# Understanding Deep Generative Models

2018. 01. 04 DMQA Lab Seminar

# Deep Generative Models

## Generative Models

Generative models  $\rightarrow$  try to learn data generating process

Motivating example: latent Dirichlet allocation





## Generative Models with Latent Variables

Introducing latent variable can make problems tractable (e.g. mixture distribution)







## Deep Generative Models

Conventional generative models are not tractable with

high-dimensional complex data

## Deep Generative Models



# GANs, GMMN, and VAE



Neural network Input → noise (from prior) Output → random sample (from model distribution)

















Adversarial learning process

Generated



Random Noise e.g. Uniform (0, 1) of 100 dimension (Latent Distribution)

| z1     | z2      | <br>z99     | z100   |
|--------|---------|-------------|--------|
| 0.8642 | -0.3331 | <br>-0.0322 | 0.1234 |

100-dimensional vector (Latent Variable)





Image

generator

Generating Process of GANs



Training of GANs (Alternating Minimization)



Neural network Input → noise (from prior) Output → random sample (from model distribution)



Random Noise e.g. Uniform (0, 1) of 100 dimension (Latent Distribution)

| z1     | z2      | <br>z99     | z100   |
|--------|---------|-------------|--------|
| 0.8642 | -0.3331 | <br>-0.0322 | 0.1234 |

100-dimensional vector (Latent Variable)





Image

generator

Generating Process of GMMN



**Discriminator** in GANs determines how true samples and generated samples are similar



In GMMN, a method called **Moment Matching** is used to measure the similarity between true samples and generated samples

## Variational Autoencoder

Gaussian Encoder – Gaussian Decoder



## Variational Autoencoder

| z1     | z2      |     | z99     | z100   |
|--------|---------|-----|---------|--------|
| 0.8642 | -0.3331 | ••• | -0.0322 | 0.1234 |

100-dimensional vector (Latent Variable)





Image

## What's Different



**9** Image





GANs

- G generates samples G is a transformation (noise to sample)
  → Implicit density / likelihood free
- Random noise distribution does not change (prior)
  - $\rightarrow$  There is no recognition model
- Min-max problem (adversarial)
- Suffers from mode collapse
- Unstable training (hard to balance G and D)
- Try to minimize the discrepancy between data distribution and model distribution
- Possible to utilize discrete random noise

#### VAE

- Decoder generates samples decoder is an inference model (latent to parameters)
  → Explicit density
- Latent variable distribution changes (posterior)
  - $\rightarrow$  There is a recognition model (encoder)
- Minimization (or maximization) problem
- Suffers from blurry image (low quality images)
- Stable training
- Try to maximize model likelihood given data
- Hard to impose discrete latent distribution

#### **Generative Adversarial Nets**

Ian J. Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, Yoshua Bengio<sup>8</sup>

Département d'informatique et de recherche opérationnelle Université de Montréal Montréal, QC H3C 3J7

#### Abstract

We propose a new framework for estimating generative models via an adversarial process, in which we simultaneously train two models: a generative model Gthat captures the data distribution, and a discriminative model D that estimates the probability that a sample came from the training data rather than G. The training procedure for G is to maximize the probability of D making a mistake. This framework corresponds to a minimax two-player game. In the space of arbitrary functions G and D, a unique solution exists, with G recovering the training data distribution and D equal to  $\frac{1}{2}$  everywhere. In the case where G and D are defined by multilayer perceptrons, the entire system can be trained with backpropagation. There is no need for any Markov chains or unrolled approximate inference networks during either training or generation of samples. Experiments demonstrate the potential of the framework through qualitative and quantitative evaluation of the generated samples.



**Generator** tries to make generated samples to be classified as real **Discriminator** tries to distinguish generated samples and real data

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

D(x) =Output of D = probability of x is determined to be real by DG(z) =Output of G = generated sample by G given a latent vector z $\theta_G, \ \theta_D =$  neural network parameters of G and D, respectively

**Generator** tries to make generated samples to be classified as real **Discriminator** tries to distinguish generated samples and real data

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

$$\min_{\theta_G} \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

$$\max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

**Generator** tries to make generated samples to be classified as real **Discriminator** tries to distinguish generated samples and real data

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

**Proposition 1.** For G fixed, the optimal discriminator D is

$$D_G^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_G(x)}$$

$$\begin{split} \min_{\theta_{G}} \max_{\theta_{D}} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))] \\ &= \min_{\theta_{G}} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D_{G}^{*}(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D_{G}^{*}(G(z)))] \\ &= \min_{\theta_{G}} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D_{G}^{*}(x)] + \mathbb{E}_{x \sim p_{G}(x)} [\log(1 - D_{G}^{*}(x))] \\ &= \min_{\theta_{G}} \mathbb{E}_{x \sim p_{\text{data}}(x)} \left[ \log \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_{G}(x)} \right] + \mathbb{E}_{x \sim p_{G}(x)} \left[ \log \frac{p_{G}(x)}{p_{\text{data}}(x) + p_{G}(x)} \right] \\ &= \min_{\theta_{G}} - \log 2 + \mathbb{E}_{x \sim p_{\text{data}}(x)} \left[ \log \frac{p_{\text{data}}(x)}{\frac{1}{2}(p_{\text{data}}(x) + p_{G}(x))} \right] - \log 2 + \mathbb{E}_{x \sim p_{G}(x)} \left[ \log \frac{p_{G}(x)}{\frac{1}{2}(p_{\text{data}}(x) + p_{G}(x))} \right] \\ &= \min_{\theta_{G}} - \log 4 + \mathcal{D}_{\text{KL}} \left( p_{\text{data}} \left\| \frac{p_{\text{data}} + p_{G}}{2} \right) + \mathcal{D}_{\text{KL}} \left( p_{G} \right\| \frac{p_{\text{data}} + p_{G}}{2} \right) \\ &= \min_{\theta_{G}} - \log 4 + 2\mathcal{D}_{\text{JS}} \left( p_{\text{data}} \right\| p_{G}) \end{split}$$

G is trained to minimize Jensen-Shannon divergence between data distribution and generator distribution!



G is trained to minimize Jensen-Shannon divergence between data distribution and generator distribution!





Generalized GANs from minimizing JS divergence to minimizing an arbitrary *f*-divergence

### *f*-GAN: Training Generative Neural Samplers using Variational Divergence Minimization

Sebastian Nowozin Machine Intelligence and Perception Group Microsoft Research Cambridge, UK Sebastian.Nowozin@microsoft.com Botond Cseke Machine Intelligence and Perception Group Microsoft Research Cambridge, UK botcse@microsoft.com

Ryota Tomioka Machine Intelligence and Perception Group Microsoft Research Cambridge, UK ryoto@microsoft.com

#### Abstract

Generative neural samplers are probabilistic models that implement sampling using feedforward neural networks: they take a random input vector and produce a sample from a probability distribution defined by the network weights. These models are expressive and allow efficient computation of samples and derivatives, but cannot be used for computing likelihoods or for marginalization. The *generative-adversarial* training method allows to train such models through the use of an auxiliary discriminative neural network. We show that the generative-adversarial approach is a special case of an existing more general variational divergence estimation approach. We show that any f-divergence can be used for training generative neural samplers. We discuss the benefits of various choices of divergence functions on training complexity and the quality of the obtained generative models.

### *f*-divergence

$$\mathcal{D}_f(p||q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx, \text{ s.t. } f(1) = 0$$

$$\mathcal{D}_{\mathrm{KL}}(p||q) = \int p(x) \log\left(\frac{p(x)}{q(x)}\right) dx \Longrightarrow f(u) = u \log u$$
  
$$\mathcal{D}_{\mathrm{RKL}}(p||q) = \int q(x) \log\left(\frac{q(x)}{p(x)}\right) dx \Longrightarrow f(u) = -\log u$$
  
$$\mathcal{D}_{\mathrm{JS}}(p||q) = \frac{1}{2} \int \left\{ p(x) \log\left(\frac{2 \cdot p(x)}{p(x) + q(x)}\right) + q(x) \log\left(\frac{2 \cdot q(x)}{p(x) + q(x)}\right) \right\} dx$$
  
$$\Longrightarrow f(u) = -(u+1) \log\frac{u+1}{2} + u \log u$$

So, how can we train GANs with f-divergences?

We want to solve the following problem:

$$\min_{\theta_G} \mathcal{D}_f \left( p_{\text{data}} \| p_G \right)$$
$$\iff \min_{\theta_G} \int p_G(x) f\left( \frac{p_{\text{data}}(x)}{p_G(x)} \right) dx$$

However, we do not know  $p_{data}$  and  $p_G$ ,

but only have samples drawn from them, respectively

### Variational Estimation of *f*-divergences

#### Estimating divergence functionals and the likelihood ratio by convex risk minimization

XuanLong Nguyen Dept. of Statistical Science Duke University xuanlong.nguyen@stat.duke.edu Martin J. Wainwright Dept. of Statistics, and Dept. of EECS University of California, Berkeley wainwrig@stat.berkeley.edu

Michael I. Jordan Dept. of Statistics, and Dept. of EECS University of California, Berkeley jordan@stat.berkeley.edu

Revised April 15, 2009

Technical Report 764 Department of Statistics University of California, Berkeley

#### Abstract

We develop and analyze M-estimation methods for divergence functionals and the likelihood ratios of two probability distributions. Our method is based on a non-asymptotic variational characterization of f-divergences, which allows the problem of estimating divergences to be tackled via convex empirical risk optimization. The resulting estimators are simple to implement, requiring only the solution of standard convex programs. We present an analysis of consistency and convergence for these estimators. Given conditions only on the ratios of densities, we show that our estimators can achieve optimal minimax rates for the likelihood ratio and the divergence functionals in certain regimes. We derive an efficient optimization algorithm for computing our estimates, and illustrate their convergence behavior and practical viability by simulations.

rXiv:0809.0853v2 [math.ST] 22 Apr 2009

Fenchel (Convex) Conjugate of f at t:  $f^*(t) = \sup_{u \in \text{dom}f} \{ut - f(u)\}$ 

$$\begin{aligned} \mathcal{D}_{f}\left(p\|q\right) &= \int q(x)f\left(\frac{p(x)}{q(x)}\right) dx \\ &= \int q(x) \sup_{t \in \text{dom}f} \left\{ t\frac{p(x)}{q(x)} - f^{*}(t) \right\} dx \\ &= \int \sup_{t \in \text{dom}f} \left\{ tp(x) - q(x)f^{*}(t) \right\} dx \\ &= \int \sup_{T \in \mathcal{T}} \left\{ p(x)T(x) - q(x)f^{*}(T(x)) \right\} dx \\ &\geq \sup_{T \in \mathcal{T}} \left\{ \int p(x)T(x)dx - \int q(x)f^{*}(T(x))dx \right\} \\ &= \sup_{T \in \mathcal{T}} \left\{ \mathbb{E}_{x \sim p(x)}[T(x)] - \mathbb{E}_{x \sim q(x)}[f^{*}(T(x))] \right\} \text{ the lower bound is tight if } T^{*}(x) = f'\left(\frac{p(x)}{q(x)}\right) \end{aligned}$$

$$\min \ \mathcal{D}_f(p \| q) \Longleftrightarrow \min \ \{\mathbb{E}_{x \sim p(x)}[T(x)] - \mathbb{E}_{x \sim q(x)}[f^*(T(x))]\}$$
$$\min_{\theta_G} \ \mathcal{D}_f(p_{\text{data}} \| p_G) \Longleftrightarrow \min_{\theta_G} \ \{\mathbb{E}_{x \sim p_{\text{data}}(x)}[T(x)] - \mathbb{E}_{x \sim p_G(x)}[f^*(T(x))]\} \qquad f\text{-GAN objective}$$

$$\begin{split} \min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))] \\ &= \min_{\theta_G} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D_G^*(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D_G^*(G(z)))] \\ &= \min_{\theta_G} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D_G^*(x)] + \mathbb{E}_{x \sim p_G(x)} [\log(1 - D_G^*(x))] \end{split}$$
 Vanilla GAN objective

| Name              | $D_f(P \  Q)$   | Generator $f(u)$                      | $T^*(x)$   |
|-------------------|---|---------------------------------------|--|
| Kullback-Leibler  | $\int p(x) \log \frac{p(x)}{q(x)} dx$   | $u \log u$                            | $1 + \log \frac{p(x)}{q(x)}$   |
| Reverse KL        | $\int q(x) \log \frac{\dot{q}(x)}{p(x)} dx$   | $-\log u$                             | $-\frac{q(x)}{p(x)}$   |
| Pearson $\chi^2$  | $\int \frac{(q(x)-p(x))^2}{p(x)} dx$  | $(u - 1)^2$                           | $2\left(\frac{p(x)}{q(x)}-1\right)$                                    |
| Squared Hellinger | $\int \left(\sqrt{p(x)} - \sqrt{q(x)}\right)^2 dx$  | $(\sqrt{u}-1)^2$                      | $\left(\sqrt{\frac{p(x)}{q(x)}}-1\right)\cdot\sqrt{\frac{q(x)}{p(x)}}$ |
| Jensen-Shannon    | $\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x) + q(x)} + q(x) \log \frac{2q(x)}{p(x) + q(x)}  \mathrm{d}x$ | $-(u+1)\log \tfrac{1+u}{2} + u\log u$ | $\log \frac{2p(x)}{p(x)+q(x)}$   |
| GAN               | $\int p(x) \log \frac{2p(x)}{p(x) + q(x)} + q(x) \log \frac{2q(x)}{p(x) + q(x)} \mathrm{d}x - \log(4)$    | $u\log u - (u+1)\log(u+1)$            | $\log \frac{p(x)}{p(x)+q(x)}$  |

| Name                  | Output activation $g_f$        | dom <sub>f*</sub> | Conjugate $f^*(t)$     | f'(1)      |
|-----------------------|--------------------------------|-------------------|------------------------|------------|
| Kullback-Leibler (KL) | v                              | R                 | $\exp(t-1)$            | 1          |
| Reverse KL            | $-\exp(-v)$                    | $\mathbb{R}_{-}$  | $-1 - \log(-t)$        | -1         |
| Pearson $\chi^2$      | v                              | $\mathbb{R}$      | $\frac{1}{4}t^{2} + t$ | 0          |
| Squared Hellinger     | $1 - \exp(-v)$                 | t < 1             | $\frac{t}{1-t}$        | 0          |
| Jensen-Shannon        | $\log(2) - \log(1 + \exp(-v))$ | $t < \log(2)$     | $-\log(2 - \exp(t))$   | 0          |
| GAN                   | $-\log(1+\exp(-v))$            | $\mathbb{R}_{-}$  | $-\log(1-\exp(t))$     | $-\log(2)$ |

# $\min_{\theta_G} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[T(x)] - \mathbb{E}_{x \sim p_G(x)}[f^*(T(x))] \right\}$



Kullback-Leibler

Reverse Kullback-Leibler

Squared Hellinger

Jensen-Shannon (Vanilla GAN)
f - GAN



(a) GAN

(b) KL



# What else?

#### Wasserstein GAN

Martin Arjovsky<sup>1</sup>, Soumith Chintala<sup>2</sup>, and Léon Bottou<sup>1,2</sup> <sup>1</sup>Courant Institute of Mathematical Sciences

<sup>2</sup>Facebook AI Research

#### 1 Introduction

The problem this paper is concerned with is that of unsupervised learning. Mainly, what does it mean to learn a probability distribution? The classical answer to this is to learn a probability density. This is often done by defining a parametric family of densities  $(P_{\theta})_{\theta \in \mathbb{R}^d}$  and finding the one that maximized the likelihood on our data: if we have real data examples  $\{x^{(i)}\}_{i=1}^m$ , we would solve the problem

$$\max_{\theta \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^m \log P_{\theta}(x^{(i)})$$



Optimal Transport Cost / Earth Mover's Distance



We have to move the mass in gray region to green region

Optimal Transport Cost / Earth Mover's Distance

transportation plan:  $\gamma(x, y) =$  amount of mass to move from x to y



Also, there is a cost to move the mass from x to y is given by a function

$$c(x, y) \mapsto [0, \infty)$$
$$c(x, y) = ||x - y||_1$$
$$c(x, y) = ||x - y||_2^2$$

Optimal Transport Cost / Earth Mover's Distance



Also, there is a cost to move the mass from *x* to *y* is given by a function

$$\cot(\gamma; c) = \int \int c(x, y) \gamma(x, y) dx dy$$

optimal 
$$\operatorname{cost}(\gamma; c) = \inf_{\gamma \in \Gamma(p,q)} \int \int c(x,y) \gamma(x,y) dx dy = \inf_{\gamma \in \Gamma(p,q)} \mathbb{E}_{(x,y) \in \gamma} [c(x,y)]$$

$$W_1(p_{\text{data}}, p_G) = \inf_{\gamma \in \Gamma(p_{\text{data}}, p_G)} \mathbb{E}_{(x,y) \sim \gamma}[\|x - y\|_1]$$

How can we minimize the loss function ???

By Kantorovich-Rubinstein duality, we have

$$W_1(p_{\text{data}}, p_G) = \sup_{\|f\|_L \le K} \left\{ \mathbb{E}_{x \sim p_{\text{data}}}[f(x)] - \mathbb{E}_{x \sim p_G}[f(x)] \right\}$$

$$W_1(p_{\text{data}}, p_G) = \sup_{\|f\|_L \le K} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[f(x)] - \mathbb{E}_{x \sim p_G(x)}[f(x)] \right\}$$

Applying generative adversarial network settings (G, D)

$$W_1(p_{\text{data}}, p_G) = \max_{\theta_D} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[D(x)] - \mathbb{E}_{x \sim p_G(x)}[D(x)] \right\}$$

$$W_1(p_{\text{data}}, p_G) = \max_{\theta_D} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[D(x)] - \mathbb{E}_{z \sim p(z)}[D(G(z))] \right\}$$

Now we have Wasserstein GAN problem that minimizes Wassersten-1 distance between data distribution and the generator distribution

$$\min_{\theta_G} W_1(p_{\text{data}}, p_G) = \min_{\theta_G} \max_{\theta_D} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[D(x)] - \mathbb{E}_{z \sim p(z)}[D(G(z))] \right\}$$

Wasserstein GAN Problem

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

Vanilla GAN Problem

So, why Wassersten-1 distance?

(Kullback-Leibler divergence)  $\mathcal{D}_{\mathrm{KL}}(p_{\theta}, p) \to 0$ (Reverse KL divergence)  $\mathcal{D}_{\mathrm{KL}}(p, p_{\theta}) \to 0$ (Jensen-Shannon divergence)  $\mathcal{D}_{\mathrm{JS}}(p_{\theta}, p) \to 0$ (Total variation distance)  $\mathrm{TV}(p_{\theta}, p) \to 0$ (We seem to in 1 distance)  $\mathrm{W}(p_{\theta}, p) \to 0$ 

(Wasserstein-1 distance)  $W_1(p_\theta, p) \to 0$  (3)

(3) is the most strict condition That is, we can find a case satisfying (1) or (2) but not satisfying (3)

So, why Wassersten-1 distance?



- GAN D learns very quickly to distinguish real and fake
- $\rightarrow$  Optimal D is locally saturated and its gradient vanishes

WGAN Critic does not saturate, and converges to a linear function

 $\rightarrow$  Optimal critic have no problem at all

Additionally, using critic does not accompany mode collapse unlike GANs

Loss function value – Visual quality (Wasserstein-1)



Loss function value – Visual quality (JSD)



#### DCGAN

#### LSGAN

## WGAN (clipping)

WGAN-GP (ours)

Baseline (G: DCGAN, D: DCGAN)



## G: No BN and a constant number of filters, D: DCGAN









# G: 4-layer 512-dim ReLU MLP, D: DCGAN









#### No normalization in either G or D









#### DCGAN

#### LSGAN

#### WGAN (clipping)

#### WGAN-GP (ours)

Gated multiplicative nonlinearities everywhere in G and D









#### $\tanh$ nonlinearities everywhere in G and D









#### 101-layer ResNet G and D











Vanilla GANs (JS Divergence)

*f*–GANs (*f*–Divergence)



Wasserstein GANs (Wasserstein-1 Distance)



Energy-Based GANs (Energy)

Published as a conference paper at ICLR 2017

#### ENERGY-BASED GENERATIVE ADVERSARIAL NET-WORKS

#### Junbo Zhao, Michael Mathieu and Yann LeCun

Department of Computer Science, New York University Facebook Artificial Intelligence Research {jakezhao, mathieu, yann}@cs.nyu.edu

#### ABSTRACT

We introduce the "Energy-based Generative Adversarial Network" model (EBGAN) which views the discriminator as an energy function that attributes low energies to the regions near the data manifold and higher energies to other regions. Similar to the probabilistic GANs, a generator is seen as being trained to produce contrastive samples with minimal energies, while the discriminator is trained to assign high energies to these generated samples. Viewing the discriminator as an energy function allows to use a wide variety of architectures and loss functionals in addition to the usual binary classifier with logistic output. Among them, we show one instantiation of EBGAN framework as using an auto-encoder architecture, with the energy being the reconstruction error, in place of the discriminator. We show that this form of EBGAN exhibits more stable behavior than regular GANs during training. We also show that a single-scale architecture can be trained to generate high-resolution images.

Energy Function: A function assigns energy (a scalar value) to every point of space (lower the better)

In unsupervised learning, low energy is assigned where data are observed





AE is trained to assign low energy (good reconstruction) to real data AE is trained to assign high energy (bad reconstruction) to generated data G is trained to assign low energy (good reconstruction) to generated data

AE is trained to assign low energy (good reconstruction) to real data AE is trained to assign high energy (bad reconstruction) to generated data G is trained to assign low energy (good reconstruction) to generated data

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}}(x)} [D(x)] + \mathbb{E}_{x \sim p_G(x)} [(m - D(x))_+] + \mathbb{E}_{x \sim p_G(x)} [D(x)]$$

$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}}(x)} [D(x)] + \mathbb{E}_{z \sim p(z)} [(m - D(G(z)))_+] + \mathbb{E}_{z \sim p(z)} [D(G(z))]$$

For optimal 
$$D^*$$
 and  $G^*$ ,  $\int \mathbb{I}_{\{x:p_{\text{data}}(x) < p_{G^*}(x)\}}(p_{\text{data}}(x) - p_{G^*}(x))dx = 0$   
that is,  $p_{\text{data}} = p_{G^*}$  a.e.

DCGAN

EBGAN







ImageNet 128 by 128



ImageNet 256 by 256

#### **BEGAN: Boundary Equilibrium Generative** Adversarial Networks

David Berthelot, Thomas Schumm, Luke Metz Google {dberth,fwiffo,lmetz}@google.com

#### Abstract

We propose a new equilibrium enforcing method paired with a loss derived from the Wasserstein distance for training auto-encoder based Generative Adversarial Networks. This method balances the generator and discriminator during training. Additionally, it provides a new approximate convergence measure, fast and stable training and high visual quality. We also derive a way of controlling the trade-off between image diversity and visual quality. We focus on the image generation task, setting a new milestone in visual quality, even at higher resolutions. This is achieved while using a relatively simple model architecture and a standard training procedure.





EBGAN (64 by 64)

BEGAN (128 by 128)



 $\mathcal{L}(x) = \|x - D(x)\|_1 \Longrightarrow \text{Reconstruction error of } x$ 

 $\mathcal{L}(x) \sim q_{\text{data}}, \ x \sim p_{\text{data}} \Longrightarrow \text{Error distribution of real samples}$  $\mathcal{L}(x) \sim q_{\text{G}}, \ x \sim p_{\text{G}} \Longrightarrow \text{Error distribution of generated samples}$ 

We want to make two error distributions similar

$$W_1(q_{\text{data}}, q_G) = \inf_{\gamma \in \Gamma(q_{\text{data}}, q_G)} \mathbb{E}_{(x,y) \sim \gamma}[|x - y|]$$

$$W_1(q_{\text{data}}, q_G) = \inf_{\gamma \in \Gamma(q_{\text{data}}, q_G)} \mathbb{E}_{(x,y) \sim \gamma}[|x - y|]$$

Instead of using the Kantorovich-Rubinstein duality, in BEGAN simply utilize lower bound

inf 
$$\mathbb{E}[|x - y|] \ge \inf |\mathbb{E}[x - y]| = |\mathbb{E}[x] - \mathbb{E}[y]|$$
  
 $W_1(q_{\text{data}}, q_G) \ge |\mathbb{E}_{x \sim q_{\text{data}}}[x] - \mathbb{E}_{y \sim q_G}[y]|$ 

$$W_1(q_{\text{data}}, q_G) \ge |\mathbb{E}_{x \sim q_{\text{data}}}[x] - \mathbb{E}_{y \sim q_G}[y]|$$

We want the discriminator to maximize the lower bound to maximize the Wassertein-1 distance

Two possible cases to maximize the lower bound

In BEGAN, the second case is selected since minimizing the reconstruction error of the real data naturally leads to autoencoder task

Finally we have,

D-loss 
$$\mathcal{L}_D = \mathbb{E}_{x \sim p_{\text{data}}(x)} [\|x - D(x)\|_1] - \mathbb{E}_{z \sim p(z)} [\|G(z) - D(G(z))\|_1]$$

G-loss 
$$\mathcal{L}_G = -\mathcal{L}_D$$

Similar to Wasserstein GANs, but two main differences

(1) BEGAN matches distributions between reconstruction errors not between samples

(2) No K-Lipschitz condition is necessary because of not using the Kantorovich-Rubinstein duality

 $\rightarrow$  Weight/gradient clipping not required

In practice it is crucial to maintain a balance between the generator and discriminator losses

In the paper, G and D are at equilibrium when

$$\mathbb{E}_{x \sim p_{\text{data}}(x)}[\mathcal{L}(x)] = \mathbb{E}_{z \sim p(z)}[\mathcal{L}(G(z))]$$

Moreover, the point of equilibrium can be tuned with a parameter gamma

$$\gamma = \frac{\mathbb{E}_{z \sim p(z)} [\mathcal{L}(G(z))]}{\mathbb{E}_{x \sim p_{\text{data}}(x)} [\mathcal{L}(x)]}$$

$$\gamma = \frac{\mathbb{E}_{z \sim p(z)} [\mathcal{L}(G(z))]}{\mathbb{E}_{x \sim p_{\text{data}}(x)} [\mathcal{L}(x)]}$$

(quality)  $0 \rightarrow 1$  (diversity)



0.7

0.5

0.3
### Boundary Equilibrium Generative Adversarial Networks

 $\mathcal{M}_{global} = \mathcal{L}(x) + |\gamma \mathcal{L}(x) - \mathcal{L}(G(z_G))|$ 

Convergence measure – Visual quality



#### InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets

Xi Chen<sup>†‡</sup>, Yan Duan<sup>†‡</sup>, Rein Houthooft<sup>†‡</sup>, John Schulman<sup>†‡</sup>, Ilya Sutskever<sup>‡</sup>, Pieter Abbeel<sup>†‡</sup> † UC Berkeley, Department of Electrical Engineering and Computer Sciences ‡ OpenAI

#### Abstract

This paper describes InfoGAN, an information-theoretic extension to the Generative Adversarial Network that is able to learn disentangled representations in a completely unsupervised manner. InfoGAN is a generative adversarial network that also maximizes the mutual information between a small subset of the latent variables and the observation. We derive a lower bound of the mutual information objective that can be optimized efficiently. Specifically, InfoGAN successfully disentangles writing styles from digit shapes on the MNIST dataset, pose from lighting of 3D rendered images, and background digits from the central digit on the SVHN dataset. It also discovers visual concepts that include hair styles, presence/absence of eyeglasses, and emotions on the CelebA face dataset. Experiments show that InfoGAN learns interpretable representations that are competitive with representations learned by existing supervised methods.





Entangled Representation (hard to interpret)



Disentangled Representation (easier to interpret)



Example: z1 axis corresponds to the "width" of digits z2 axis corresponds to the "type" of digits



$$\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}(x)}} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

# $\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z), c \sim p(c)} [\log(1 - D(G(z, c)))]$

Mutual Information: Measure of dependence between two random variables  $\rightarrow$  amount of information obtained about *X* through observing *Y* 

$$I(X;Y) = H(Y) - H(Y|X) = H(X) - H(X|Y)$$



InfoGAN tries to maximize the mutual information of the latent code c and the output of G

 $\min_{\theta_G} \max_{\theta_D} \mathbb{E}_{x \sim p_{\text{data}}(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z), c \sim p(c)} [\log(1 - D(G(z, c)))] - \lambda \cdot I(c; G(z, c)))$ 

$$I(c; G(z, c)) = H(G(z, c)) - H(G(z, c); c) = H(c) - H(c; G(z, c))$$

Have no idea of probability density of G(z,c), but we know p(c)

Variational Mutual Information Maximization

→ We can obtain a lower bound of the posterior  $p(c|\underline{G}(z,c))$ 

Let q(c|x) be an approximation of p(c|x)

$$I(c; G(z, c)) = -H(c|G(z, c)) + H(c)$$
  

$$= \mathbb{E}_{x \sim G(z, c)} \mathbb{E}_{c' \sim p(c|x)} [\log p(c'|x)] + H(c)$$
  

$$= \mathbb{E}_{x \sim G(z, c)} \left[ \mathcal{D}_{\mathrm{KL}}(p(c|x)) ||q(c|x)) + \mathbb{E}_{c' \sim p(c|x)} [\log q(c'|x)] \right] + H(c)$$
  

$$\geq \mathbb{E}_{x \sim G(z, c)} \mathbb{E}_{c' \sim p(c|x)} [\log q(c'|x)] + H(c)$$
  

$$= \mathbb{E}_{c \sim p(c), x \sim G(z, c)} \log q(c|x) + H(c)$$
  

$$= L_I(G, q)$$

q is parameterized by an additional neural network

$$\min_{\theta_G, \theta_q} \max_{\theta_D} \mathbb{E}_{x \sim p_{data}(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z), c \sim p(c)} [\log(1 - D(G(z, c)))] - \lambda \cdot L_I(G, q)$$







q (a) Varying  $c_1$  on InfoGAN (Digit type) (b) Varying  $c_1$  on regular GAN (No clear meaning) K ŏ ð .5

(c) Varying  $c_2$  from -2 to 2 on InfoGAN (Rotation)

(d) Varying  $c_3$  from -2 to 2 on InfoGAN (Width)

佰 3 E E E E ie (a T. 140 e, J. 15 1 2 2 0

(a) Azimuth (pose)

(b) Elevation



#### Generative Moment Matching Networks

Yujia Li<sup>1</sup> Kevin Swersky<sup>1</sup> Richard Zemel<sup>1,2</sup> YUJIALI@CS.TORONTO.EDU KSWERSKY@CS.TORONTO.EDU ZEMEL@CS.TORONTO.EDU

<sup>1</sup>Department of Computer Science, University of Toronto, Toronto, ON, CANADA <sup>2</sup>Canadian Institute for Advanced Research, Toronto, ON, CANADA

#### Abstract

We consider the problem of learning deep generative models from data. We formulate a method that generates an independent sample via a single feedforward pass through a multilayer preceptron, as in the recently proposed generative adversarial networks (Goodfellow et al., 2014). Training a generative adversarial network, however, requires careful optimization of a difficult minimax program. Instead, we utilize a technique from statistical hypothesis testing known as maximum mean discrepancy (MMD), which leads to a simple objective that can be interpreted as matching all orders of statistics between a dataset and samples from the model, and can be trained by backpropagation. We further boost the performance of this approach by combining our generative network with an auto-encoder network, using MMD to learn to generate codes that can then be decoded to produce samples. We show that the combination of these techniques yields excellent generative models compared to baseline approaches as measured on MNIST and the Toronto Face Database.

Kiros et al., 2014), machine translation (Cho et al., 2014; Sutskever et al., 2014), and more. Despite their successes, one of the main bottlenecks of the supervised approach is the difficulty in obtaining enough data to learn abstract features that capture the rich structure of the data. It is well recognized that a promising avenue is to use unsupervised learning on unlabelled data, which is far more plentiful and cheaper to obtain.

A long-standing and inherent problem in unsupervised learning is defining a good method for evaluation. Generative models offer the ability to evaluate generalization in the data space, which can also be qualitatively assessed. In this work we propose a generative model for unsupervised learning that we call generative moment matching networks (GMMNs). GMMNs are generative neural networks that begin with a simple prior from which it is easy to draw samples. These are propagated deterministically through the hidden layers of the network and the output is a sample from the model. Thus, with GMMNs it is easy to quickly draw independent random samples, as opposed to expensive MCMC procedures that are necessary in other models such as Boltzmann machines (Ackley et al., 1985; Hinton, 2002; Salakhutdinov & Hinton, 2009). The structure of a GMMN is most analogous to the recently pro-



Maximum Mean Discrepancy

$$x_1, \cdots, x_n \sim p_x$$
  
 $y_1, \cdots, y_m \sim p_y$   $\implies$  want to test  $p_x = p_y$ 

$$\mathcal{L}_{\text{MMD}}(p_x, p_y; f) = \left\| \frac{1}{n} \sum_{i=1}^n f(x_i) - \frac{1}{m} \sum_{i=1}^m f(y_i) \right\|_2^2$$

if 
$$f(x) = x \implies \left\| \frac{1}{n} \sum_{i=1}^{n} x_i - \frac{1}{n} \sum_{i=1}^{m} y_i \right\|$$
 (difference of sample mean)

if 
$$f(x) = x^2 \implies \left\| \frac{1}{n} \sum_{i=1}^n x_i^2 - \frac{1}{n} \sum_{i=1}^m y_i^2 \right\|$$
 (difference of the second moment)

Maximum Mean Discrepancy

$$\mathcal{L}_{\text{MMD}}(p_x, p_y; f) = \left\| \frac{1}{n} \sum_{i=1}^n f(x_i) - \frac{1}{m} \sum_{i=1}^m f(y_i) \right\|_2^2$$

$$= \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n f(x_i)^T f(x_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m f(x_i)^T f(y_j) + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m f(y_i)^T f(y_j)$$

$$= \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, x_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m k(x_i, y_j) + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(y_i, y_j)$$

using  $k(x,y) = \exp\left(-\frac{1}{2\sigma}(x-y)^2\right) \Longrightarrow$  difference of moments of all the orders

with Gaussian kernel, k,

Moment Matching

$$p_x = p_y \iff \mathcal{L}_{MMD}(p_x, p_y; f) = 0$$

# Training

| AI                 | gontann 1. Olvnvn v minioaten training   |
|--------------------|--|
| I                  | <b>nput</b> : Dataset $\{\mathbf{x}_1^d,, \mathbf{x}_N^d\}$ , prior $p(\mathbf{h})$ , network  |
|                    | $f(\mathbf{h}; \mathbf{w})$ with initial parameter $\mathbf{w}^{(0)}$  |
| (                  | <b>Dutput</b> : Learned parameter w*   |
|                    |  |
| 1 V                | while Stopping criterion not met do  |
| 1 V<br>2           | while Stopping criterion not met <b>do</b><br>Get a minibatch of data $\mathbf{X}^d \leftarrow {\mathbf{x}_{i_1}^d,, \mathbf{x}_{i_b}^d}$  |
| 1 V<br>2<br>3      | while Stopping criterion not met <b>do</b><br>Get a minibatch of data $\mathbf{X}^d \leftarrow \{\mathbf{x}_{i_1}^d,, \mathbf{x}_{i_b}^d\}$<br>Get a new set of samples $\mathbf{X}^s \leftarrow \{\mathbf{x}_1^s,, \mathbf{x}_b^s\}$  |
| 1 V<br>2<br>3<br>4 | while Stopping criterion not met <b>do</b><br>Get a minibatch of data $\mathbf{X}^d \leftarrow \{\mathbf{x}_{i_1}^d,, \mathbf{x}_{i_b}^d\}$<br>Get a new set of samples $\mathbf{X}^s \leftarrow \{\mathbf{x}_1^s,, \mathbf{x}_b^s\}$<br>Compute gradient $\frac{\partial \mathcal{L}_{\text{MMD}}}{\partial \mathbf{w}}$ on $\mathbf{X}^d$ and $\mathbf{X}^s$ |





(a) MNIST interpolation

(b) TFD interpolation

#### MMD – GAN

#### MMD GAN: Towards Deeper Understanding of Moment Matching Network

Chun-Liang Li<sup>1,\*</sup> Wei-Cheng Chang<sup>1,\*</sup> Yu Cheng<sup>2</sup> Yiming Yang<sup>1</sup> Barnabás Póczos<sup>1</sup> <sup>1</sup> Carnegie Mellon University, <sup>2</sup>AI Foundations, IBM Research {chunlial,wchang2,yiming,bapoczos}@cs.cmu.edu chengyu@us.ibm.com (\* denotes equal contribution)

#### Abstract

Generative moment matching network (GMMN) is a deep generative model that differs from Generative Adversarial Network (GAN) by replacing the discriminator in GAN with a two-sample test based on kernel maximum mean discrepancy (MMD). Although some theoretical guarantees of MMD have been studied, the empirical performance of GMMN is still not as competitive as that of GAN on challenging and large benchmark datasets. The computational efficiency of GMMN is also less desirable in comparison with GAN, partially due to its requirement for a rather large batch size during the training. In this paper, we propose to improve both the model expressiveness of GMMN and its computational efficiency by introducing adversarial kernel learning techniques, as the replacement of a fixed Gaussian kernel in the original GMMN. The new approach combines the key ideas in both GMMN and GAN, hence we name it MMD GAN. The new distance measure in MMD GAN is a meaningful loss that enjoys the advantage of weak\* topology and can be optimized via gradient descent with relatively small batch sizes. In our evaluation on multiple benchmark datasets, including MNIST, CIFAR-10, CelebA and LSUN, the performance of MMD GAN significantly outperforms GMMN, and is competitive with other representative GAN works.

Generative Moment Matching Network:  $\min_{\theta_G} \mathcal{L}_{\text{MMD}}(p_{\text{data}}, p_G; k)$ 

Better results with:  $\min_{\theta_G} \max_{k \in \mathcal{K}} \mathcal{L}_{\text{MMD}}(p_{\text{data}}, p_G; k)$ 

Apply adversarial learning & NN:  $\min_{\theta_G} \max_{\theta_f} \mathcal{L}_{\text{MMD}}(p_{\text{data}}, p_G; k \circ f)$ 

Feature extraction before apply kernel trick





(d) GMMN-D CIFAR-10

(e) GMMN-C CIFAR-10

(f) MMD GAN CIFAR-10



(d) MMD GAN MNIST

(e) MMD GAN CelebA

(f) MMD GAN LSUN

MMD - GAN



# Variational Autoencoder

(1) Bayesian Inference Problem with Latent Variables



(1) Bayesian Inference Problem with Latent Variables



(2) Bayesian Approximate Inference

Monte Carlo Methods

 $z_1, z_2, \cdots, z_n \sim p(z|x)$ samples

Approximate Inference

 $q(z) \approx p(z|x)$ 

(2) Bayesian Approximate Inference

Monte Carlo Methods

 $z_1, z_2, \cdots, z_n \sim p(z|x)$ samples

Approximate Inference

 $q(z) \approx p(z|x)$ 

Family of q Measure of proximity

(2) Bayesian Approximate Inference

|                       | Naïve Monte Carlo       | Metropolis-Hastings |
|-----------------------|-------------------------|---------------------|
| Monte Carlo Methods   | Rejection Sampling      | Gibbs Sampling      |
|                       | Importance Sampling     | Reversible-Jump     |
|                       | <b></b> ]               |                     |
|                       | Laplace Approximation   |                     |
| Approximate Inference | Expectation Propagation |                     |
|                       | Variational Inference   |                     |

(3) Variational Inference

What we do not know

**→** ????

(3) Variational Inference

$$\mathcal{D}_{\mathrm{KL}}(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z|x)} dz$$
  

$$= \int q(z) \log q(z) dz - \int q(z) \log p(z|x) dz$$
  

$$= \mathbb{E}_{z \sim q(z)} [\log q(z)] - \mathbb{E}_{z \sim q(z)} [\log p(z|x)]$$
  

$$= \mathbb{E}_{z \sim q(z)} [\log q(z)] - \mathbb{E}_{z \sim q(z)} \left[ \log \frac{p(z,x)}{p(x)} \right]$$
  

$$= \mathbb{E}_{z \sim q(z)} [\log q(z)] - \mathbb{E}_{z \sim q(z)} [\log p(z,x)] + \log p(x)$$
  

$$= \mathbb{E}_{z \sim q(z)} [\log q(z)] - \mathbb{E}_{z \sim q(z)} [\log p(z)p(x|z)] + \log p(x)$$

(3) Variational Inference

$$\min_{q \in \mathcal{Q}} \mathcal{D}_{\mathrm{KL}}(q(z)||p(z|x)) \iff \min_{q \in \mathcal{Q}} \mathbb{E}_{z \sim q(z)}[\log q(z)] - \mathbb{E}_{z \sim q(z)}[\log p(z)p(x|z)]$$

Now we can solve the problem!

If q is parametrized by  $\phi$ ,

$$\min_{\phi} \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z)||p(z|x)) \iff \min_{\phi} \mathbb{E}_{z \sim q_{\phi}(z)}[\log q_{\phi}(z)] - \mathbb{E}_{z \sim q_{\phi}(z)}[\log p(z)p(x|z)]$$
## Variational Inference

(3) Variational Inference

$$\mathcal{D}_{\mathrm{KL}}(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z|x)} dz$$

$$= \mathbb{E}_{z \sim q(z)} [\log q(z)] - \mathbb{E}_{z \sim q(z)} [\log p(z)p(x|z)] + \log p(x)$$



### **Auto-Encoding Variational Bayes**

Diederik P. Kingma Machine Learning Group Universiteit van Amsterdam dpkingma@gmail.com Max Welling Machine Learning Group Universiteit van Amsterdam welling.max@gmail.com

#### Abstract

How can we perform efficient inference and learning in directed probabilistic models, in the presence of continuous latent variables with intractable posterior distributions, and large datasets? We introduce a stochastic variational inference and learning algorithm that scales to large datasets and, under some mild differentiability conditions, even works in the intractable case. Our contributions is two-fold. First, we show that a reparameterization of the variational lower bound yields a lower bound estimator that can be straightforwardly optimized using standard stochastic gradient methods. Second, we show that for i.i.d. datasets with continuous latent variables per datapoint, posterior inference can be made especially efficient by fitting an approximate inference model (also called a recognition model) to the intractable posterior using the proposed lower bound estimator. Theoretical advantages are reflected in experimental results.





(1) VAE problem includes not only posterior (approximate) inference

(2) But also involves maximum likelihood inference of the generating process

Based on the maximum likelihood principle, we want to maximize the marginal likelihood of \theta given data x

$$\log p_{\theta}(x) = \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)) || p_{\mathrm{true}}(z|x)) + \mathbb{E}_{z \sim q_{\phi}(z|x)}[-\log q_{\phi}(z|x) + \log p(z) + \log p_{\theta}(x|z)]$$

$$\log p_{\theta}(x) \ge \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ -\log q_{\phi}(z|x) + \log p(z) + \log p_{\theta}(x|z) \right]$$

$$\max_{\theta,\phi} \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ -\log q_{\phi}(z|x) + \log p(z) + \log p_{\theta}(x|z) \right]$$

Maximizing the ELBO implies the following two:

- a) Maximizing the marginal likelihood (for generating process, or the decoder)
- b) Minimizing the KL divergence of the approximate from the true posterior

 $\mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ -\log q_{\phi}(z|x) + \log p(z) + \log p_{\theta}(x|z) \right] = -\mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log q_{\phi}(z|x) - \log p(z) \right] + \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log p_{\theta}(x|z) \right]$  $= -\mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log \frac{q_{\phi}(z|x)}{p(z)} \right] + \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log p_{\theta}(x|z) \right]$  $= -\mathcal{D}_{\mathrm{KL}} (q_{\phi}(z|x)) ||p(z)) + \mathbb{E}_{z \sim q_{\phi}(z|x)} \left[ \log p_{\theta}(x|z) \right]$ 

$$\max_{\theta,\phi} - \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)||p(z)) + \mathbb{E}_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

$$\min_{\theta,\phi} \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)||p(z)) - \mathbb{E}_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

- (1) Guide variational approximate posterior to match the prior p(z)
- (2) Maximize the expected likelihood of the generative model given data x (or guide encoder-decoder to reconstruct the data)



$$\min_{\theta,\phi} \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)||p(z)) - \mathbb{E}_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

Example 1: Gaussian Encoder – Gaussian Decoder VAE



 $q_{\phi}(z_i|x_i) = \mathcal{N}(z_i; \mu(x_i), \sigma(x_i)^2 \mathbf{I}) \qquad p_{\theta}(x_i|z_i) = \mathcal{N}(x_i; \mu(z_i), \sigma(z_i)^2 \mathbf{I})$ 

Example 2: Gaussian Encoder – Bernoulli Decoder VAE



 $q_{\phi}(z_i|x_i) = \mathcal{N}(z_i; \mu(x_i), \sigma(x_i)^2 \mathbf{I}) \qquad p_{\theta}(x_i|z_i) = \text{Bernoulli}(x_i; p(z_i))$ 



# $\beta$ -VAE: LEARNING BASIC VISUAL CONCEPTS WITH A CONSTRAINED VARIATIONAL FRAMEWORK

Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, Alexander Lerchner Google DeepMind {irinah,lmatthey,arkap,cpburgess,glorotx, botvinick,shakir,lerchner}@google.com

#### ABSTRACT

Learning an interpretable factorised representation of the independent data generative factors of the world without supervision is an important precursor for the development of artificial intelligence that is able to learn and reason in the same way that humans do. We introduce  $\beta$ -VAE, a new state-of-the-art framework for automated discovery of interpretable factorised latent representations from raw image data in a completely unsupervised manner. Our approach is a modification of the variational autoencoder (VAE) framework. We introduce an adjustable hyperparameter  $\beta$  that balances latent channel capacity and independence constraints with reconstruction accuracy. We demonstrate that  $\beta$ -VAE with appropriately tuned  $\beta > 1$  qualitatively outperforms VAE ( $\beta = 1$ ), as well as state of the art unsupervised (InfoGAN) and semi-supervised (DC-IGN) approaches to disentangled factor learning on a variety of datasets (celebA, faces and chairs). Furthermore, we devise a protocol to quantitatively compare the degree of disentanglement learnt by different models, and show that our approach also significantly outperforms all baselines quantitatively. Unlike InfoGAN,  $\beta$ -VAE is stable to train, makes few assumptions about the data and relies on tuning a single hyperparameter  $\beta$ , which can be directly optimised through a hyperparameter search using weakly labelled data or through heuristic visual inspection for purely unsupervised data.



More weights on KL divergence term





Entangled Representation (hard to interpret)

Disentangled Representation (easier to interpret)





### **Adversarial Autoencoders**

Alireza Makhzani University of Toronto makhzani@psi.toronto.edu

Ian Goodfellow OpenAI goodfellow.ian@gmail.com Jonathon Shlens & Navdeep Jaitly Google Brain {shlens,ndjaitly}@google.com

> Brendan Frey University of Toronto frey@psi.toronto.edu

#### Abstract

In this paper, we propose the "adversarial autoencoder" (AAE), which is a probabilistic autoencoder that uses the recently proposed generative adversarial networks (GAN) to perform variational inference by matching the aggregated posterior of the hidden code vector of the autoencoder with an arbitrary prior distribution. Matching the aggregated posterior to the prior ensures that generating from any part of prior space results in meaningful samples. As a result, the decoder of the adversarial autoencoder learns a deep generative model that maps the imposed prior to the data distribution. We show how the adversarial autoencoder can be used in applications such as semi-supervised classification, disentangling style and content of images, unsupervised clustering, dimensionality reduction and data visualization. We performed experiments on MNIST, Street View House Numbers and Toronto Face datasets and show that adversarial autoencoders achieve competitive results in generative modeling and semi-supervised classification tasks.



VAE 
$$\min_{\theta,\phi} \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)||p(z)) - \mathbb{E}_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

Minimize the discrepancy between prior p(z) and posterior q(z|x)

AAE 
$$\min_{\theta,\phi} \max_{\psi} \mathbb{E}_{z \sim p(z)} [\log D(z)] + \mathbb{E}_{z \sim q(z)} [\log(1 - D(z))] - \mathbb{E}_{z \sim q_{\phi}(z|x)} [\log p_{\theta}(x|z)]$$

Minimize the discrepancy between prior p(z) and **aggregated** posterior q(z)

$$q(z) = \int q_{\phi}(z|x) p_{\text{data}}(x) dx \rightarrow \text{aggregated posterior distribution}$$

### Adversarial Autoencoder



### Variational Autoencoder





(a) VAE



 $\min_{\theta,\phi} \mathcal{D}_{\mathrm{KL}}(q_{\phi}(z|x)||p(z)) - \mathbb{E}_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$ 

(b) WAE and AAE



 $\min_{\theta,\phi,\psi} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q_{\phi}(z|x)} [c(x, G_{\theta}(z))] + \lambda \cdot \mathcal{D}_{\psi}(q_{z}||p_{z})$ 



AAE Basic Form



Supervised AAE



Semi-Supervised AAE



**Dimensionality Reduction AAE** 

### Wasserstein Auto-Encoders

Ilya Tolstikhin<sup>1</sup>, Olivier Bousquet<sup>2</sup>, Sylvain Gelly<sup>2</sup>, and Bernhard Schölkopf<sup>1</sup>

<sup>1</sup>Max Planck Institute for Intelligent Systems <sup>2</sup>Google Brain

#### Abstract

We propose the Wasserstein Auto-Encoder (WAE)—a new algorithm for building a generative model of the data distribution. WAE minimizes a penalized form of the Wasserstein distance between the model distribution and the target distribution, which leads to a different regularizer than the one used by the Variational Auto-Encoder (VAE) [1]. This regularizer encourages the encoded training distribution to match the prior. We compare our algorithm with several other techniques and show that it is a generalization of adversarial auto-encoders (AAE) [2]. Our experiments show that WAE shares many of the properties of VAEs (stable training, encoder-decoder architecture, nice latent manifold structure) while generating samples of better quality, as measured by the FID score.

$$W_1(p_{\text{data}}, p_G) = \inf_{\gamma \in \Gamma(p_{\text{data}}, p_G)} \mathbb{E}_{(x,y) \sim \gamma}[\|x - y\|_1]$$

$$W_1(p_{\text{data}}, p_G) = \sup_{\|f\|_L \le K} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[f(x)] - \mathbb{E}_{x \sim p_G(x)}[f(x)] \right\}$$

$$W_1(p_{\text{data}}, p_G) = \max_{\theta_D} \left\{ \mathbb{E}_{x \sim p_{\text{data}}(x)}[D(x)] - \mathbb{E}_{z \sim p(z)}[D(G(z))] \right\}$$

$$W_{c}(p_{\text{data}}, p_{G}) = \inf_{\substack{\gamma \in \Gamma(p_{\text{data}}, p_{G})}} \mathbb{E}_{(x, y) \sim \gamma}[c(x, y)]$$
$$= \inf_{\{q: q_{z} = p_{z}\}} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q(z|x)}[c(x, G(z))$$

 $q_z$  is the aggregated posterior when  $x \sim p_{data}(x)$  and  $z \sim q(z|x)$ 

$$\inf_{q(z|x)} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q(z|x)} [c(x, G(z))] + \lambda \cdot \mathcal{D}(q_z || p_z)$$

WAE problem 
$$\min_{\theta,\phi,\psi} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q_{\phi}(z|x)} [c(x, G_{\theta}(z))] + \lambda \cdot \mathcal{D}_{\psi}(q_{z}||p_{z})$$

WAE problem 
$$\min_{\theta,\phi,\psi} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q_{\phi}(z|x)} [c(x, G_{\theta}(z))] + \lambda \cdot \mathcal{D}_{\psi}(q_{z}||p_{z})$$

### WAE-GAN

 $\min_{\theta,\phi} \max_{\psi} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q_{\phi}(z|x)} [c(x, G_{\theta}(z))] + \lambda \cdot (\mathbb{E}_{z \sim p_{z}(z)} [\log D_{\psi}(z)] + \mathbb{E}_{z \sim q_{z}(z)} [\log(1 - D_{\psi}(z))])$ 

### WAE – MMD

$$\min_{\theta,\phi} \mathbb{E}_{x \sim p_{\text{data}}(x)} \mathbb{E}_{z \sim q_{\phi}(z|x)} [c(x, G_{\theta}(z))] + \lambda \cdot \mathcal{L}_{\text{MMD}}(q_z, p_z)$$

VAE

WAE-MMD

WAE-GAN

