.92) | 0.1929 (0.0366) |

Figure 1: Reconstructions from bidirectional generative models on the MoG dataset using various divergences as the objective.

Minority modes could be easily lost. The other is the stacked MNIST dataset [16, 17], which is constructed by stacking three randomly sampled MNIST digits. Hence it has 1000 modes with uniform probabilities.

**Metrics** We use two previously used metrics. One is the number of modes captured by a generator. For the above two labelled datasets, we can compute this number using pre-trained classifiers. Another metric is the reverse KL divergence (since the KL divergence is infinity when some mode is missing) between the mode distribution of generated samples and the real mode distribution.

**Methods for comparison** We mainly focus on different choices of divergence as the objective with AGE for optimization. We compare KL, JS, Reverse KL, and Squared Hellinger distance. In addition, we also conduct our proposed AGE-ALL, non-saturating BiGAN with the “logD” trick (abbreviated as logD-GAN) and Hinge loss used in BigBiGAN [18] for comparison.

### 5.2.1 MoG

We use deterministic encoders and generators in this experiment. The results are reported in Table 4 from which we can see that KL divergence has a significant benefit in mode capturing over other divergences or formulations. Reverse KL performs far worse than KL, and the Squared Hellinger distance which is defined in between KL and reverse KL performs moderately. AGE-KL tends to be better and more stable than f-GAN-KL, which is consistent with the results in Section 5.1. AGE-ALL is slightly worse than several divergences on this toy dataset, but still covers more modes than Reverse KL, logD-GAN and Hinge. Figure 1 visually shows the reconstruction performance of various divergences with additional results given in Appendix F, where we can clearly observe how mode collapse occurs for all divergences except KL.

### 5.2.2 Stacked MNIST

On real datasets, we find that scaling clipping is necessary in order to maintain stable gradients. In appendix D we show how the AGE algorithms behave with varying clipping ranges and conclude that AGE-ALL generally performs well and stably. Thus, for real data tasks we adopt AGE-ALL that approximately...
Table 5: Two measures of mode collapse and reconstruction accuracy on Stacked MNIST. All results are averaged over 10 trials shown with the standard error.

| Method          | Modes   | KL       | Recon. (%) |
|-----------------|---------|----------|------------|
| AGE-ALL(d)      | 971.7 (20.1) | 0.42 (0.10) | 81.7 (1.8) |
| AGE-ALL         | 981.2 (9.5)  | 0.36 (0.05) | 86.5 (1.6) |
| f-GAN-KL        | 466 (452.5)  | 3.49 (2.45) | 27.8 (1.6) |
| GAN (JS)        | 954.2 (17.3) | 0.71 (0.08) | 64.2 (2.2) |
| logD-GAN        | 932.1 (59.8) | 0.55 (0.14) | 81.3 (2.3) |
| Hinge           | 959.9 (17.1) | 0.53 (0.10) | 84.1 (1.8) |

minimizes several $f$-divergences (including KL) simultaneously with stable training. We try a deterministic encoder and generator called “AGE-ALL(d)” and use a Gaussian encoder and an implicit generator for all other methods.

The results in Table 5 demonstrate the effectiveness of AGE-ALL in diminishing mode collapse on Stacked MNIST. Furthermore, we observe advantages of stochastic encoders and generators over deterministic ones in both mode covering and reconstruction accuracy (discussed later in Section 5.3). This is consistent with the arguments that stochasticity in transformations increases the expressiveness of generative models and adding noise to the generator helps alleviate mode collapse. We notice that $f$-GAN-KL tends to perform poorly and even collapse on this dataset, leading to a far worse result.

5.3 Real data generation and representation

In this section we apply our method on real datasets of digits (Stacked MNIST), human faces (CelebA) and natural images (ImageNet) to extensively evaluate the performance of our method in data generation and representation. Stacked MNIST is an elementary dataset; CelebA contains a large number of well-aligned face images with large variations of attributes; ImageNet contains real-world images with a huge diversity and thus is one of the most elusive tasks in image synthesis.

For fair comparison, we mainly consider three approaches with non-saturating losses and high training stability on real datasets: AGE-ALL (proposed), Hinge (BigBiGAN) and logD-GAN (BiGAN). For all methods, we apply Gaussian encoders and implicit generator distributions. Due to limited computational resource, we resize the images from CelebA and ImageNet to the resolution of $64 \times 64$ and use relatively small network architecture and training scale with details given in Appendix E. For ImageNet, we only use Hinge following BigBiGAN as our baseline because we observe from previous experiments that Hinge generally outperforms logD-GAN, and experiments on ImageNet are quite expensive.

5.3.1 Generation

Generated samples on three datasets are shown in Figure 2 with the Fréchet Inception Distances (FIDs) reported in Table 6. Additional samples are presented in Appendix F. The results demonstrate the advantage of our method to generate images with high fidelity, which is a consequence of effective optimization and merits of our bidirectional generative formulation.

Furthermore, we find that the bidirectional generative models (BGMs) achieve comparable performance to unidirectional generative models (UGMs, row 1 in Table 6). One explanation is our justification on the advantage of the bidirectional formulation in unidirectional generation. For ImageNet with such a huge diversity, the generator in a BGM benefits from the encoder and achieves even better performance than that in a UGM. Hence, bidirectional generative models should be favored over unidirectional ones since they can achieve the goal of the latter while additionally learn an inference model which is useful in many applications.

5.3.2 Representation

In order to explore the property of the latent representations learned by our BGM, we investigate the reconstruction performance, latent space interpolation, and nearest neighbors.
We would like to investigate how much information, especially high-level semantics, is preserved in the inferred representation $E(x)$ by looking at the reconstruction $G(E(x))$. Since our concern is not in the pixel level, we measure the reconstruction performance by how much high-level features or attributes it can retain. We use both qualitative illustration and quantitative metrics. The last column of Table 5 reports the classification accuracy of the reconstructions on Stacked MNIST and shows the advantage of AGE in preserving category information. Figure 3 and 4 present the reconstructions on CelebA and ImageNet validation sets, with additional samples given in Appendix F. AGE achieves much more faithful reconstructions than other methods, which supports our theoretical justifications on cycle consistency in Section 2.2. Although the reconstructions are generally not perfect in the pixel level, our method is able to capture high-level attributes and semantics. This property is essentially demanded in learning high-level representations such as disentangling and is worth investigating in future work.

Figure 5(a) shows latent space interpolations between validation samples which exhibit smooth semantic transitions, verifying the smooth and well-dispersed latent space learned by our model. As shown in Figure 5(b), the neighbors in the latent space often share the same high-level features with the query image, indicating that the learned representations are mostly consistent with visual semantics. Results from other methods in Appendix F suggest the advantage of ours.
Figure 4: Reconstructions on ImageNet. The reconstructions from AGE are more often belonging to the same category as the original images with similar texture, position, and pose.

Figure 5: (a) Latent space interpolations on CelebA validation set using AGE. The left and right columns are real images; the columns in between are generated from the latent variables interpolated linearly from the two inferred representations of the real. (b) Nearest neighbors in the learned latent space. The one in the red rectangle is a query image, and the remaining ones are its four nearest neighbors. All images are from the validation set.

6 Related work

6.1 Bidirectional generative modeling

VAE is often regarded to be far different from GANs. We point out in Section 4 that both are special cases of our bidirectional generative modeling optimized using AGE. Both are limited to specific objectives and model assumptions, and hence do not apply to the general $f$-divergence formulation with more expressive generator/encoder distributions.

Along the extensions, apart from AVB [6] which is also a special case of ours involving partial gradient estimation, approaches like VAE-GAN [20] and AAE [21] or more general WAE [22] enhance VAE using unidirectional GANs. The former uses a GAN to match the data distributions while the latter uses one in the latent space. These formulations are mainly motivated by certain specific concerns and modify the loss accordingly, and thus are not as principled as ours. Other methods including ALICE [11] and VEEGAN [7] can be regarded as variants of our fundamental formulation by adding special regularizers like conditional entropy or reconstruction error on the latent space. Recently, BigBiGAN [18] is proposed to implement the formulation of BiGAN using the BigGAN architectures. Its main contribution is to translate the progress in image generation to representation learning, especially the network architectures with much more capacity and benefits of scaling up training. In contrast, our work only considers small training scale while focus on the formulation and algorithm, and thus is orthogonal to it.

6.2 Adversarial approach for $f$-divergence minimization

There is a number of work involving adversarial approach for $f$-divergence minimization. One principled approach is the $f$-GAN [4] which is based on the variational representation of $f$-divergences. We investigate clearly the differences and advantages of our AGE over $f$-GAN in Section 3.3 and experiments.

Several papers propose to use discriminator-based approaches for minimizing the KL divergence where
the discriminator is obtained using Logistic regression [6][9]. Unlike our proposed gradient estimation, they
directly express the objective function by plugging in the discriminator in which way the discriminator itself
still depends on the generator (and encoder) parameters. However when evaluating the gradients of the
objective they simply ignore this dependence in the discriminator while only consider the dependence in data.
Their consequent gradient estimations are generally different from ours given the same objective. Therefore
the accuracy of their approaches requires further investigation. Since we provide clear and rigorous theoretical
justifications of the adversarial gradient estimation, our approach is more principled, and applicable to all
formulations that require $f$-divergence minimization.

7 Conclusion

This paper considers the general $f$-divergence formulation of bidirectional generative modeling and discuss
its advantages. We propose a new optimization method, AGE, for this formulation, where the gradient is
computed using an adversarially learned discriminator. In our framework, we show that different divergences
induce similar algorithms in terms of gradient evaluation, except with different scaling. This unifies the
treatment of $f$-divergence GAN. Therefore this paper proposes a general recipe for a class of principled
$f$-divergence based generative modeling methods. We further propose the scaling clipping technique and
obtain an algorithm which locally minimizes several divergences simultaneously with a lower variance and
higher training stability.

Extensive empirical studies are conducted to demonstrate the advantages of our approach over existing
methods, including effective divergence optimization, alleviating mode collapse, and promising performance
in real data generation and representation. The potential of our method in more applications such as
disentanglement, image translation and downstream classification tasks, and the benefits after scaling up are
worth further exploration.

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Appendix A  Proofs

A.1 Proof of equivalent expressions of the joint KL

Proof of (6). By the definition of KL divergence, we have
\[
D_{\text{KL}}(p_e(x, z), p_g(x, z)) = \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_e(x, z)}{p_g(x, z)} p_g(z|x) \right] = \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_r(x) p_e(z|x)}{p_g(x) p_g(z|x)} \right]
\]
\[
= \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_r(x)}{p_g(x)} + \log \frac{p_e(z|x)}{p_g(z|x)} \right] + \mathbb{E}_{p_e(x)} \left[ \log p_r(x) \right] + \mathbb{E}_{p_e(z|x)} \left[ \log \frac{p_e(z|x)}{p_g(z|x)} \right] = D_{\text{KL}}(p_r(x), p_g(x)) + \mathbb{E}_{x \sim p_r(x)} [D_{\text{KL}}(p_e(z|x), p_g(z|x))].
\]

Proof of (9). By the definition of KL divergence, we have
\[
D_{\text{KL}}(p_e(x, z), p_g(x, z)) = \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_e(x, z)}{p_g(x, z)} p_g(z|x) \right] = \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_r(x) p_e(z|x)}{p_g(x) p_g(z|x)} \right]
\]
\[
= \mathbb{E}_{p_e(x, z)} \left[ \log \frac{p_r(x)}{p_g(x)} + \log \frac{p_e(z|x)}{p_g(z|x)} \right] + \mathbb{E}_{p_e(x)} \left[ \log p_r(x) \right] + \mathbb{E}_{p_e(z|x)} \left[ \log \frac{p_e(z|x)}{p_g(z|x)} \right] = D_{\text{KL}}(p_r(x), p_g(x)) + \mathbb{E}_{x \sim p_r(x)} [D_{\text{KL}}(p_e(z|x), p_g(z|x))].
\]

A.2 Proof of Theorem 1

The proof technique is inspired by that of CFG-GAN [23]. Let $\| \cdot \|$ denote the vector 2-norm. Given a differentiable vector function $g(x): \mathbb{R}^k \to \mathbb{R}^k$, we use $\nabla \cdot g(x)$ to denote its divergence, defined as
\[
\nabla \cdot g(x) := \sum_{j=1}^{k} \frac{\partial [g(x)]_j}{\partial x_j},
\]
where $[x]_j$ denotes the $j$-th component of $x$. We know that
\[
\int \nabla \cdot g(x) dx = 0
\]
for all vector function $g(x)$ such that $g(\infty) = 0$. Given a matrix function $w(x) = (w_1(x), \ldots, w_l(x)) : \mathbb{R}^k \to \mathbb{R}^{k \times l}$ where each $w_i(x), i = 1 \ldots, l$ is a $k$-dimensional differentiable vector function, its divergence is defined as $\nabla \cdot w(x) = (\nabla \cdot w_1(x), \ldots, \nabla \cdot w_l(x))$.

To prove Theorem 1, we need the following lemma which specifies the dynamics of the generator joint distribution $p_g(x, z)$ and the encoder joint distribution $p_e(x, z)$, denoted by $p_\theta(x, z)$ and $p_\phi(x, z)$ here.

Lemma 1. Using the definitions and notations in Theorem 1, we have
\[
\nabla_\theta p_\theta(x, z) = \nabla_x p_\theta(x, z)^\top g_\theta(x) - p_\theta(x, z) \nabla \cdot g_\theta(x), \quad (9)
\]
\[
\nabla_\phi p_\phi(x, z) = \nabla_z p_\phi(x, z)^\top e_\phi(z) - p_\phi(x, z) \nabla \cdot e_\phi(z), \quad (10)
\]
for all data $x$ and latent variable $z$, where $g_\theta(G_\theta(z, \epsilon)) = \nabla_\theta G_\theta(z, \epsilon)$ and $e_\phi(E_\phi(x, \epsilon)) = \nabla_\phi E_\phi(x, \epsilon)$.

Proof of Lemma 1. Let $l$ be the dimension of parameter $\theta$. To simplify notation, let random vector $X = G_\theta(Z, \epsilon) \in \mathbb{R}^d$ and $Y = (X, Z) \in \mathbb{R}^{d+k}$, and let $p$ be the probability density of $Y$. For each $i = 1, \ldots, l$, let $\Delta = \delta e_i$ where $e_i$ is a $l$-dimensional unit vector whose $i$-th component is one and all the others are zero, and $\delta$ is a small scalar. Let $X' = G_{\theta + \Delta}(Z, \epsilon)$ and $Y' = (X', Z)$ so that $Y'$ is a random variable transformed from $Y$ by
\[
Y' = Y + \begin{pmatrix} g(X) \\ 0 \end{pmatrix} \Delta + o(\delta)
\]
where \( g(X) \in \mathbb{R}^{d \times 1} \) and let \( p' \) be the probability density of \( Y' \). For an arbitrary \( y' = (x', z) \in \mathbb{R}^{d + k} \), let \( x = x' + g(x)\Delta + o(\delta) \) and \( y = (x, z) \). Then we have

\[
p'(y') = p(y) |\det(dy'/dy)|^{-1} \\
= p(y) |\det(1 + \nabla g(x)\Delta + o(\delta))|^{-1} \\
= p(y)(1 + \Delta^\top \nabla \cdot g(x) + o(\delta))^{-1} \\
= p(y) - \Delta^\top p(y') \nabla \cdot g(x') + o(\delta) \\
= p(y') - \Delta^\top g(x')^\top \nabla_x p(x', z) - \Delta^\top p(y') \nabla \cdot g(y') + o(\delta).
\]

(11)

The first three equalities use the multivariate change of variables formula for probability densities for the change from \( Y \) to \( Y' \) and the definition of determinant with terms explicitly expanded up to \( O(\delta) \). (11) uses the Taylor expansion of \((1 + \xi)^{-1} = 1 - \xi + o(\xi)\) with \( \xi = \Delta^\top \nabla \cdot g(y) \). (12) follows from the fact that \( p(y') = p(y) + o(1) \) and \( \nabla \cdot g(x') = \nabla \cdot g(x) + o(1) \). (13) is due to \( p(y) = p(y') - (y' - y)^\top \nabla p(y') + o(\delta) \).

Since \( y' \) is arbitrary, above implies that 

\[
p'(x, z) = p(x, z) - \Delta^\top g(x)^\top \nabla_x p(x, z) - \Delta^\top p(x, z) \nabla \cdot g(x) + o(\|\delta\|)
\]

for all \( x \in \mathbb{R}^d, z \in \mathbb{R}^k \) and \( i = 1, \ldots, l \), leading to (9) by taking \( \delta \to 0 \), setting \( g(x) = g_\theta(x) \), and noting that \( p = p_\theta \) as both are the density of \((G_{\theta}(Z, \epsilon), z)\) and \( p' = p_{\theta + \Delta} \) as both are the density of \((G_{\theta + \Delta}(Z, \epsilon), z)\). Similarly we can obtain (10).

**Proof of Theorem 7**  Let \( \ell'_2(p_\epsilon, p_\theta) = \partial \ell_2(p_\epsilon, p_\theta) / \partial p_\theta \). Using the chain rule and Lemma 1 we have

\[
\nabla_\theta \ell_2(p_\epsilon(x, z), p_{\theta}(x, z)) = \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) \nabla_\theta p_{\theta}(x, z) \\
= \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) \left(-\nabla_x p_{\theta}(x, z)^\top g_\theta(x) - p_\theta(x, z) \nabla \cdot g_\theta(x) \right) \\
= p_\theta(x, z) \nabla_x \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z))^\top g_\theta(x) - \nabla_x \cdot \left[ \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) p_{\theta}(x, z) g_{\theta}(x) \right],
\]

(14)

where the third equality is obtained by applying the product rule as follows

\[
\nabla_x \cdot \left[ \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) p_{\theta}(x, z) g_{\theta}(x) \right] = \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) p_{\theta}(x, z) \nabla \cdot g_{\theta}(x) \\
+ \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) \nabla_x p_{\theta}(x, z)^\top g_{\theta}(x) \\
+ p_\theta(x, z) \nabla_x \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z))^\top g_{\theta}(x).
\]

By integrating (14) over \( x \) and \( z \), and by using the fact that \( \int \nabla \cdot f(x) dx = 0 \) with \( f(x) = \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) p_{\theta}(x, z) g_{\theta}(x) \), we have

\[
\nabla_\theta L(\theta, \phi) = \int \nabla_\theta \ell_2(p_\epsilon(x, z), p_{\theta}(x, z)) dx dz = \int p_{\theta}(x, z) \nabla_x \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z))^\top g_{\theta}(x) dx dz.
\]

According to the definition (2) of \( f \)-divergences, we have

\[
\nabla_x \ell'_2(p_\epsilon(x, z), p_{\theta}(x, z)) = \tilde{f}''' \left( \frac{1}{r(x, z)} \right) \nabla_{x} \frac{1}{r(x, z)} = \tilde{f}''' \left( \frac{1}{r(x, z)} \right) \frac{1}{r(x, z)} \nabla_x D(x, z).
\]

(15)

Further by reparametrization and noting that \( r(x, z) = e^{D(x, z)} \), we obtain

\[
\nabla_\theta L(\theta, \phi) = -\mathbb{E}_{(x, z) \sim p_\theta}(x, z) \left[ \tilde{f}''' \left( \frac{1}{r(x, z)} \right) \frac{1}{r(x, z)} \nabla_x D(x, z)^\top g_{\theta}(x) \right] \\
= -\mathbb{E}_{z \sim p_\phi(z), \epsilon \sim p_\epsilon} \left[ \tilde{f}''' \left( \frac{1}{r(G_{\theta}(z, \epsilon), z)} \right) \frac{1}{r(G_{\theta}(z, \epsilon), z)} \nabla_x D(G_{\theta}(z, \epsilon), z)^\top \nabla_\theta G_{\theta}(z, \epsilon) \right].
\]
Theorem 2. Let encoder and generator transformations which are essentially degenerated cases in the sense that Stochastic encoders and generators have benefits. On the other hand, BiGAN uses deterministic improper Gaussian assumption rather than KL as the objective. random samples are noisy and far away from the true data distribution. The reason we suggest is due to the Gaussian generator rather than random samples. For images, the means tend to be blurry while the approximately minimizes several likelihood estimator for the gradients. Similar to bidirectional AGE-ALL, we obtain an algorithm that different algorithms given the same f-divergence as the objective. The following theorem enables us to evaluate the gradient of f-divergence w.r.t. the generator parameter.

Theorem 2. Let \( r(x) = p_r(x)/p_\theta(x) \) and \( D(x) = \log(p_r(x)/p_\theta(x)) \). We have

\[
\nabla_\theta L_{\text{uni}}(\theta) = -E_{z \sim p_z, \epsilon \sim p_\epsilon} \left[ s(G_\theta(z, \epsilon)) D(G_\theta(z, \epsilon))^\top \nabla_\theta G_\theta(z, \epsilon) \right],
\]

(16)

where \( s(x) = \tilde{f}''(1/r(x))/r(x) \).

Proof. Similar to the proof of Theorem 1. □

Let \( D(x) \) be the solution to the empirical Logistic regression that distinguishes the generated data from the real data:

\[
D(x) = \arg\min_{D'} \left[ \frac{1}{|S_r|} \sum_{i \in S_r} \log(1 + e^{-D'(x)}) + \frac{1}{|S_g|} \sum_{i \in S_g} \log(1 + e^{D'(x)}) \right]
\]

where \( S_r \) and \( S_g \) are finite samples from \( p_r(x) \) and \( p_\theta(x) \) respectively. Similarly we know \( D(x) \approx D(x) \). Replacing \( D(x) \) and \( r(x) \) in the gradients \( \{16\} \) with \( D(x) \) and \( \tilde{r}(x) = e^{D(x)} \), we obtain the maximum likelihood estimator for the gradients. Similar to bidirectional AGE-ALL, we obtain an algorithm that approximately minimizes several \( f \)-divergences between \( p_r(x) \) and \( p_\theta(x) \) simultaneously by setting \( s(x) = 1 \).

Appendix C  Choice for encoder and generator distributions

In this section we discuss the conventional choices for encoder and generator distributions in VAEs and GANs along with our suggestions.

Gaussian generators may not be suitable. While AVB extends the Gaussian encoder in VAE to an implicit distribution, we argue that the more crucial model element is the choice for the generator distribution. A Gaussian generator used in VAE and AVB is not suitable to model more complex real data like images. One intuitive explanation is that the complex space (e.g., pixels) is usually of very high dimension and may have some properties which can not be suited well in the Euclidean space with a Gaussian distribution. In practice when generating new data from VAE/AVB, after sampling \( z \sim p_z \), people always use the mean of the Gaussian generator rather than random samples. For images, the means tend to be blurry while the random samples are noisy and far away from the true data distribution. The reason we suggest is due to the improper Gaussian assumption rather than KL as the objective.

Stochastic encoders and generators have benefits. On the other hand, BiGAN uses deterministic encoder and generator transformations which are essentially degenerated cases in the sense that \( p_r(z|x) \) and \( p_g(x|z) \) can only capture one-point distributions. ALI and BigBiGAN use a deterministic generator and a
stochastic encoder which causes some asymmetry. In contrast, we suggest that stochasticity in transformations increases model expressiveness and helps with mode covering.

**We suggest an implicit generator distribution.** Usually in unidirectional GANs, people use “deterministic” generators but a relatively high dimensional latent vector. For example the progressive GAN [24] sets the latent dimensionality to 512. We can think of the latent vector as a composition of latent factors to represent high-level features and random noises to capture stochastic variation. Then with the nonlinear transformation over the random noises, the conditional distribution of generated data given the high-level features is implicit. However in bidirectional models, the desired latent representation should only include high-level features. Thus we separate random noises $\epsilon$ as the source of randomness and follow the idea of expressive implicit distributions. With an implicit generator distribution, both VAE and AVB do not apply and hence we are motivated to employ the proposed AGE for optimization.

**Details of the implicit generator.** To construct a generator with an implicit distribution, we adopt the similar idea as the StyleGAN generator [29]. We generate some single-channel feature maps consisting of uncorrelated Gaussian noises, one for each layer of the generator network except the final output image, with the same resolution as the output feature map of that layer. Each noise feature map is broadcasted to all channels using learned per-pixel scaling factors and then added to the output of the corresponding convolution. In this manner, each convolution layer in the generator produces a conditional Gaussian distribution given all the previous layers. After the consequent nonlinear transformations, the final output image conditional on the input latent variable is an implicit distribution.

**Appendix D Additional experiments on scaling clipping**

In this section, we explore how the AGE algorithms behave with varying clipping ranges. Following Section 3.2, we clip the scaling factors into a range of $[r_0, 1/r_0]$ with a specified lower bound $r_0 \in [0, 1]$. The case of $r_0 = 0$ means no clipping while $r_0 = 1$ is the extreme case where all AGE algorithms for different divergences converge to AGE-ALL.

Figure 6 exhibits how various metrics vary with the lower bound of scaling clipping $r_0$ increasing from 0 to 1 on Stacked MNIST. Experiments show that without SC, AGEs for all divergences tend to suffer from the vanishing or exploding gradient problem and perform poorly. Reverse KL is the most stable one in this case. We notice that some divergences perform better in certain metrics with certain clipping ranges while some perform better in other cases. For example, AGE-KL-SC has advantages in mode covering over other divergences, which coincides with the results on the MoG dataset. With heavy enough scaling clipping, different divergences do not differ too much on this dataset in reconstruction and generation. As we narrow the clipping range (increase $r_0$), the behaviors of different divergences converge to the same one. The extreme AGE-ALL performs stably and sufficiently well in all metrics, for which reason we adopt AGE-ALL on real datasets in the main text.

We observe that $r_0 \approx 0.5$ is probably a decent choice where the AGE algorithms for different divergences significantly differ from each other and can preserve the distinctive property of each divergence, while avoid vanishing or exploding gradient. We hence report the detailed results of AGE-SC with a clipping range of $[0.5, 2]$ on Stacked MNIST and CelebA in Table 7. We see that equipped with the scaling clipping technique, AGE algorithms for various divergences generally perform well and stably on real datasets.

| Divergence | Modes   | KL     | Recon. (%) | Modes   | KL     | Recon. (%) |
|------------|---------|--------|------------|---------|--------|------------|
| ALL        | 981.2 (9.5) | 0.3574 (0.05) | 86.53 (1.58) | 4.40 | 8.08 |
| KL         | 983.5 (8.7)  | 0.3503 (0.04) | 84.84 (1.51) | 4.68 | 7.57 |
| Hellinger  | 982.5 (10.2) | 0.3497 (0.08) | 85.58 (0.92) | 5.04 | 7.96 |
| JS         | 977.7 (17.7) | 0.3600 (0.05) | 83.70 (2.25) | 5.36 | 8.59 |
| RevKL      | 976.9 (12.1) | 0.3690 (0.07) | 84.73 (1.26) | 5.06 | 8.68 |
(a) Number of modes covered in generations (larger is better)  
(b) RevKL of real/generated mode dist. (smaller is better)  
(c) Reconstruction accuracy (higher is better)  
(d) FID (smaller is better)

Figure 6: Behavior of AGE algorithms with scaling clipping (AGE-SC) on Stacked MNIST in mode covering, data reconstruction and generation. We repeat each experiment 10 times with the standard error shown by the error bar.

Appendix E Experimental details

In this section we state the details of experimental setup and the network architectures used for all experiments. In experiments on one dataset, we adopt exactly the same network architecture and experimental settings for different methods.

E.1 MoG

For both 9-Gaussians and 25-Gaussians datasets, each majority class contains 10,000 samples and each minority class contains 500 samples. The standard deviation is 0.3 for all classes. The generator and encoder have two and three fully connected layers respectively with 500 units in each layer with batch-normalization and ReLU as the activation function. The discriminator consists of three modules of two fully connected layers with 400 units each and Leaky-ReLU as the activation function to extract features from $x$, $z$ and their concatenated features. We use the Adam optimizer with a learning rate of $1 \times 10^{-4}$ for $D$ and $5 \times 10^{-5}$ for $E$ and $G$ and a mini-batch size of 500. The models on 25-Gaussians are trained for 30 epochs before evaluation. We use 30 $D$ steps per $G/E$ step on 9-Gaussians to retain a nearly optimal $D$, and 5 $D$ steps per $G/E$ step on 25-Gaussians to make it a harder task.
E.2 Stacked MNIST

We adopt the DCGAN [27] architecture for Stacked MNIST. When following exactly the same experimental setup reported in PacGAN [17] and VEEGAN [7], we find that all of the algorithms can cover all modes. Hence we reduce the model capacity to make it a harder task. Specifically, details for networks are given below in Table 8-10. We use a pre-trained MNIST classifier to classify simulated samples on each of the three stacked channels. We train all models on 128,000 samples, with a mini-batch size of 64, for 50 epochs. We use Adam with a learning rate of 0.0001 and update all three networks once on each mini-batch. Evaluation for mode covering is done on 26,000 test samples. In all experiments, we use 50k generated images for evaluating FIDs.

Table 8: Generator network for Stacked-MNIST. With batch-normalization. With one Gaussian feature map added to each conv layer.

| Layer                     | Number of outputs | Kernel size | Stride | Activation function |
|---------------------------|-------------------|-------------|--------|---------------------|
| Input \( z \sim \mathcal{N}(0, I)^8 \) | 8                 | -           | -      | -                   |
| Fully-connected           | 4 x 4 x 256       | -           | -      | ReLU                |
| Transposed convolution    | 7 x 7 x 128       | 5 x 5       | 2      | ReLU                |
| Transposed convolution    | 14 x 14 x 64      | 5 x 5       | 2      | ReLU                |
| Transposed convolution    | 28 x 28 x 3       | 5 x 5       | 2      | Tanh                |

Table 9: Encoder network for Stacked-MNIST. With batch-normalization. The number of outputs is twice the latent dimension with a Gaussian encoder.

| Layer                     | Number of outputs | Kernel size | Stride | Activation function |
|---------------------------|-------------------|-------------|--------|---------------------|
| Input \( x \)             | 28 x 28 x 3       | -           | -      | -                   |
| Convolution               | 14 x 14 x 64      | 5 x 5       | 2      | ReLU                |
| Convolution               | 7 x 7 x 128       | 5 x 5       | 2      | ReLU                |
| Convolution               | 4 x 4 x 256       | 5 x 5       | 2      | ReLU                |
| Fully-connected           | 8 or 16           | -           | -      | -                   |

Table 10: Discriminator network for Stacked-MNIST. Without batch-normalization.

| Layer                     | Number of outputs | Kernel size | Stride | Activation function |
|---------------------------|-------------------|-------------|--------|---------------------|
| Input \( x \)             | 28 x 28 x 3       | -           | -      | -                   |
| Convolution               | 14 x 14 x 64      | 5 x 5       | 2      | LeakyReLU           |
| Convolution               | 7 x 7 x 128       | 5 x 5       | 2      | LeakyReLU           |
| Convolution               | 4 x 4 x 256       | 5 x 5       | 2      | LeakyReLU           |
| Flatten                   | -                 | -           | -      | -                   |
| Concatenate \( z \)       | -                 | -           | -      | -                   |
| Fully-connected           | 1024              | -           | -      | LeakyReLU           |
| Fully-connected           | 1                 | -           | -      | -                   |

E.3 CelebA and ImageNet

We pre-process the images by taking a center crops of 128 x 128 for CelebA and 73 x 73 for ImageNet and resizing to the 64 x 64 resolution. For such complex datasets, we adopt the SAGAN [25][26] architecture for \( D \) and \( G \). For the discriminator, we adopt the similar idea in BigBiGAN, where we the \( D \) network consists of three modules (Figure 7) where \( D_x \) is the normal SAGAN discriminator with data \( x \) as input and feature \( f_x \) and score \( s_x \) as output, \( D_z \) is an MLP with latent \( z \) as input and score \( s_z \) as output, and \( D_xz \) is an MLP with concatenated feature \( (f_x, f_z) \) as input and score \( s_{xz} \) as output. Unlike BigBiGAN which introduces additional unary terms in the \( D \) loss, we use a single output of \( D \) as the average \( (s_x + s_z + s_{xz})/3 \) and keep the formulation of \( D(x, z) - \) Logistic regression between joint distributions \( p_x(x, z) \) and \( p_g(x, z) \). In this sense, involving unary scores here is just an architectural design for \( D \) while in BigBiGAN makes it deviate from the original formulation [1]. Details for newtork \( G \) and \( D_x \) are given in Figure 8 and Table 11.
The encoder architecture is the ResNet50 [28] followed by a 4-layer MLP (size 1024 for CelebA and 2048 for ImageNet) with skip connections after ResNet’s global average pooling layer.

We use Adam with $\beta_1 = 0$, $\beta_2 = 0.999$, and a learning rate of $1 \times 10^{-4}$ for $D$ and $5 \times 10^{-5}$ for $E$ and $G$. Due to limited computational resource, we use a mini-batch size of 256 for CelebA and 240 for ImageNet. We update all three networks once on each mini-batch. Models were trained for around 50 epochs on CelebA and more than 100 epochs on ImageNet on NVIDIA RTX 2080 Ti.

Table 11: SAGAN architecture. CelebA uses $k = 100$ and $ch = 32$; ImageNet uses $k = 140$ and $ch = 64$.

| (a) Generator | (b) Discriminator module $D_x$ |
|----------------|--------------------------------|
| Input: $z \in \mathbb{R}^k \sim \mathcal{N}(0, I)$ | Input: RGB image $x \in \mathbb{R}^{64 \times 64 \times 3}$ |
| Linear $\rightarrow$ $4 \times 4 \times 16ch$ | ResBlock down $ch \rightarrow 2ch$ |
| ResBlock up $16ch \rightarrow 16ch$ | Non-Local Block ($64 \times 64$) |
| ResBlock up $16ch \rightarrow 8ch$ | ResBlock down $2ch \rightarrow 4ch$ |
| ResBlock up $8ch \rightarrow 4ch$ | ResBlock down $4ch \rightarrow 8ch$ |
| Non-Local Block ($64 \times 64$) | ResBlock down $8ch \rightarrow 16ch$ |
| ResBlock up $4ch \rightarrow 2ch$ | ResBlock $16ch \rightarrow 16ch$ |
| BN, ReLU, $3 \times 3$ Conv $2ch \rightarrow 3$ | ReLU, Global average pooling ($f_x$) |
| Tanh | Linear $\rightarrow 1$ ($s_x$) |
Appendix F  Additional samples and reconstructions

Figure 9: Generations, reconstructions and latent space from bidirectional generative models on the MoG dataset using various divergences as the objective. Shown top to bottom, left to right are AGE-KL, AGE-$H^2$, $f$-GAN-KL, AGE-ALL, AGE-RevKL, GAN (AGE-JS), logD-GAN, Hinge. We can clearly observe that mode collapse occurs for all divergences except KL. Moreover, the encoder learned by AGE-KL matches the aggregated posterior $p_e(z)$ and prior $p_z(z)$ the best. Apart from better mode covering, another reason for this is due to the justification of our formulation in unidirectional generative modeling.

Figure 10: Generations on Stacked MNIST by the BGM trained using various methods.
Figure 11: Generations on CelebA by the BGM trained using AGE.

Figure 12: Generations on ImageNet by the BGM trained using AGE.
Figure 13: Reconstructions on CelebA using AGE-ALL. Odd columns are real images from the validation set and even columns are the corresponding reconstructions.

Figure 14: Reconstructions on ImageNet using AGE-ALL. Odd columns are real images from the validation set and even columns are the corresponding reconstructions.
Figure 15: Latent space interpolations on CelebA validation set using various methods. The left and right columns are real images; the columns in between are generated from the latent variables interpolated linearly from the two inferred representations from the real. In contrast to other methods, AGE-ALL is able to generate smoother, more faithful and meaningful intermediate images from the interpolated latent representations between two real images.