Spread Divergence

Mingtian Zhang 1  Peter Hayes 1  Tom Bird 1  Raza Habib 1  David Barber 1

Abstract
For distributions \( P \) and \( Q \) with different supports or undefined densities, the divergence \( D(\mathbb{P}||\mathbb{Q}) \) may not exist. We define a Spread Divergence \( \hat{D}(\mathbb{P}||\mathbb{Q}) \) on modified \( P \) and \( Q \) and describe sufficient conditions for the existence of such a divergence. We demonstrate how to maximize the discriminatory power of a given divergence by parameterizing and learning the spread. We also give examples of using a Spread Divergence to train implicit generative models, including linear models (Independent Components Analysis) and non-linear models (Deep Generative Networks).

1. Introduction
For distributions \( P \) and \( Q \), a divergence \( D(\mathbb{P}||\mathbb{Q}) \) is a measure of their difference (Dragomir, 2005) provided it satisfies the properties\(^1\)
\[
D(\mathbb{P}||\mathbb{Q}) \geq 0 \quad \text{and} \quad D(\mathbb{P}||\mathbb{Q}) = 0 \iff P = Q. \tag{1}
\]

For absolutely continuous distributions\(^2\) \( P \) and \( Q \) and probability density functions \( p(x), q(x) \), the \( f \)-divergence is
\[
D_f(\mathbb{P}||\mathbb{Q}) = D_f(p||q) = \mathbb{E}_{q(x)} \left[ f \left( \frac{p(x)}{q(x)} \right) \right], \tag{2}
\]
where \( f(x) \) is a convex function with \( f(1) = 0 \). When \( p \) and \( q \) have the same support\(^3\),
\[
D_f(p||q) = 0 \iff p = q \ a.e. \iff \mathbb{P} = \mathbb{Q}, \tag{3}
\]
where \( \mathbb{P} \) and \( \mathbb{Q} \) are the probabilities to data.

\(^1\)Department of Computer Science, University College London, UK. Correspondence to: Mingtian Zhang <mingtian.zhang.17@ucl.ac.uk>.

\(^2\)Two distributions being equal \( \mathbb{P} = \mathbb{Q} \) can be interpreted to mean that the cdfs (cumulative distribution functions) of the two distributions match.

\(^3\)A distribution is absolutely continuous if its cdf is absolutely continuous. In this case, it has a density function. See also Tao (2011, p. 172).

\(^4\)We use 'generalised density' to include implicit generative models. This includes also the special case \( p(x) = \delta(x - \mu) \), where \( p(x) \) represents a (Dirac) delta distribution with support \( \{\mu\} \). In general we cannot define an \( f \)-divergence based on generalised densities, but can do so if the distribution is absolutely continuous - see section 2.1.2 for details.

---

**Abstract**

For distributions \( P \) and \( Q \) with different supports or undefined densities, the divergence \( D(\mathbb{P}||\mathbb{Q}) \) may not exist. We define a Spread Divergence \( \hat{D}(\mathbb{P}||\mathbb{Q}) \) on modified \( P \) and \( Q \) and describe sufficient conditions for the existence of such a divergence. We demonstrate how to maximize the discriminatory power of a given divergence by parameterizing and learning the spread. We also give examples of using a Spread Divergence to train implicit generative models, including linear models (Independent Components Analysis) and non-linear models (Deep Generative Networks).

**1. Introduction**

For distributions \( P \) and \( Q \), a divergence \( D(\mathbb{P}||\mathbb{Q}) \) is a measure of their difference (Dragomir, 2005) provided it satisfies the properties\(^1\)
\[
D(\mathbb{P}||\mathbb{Q}) \geq 0 \quad \text{and} \quad D(\mathbb{P}||\mathbb{Q}) = 0 \iff P = Q. \tag{1}
\]

For absolutely continuous distributions\(^2\) \( P \) and \( Q \) and probability density functions \( p(x), q(x) \), the \( f \)-divergence is
\[
D_f(\mathbb{P}||\mathbb{Q}) = D_f(p||q) = \mathbb{E}_{q(x)} \left[ f \left( \frac{p(x)}{q(x)} \right) \right], \tag{2}
\]
where \( f(x) \) is a convex function with \( f(1) = 0 \). When \( p \) and \( q \) have the same support\(^3\),
\[
D_f(p||q) = 0 \iff p = q \ a.e. \iff \mathbb{P} = \mathbb{Q}, \tag{3}
\]
where \( \mathbb{P} \) and \( \mathbb{Q} \) are the probabilities to data.

\(^1\)Department of Computer Science, University College London, UK. Correspondence to: Mingtian Zhang <mingtian.zhang.17@ucl.ac.uk>.

\(^2\)Two distributions being equal \( \mathbb{P} = \mathbb{Q} \) can be interpreted to mean that the cdfs (cumulative distribution functions) of the two distributions match.

\(^3\)A distribution is absolutely continuous if its cdf is absolutely continuous. In this case, it has a density function. See also Tao (2011, p. 172).

\(^4\)We use 'generalised density' to include implicit generative models. This includes also the special case \( p(x) = \delta(x - \mu) \), where \( p(x) \) represents a (Dirac) delta distribution with support \( \{\mu\} \). In general we cannot define an \( f \)-divergence based on generalised densities, but can do so if the distribution is absolutely continuous - see section 2.1.2 for details.
A common approach to enable maximum likelihood to be evaluated. As we adjust \( \theta \) the likelihood of generating a data point off the manifold is zero meaning that the likelihood will in general be a non-continuous function of the parameters defining the manifold.

The likelihood is discontinuous in \( \theta \) typically increase to a finite non-zero value, meaning that the (log) likelihood will in general be a non-continuous function of the parameters defining the manifold.

This approach does not guarantee a consistent estimator. To see this, consider the simple implicit generative model \( Q \) with the model \( q(x) \) only has limited support, see figure(1).

Strictly speaking, this does not define a density over the real space \( \mathbb{R}^{\text{dim}(X)} \) since \( X \) is not absolutely continuous. Nevertheless, this does define a distribution \( Q \). To generate a sample from \( Q \), one first samples \( z \) from \( q(z) \) and then passes this through the ‘generator’ function \( g_\theta(z) \).

In this case, gradient based maximum likelihood learning is problematic since \( L(\theta) \) is typically not a continuous function of \( \theta \). Furthermore, the Expectation Maximisation algorithm (Dempster et al., 1977) is not available for models of the form in eq(6) since EM assumes that \( \log q(x|z) \) is well defined, which is not the case when \( q(x|z) = \delta(x - g_\theta(z)) \) (Bermond & Cardoso, 1999). Equally, in eq(4) the ratio \( p(x)/q(x) \) may represent a division by zero; the KL divergence between the model and the data generating process is thus ill-defined.

It is natural to consider transforming two distributions \( \mathbb{P} \) and \( Q \) to have common support by using a mixture model \( \mathbb{P} = \alpha \mathbb{P} + (1 - \alpha) N \), \( Q = \alpha Q + (1 - \alpha) N \), where \( N \) is an absolutely continuous noise distribution with full support. However, as we explain in appendix(E) this approach is not useful in the context of training implicit generative models since \( Q \) does not have a density which can be numerically evaluated.

1.1.1. MODEL NOISE IS NOT ENOUGH

A common approach to enable maximum likelihood to be used to train implicit generative models is to simply add noise to the model so that it has full support (and a valid density), see for example (Wu et al., 2016). However, this approach does not guarantee a consistent estimator. To see this, consider the simple implicit generative model \( Q \) with

\[
q(x) = \int \delta(x - z\theta_q) N(z|0,1) \, dz,
\]

where the latent \( Z \) is univariate and \( \text{dim}(X) > 1 \). Here the vector \( \theta_q \) defines a one-dimensional line in the \( X \)-space. For \( D \)-dimensional \( X \), adding independent Gaussian noise with mean zero and isotropic covariance \( \sigma^2 I_D \) to \( X \) results in the noised distribution with density

\[
\tilde{q}(x) = N(x|0_D, \Sigma), \quad \Sigma \equiv \theta_q\theta_q^T + \sigma^2 I_D.
\]

For observed training data \( x_1, \ldots, x_N \) the log likelihood under this model is

\[
\frac{1}{N} \mathcal{L}(\theta_q) = -\frac{1}{N} \sum_{n=1}^N x_n^T \Sigma^{-1} x_n - \log \det \Sigma + \text{const.}
\]

We assume that the training data \( x_n \) is iid sampled from the distribution \( \mathbb{P} \) with generalised density

\[
p(x) = \int \delta(x - z\theta_p) N(z|0,1) \, dz.
\]

Hence \( \mathbb{P} \) and \( Q \) are from the same parametric distribution but with different parameters. By the law of large numbers, in the large \( N \) limit, the log likelihood eq(9) tends to

\[
-\theta_p^T \Sigma^{-1} \theta_p - \log \det \Sigma + \text{const.}
\]

which has an optimum when \(^6\) (see appendix(A))

\[
\theta_q = \sqrt{\frac{\theta_p^2 - \sigma^2}{\theta_p^2}} \theta_p.
\]

Thus adding noise to the model \( Q \) and training using maximum likelihood does not form a consistent estimator; it has an optimum at \( \theta_q \neq \theta_p \), resulting in an incorrect estimate of the data generating process. In appendix(A) we explain why annealing the noise \( \sigma^2 \) towards zero during numerical optimisation will not directly heal this problem.

Another well-known failure case of trying to learn an implicit generative model by adding noise only to the model is deterministic ICA, which we discuss at length in section(4.1).

For this reason alternative (non-likelihood, non-KL) approaches to measure the difference between distributions are commonly used in training implicit generative models (see for example Mohamed & Lakshminarayanan (2016), such as Maximum Mean Discrepancy (Gretton et al., 2012) and Wasserstein distance (Arjovsky et al., 2017; Peyré et al., 2019).

In the next section we introduce the Spread Divergence which defines a valid divergence even when the noise.\(^5\)

\(^5\)For a point \( x_n \) that is not on the model manifold, \( q(x_n) = 0 \). As we adjust \( \theta \) such that \( x_n \) becomes on the manifold, \( q(x_n) \) will typically increase to a finite non-zero value, meaning that the (log) likelihood is discontinuous in \( \theta \).

\(^6\)\( \theta_p^2 \) is shorthand for the squared length \( \| \theta_p \|^2 \).
supports of the distributions do not match or the distributions do not have a valid density. As we will demonstrate, the Spread Divergence allows one to use maximum likelihood based approaches to train implicit generative models, whilst resulting in a consistent estimator.

2. Spread Divergence

For distributions \( Q \) and \( P \) with generalised densities \( q(x) \) and \( p(x) \) we first need to define \( \tilde{q}(y) \) and \( \tilde{p}(y) \) that (i) are valid probability density functions and (ii) have the same support. In contrast to simply noising \( Q \) we define ‘noisy’ densities for both distributions

\[
\tilde{p}(y) = \int p(y|x)p(x)dx, \quad \tilde{q}(y) = \int p(y|x)q(x)dx
\]  

(13)

The ‘noise’ \( p(y|x) \) must ‘spread’ \( P \) and \( Q \) such that \( \tilde{p}(y) \) and \( \tilde{q}(y) \) satisfy the above two requirements. The choice of \( p(y|x) \) must also ensure that \( D(\tilde{p}|\tilde{q}) = 0 \iff P = Q \). If we can define the noise appropriately, this would allow us to define the Spread Divergence

\[
D(P||Q) = D(\tilde{p}||\tilde{q}),
\]  

(14)

which satisfies the divergence requirement \( D(P||Q) \geq 0 \) and \( D(P||Q) = 0 \iff P = Q \). In the following we discuss appropriate choices for the noise distribution \( p(y|x) \). We focus on stationary spread noise \( p(y|x) = k(y-x) \) since this is simple to implement by adding independent noise to a variable. Non-stationary spread distributions can be easily constructed using a mixture of stationary noise distributions, or through Mercer kernels – these are left for future study. The case of discrete \( X \) is discussed in appendix(B).

2.1. Stationary Spread Divergence

For a random variable \( X \) we define a new ‘stationary spread’ random variable \( Y \) by adding to \( X \) random noise \( K \). In order to ensure that \( Y \) has a valid probability density function and required support, we assume that \( K \) is absolutely continuous with density \( k(x) > 0, x \in \mathbb{R} \). We then define a random variable \( Y = X + K \). In the context of eq(13) this corresponds to using noise of the form \( p(y|x) = k(y-x) \).

2.1.1. Absolutely Continuous Distributions

For two absolutely continuous distributions \( P \) and \( Q \) with densities \( p(x) \) and \( q(x) \). We define \( \tilde{p} \) and \( \tilde{q} \) as a convolution

\[
\tilde{p}(y) = \int k(y-x)p(x)dx = (k*p)(y),
\]  

(15)

\[
\tilde{q}(y) = \int k(y-x)q(x)dx = (k*q)(y).
\]  

(16)

Since \( k>0 \), \( \tilde{p} \) and \( \tilde{q} \) have common support \( \mathbb{R} \).

Since all densities \( p(x) \) are absolutely integrable, the Fourier transforms \( F\{p\} \) and \( F\{q\} \) exist. Assuming \( F\{k\} \) also exists, we can then use the convolution theorem to write

\[
F\{\tilde{p}\} = F\{k\}F\{p\}, \quad F\{\tilde{q}\} = F\{k\}F\{q\}.
\]  

(17)

Let \( F\{k\} \neq 0 \). Then

\[
F\{k\}F\{p\} = F\{k\}F\{q\} \Rightarrow F\{p\} = F\{q\}.
\]  

(18)

Using this we can show that the stationary Spread Divergence is valid. A sketch of the proof is as follows:

\[
D(p||q) = 0 \iff D(\tilde{p}||\tilde{q}) = 0
\]  

(19)

\[
\iff \tilde{p} = \tilde{q} \text{ a.e.}
\]  

(20)

\[
\iff F\{k\}F\{p\} = F\{k\}F\{q\}
\]  

(21)

\[
\iff F\{p\} = F\{q\}
\]  

(22)

\[
\iff p = q \text{ a.e.} \iff P = Q,
\]  

(23)

where we used the invertibility of the Fourier transform.

Hence we can define a valid Spread Divergence provided (i) \( k(x) \) is a positive probability density function with support \( \mathbb{R} \) and (ii) \( F\{k\} \neq 0 \).

As an example consider Gaussian additive spread noise \( k(x) = \mathcal{N}(x|0, \sigma^2) \). This has Fourier transform

\[
F\{k\}(\omega) = e^{-\frac{\omega^2\sigma^2}{2}} > 0.
\]  

(24)

Similarly, for Laplace noise \( k(x) = \frac{1}{2\pi}e^{-\frac{|x|}{\gamma}} \),

\[
F\{k\}(\omega) = \sqrt{\frac{2}{\pi}} \frac{1}{b^2 + \omega^2} > 0.
\]  

(25)

In both cases \( k>0 \) and \( F\{k\}>0 \). Additive Gaussian and Laplace noise can therefore be used to define a valid Spread Divergence. That is, if the divergence between the spreaded distributions is zero, then the original distributions are equal.

2.1.2. General Stationary Case

The previous additive noise setting assumed that \( X \) is absolutely continuous. In appendix(C) we show how to extend this to all distributions, including implicit generative models. We show that adding absolutely continuous noise \( K \) to \( X \) defines an absolutely continuous random variable \( X + K \), even if \( X \) is itself not absolutely continuous (which is the case for implicit generative models). Applying the same additive noise process to both \( P \) and \( Q \) then results in absolutely continuous distributions that have densities \( \tilde{p} \) and \( \tilde{q} \) and common support. We further show that, provided the characteristic function of the additive random noise variable

\[\text{In fact the more general proof in appendix(C) shows that only the weaker condition that } F\{k\} \neq 0 \text{ on a countable set is needed.}\]
Spread Divergence

Figure 2. (a) Delta distributions $p(x) = \delta(x - \mu_p)$, $q(x) = \delta(x - \mu_q)$ where $\mu_p = 0$, $\mu_q = 1$. (b) Spreaded distributions $\tilde{p}(y) = \int p(y|x)p(x)dx$, $\tilde{q}(y) = \int p(y|x)q(x)dx$, where $p(y|x) = \mathcal{N}(y|x, \sigma^2 = 0.5)$. (c) The Spread KL divergence as a function of $\mu_q$.

As an illustration, consider the extreme case of two delta distributions $\mathbb{P}$ and $\mathbb{Q}$ with generalised densities

$$
    p(x) = \delta(x - \mu_p), \quad q(x) = \delta(x - \mu_q).
$$

In this case $\text{KL}(p||q)$ is not well defined. For stationary Gaussian noise $p(y|x) = \mathcal{N}(y|x, \sigma^2)$, the 'spreaded' distributions are:

$$
    \tilde{p}(y) = \int \delta(x - \mu_p)\mathcal{N}(y|x, \sigma^2) \, dx = \mathcal{N}(y|\mu_p, \sigma^2),
$$

$$
    \tilde{q}(y) = \int \delta(x - \mu_q)\mathcal{N}(y|x, \sigma^2) \, dx = \mathcal{N}(y|\mu_q, \sigma^2).
$$

For noise variance $\sigma^2 = 0.5$ this gives:

$$
    \text{KL}(\tilde{p}||\tilde{q}) = ||\mu_p - \mu_q||_2^2.
$$

Hence $\text{KL}(\tilde{p}||\tilde{q}) = 0 \iff \mathbb{P} = \mathbb{Q}$. It is also worth noting that the spread KL divergence in this case is equal to the squared 2-Wasserstein distance (Peyré et al., 2019; Gellrich, 1990). Treating $\mu_q$ as a variable, figure(2) illustrates the spread KL divergence converging to 0 as $\mu_q$ tends to $\mu_p = 0$.

This treatment of generalised densities allows us to define a divergence for implicit generative models and, by extension, an associated training algorithm, as we describe below.

2.2. Spread Maximum Likelihood Estimation

In section(1.1.1) we noted that in the context of fitting an implicit generative model $\mathbb{Q}$ to training data, simply adding noise to the model distribution $\mathbb{Q}$ and using maximum likelihood does not result in a consistent estimator. In the Spread Divergence case, for data $x_1, \ldots, x_N$ we define the empirical (generalised) density as

$$
    p(x) = \frac{1}{N} \sum_{n=1}^N \delta(x - x_n).
$$

For spread noise $p(y|x)$ we then spread both the model $\mathbb{Q}$ and empirical density using

$$
    \tilde{q}(y) = \int p(y|x)q(x)dx, \quad \tilde{p}(y) = \int p(y|x)p(x)dx. \quad (29)
$$

We then define the spread log likelihood using

$$
    \tilde{L} = \int \tilde{p}(y) \log \tilde{q}(y)dy. \quad (30)
$$

We consider that the data $x_1, \ldots, x_N$ is generated from the same underlying parametric implicit distribution as the model $\mathbb{Q}$

$$
    m(x; \theta_q) = \int \delta(x - g_{\theta_q}(z))q(z)dz,
$$

but with a different parameters $\theta_p$. Then as $N \to \infty$ (using the law of large numbers) the spread log likelihood becomes

$$
    \lim_{N \to \infty} \tilde{L} = \int \tilde{m}(y; \theta_p) \log \tilde{m}(y; \theta_q)dy, \quad (32)
$$

where

$$
    \tilde{m}(y; \theta) = \int p(y|x)m(x; \theta)dx. \quad (33)
$$

Up to an additive constant this is $-\text{KL}(\tilde{m}(y; \theta_p)||\tilde{m}(y; \theta_q))$. The spread log likelihood eq(32) therefore has a maximum when the spread KL divergence has a minimum. This occurs when the two spread distributions match $\tilde{m}(y; \theta_p) = \tilde{m}(y; \theta_q)$. Furthermore, by the property of the Spread Divergence, this means that the spread log likelihood has a maximum when the distributions match $m(y; \theta_p) = m(y; \theta_q)$.

K is non-zero\(^8\), the noise $K$ can be used to define a valid Spread Divergence between any two distributions with the property that $D_f(\mathbb{P}||\mathbb{Q}) = 0 \iff \mathbb{P} = \mathbb{Q}$. This non-zero requirement for the characteristic function is analogous to the characteristic condition on kernels such that the Maximum Mean Discrepancy MMD($\mathbb{P}, \mathbb{Q}$) = 0 $\iff \mathbb{P} = \mathbb{Q}$, see (Sriperumbudur et al., 2011; 2012; Gretton et al., 2012).

\(^8\)See appendix(C) for a weaker condition.
which occurs when $\theta_q = \theta_p$. Hence, the spread log likelihood defines a consistent estimator. In practice we typically cannot carry out the integral in eq(30) exactly, and resort to a sample approximation, sampling $L$ noisy versions $y_{n,l}$, $l = 1, \ldots, L$ of each datapoint $x_n$ to give

$$\hat{L} \approx \frac{1}{LN} \sum_{n=1}^{N} \sum_{l=1}^{L} \log \tilde{q}(y_{n,l}).$$

(34)

The Maximum Likelihood Estimator (MLE) is a cherished approach due to its consistency (convergence to the true parameters in the large data limit) and asymptotic efficiency (achieves the Cramér-Rao lower bound on the variance of any unbiased estimator) - see Casella & Berger (2002) for an introduction. An interesting question for future study is whether these properties also carry over to the spread MLE. In appendix(F), we demonstrate that spread MLE (for a certain family of spread noise) has weaker sufficient conditions than MLE for both consistency and asymptotic efficiency. Furthermore, a sufficient condition for the existence of the MLE is that the likelihood function is continuous over a compact parameter space $\Theta$. We provide an example in appendix(F.1) where the maximum likelihood estimator may not exist (since it violates the compactness requirement), but the spread maximum likelihood estimator still exists.

3. Maximising Discriminatory Power

Intuitively, spreading out distributions makes them more similar. More formally, from the data processing inequality (see appendix(D)), using spread noise will always decrease the $f$-divergence $D_f(\tilde{p}||\tilde{q}) \leq D_f(p||q)$ (when $D_f(p||q)$ is well defined). If we use spread MLE to train a model, too much noise may make the spreaded empirical and spreaded model distributions so similar that it becomes difficult to numerically distinguish them. It is useful therefore to learn spread noise $p_\psi(y|x)$ (parameterised by $\psi$) to maximally discriminate between the distributions $\max_\psi D(\tilde{p}||\tilde{q})$. In general we need to constrain the spread noise to ensure that the divergence remains bounded. The learned noise will discourage overlap between the two spreaded distributions.

We discuss below two complementary approaches to adjust $p_\psi(y|x)$. The first adjusts the covariance for Gaussian $p(y|x)$ and the second uses a mean transformation. In principle, both approaches can be combined and easily generalised to other noise distributions, such as the Laplace distribution. In section(4.2), we empirically investigate the benefit of these approaches when scaling the application of Spread Divergence to complex high dimensional problems.

3.1. Learning the Gaussian Noise Covariance

In learning Gaussian stationary spread noise $p(y|x) = \mathcal{N}(y|x, \Sigma)$, the number of parameters in the covariance matrix $\Sigma$ scales quadratically with the data dimension $D$. We therefore define $\Sigma = \sigma^2 I + UU^T$ where $\sigma^2 > 0$ is fixed (to ensure bounded Spread Divergence) and $U$ is a learnable $D \times R$ matrix with $R \ll D$.

As a simple example that can be computed exactly, we consider a implicit generative models with generalised densities $p$ and $q$ that generate data in separated linear subspaces,

$$p(x) = \int \delta(x - a - Az) p(z) dz$$

(35)

$$q(x) = \int \delta(x - b - Bz) p(z) dz,$$

(36)

with $p(z) = \mathcal{N}(z|0, I_D)$. The spreaded densities are then

$$\tilde{p}(y) = \mathcal{N}(y|a, AA^T + \Sigma), \quad \tilde{q}(y) = \mathcal{N}(y|b, BB^T + \Sigma).$$

As $\Sigma$ tends to zero, $\text{KL}(\tilde{p}||\tilde{q})$ tends to infinity. We therefore constrain $\Sigma = \sigma^2 I + uu^T$, where $\sigma^2$ is fixed and $u^T u = 1$. Also, for calculational simplicity, we assume $A = B$. The Spread Divergence $\text{KL}(\tilde{p}||\tilde{q})$ is then maximised for the noise direction $u$ pointing orthogonal to the vector $(AA^T + \sigma^2 I)^{-1} (b-a)$. The noise thus concentrates along directions defined by $p$ and $q$, as denoted by the ellipses.

3.2. Learning a Mean Transformation

Consider spread noise $p(y|x) = k(y - f(x))$ for injective\(^9\) $f$ and stationary $k$. Then, we define

$$\tilde{p}(y) = \int k(y - f(x)) p_x(x) dx.$$

(37)

Using a change of variables $s = f(x)$

$$\tilde{p}(y) = \int k(y - s) p_s(s) ds,$$

(38)

$$p_s(s) = p_x(f^{-1}(s))/J(x = f^{-1}(s)),$$

\(^9\)Since the co-domain of $f$ is determined by its range, injective indicates invertible in this case.
where \( J \) is the absolute Jacobian of \( f \). This is a valid Spread Divergence since eq(38) is in the form of standard stationary spread noise, but on an invertible transformed variable \( s \). Hence, \( \text{D}(p_\theta || q_\theta) = 0 \iff p_s = q_s \iff p_x = q_x \). Each injective \( f \) gives a different noise \( p(y|x) \) and hence we can search for the best noise implicitly by learning \( f \).

4. Applications

As an application of the spread MLE, we use it to train implicit generative models with generalised density

\[
p_\theta(x) = \int \delta(x - g_\theta(z)) p(z) dz,\]

where \( \theta \) are the parameters of the encoder \( g \). We show that, despite the likelihood gradient not being available, we can nevertheless successfully train such models using slightly modified versions of standard likelihood based training approaches, such as variational algorithms (Barber, 2012). In particular we discuss learning a low dimensional linear ICA model and a high dimensional deep generative model.

4.1. Implicit Linear Models: Deterministic ICA

ICA (Independent Components Analysis) corresponds to the model \( p(x,z) = p(x|z) \prod_i p(z_i) \), where the independent components \( z_i \) follow a non-Gaussian distribution. For Gaussian noise ICA an observation \( x \) is assumed to be generated by the process \( p(x|z) = \prod_j \mathcal{N}(x_j | g_j(z), \gamma^2) \) where \( g_j(z) \) mixes the independent latent process \( z \). In linear ICA, \( g_j(z) = a_j^T z \) where \( a_j \) is the \( j \)th column on the mixing matrix \( A \). For zero observation noise \( \gamma^2 = 0 \) this corresponds to a linear implicit generative model. For training data \( x_1, \ldots, x_N \) a standard maximum likelihood approach to learning \( A \) is to maximise

\[
\mathbb{E}_{p(y)} [\log p(y)],
\]

where \( p(x) \) is the marginal of the joint \( p(x,z) \) and we define the empirical distribution

\[
\hat{p}(x) = \frac{1}{N} \sum_{n=1}^N \delta(x - x_n).
\]

Since this is a latent variable model, it is natural to apply the EM algorithm (Dempster et al., 1977) to learn \( A \). However, for zero, or even small observation noise \( \gamma^2 \), it is well known that EM is ineffective (Bermond & Cardoso, 1999; Winther & Petersen, 2007). To see this, consider \( \text{dim}(X) = \text{dim}(Z) \) (where \( \text{dim}(X) \) and \( \text{dim}(Z) \) are the dimension of the data and latents respectively) and invertible \( A \). At iteration \( k \) the EM algorithm has an estimate \( A_k \) of the mixing matrix. It is straightforward to show that the M-step updates \( A_k \) to

\[
A_{k+1} = \mathbb{E} [zz^T] \mathbb{E} [zz^T]^{-1},
\]

where, for zero observation noise (\( \gamma = 0 \),

\[
\mathbb{E} [xz^T] = \frac{1}{N} \sum_{n=1}^N x_n (A_k^{-1} x_n^T) = \check{S} A_k^{-T},
\]

\[
\mathbb{E} [zz^T] = A_k^{-1} \check{S} A_k^{-T},
\]

and \( \check{S} \equiv \frac{1}{N} \sum_k x_n x_n^T \) is the moment matrix of the data. Thus, \( A_{k+1} = \check{S} A_k^{-T} (A_k^{-1} \check{S} A_k^{-T})^{-1} = A_k \) and the algorithm ‘freezes’. Similarly, for low noise \( \gamma \ll 1 \), progress critically slows down. Thus trying to train a deterministic ICA model by simply adding noise to the model will not help directly (see also section(1.1.1)).

To deal with small noise and the limiting case of a deterministic model (\( \gamma = 0 \)), we consider Gaussian spread noise \( p(y|x) = \mathcal{N}(y|x, \sigma^2 I_X) \) to give

\[
p(y, z) = \int p(y|x)p(x, z) dx = \prod_j \mathcal{N}(y_j | g_j(z), (\gamma^2 + \sigma^2) I_X) \prod_i p(z_i). \]

Using spread noise, the empirical distribution is replaced by the spread empirical distribution

\[
\hat{p}(y) = \frac{1}{N} \sum_n \mathcal{N}(y_n | x^n, \sigma^2 I_X).
\]

We then learn the model parameters by maximising the spread log likelihood (see section(2.2))

\[
\mathbb{E}_{\hat{p}(y)} [\log p(y)].
\]

Since this is of the form of a latent variable model, we can use an EM algorithm to maximise eq(49). The M-step to maximise the spread log likelihood has the same form as eq(43) but with modified statistics

\[
\mathbb{E} [yz^T] = \frac{1}{N} \sum_{n=1}^N \int p(y, z|n)yz^T dz dy,
\]

\[
\mathbb{E} [zz^T] = \frac{1}{N} \sum_{n=1}^N \int p(y, z|n)zz^T dz dy.
\]

where

\[
p(y, z|n) = \mathcal{N}(y | x^n, \sigma^2) p(z|y)
\]

with

\[
p(z|y) = \frac{1}{Z_q(y)} \mathcal{N}(z | \mu(y), \Sigma) \prod_i p(z_i),
\]

\[
Z_q(y) = \int \mathcal{N}(z | \mu(y), \Sigma) \prod_i p(z_i) dz,
\]

Here \( Z_q(y) \) is a normaliser and

\[
\Sigma = (\gamma^2 + \sigma^2) (A^T A)^{-1}, \quad \mu(y) = (A^T A)^{-1} A y.
\]
Since the posterior $p(z|y)$ peaks around $\mathcal{N}(z|\mu(y), \Sigma)$, we rewrite eq\((50)\) as

$$
\mathbb{E}[yz^T] = \frac{1}{N} \sum_{n} \int \mathcal{N}(y|x^n, \sigma^2 I_X) \mathcal{N}(z|\mu(y), \Sigma) \times \prod_{i} p(z_i) \frac{1}{Z_q(y)} yz^T dz dy
$$

and similarly for $\mathbb{E}[zz^T]$. Writing the expectations with respect to $\mathcal{N}(z|\mu(y), \Sigma)$ allows for a simple but effective importance sampling approximation focused on regions of high probability. We implement this update by drawing $S_y$ samples from $\mathcal{N}(y|x^n, \sigma^2 I_X)$ and, for each $y$ sample, we draw $S_z$ samples from $\mathcal{N}(z|\mu(y), \Sigma)$. This scheme has the advantage over more standard variational approaches, see for example (Winther & Petersen, 2007), in that we obtain a consistent estimator of the M-step update for $A$.

We show results for a toy experiment in figure\((4)\), learning the mixing matrix $A$ in a deterministic non-square setting. Note that standard algorithms such as FastICA (Hyvärinen, 1999) fail in this case. The spread noise is set to $\sigma = \max(0.001, 2.5 * \text{sqrt}($mean$(AA^T)))$. This modified EM algorithm thus learns a good approximation of $A$, with no critical slowing down.

### 4.2. Non-linear Implicit Models: $\delta$-VAE

A deep implicit generative model has generalised density

$$
p_\theta(x) = \int \delta(x - g_\theta(z)) p(z) dz,
$$

where $g_\theta$ is a deep neural network, see for example (Goodfellow et al., 2014). As discussed, for $\dim(Z) < \dim(X)$ we cannot use standard maximum likelihood approaches to train this model. To address this, we consider using the spread MLE approach section\((2.2)\). For training data $x_1, \ldots, x_N$ the empirical distribution is

$$
\hat{p}(x) = \frac{1}{N} \sum_{n=1}^{N} \delta(x - x_n).
$$

For Gaussian spread noise $p(y|x) = \mathcal{N}(y|x, \sigma^2 I_X)$, the spreaded empirical distribution is

$$
\hat{p}(y) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(y|x_n, \sigma^2 I_X),
$$

and the spreaded model is

$$
\tilde{p}_\theta(y) = \int \mathcal{N}(y|g_\theta(z), \sigma^2 I_X) p(z) dz
$$

$$
= \int p_\theta(y|z)p(z) dz.
$$

We then maximise the spread log likelihood

$$
\int \hat{p}(y) \log \tilde{p}_\theta(y) dy.
$$

Typically, the integral over $y$ is intractable, in which case we resort to a sampling estimation

$$
\frac{1}{NS} \sum_{n=1}^{N} \sum_{s=1}^{S} \log \tilde{p}_\theta(y^s_n),
$$

where $\gamma$ is the observation noise.

### Figure 4

Relative error $|A^{est}_{ij} - A^{true}_{ij}| / |A^{true}_{ij}|$ versus observation noise (a) and number of training points (b). (a) For $\dim(X) = 20$ dimensional observations and $\dim(Z) = 10$ dimensional latent variables, we generate $N=20000$ data points from the model $x = Az + \gamma \mathcal{N}(0, I_X)$, for independent zero mean unit variance Laplace $z$. The elements of $A$ are uniform random $\pm 1$. We use $S_y=1$, $S_z=1000$ samples and 2000 EM iterations to estimate $A$. The error is averaged over all $i, j$ and 10 experiments. We also plot standard errors around the mean relative error. In blue we show the error in learning $A$ using the standard EM algorithm. As $\gamma \to 0$, the error blows up as the EM algorithm ‘freezes’. In orange we plot the error for spread noise EM; no slowing down occurs as the observation noise $\gamma$ decreases. In (b), apart from small $N$, the spread EM algorithm error is lower than for the standard EM algorithm. Here $\dim(Z) = 5$, $\dim(X) = 10$, $S_y=1, S_z=1000$, $\gamma = 0.2$, with 500 EM updates used. Results are averaged over 50 runs of randomly drawn $A$. 

Note that standard algorithms such as FastICA (Hyvärinen, 1999) fail in this case.
Figure 5. Samples from a deep implicit generative model trained using $\delta$-VAE with (a) Laplace spread noise with fixed covariance, (b) Gaussian spread noise with fixed covariance and (c) Gaussian spread noise with learned covariance. We first train with one epoch a standard VAE as initialization to all models and keep the latent code $z \sim \mathcal{N}(z|0, I_Z)$ fixed when sampling from these models thereafter, so we can more easily compare the sample quality. See also figure(8) for further samples.

Figure 6. Samples from a deep implicit generative model trained using $\delta$-VAE with (a) fixed and (b) learned spread with the mean transformation method. See also figure(9) for more samples. We use a similar sampling strategy as in the MNIST experiment to facilitate sample comparison between the different models – see appendix(I).

where $y^n$ is a sample from $p(y^n|x_n) = \mathcal{N}(y^n|x_n, \sigma^2 I_X)$.

For non-linear $g$, the distribution $p_{\theta}(y)$ is usually intractable and we therefore use the variational lower bound

$$\log \hat{p}_\theta(y) \geq \int q_\phi(z|y) \left(-\log q_\phi(z|y) + \log (p_\theta(y|z)p(z))\right) dz. \quad (64)$$

This approach is a straightforward extension of the standard variational autoencoder (VAE) method (Kingma & Welling, 2013) and in appendix(G) we derive a lower variance objective and detail the learning procedure. We dub this model and associated Spread Divergence training the ‘$\delta$-VAE’.

For learning the spread noise we use the approach outlined in section(3). To learn the mean transformation function, we used an invertible residual network (Behrmann et al., 2018) $f_\psi : \mathbb{R}^D \rightarrow \mathbb{R}^D$ where $f_\psi = (f_{x_1}^\psi \circ \ldots \circ f_{x_T}^\psi)$ denotes a ResNet with blocks $f_{x_t}^\psi = I(\cdot) + g_{\psi_t}(\cdot)$. Then $f_\psi$ is invertible if the Lipschitz-constants $\text{Lip}(g_{\psi_t}) < 1$, for all $t \in \{1, \ldots, T\}$. Note that when using the Spread Divergence for training we only need samples from $p(y)$ which can be obtained from eq(37) by first sampling $x$ from $p_x(x)$ and then $y$ from $p(y|x) = k(y-f(x))$; this does not require computing the Jacobian or inverse $f_\psi^{-1}$.

**MNIST Experiment:** We trained a $\delta$-VAE on MNIST (Le-Cun et al., 2010) with (i) fixed Laplace spread noise, as in eq(25), (ii) fixed Gaussian spread noise, as in eq(24) and (iii) Gaussian noise with learned covariance, as in section(3.1), with rank $R = 20$; $g_\theta(\cdot)$ is a neural network that contains 3 feed forward layers. See appendix(H) for further details.

Figures 5(a,b,c) show samples from $p_\theta(x)$ for these models. MNIST is a relatively easy problem in the sense that it is hard to distinguish between the quality of the fixed and learned noise samples. We speculate that Laplace noise appears to improve image sharpness since this noise focuses attention on discriminating between points close to the data manifold (since the Laplace distribution is leptokurtic and has a higher probability of generating points close to the data manifold than the Gaussian distribution).

**CelebA Experiment:** We trained a $\delta$-VAE on the CelebA dataset (Liu et al., 2015) with (i) fixed and (ii) learned spread using the mean transformation method as discussed in section(3.2). We compare to results from a standard VAE with fixed Gaussian noise $p(x|z) = \mathcal{N}(x|g_\theta(z), 0.5 I_X)$ (Tolstikhin et al., 2017), where $g_\theta(\cdot)$ is a neural network contains 4 convolutional layers.

For (i) the fixed Spread Divergence uses Gaussian noise $\mathcal{N}(y|x, 0.25 I_X)$. For (ii) we use Gaussian noise with a learned injective function in the form of a ResNet: $f_\psi(\cdot) = I(\cdot) + g_\psi(\cdot)$ - see appendix(I) for details. Figure 6 shows samples from our $\delta$-VAE for (i) and (ii) (with $g_\theta(z)$ initialised to the fixed-noise setting). It is notable how the ‘sharpness’ of the image samples substantially increases when learning the spread noise. Table 1 shows Frechet Inception Distance (FID) (Heusel et al., 2017) score comparisons between different baseline algorithms for implicit generative model training.\(^{10}\) The $\delta$-VAE significantly improves on the standard VAE result. Learning the mean transformation improves on the fixed-noise $\delta$-VAE. Indeed the mean transformation $\delta$-VAE results are comparable to popular GAN and WAE models (Gulrajani et al., 2017; Berthelot et al., 2017; Arjovsky et al., 2017; Kodali et al., 2017; Mao et al., 2017; Fedus et al., 2017; Tolstikhin et al., 2017). Whilst the $\delta$-VAE results are not state-of-the-art, we believe\(^{10}\) FID scores were computed using github.com/bioinf-jku/TTUR based on 10000 samples.
Table 1. CelebA FID Scores. The $\delta$-VAE results are the average over 5 independent measurements. The scores of the GAN models are based on a large-scale hyperparameter search and take the best FID obtained (Lucic et al., 2018). The results of the VAE model and both WAE-based models are from (Tolstikhin et al., 2017).

| Encoder-Decoder Models | FID | GAN Models | FID |
|------------------------|-----|------------|-----|
| VAE                    | 63.0| WGAN GP    | 30.0|
| $\delta$-VAE with fixed spread | 52.7| BEGAN      | 38.9|
| $\delta$-VAE with learned spread | 46.5| WGAN       | 41.3|
| WAE-MMD                | 55.0| DRAGAN     | 42.3|
| WAE-GAN                | 42.0| LSGAN      | 53.9|
|                        |      | NS GAN     | 55.0|
|                        |      | MM GAN     | 65.6|

it is the first time that implicit models have been trained using a principled maximum likelihood based approach. By increasing the complexity of the generative model $g_\theta$ and injective function $f_\psi$, or using better choices of noise, the results may become more competitive with state-of-the-art GAN models.

5. Related Work

**Instance noise:** The instance noise trick to stabilize GAN training (Roth et al., 2017; Sonderby et al., 2016) is a special case of Spread Divergence using fixed Gaussian noise. Whilst other similar tricks, e.g. (Furmston & Barber, 2009), have been proposed previously, we believe it is important to state the more general utility of the spread noise approach.

**$\delta$-VAE versus WAE:** The Wasserstein Auto-Encoder (Tolstikhin et al., 2017) is another implicit generative model that uses an encoder-decoder architecture. The major difference to our work is that the $\delta$-VAE is based on the KL divergence, which corresponds to MLE, whereas the WAE uses the Wasserstein distance.

**$\delta$-VAE versus denoising VAE:** The denoising VAE (Im et al., 2017) uses a VAE with noise added to the data only. In contrast, for our $\delta$-VAE, spread MLE adds noise to both the data and the model. Therefore, the denoising VAE cannot recover the true data distribution, whereas in principle the $\delta$-VAE with spread MLE can.

**MMD GAN with kernel learning:** Learning a kernel to increase discrimination is also used in MMD GAN (Li et al., 2017). Similar to ours, the kernel in MMD GAN is constructed by $k = k \circ f_\psi$, where $k$ is a fixed kernel and $f_\psi$ is a neural network. To ensure the MMD distance $M_{f_\psi}(p, q) = 0 \Leftrightarrow p = q$, this requires $f_\psi$ to be injective (Gretton et al., 2012). However, in this framework, $f_\psi(x)$ usually maps $x$ to a lower dimensional space. This is crucial for MMD because the amount of data required to produce a reliable estimator grows with the data dimension (Ramdas et al., 2015) and the computational cost of MMD scales quadratically with the amount of data. Whilst using a lower-dimensional mapping makes MMD more practical it also makes it difficult to construct an injective function $f$. For this reason, heuristics such as the auto-encoder regularizer (Li et al., 2017) are considered. In contrast, for the $\delta$-VAE with spread MLE, the cost of estimating the divergence is linear in the number of data points. Therefore, there is no need for $f_\psi$ to be a lower-dimensional mapping: guaranteeing that $f_\psi$ is injective is straightforward for the $\delta$-VAE.

**Flow-based generative models:** Invertible flow-based functions (Rezende & Mohamed, 2015) have been used to boost the representation power of generative models. Our use of injective functions is quite distinct from the use of flow-based functions to boost generative model capacity. In our case, the injective function $f$ does not change the model - it only changes the divergence. For this reason, the Spread Divergence doesn’t require the log determinant of the Jacobian, which is required in (Rezende & Mohamed, 2015; Behrmann et al., 2018), meaning that more general invertible functions can be used to boost the discriminatory power of a Spread Divergence.

6. Summary

We described how to define a divergence even when two distributions don’t have valid probability density functions or have the same support. We showed that defining divergences this way enables us to train implicit generative models using standard likelihood based approaches. In principle, we can learn the true data generating implicit generative model by using any valid Spread Divergence. In practice, however, the quality of the learned model can depend strongly on the choice of spread noise. We therefore investigated learning spread noise to maximally discriminate between two distributions. We found that the resulting training approach is numerically stable and that it can significantly improve the quality of the learned model.

There are several directions for further investigation: (i) the broader family of spread noise and their properties, including statistical efficiency; (ii) optimal noise selection for different tasks; (iii) the connections between Spread Divergence and other distance (or divergence) measures, e.g. MMD, Wasserstein Distance.

Acknowledgments

We would like to thank a reviewer for improving our consideration of non-absolutely continuous distributions and Li Zhu for useful discussions.

11 We also tried learning the image generator using Laplace spread noise. However, the colour of the sampled images becomes overly intense and we leave it to future work to address this.
References

Ali, S. and Silvey, S. A General Class of Coefficients of Divergence of one Distribution from Another. *Journal of the Royal Statistical Society: Series B (Methodological)*, 28(1):131–142, 1966.

Arjovsky, M., Chintala, S., and Bottou, L. Wasserstein GAN. *arXiv:1701.07875*, 2017.

Burber, D. *Bayesian Reasoning and Machine Learning*. Cambridge University Press, 2012.

Behrmann, J., Duvenaud, D., and Jacobsen, J. Invertible Residual Networks. *arXiv:1811.00995*, 2018.

Bermond, O. and Cardoso, J. Approximate Likelihood for Noisy Mixtures. In *Proc. ICA ’99*, pp. 325–330, 1999.

Berthelot, D., Schumm, T., and Metz, L. Began: Boundary Equilibrium Generative Adversarial Networks. *arXiv:1703.10717*, 2017.

Casella, G. and Berger, R. *Statistical Inference*, volume 2. Duxbury Pacific Grove, CA, 2002.

Cramér, H. *Mathematical Methods of Statistics*, volume 9. Princeton University Press, 1999.

Csiszár, I. Information-type Measures of Difference of Probability Distributions and Indirect Observation. *studia scientiarum Mathematicarum Hungarica*, 2:229–318, 1967.

Csiszár, I. A Class of Measures of Informativity of Observation Channels. *Periodica Mathematica Hungarica*, 2(1-4):191–213, 1972.

Dempster, A., Laird, N., and Rubin, D. Maximum Likelihood from Incomplete Data via the EM algorithm. *Journal of the Royal Statistical Society: Series B (Methodological)*, 39(1):1–22, 1977.

Dragomir, S. Some General Divergence Measures for Probability Distributions. *Acta Mathematica Hungarica*, 109(4):331–345, Nov 2005. ISSN 1588-2632. doi: 10.1007/s10474-005-0251-6.

Durrett, R. *Probability: Theory and Examples*, volume 49. Cambridge university press, 2019.

Fedus, W., Rosca, M., Lakshminarayanan, B., Dai, A., Mohamed, S., and Goodfellow, I. Many Paths to Equilibrium: GANs Do Not Need to Decrease a Divergence at Every Step. *arXiv:1710.08446*, 2017.

Ferguson, T. An Inconsistent Maximum Likelihood Estimate. *Journal of the American Statistical Association*, 77(380):831–834, 1982.

Furmston, T. and Barber, D. Solving Deterministic Policy (PO)MPDs using Expectation-Maximisation and Antifreeze. In *First international workshop on learning and data mining for robotics (LEMIR)*, pp. 56–70, 2009. In conjunction with ECML/PKDD-2009.

Gelbrich, M. On a Formula for the L2 Wasserstein Metric Between Measures on Euclidean and Hilbert Spaces. *Mathematische Nachrichten*, 147(1):185–203, 1990.

Gerchinovitz, S., Ménard, P., and Stoltz, G. Fano’s Inequality for Random Variables. *arXiv*, 2018. doi: arXiv:1702.05985v2.

Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., Courville, A., and Bengio, Y. Generative Adversarial Nets. In *Advances in Neural Information Processing Systems*, pp. 2672–2680, 2014.

Gretton, A., Borgwardt, K., Rasch, M., Schölkopf, B., and Smola, A. A Kernel Two-Sample Test. *Journal of Machine Learning Research*, 13(Mar):723–773, 2012.

Gulrajani, I., Ahmed, F., Arjovsky, M., Dumoulin, V., and Courville, A. Improved Training of Wasserstein GANs. In *Advances in Neural Information Processing Systems*, pp. 5767–5777, 2017.

Heusel, M., Ramsauer, H., Unterthiner, T., Nessler, B., and Hochreiter, S. GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium. In *Advances in Neural Information Processing Systems*, pp. 6626–6637, 2017.

Hyvärinen, A. Fast and Robust Fixed-point Algorithms for Independent Component Analysis. *IEEE Transactions on Neural Networks*, 10(3):626–634, May 1999. ISSN 1045-9227. doi: 10.1109/72.761722.

Im, D., Ahn, S., Memisevic, R., and Bengio, Y. Denoising Criterion for Variational Auto-Encoding Framework. In *Thirty-First AAAI Conference on Artificial Intelligence*, 2017.

Ioffe, S. and Szegedy, C. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. *arXiv:1502.03167*, 2015.

Kallenberg, O. *Foundations of Modern Probability*. Springer Science & Business Media, 2006.

Kingma, D. and Ba, J. Adam: A Method for Stochastic Optimization. *arXiv:1412.6980*, 2014.

Kingma, D. and Welling, M. Auto-Encoding Variational Bayes. *arXiv:1312.6114 [stat.ML]*, 2013.

Kodali, N., Abernethy, J., Hays, J., and Kira, Z. On Convergence and Stability of GANs. *arXiv:1705.07215*, 2017.
LeCun, Y., Cortes, C., and Burges, C. MNIST Handwritten Digit Database. AT&T Labs [Online]. Available: http://yann.lecun.com/exdb/mnist, 2:18, 2010.

Lehmann, E. Elements of Large-sample Theory. Springer Science & Business Media, 2004.

Li, C., Chang, W., Cheng, Y., Yang, Y., and Póczos, B. MMD GAN: Towards Deeper Understanding of Moment Matching Network. In Advances in Neural Information Processing Systems, pp. 2203–2213, 2017.

Liu, Z., Luo, P., Wang, X., and Tang, X. Deep Learning Face Attributes in the Wild. In Proceedings of International Conference on Computer Vision (ICCV), 2015.

Lucic, M., Kurach, K., Michalski, M., Gelly, S., and Bousquet, O. Are GANs Created Equal? A Large-Scale Study. In Advances in Neural Information Processing Systems, pp. 700–709, 2018.

Mao, X., Li, Q., Xie, H., Lau, R., Wang, Z., and S., P. Least Squares Generative Adversarial networks. In Proceedings of the IEEE International Conference on Computer Vision, pp. 2794–2802, 2017.

Miyato, T., Kataoka, T., Koyama, M., and Yoshida, Y. Spectral Normalization for Generative Adversarial Networks. arXiv:1802.05957, 2018.

Mohamed, S. and Lakshminarayanan, B. Learning in Implicit Generative Models. arXiv, 2016. doi: arXiv: 1610.03483.

Peyré, G., Cuturi, M., et al. Computational Optimal Transport. Foundations and Trends® in Machine Learning, 11 (5-6):355–607, 2019.

Ramdas, A., Reddi, S., Póczos, B., Singh, A., and Wasserman, L. On the Decreasing Power of Kernel and Distance Based Nonparametric Hypothesis Tests in High Dimensions. In Twenty-Ninth AAAI Conference on Artificial Intelligence, 2015.

Rezende, J. and Mohamed, S. Variational Inference with Normalizing Flows. arXiv:1505.05770, 2015.

Roth, K., Lucchi, A., Nowozin, S., and Hofmann, T. Stabilizing Training of Generative Adversarial Networks through Regularization. pp. 2018–2028, 2017.

Sønderby, C., Caballero, J., Theis, L., Shi, W., and Huszár, F. Amortised Map Inference for Image Super-Resolution. arXiv:1610.04490, 2016.

Sriperumbudur, B., Fukumizu, K., and Lanckriet, G. Universality, Characteristic Kernels and RKHS Embedding of Measures. J. Mach. Learn. Res., 12:2389–2410, July 2011. ISSN 1532-4435.

Tao, T. An Introduction to Measure Theory. 2011.

Tolstikhin, I., Bousquet, O., Gelly, S., and Schölkopf, B. Wasserstein Auto-Encoders. arXiv:1711.01558, 2017.

Wald, A. Note on the Consistency of the Maximum Likelihood Estimate. The Annals of Mathematical Statistics, 20(4):595–601, 1949.

Winther, O. and Petersen, K. Bayesian Independent Component Analysis: Variational Methods and Non-negative Decompositions. Digital Signal Processing, 17(5):858 – 872, 2007. ISSN 1051-2004. Special Issue on Bayesian Source Separation.

Wu, Y., Burda, Y., Salakhutdinov, R., and Grosse, R. On the Quantitative Analysis of Decoder-based Generative Models. arXiv:1611.04273, 2016.

Zhang, M., Bird, T., Habib, R., Xu, T., and Barber, D. Variational f-Divergence Minimization. arXiv:1907.11891, 2018.
A. Annealing the Noise

In section(1.1.1) we discussed the common approach to first adding noise to a model $Q$ in order to define a proper density and then using maximum likelihood to fit that 'noised model' to data.

We can use standard Woodberry identities to rewrite the expected log likelihood eq(11) as

$$-\frac{\theta_p^2}{\sigma^2} + \frac{(\theta_p^T\theta_q)^2}{\sigma^2(\sigma^2 + \theta_q^2)} - \log \left(1 + \frac{\theta_q^2}{\sigma^2}\right) - D \log \sigma^2.$$  (65)

where $D = \text{dim}(\theta_p)$.

Differentiating wrt $\theta_q$, we note that the optimal solution is given when

$$\theta_q = \gamma \theta_p,$$  (66)

for scalar $\gamma$. Plugging this form back into eq(65) we find that the optimum is obtained when

$$\theta_q = \sqrt{\frac{\theta_p^2 - \sigma^2}{\theta_p^2}} \theta_p.$$  (67)

For finite Gaussian noise $\sigma^2 > 0$ the resulting estimator for the toy model in section(1.1.1) is therefore not consistent.

A natural question is what would happen if one uses a numerical optimisation of eq(65) but anneals the noise $\sigma^2$ to zero during the optimisation process? As $\sigma^2$ tends to zero, the expression eq(65) blows up. This means that a naive approach to annealing $\sigma^2$ towards zero whilst using a standard optimisation technique is unlikely to result in $\theta_q$ converging to $\theta_p$.

However, if one considers removing the additive constant $D \log \sigma^2$ and multiplying the remaining objective by $\sigma^2$, the resulting quantity

$$\frac{(\theta_p^T\theta_q)^2}{(\sigma^2 + \theta_q^2)} - \sigma^2 \log \left(1 + \frac{\theta_q^2}{\sigma^2}\right),$$  (68)

is well-behaved as $\sigma^2 \to 0$, as plotted in figure(7).

![Figure 7](image_url)

*Figure 7.* The (modified) expected log likelihood eq(68) when adding noise $\sigma^2$ to the model only and for unit length true data generating parameter $\theta_p^2 = 1$. The $x$-axis is the value $\gamma^2$ assuming that the optimal $\theta_q$ is of the form $\theta_q = \gamma \theta_p$. As we see, as $\sigma^2 \to 0$ the scaled objective becomes flat around the optimum point $\gamma^2 = 1$. 
Spread Divergence

Nevertheless, the objective eq(68) becomes flat (with respect to \( \theta_q \)) around the optimum as \( \sigma^2 \to 0 \). In figure(7) we plot the scaling behaviour of the objective eq(68), assuming \( \theta_q = \gamma \theta_p \), showing how it becomes flat with respect to \( \gamma \) as \( \sigma^2 \) is annealed towards zero. This means that a standard first-order numerical optimisation approach, even for this modified objective, will result in a ‘critical slowing down’ phenomenon, leading to \( \theta_q \) not updating. This might be fixable by taking the curvature of the objective into consideration.

However, addressing all the above issues requires an understanding of the small \( \sigma^2 \) behaviour of the original objective; dealing with arbitrarily large constants, arbitrarily large scaling and loss of curvature. In general, such insight is unlikely to be available for any given implicit generative model. Thus, we are doubtful that it will be possible to find an annealing schedule and associated general numerical optimisation procedure that will result in a consistent estimator.

B. Noise Requirements for Discrete Distributions

Our main interest is to define a new divergence in situations where the original divergence \( D(p||q) \) is itself not defined. For discrete variables \( x \in \{1, \ldots, n\} \), \( y \in \{1, \ldots, n\} \), the spread \( P_{ij} = p(y = i|x = j) \) must be a distribution; \( \sum_j P_{ij} = 1 \), \( P_{ij} \geq 0 \), and

\[
\tilde{p}_i \equiv \sum_j P_{ij} p_j = \sum_j P_{ij} q_j \equiv \tilde{q}_i \quad \forall i
\]

\[
\Rightarrow \quad p_j = q_j \quad \forall j,
\]

which is equivalent to the requirement that the matrix \( P \) is invertible. In addition, for the Spread Divergence to exist in the case of \( f \)-divergences, \( \tilde{p} \) and \( \tilde{q} \) must have the same support. This requirement is guaranteed if

\[
\sum_j P_{ij} p_j > 0, \quad \sum_j P_{ij} q_j > 0 \quad \forall i,
\]

which is satisfied if \( P_{ij} > 0 \). Therefore, in general there is a space of spread distributions \( p(y|x) \) that define a valid Spread Divergence in the discrete case.

C. Validity of Stationary Spread \( f \)-Divergence

**Lemma 1.** Let \( X \) and \( Y \) be two random variables with Borel probability measure \( \mathbb{P}_X \) and \( \mathbb{P}_Y \). Let \( K \) be an absolutely continuous random variable that is independent of \( X \) and \( Y \) and has density function \( p_K(x) \). We define \( \tilde{X} \) and \( \tilde{Y} \) as

\[
\tilde{X} = X + K, \quad \tilde{Y} = Y + K,
\]

with distribution \( \mathbb{P}_{\tilde{X}} \) and \( \mathbb{P}_{\tilde{Y}} \). Then \( \tilde{X} \) and \( \tilde{Y} \) are absolutely continuous with density functions

\[
p_{\tilde{X}}(\tilde{x}) = \int_x p_K(\tilde{x} - x)d\mathbb{P}_X, \quad p_{\tilde{Y}}(\tilde{y}) = \int_y p_K(\tilde{y} - y)d\mathbb{P}_Y.
\]

**Proof.** The proof can be found in Durrett (2019, Theorem 2.1.16). \( \square \)

**Theorem 1.** Let \( X \) and \( Y \) be two random variables\(^{12}\) with Borel probability measure \( \mathbb{P}_X \) and \( \mathbb{P}_Y \). Let the stationary spread noise \( K \) be an absolutely continuous random variable that is independent of \( X \) and \( Y \), and its density function \( p_K(x) \) has support\(^ {13} \) \( \mathbb{R} \). Using lemma(1) we define spreaded random variables \( \tilde{X} = X + K, \tilde{Y} = Y + K \) with density functions \( p_{\tilde{X}}, \ p_{\tilde{Y}} \). We then define the stationary spread \( f \)-divergence between \( \mathbb{P}_X \) and \( \mathbb{P}_Y \) as

\[
\tilde{D}_f(\mathbb{P}_X||\mathbb{P}_Y) \equiv D_f(p_{\tilde{X}}||p_{\tilde{Y}}) = \int f(\frac{p_{\tilde{X}}(x)}{p_{\tilde{Y}}(x)}) p_{\tilde{Y}}(x)dx.
\]

Furthermore, denote the characteristic function\(^ {14} \) of the spread noise \( K \) by \( \phi_K \). Given \( \phi_K \neq 0 \) or \( \phi_K > 0 \) on at most a countable set, then the stationary spread \( f \)-divergence is a valid divergence with the properties

\[
\tilde{D}_f(\mathbb{P}_X||\mathbb{P}_Y) \geq 0, \quad \tilde{D}_f(\mathbb{P}_X||\mathbb{P}_Y) = 0 \iff \mathbb{P}_X = \mathbb{P}_Y.
\]

\(^{12}\)We don’t require \( X \) (or \( Y \)) to be absolutely continuous.

\(^{13}\)The extension to higher dimensions is straightforward.

\(^{14}\)When a distribution \( \mathbb{P}_X \) allows a density function \( p_X \), its characteristic function is equal to the Fourier transform of the density function: \( \phi_X = \mathcal{F}(p_X) \), so the Fourier transform treatment used in the main text can be seen as a special case of the characteristic function treatment.
Proof. The proof contains the following two steps.

First step: We show that if $K$ is an absolutely continuous random variable and its density function $p_K$ has support $\mathbb{R}$, then $\tilde{D}_f(P_X||P_Y) = 0 \Leftrightarrow P_X = P_Y$. By Lemma 1, we have $\tilde{X}$ and $\tilde{Y}$ are absolutely continuous and allow probability density functions $p_\tilde{X}$ and $p_\tilde{Y}$. Since $p_K$ has support $\mathbb{R}$, $p_\tilde{X}$ and $p_\tilde{Y}$ will also have support $\mathbb{R}$. The $f$-divergence between two absolutely continuous distributions with common support is equal to zero if and only if two distributions are equal (Csiszar, 1967; 1972). We have $D_f(p_\tilde{X}||p_\tilde{Y}) = 0 \Leftrightarrow P_\tilde{X} = P_\tilde{Y}$. Therefore,

$$\tilde{D}_f(P_X||P_Y) = 0 \Leftrightarrow P_X = P_Y.$$

Second step: We show that if the characteristic function of the spread noise $\phi_K \neq 0$ or $\phi_K = 0$ on at most a countable set then $P_\tilde{X} = P_\tilde{Y} \Leftrightarrow P_X = P_Y$.

The characteristic function of a probability measure $P_X$ is defined as $\phi_X(w) = \int e^{iwx} dP_X$. Since a probability measure is uniquely determined by its characteristic function (Kallenberg, 2006, Theorem 4.3), we have

$$P_\tilde{X} = P_\tilde{Y} \Leftrightarrow \phi_\tilde{X} = \phi_\tilde{Y}.$$

Using the fact that the characteristic function of the sum of two random variables is equal to the product of their characteristic functions (Durrett, 2019, Theorem 3.3.2), we can write

$$\phi_X = \phi_Y \Leftrightarrow \phi_X \phi_K = \phi_Y \phi_K.$$

When $\phi_K \neq 0$, we have $\phi_X \phi_K = \phi_Y \phi_K \Leftrightarrow \phi_X = \phi_Y$.

When $\phi_K = 0$ on at most a countable set $\mathcal{C}$, we show that $\phi_X \phi_K = \phi_Y \phi_K \Leftrightarrow \phi_X = \phi_Y$ still holds. We prove this by contradiction:

We assume there is a point $w_0 \in \mathcal{C}$ where $\phi_X(w_0) \neq \phi_Y(w_0)$. Without loss of generality, we assume $\phi_X(w_0) - \phi_Y(w_0) = \delta > 0$. For points $w_0 + h$ that are not in $\mathcal{C}$, we have $\phi_K(w_0 + h) \neq 0$, so $\phi_X \phi_K = \phi_Y \phi_K$ implies $\phi_X(w_0 + h) - \phi_Y(w_0 + h) = 0$. Since the characteristic function of a distribution is uniform continuous (Durrett, 2019, Theorem 3.3.1), we have $\delta = \phi_X(w_0 + h) - \phi_Y(w_0 + h) \rightarrow 0$ when $h \rightarrow 0$, which leads to a contradiction (since $\delta$ cannot be zero). Therefore, $\phi_X \phi_K = \phi_Y \phi_K \Leftrightarrow \phi_X = \phi_Y$.

By the uniqueness of the characteristic function (Kallenberg, 2006, Theorem 4.3), we have

$$\phi_X = \phi_Y \Leftrightarrow P_X = P_Y.$$

Using the results of the two steps, we can conclude

$$\tilde{D}_f(P_X||P_Y) = 0 \Leftrightarrow P_X = P_Y \Leftrightarrow P_\tilde{X} = P_\tilde{Y}.$$

D. Spread Noise Makes Distributions More Similar

The data processing inequality for $f$-divergences (Gerchinovitz et al., 2018) states that $D_f(\tilde{p}(y)||\tilde{q}(y)) \leq D_f(p(x)||q(x))$. For completeness, we provide here an elementary proof of this result. We consider the following joint distributions with densities

$$q(y, x) = p(y|x)q(x), \quad p(y, x) = p(y|x)p(x),$$

whose marginals are the spreaded distributions

$$\tilde{p}(y) = \int p(y|x)p(x)dx, \quad \tilde{q}(y) = \int p(y|x)q(x)dx.$$

The divergence between the two joint distributions is

$$D_f(p(y, x)||q(y, x)) = \int q(y, x)f\left(\frac{p(y|x)p(x)}{p(y|x)q(x)}\right)dxdy = D_f(p(x)||q(x)).$$
More generally, the $f$-divergence between two marginal distributions is no larger than the $f$-divergence between the joint (Zhang et al., 2018). To see this, consider

$$D_f(p(u,v)||q(u,v)) = \int q(u) \int q(v|u) f \left( \frac{p(u,v)}{q(u,v)} \right) du dv$$

(75)

$$\geq \int q(u) f \left( \int q(v|u) \frac{p(u,v)}{q(v|u)q(u)} du \right) dv$$

(76)

$$= \int q(u) f \left( \frac{p(u)}{q(u)} \right) du = D_f(p(u)||q(u)).$$

(77)

Hence,

$$D_f(q(x)||p(x)) = D_f(\hat{p}(y)||\hat{q}(y)) \leq D_f(p(y,x)||q(y,x)) = D_f(p(x)||q(x)).$$

(78)

Intuitively, spreading two distributions increases their overlap, reducing the divergence. When the distributions $P$ and $Q$ are absolutely continuous and their densities $p$ and $q$ have the same support, the spread $f$-divergence is always a lower bound of $f$-divergence. When the densities do not have the same support or are not well defined, then $D_f(P||Q)$ is not well-defined.

E. Mixture Divergence

We motivated the Spread Divergence between distribution $P$ and $Q$ by the requirement to produce a divergence that satisfying $D(P||Q) = 0 \Rightarrow P = Q$, where the original $D(P||Q)$ does not exist. We briefly discuss the case that $P$ and $Q$ are absolutely continuous but their density functions $p$ and $q$ have different supports, so $f$-divergence $D_f(P||Q) = D(p||q)$ is still not defined. For example, $P$ and $Q$ can be two uniform distributions with different supports. We mention here an alternative divergence that also can be used, namely a mixture divergence, and discuss why we focus on the Spread Divergence thereafter. Specifically, we can define a mixture model with density $\tilde{p}(x)$ of the original distribution and a ‘noise’ distribution with density function $n(x)$:

$$\tilde{p}(x) = \alpha p(x) + (1 - \alpha)n(x)$$

(79)

for $0 < \alpha < 1$. Provided $n(x)$ is non-zero, then $\tilde{p}(x)$ has support everywhere. Similarly, we can define

$$\tilde{q}(x) = \alpha q(x) + (1 - \alpha)n(x).$$

(80)

As with the Spread Divergence formulation presented previously, this will usually enable us to define a divergence $D(\tilde{p}||\tilde{q})$ when supp$(p) \neq $ supp$(q)$. Furthermore, provided the divergence between $\tilde{p}$ and $\tilde{q}$ is zero, then the two distributions $\tilde{p}$ and $\tilde{q}$ match, as do the original distributions $p$ and $q$ since

$$\tilde{p}(x) = \tilde{q}(x) \Leftrightarrow \alpha p(x) + (1 - \alpha)n(x) = \alpha q(x) + (1 - \alpha)n(x) \Leftrightarrow p(x) = q(x).$$

(81)

Therefore, creating a mixture model in this way also allows us to define a divergence between absolutely continuous distributions that otherwise would not have an appropriate divergence\(^{15}\). However, in contrast to the Spread Divergence formulation, we cannot use this approach for distributions that are not absolutely continuous, which for many applications of interest cannot be achieved. As a simple example, consider generalised densities $p(x) = \delta(x - \mu_p)$, $q(x) = \delta(x - \mu_q)$ with

$$\tilde{p}(x) = \alpha \delta(x - \mu_p) + (1 - \alpha)n(x), \quad \tilde{q}(x) = \alpha \delta(x - \mu_q) + (1 - \alpha)n(x).$$

(82)

In this case, the divergence $D(\tilde{p}(x)||\tilde{q}(x))$ is not defined since neither $\tilde{p}(x)$ nor $\tilde{q}(x)$ is a valid probability density. A similar issue arises in training implicit generative models in which a value cannot be feasibly computed for $\tilde{p}$ or $\tilde{q}$; see section(4.2). Hence, for implicit models in, we cannot feasibly assign a value to this mixture divergence. As such it appears to have only limited value in training continuous variable models.

One can combine the spread and the mixture approaches to produce a more general affine divergence

$$\tilde{p}(y) = \alpha \int p(y|x)p(x)dx + (1 - \alpha)n(y),$$

(83)

\(^{15}\)This approach is equivalent to the ‘anti-freeze’ method used in (Furmston & Barber, 2009), which was used to enable EM style training in deterministic transition Markov Decision Processes of discrete states - see also (Barber, 2012).
for spread \( p(y|x) \) and (generalised) density \( p(x) \). It follows for this case that \( D(\bar{p}||\bar{q}) = 0 \iff P = Q \); however, the benefit of the mixture noise over the spread noise is not clear. Our central interest in this work is to train implicit models and, as such, we focus interest only on the first ‘spread’ term \( \int_x p(y|x)p(x) \) in eq(83) and leave the study of the potential additional benefits of including a mixture component \( n(y) \) for future work.

F. Statistical Properties of Maximum Likelihood Estimator

F.1. Existence of Spread MLE

In some situations there may not exist a Maximum Likelihood Estimator (MLE) for \( p(x|\theta) \), but there can exist a MLE for the spread model \( p(y|\theta) = \int p(y|x)p(x|\theta)dx \). For example, suppose that \( X \sim \mathcal{N}(\mu, \sigma^2) (\mu, 0 < \sigma^2 < \infty) \). So \( \theta = (\mu, \sigma^2) \in \mathbb{R} \times \mathbb{R}^+ \). Assume we only have one data point \( x \). Then the log-likelihood function is \( L(x; \theta) \propto -\log \sigma - \frac{1}{2\sigma^2}(x - \mu)^2 \). Maximising with respect to \( \mu \), we have \( \mu = x \) and the log-likelihood becomes unbounded as \( \sigma^2 \to 0 \). In this sense, the MLE for \( (\mu, \sigma^2) \) does not exist, see (Casella & Berger, 2002) for more discussions.

In contrast, we can check whether the MLE for \( p(y|\theta) \) exists. We assume Gaussian spread noise with fixed variance \( \sigma_2^2 \). Since we only have one data point \( x \), the spread data distribution becomes \( p(y|x) = \mathcal{N}(y|x, \sigma_2^2) \), and the model is \( p(y|\theta) = \mathcal{N}(y|\mu, \sigma^2 + \sigma_2^2) \). We can sample \( N \) points from the spread model, so the spread log likelihood function is (neglecting constants) \( L(y_1, \ldots, y_N; \theta) = -\frac{N}{2} \log(\sigma^2 + \sigma_2^2) - \frac{1}{2(\sigma^2 + \sigma_2^2)} \sum_{i=1}^N (y_i - \mu)^2 \). The MLE solution for \( \mu \) is \( \mu = \frac{1}{N} \sum_{i=1}^N y_i \); the MLE solution for \( \sigma^2 \) is \( \sigma^2 = \frac{1}{N} \sum_i (y_i - \mu)^2 - \sigma_2^2 \), which has bounded spread likelihood value. Note that in the limit of a large number of spread samples \( N \to \infty \), the MLE \( \sigma^2 = \frac{1}{N} \sum_i (y_i - \mu)^2 \) tends to 0. Throughout, however, the (scaled by \( N \)) log likelihood remains bounded.

F.2. Consistency

Consistency of an estimator is an important property that guarantees the validity of the resulting estimate at convergence as the number of data points tends to infinity. In what follows, we outline the sufficient conditions for a consistent MLE estimator, before addressing the question of whether using spread MLE is also consistent and under what conditions.

F.2.1. Consistency for MLE

Sufficient conditions for the MLE being consistent and converging to the global maximum are given in (Wald, 1949). However, they are usually difficult to check even for some standard distributions. The sufficient conditions for MLE being consistent and converging to a local maxima are given in (Cramér, 1999) and are more straightforward to check:

C1. (Identifiable): \( p(x|\theta_1) = p(x|\theta_2) \to \theta_1 = \theta_2 \).

C2. The parameter space \( \Theta \) is an open interval \( (\theta, \bar{\theta}), \Theta : -\infty < \theta < \bar{\theta} < \infty \).

C3. \( p(x|\theta) \) is continuous in \( \theta \) and differentiable with respect to \( \theta \) for all \( x \).

C4. The set \( A = \{x : p_\theta(x) > 0\} \) is independent of \( \theta \).

Let \( X_1, X_2, \ldots \) be i.i.d with density \( p(x|\theta_0) (\theta \in \Theta) \) satisfying conditions C1–C4, then there exists a sequence \( \hat{\theta}_n = \hat{\theta}_n(X_1, \ldots, X_n) \) of local maxima of the likelihood function \( L(\theta_0) = \prod_{i=1}^n p(x_i|\theta_0) \) which is consistent:

\[ \hat{\theta} \xrightarrow{P} \theta_0 \text{ for all } \theta \in \Theta. \]

The proof can be found in (Lehmann, 2004) or (Cramér, 1999).

F.2.2. Consistency of Spread MLE

We provide the necessary conditions for Spread MLE being consistent.

C1. (Identifiable): \( p(x|\theta) \) is identifiable. From section(2.1) it follows immediately that \( p(y|\theta_1) = p(y|\theta_2) \to p(x|\theta_1) = p(x|\theta_2) \to \theta_1 = \theta_2 \), where the final implication follows from the assumption that \( p(x|\theta) \) is identifiable. Hence if \( p(x|\theta) \) is identifiable, so is \( p(y|\theta) \).
C2. The parameter space $\Theta$ is an open interval $(\bar{\theta}, \bar{\theta})$, $\Theta: -\infty \leq \theta < \bar{\theta} \leq \infty$. This condition is unchanged for $p(y|\theta)$.

C3. On $p(y|\theta)$, we require the same condition on $p(x|\theta)$ as in MLE; $p(y|\theta)$ is continuous in $\theta$ and differentiable with respect to $\theta$ for all $y$.

C4. For spread noise $p(y|x)$ who has full support on $\mathbb{R}^d$ (for example Gaussian noise), $p(y|\theta)$ is greater than zero everywhere and hence the original condition C4 is automatically guaranteed.

The conditions that guarantee consistency for spread MLE are weaker for the spread model $p(y|\theta)$ than for the standard model $p(x|\theta)$, since C4 is automatically satisfied. (Ferguson, 1982) gives an example for which MLE exists but is not consistent by violating condition C4, whereas spread MLE can be used to obtain a consistent estimator.

F.3. Asymptotic Efficiency

A key desirable property of any estimator is that it is efficient. The Cramer-Rao bound places a lower bound on the variance of any unbiased estimator and an efficient estimator must reach this minimal value in the limit of a large amount of data. Under certain conditions (see below) the Maximum Likelihood Estimator attains this minimal variance value meaning that there is no better estimator possible (in the limit of a large amount of data). This is one of the reasons that the maximum likelihood is a cherished criterion.

F.3.1. Asymptotic Efficiency for MLE

Building upon conditions C1-C4, additional conditions on $p(x|\theta)$ are required to show MLE is asymptotical efficient:

C5. For all $x$ in its support, the density $p_0(x)$ is three times differentiable with respect to $\theta$ and the third derivative is continuous.

C6. The derivatives of the integral $\int p_0(x)dx$ respect to $\theta$ can be obtained by differentiating under the integral sign, that is:
\[
\nabla_\theta \int p_0(x)dx = \int \partial_\theta p_0(x)dx.
\]

C7. There exists a positive number $c(\theta_0)$ and a function $M_{\theta_0}(x)$ such that
\[
\left| \frac{\partial^3}{\partial \theta^3} \log p_0(x) \right| \leq M_{\theta_0}(x) \quad \text{for all } x \in A, |\theta - \theta_0| < c(\theta_0),
\]
where $A$ is the support set of $x$ and $\mathbb{E}_{\theta_0} [M_{\theta_0}(x)] < \infty$.

Let $X_1, ..., X_n$ be i.i.d with density $p_0(x)$ and satisfy conditions C1-C7, then any consistent sequence $\hat{\theta} = \hat{\theta}_n (X_1, ..., X_n)$ of roots of the likelihood equation satisfies
\[
\sqrt{n}(\hat{\theta} - \theta_0) \xrightarrow{d} \mathcal{N}(0, F(\theta_0)^{-1}),
\]
where $F^{-1}(\theta_0)$ is the inverse of Fisher information matrix (also called Cramér-Rao Lower Bound, which is a lower bound on variance of any unbiased estimators). The conditions and proof can be found in (Lehmann, 2004).

F.3.2. Asymptotic Efficiency for MLE

As with MLE above, we require further conditions on $p(y|\theta)$ for ensuring spread MLE is asymptotically efficient:

C5. On $p(y|\theta)$, we require the same condition as applied to $p(x|\theta)$ in the MLE case; for all $y$ in its support, the density $p_0(y)$ is three times differentiable with respect to $\theta$ and the third derivative is continuous.

C6. For spread noise $p(y|x)$, which has full support on $\mathbb{R}^d$ (for example Gaussian noise), the support of $y$ is independent of $\theta$, Leibniz’s rule\(^{16}\) allows us to differentiate under the integral: $\nabla_\theta \int p(y)dy = \int \partial_\theta p(y)dy$, so this condition is automatically satisfied.

\(^{16}\)Leibniz’s rule tells us: $\frac{d}{d\theta} \int_a^b y^{(\theta)}(x)dx = \int_a^b y^{(\theta)}(x)dx + p(b(\theta), \theta) \frac{d}{d\theta} b(\theta) - p(a(\theta), \theta) \frac{d}{d\theta} a(\theta)$, so if $a(\theta)$ and $b(\theta)$ are independent of $\theta$, then $\frac{d}{d\theta} \int_a^b p(x, \theta)dx = \int_a^b \partial_\theta p(x, \theta)dx$. 

According to our general theory, typically the integral over \( p(x|\theta) \) will be intractable and we resort to an unbiased sampled estimate (though see below for Gaussian \( q \)). Neglecting constants, the KL divergence estimator is

\[
\frac{1}{NS} \sum_{n=1}^{S} \sum_{s=1}^{N} \log \tilde{p}_\theta(y^n_s),
\]

where \( y^n_s \) is a perturbed version of \( x_n \). For example \( y^n_s \sim \mathcal{N}(y^n_s|x_n,\sigma^2 I_X) \) for the fixed Gaussian noise case. In most cases of interest, with non-linear \( g \), the distribution \( \tilde{p}_\theta(y) \) is intractable. We therefore use the variational lower bound

\[
\log \tilde{p}_\theta(y) \geq \int q_\phi(z|y) \left( -\log q_\phi(z|y) + \log (p_\theta(y|z)p(z)) \right) dz.
\]

Thus the conditions that guarantee asymptotic efficiency for the spread model \( p(y|\theta) \) are weaker than for the standard model \( p(x|\theta) \), since C4 and C6 are automatically satisfied.

### G. Spread Divergence for Deterministic Deep Generative Models

Instead of minimising the likelihood, we train an implicit generative model by minimising the Spread Divergence

\[
\min_{\theta} \text{KL}(\tilde{p}(y)||\tilde{p}_\theta(y)).
\]

For Gaussian noise with fixed diagonal noise \( p(y|x) = \mathcal{N}(y|x,\sigma^2 I_X) \), we can write

\[
\tilde{p}(y) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(y|x_n,\sigma^2 I_X).
\]

and

\[
\tilde{p}_\theta(y) = \int p(y|x)p_\theta(x)dx = \int \mathcal{N}(y|y_\theta(z),\sigma^2 I_X) p(z)dz = \int p(y|z)p(z)dz.
\]

For the Spread Divergence with learned covariance Gaussian noise, which is discussed in section(3.1), we can write

\[
p_\phi(y|x) = \mathcal{N}(y|f_\phi(x),\sigma^2 I_X), \quad \tilde{p}(y) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(y|x_n,\Sigma_\phi)
\]

and Spread Divergence with a learned injective function as discussed in section(3.2)

\[
p_\phi(y|x) = \mathcal{N}(y|f_\phi(x),\sigma^2 I_X), \quad \tilde{p}(y) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{N}(y|f_\phi(x),\sigma^2 I_X).
\]

According to our general theory,

\[
\min_{\theta} \text{KL}(\tilde{p}(y)||\tilde{p}_\theta(y)) = 0 \iff p(x) = p_\theta(x).
\]

Here

\[
\text{KL}(\tilde{p}(y)||\tilde{p}_\theta(y)) = -\int \tilde{p}(y) \log \tilde{p}_\theta(y)dy + \text{const}.
\]

Typically, the integral over \( y \) will be intractable and we resort to an unbiased sampled estimate (though see below for Gaussian \( q \)). Neglecting constants, the KL divergence estimator is

\[
\frac{1}{NS} \sum_{n=1}^{S} \sum_{s=1}^{N} \log \tilde{p}_\theta(y^n_s),
\]

where \( y^n_s \) is a perturbed version of \( x_n \). For example \( y^n_s \sim \mathcal{N}(y^n_s|x_n,\sigma^2 I_X) \) for the fixed Gaussian noise case. In most cases of interest, with non-linear \( g \), the distribution \( \tilde{p}_\theta(y) \) is intractable. We therefore use the variational lower bound

\[
\log \tilde{p}_\theta(y) \geq \int q_\phi(z|y) \left( -\log q_\phi(z|y) + \log (p_\theta(y|z)p(z)) \right) dz.
\]
Parameterizing the variational distribution as a Gaussian,

\[ q_\phi(z|y) = \mathcal{N}(z|\mu_\phi(y), \Sigma_\phi(y)), \] (94)

we can then use the reparameterization trick (Kingma & Welling, 2013) and write

\[
\log \tilde{p}_\theta(y) \geq H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \log \tilde{p}_\theta(y|z = h_\phi(y, \epsilon)) + \log p(z = h_\phi(y, \epsilon)) \right],
\] (95)

where \( h_\phi(y, \epsilon) = \mu_\phi(y) + C_\phi(y) \epsilon \) and \( H(\Sigma_\phi(y)) \) is the entropy of a Gaussian with covariance \( \Sigma_\phi(y) \), where \( C_\phi(y) \) is the Cholesky decomposition of \( \Sigma_\phi(y) \). For fixed covariance Gaussian spread noise in \( D \) dimensions, this is (ignoring the constant)

\[
\log \tilde{p}_\theta(y) \geq H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ -\frac{1}{(2\sigma^2)^{D/2}} (y - g_\theta(h_\phi(y, \epsilon)))^2 + \log p(z = h_\phi(y, \epsilon)) \right].
\] (96)

We can integrate the above equation over \( y \) to give the bound (ignoring the constant)

\[
\int \mathcal{N}(y|x, \sigma^2 I_x) \log \tilde{p}_\theta(y) \geq \mathbb{E}_{\mathcal{N}(y|x, \sigma^2 I_x)} \left[ H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \log p(z = h_\phi(y, \epsilon)) \right] \right]
\]

\[- \frac{1}{(2\sigma^2)^{D/2}} \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \mathbb{E}_{\mathcal{N}(\epsilon|x, \sigma^2 I_x)} \left[ (y - g_\theta(h_\phi(y, \epsilon)))^2 \right] \right],
\] (97)

where

\[
\mathbb{E}_{\mathcal{N}(\epsilon|x,\sigma^2 I_x)}[(y - g_\theta(h_\phi(y, \epsilon)))^2] = \sigma^2 - 2\mathbb{E}_{\mathcal{N}(\epsilon|x,\sigma^2 I_x)}[\epsilon_x g_\theta(h_\phi(x + \sigma \epsilon_x, \epsilon))]
\]

\[- \mathbb{E}_{\mathcal{N}(\epsilon|x,\sigma^2 I_x)}[(x - g_\theta(h_\phi(x + \sigma \epsilon_x, \epsilon)))^2].
\] (98)

We notice that the second term is zero, so the final bound for the fixed Gaussian spread KL divergence is (ignoring the constant)

\[
\int \mathcal{N}(y|x, \sigma^2 I_x) \log \tilde{p}_\theta(y) \geq \mathbb{E}_{\mathcal{N}(y|x, \sigma^2 I_x)} \left[ H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \log p(z = h_\phi(y, \epsilon)) \right] \right]
\]

\[- \frac{1}{(2\sigma^2)^{D/2}} \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \mathbb{E}_{\mathcal{N}(\epsilon|x, \sigma^2 I_x)} \left[ (x - g_\theta(h_\phi(x + \sigma \epsilon_x, \epsilon)))^2 \right] \right].
\] (99)

By analogy, for spread KL divergence with learned variance, the bound is (ignoring the constant)

\[
\int \mathcal{N}(y|x, \Sigma_\psi) \log \tilde{p}_\theta(y) \geq \mathbb{E}_{\mathcal{N}(y|x, \Sigma_\psi)} \left[ H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \log p(z = h_\phi(y, \epsilon)) \right] \right]
\]

\[- \mathbb{E}_{\mathcal{N}(\epsilon|0,1, \Sigma_\psi)} \left[ \mathbb{E}_{\mathcal{N}(\epsilon|x, \Sigma_\psi)} \left[ (x - g_\theta(h_\phi(x + S_\psi \epsilon_x, \epsilon)))^T \Sigma_\psi^{-1} (x - g_\theta(h_\phi(x + S_\psi \epsilon_x, \epsilon))) \right] \right],
\] (100)

where \( S_\psi \) is the cholesky decomposition of \( \Sigma_\psi \).

For spread KL divergence with a learned injective function, the bound is (ignoring the constant)

\[
\int \mathcal{N}(y|f_\psi(x), \sigma^2 I_x) \log \tilde{p}_\theta(y) \geq \mathbb{E}_{\mathcal{N}(y|f_\psi(x), \sigma^2 I_x)} \left[ H(\Sigma_\phi(y)) + \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \log p(z = h_\phi(y, \epsilon)) \right] \right]
\]

\[- \frac{1}{(2\sigma^2)^{D/2}} \mathbb{E}_{\mathcal{N}(\epsilon|0,1)} \left[ \mathbb{E}_{\mathcal{N}(\epsilon|x, \sigma^2 I_x)} \left[ (f_\psi(x) - f_\psi(g_\theta(h_\phi(x + \sigma \epsilon_x, \epsilon))))^2 \right] \right].
\] (101)

The overall procedure is therefore a straightforward modification of the standard VAE method (Kingma & Welling, 2013) with an additional sub-routine for learning the spread online to maximize the divergence:

1. Choose a noise distribution \( p(y|x) \).
2. Choose a tractable family for the variational distribution, for example \( q_\phi(z|y) = \mathcal{N}(z | \mu_\phi(y), \Sigma_\phi(y)) \), and initialise \( \phi \).

3. Sample a \( y_n \) for each data point (if we’re using \( S = 1 \) samples).

4. If learning the spread noise:
   
   (a) Draw samples \( \epsilon \) to estimate \(- \log \tilde{p}_\theta(y_n)\) according to the corresponding bound.
   
   (b) Do a gradient ascent step in \( \psi \).

5. Draw samples \( \epsilon \) to estimate \( \log \tilde{p}_\theta(y_n) \) according to the corresponding bound.

6. Do a gradient ascent step in \( (\theta, \phi) \).

7. Go to 3 and repeat until convergence.

H. MNIST Experiment

We first scaled the MNIST data to lie in \([0, 1]\). We use Laplace spread noise with \( \sigma = 0.3 \) and Gaussian spread noise with \( \sigma = 0.3 \) for the \( \delta \)-VAE case. Both the encoder and the decoder networks contain 3 feed-forward layers, each layer has 400 units and use ReLu activation functions. The latent dimension is \( Z = 64 \). The variational inference network \( q_\phi(z|y) = \mathcal{N}(z | \mu_\phi(y), \sigma^2_\phi I_Z) \) has a similar structure for the mean network \( \mu_\phi(y) \). For fixed spread \( \delta \)-VAE, learning was done using the Adam (Kingma & Ba, 2014) optimizer with learning rate \( 5\times 10^{-4} \) for 200 epochs. For \( \delta \)-VAE with learned spread (learned covariance), we interleave 2 covariance training epochs with 10 model training epochs (using the Adam optimizer with learning rate \( 5\times 10^{-5} \)).

I. CelebA Experiment

We pre-processed CelebA images by first taking 140x140 centre crops and then resizing to 64x64. Pixel values were then rescaled to lie in \([0, 1]\). For the learned spread we use Gaussian noise with a learned injective function ResNet \( f_\psi(\cdot) = I(\cdot) + g_\psi(\cdot) \), where \( g_\psi(\cdot) \) is a one layer convolutional neural net with kernel size \( 3 \times 3 \), with stride length 1. We use spectral normalization (Miyato et al., 2018) to satisfy the Lipschitz constraint. That is, we replace the weight matrix \( w \) of the convolution kernel by \( wSN(w) := c \times w / \sigma(w) \), where \( \sigma(w) \) is the spectral norm of \( w \) and \( c \in (0, 1) \). This guarantees that \( f_\psi \) is invertible - see (Behrmann et al., 2018).

The encoder and decoder are 4-layer convolutional neural networks with batch norm (Ioffe & Szegedy, 2015). Both networks use a fully convolutional architecture with \( 5 \times 5 \) convolutional filters with stride length 2 in both vertical and horizontal directions, except the last deconvolution layer where we use stride length 1. \( \text{Conv}_k \) represents a convolution with \( k \) filters and \( \text{DeConv}_k \) represents a deconvolution with \( k \) filters, BN for the batch normalization (Ioffe & Szegedy, 2015), Relu for the rectified linear units, and FC\(_k\) for the fully connected layer mapping to \( \mathbb{R}^k \).

\[
\begin{align*}
  x & \in \mathbb{R}^{64 \times 64 \times 3} \rightarrow \text{injective} f(\cdot) \in \mathbb{R}^{64 \times 64 \times 3} \\
  & \rightarrow \text{Conv}_{128} \rightarrow \text{BN} \rightarrow \text{Relu} \\
  & \rightarrow \text{Conv}_{256} \rightarrow \text{BN} \rightarrow \text{Relu} \\
  & \rightarrow \text{Conv}_{512} \rightarrow \text{BN} \rightarrow \text{Relu} \\
  & \rightarrow \text{Conv}_{1024} \rightarrow \text{BN} \rightarrow \text{Relu} \rightarrow \text{FC}_{100}
\end{align*}
\]

\[
\begin{align*}
  z & \in \mathbb{R}^{100} \rightarrow \text{FC}_{10 \times 10 \times 1024} \\
  & \rightarrow \text{DeConv}_{128} \rightarrow \text{BN} \rightarrow \text{Relu} \\
  & \rightarrow \text{DeConv}_{256} \rightarrow \text{BN} \rightarrow \text{Relu} \\
  & \rightarrow \text{DeConv}_{128} \rightarrow \text{BN} \rightarrow \text{Relu} \rightarrow \text{DeConv}_{3} \rightarrow \text{sigmoid}(\cdot) \\
  & \rightarrow \text{injective} f(\cdot) \in \mathbb{R}^{64 \times 64 \times 3}
\end{align*}
\]

We use batch size 100 and latent dimension \( \text{dim}(Z) = 100 \) in all CelebA experiments. For the \( \delta \)-VAE with fixed spread, we use the fixed Gaussian noise with 0 mean and \((0.5)^2 I\) covariance. We train the model for 500 epochs using Adam optimizer with learning rate \( 1e^{-4} \). We decay the learning rate with scaling factor 0.9 every 100000 iterations.
For the \(\delta\)-VAE with learned spread we first train a \(\delta\)-VAE with fixed \(f(x) = x\) and fixed Gaussian noise with 0 mean and 
\((0.5)^2 I\) diagonal covariance for 300 epochs. We decay the learning with scaling factor 0.9 every 100000 iterations. We start
iterative training by doing one step inner maximisation over the Spread Divergence parameters \(\psi\) using Adam optimizer
with learning rate \(1e^{-5}\) and one step minimization over the model parameter’s \((\theta, \phi)\) using Adam optimizer for additional
200 epochs. We can share the first 300 epochs between the two models. When we sample form two models, we first sample
from a 100 dimensional standard Gaussian distribution \(z \sim N(0, I)\) and use the same latent code \(z\) to get samples from
both \(\delta\)-VAE with fixed and learned spread, so we can easily compare the sample quality between two models.

Figure 8. Samples from an implicit generative model trained using \(\delta\)-VAE with (a) Laplace noise with fixed covariance, (a) Gaussian
noise with fixed covariance and (c) Gaussian noise with learned covariance.
Figure 9. Samples from an implicit generative model trained using $\delta$-VAE with (a) fixed and (b) learned spread with injective mean transformation.