

Generative Modeling

Generative adversarial networks

Laboratory for methods of big data analysis



In this Lecture

- ▶ Generative Adversarial Networks
 - algorithm statement;
 - ideal case;
 - shortcomings of vanilla algorithm;
 - proposed shortcuts.

Idea



Reminder: f -divergence

- ▶ For convex $f(\cdot)$, P and Q some distributions, we define f -divergence:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

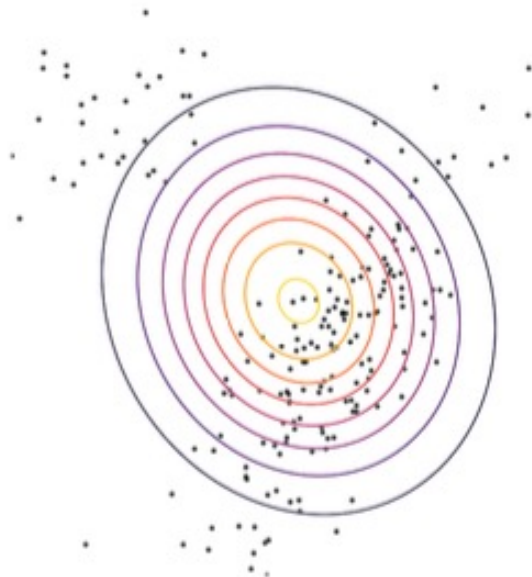
Reminder: f -divergence

- For convex $f(\cdot)$, P and Q some distributions, we define f -divergence:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

$$KL = \int p(x) \log \frac{p(x)}{q_\theta(x)} dx$$

$$rKL = \int q(x) \log \frac{q_\theta(x)}{p(x)} dx$$



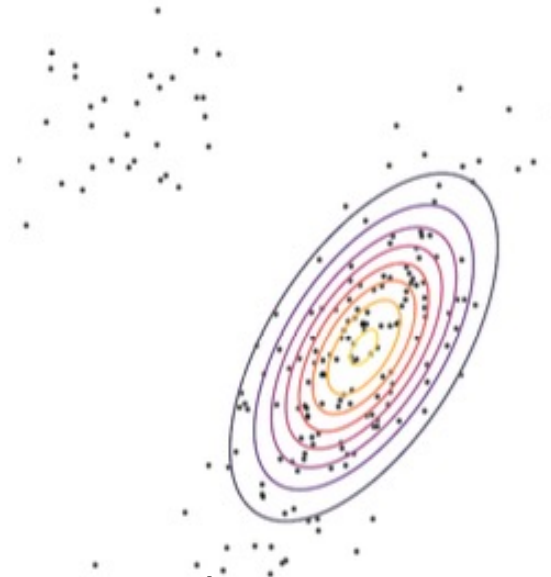
Reminder: f -divergence Convergence

- For convex $f(\cdot)$, P and Q some distributions, we define f -divergence:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

$$rKL = \int q(x) \log \frac{q_\theta(x)}{p(x)} dx$$

$$\begin{aligned} \theta^* &= \operatorname{argmin}_{\theta} KL(q_\theta(x)||p(x)) \\ &= \operatorname{argmax}_{\theta} (-\mathbb{E}_{\tilde{x} \sim q_\theta} [\log q_\theta(x)] + \mathbb{E}_{\tilde{x} \sim q_\theta} [\log p(x)]) \end{aligned}$$



Reminder: Variational Lower Bound

- ▶ For convex $f(\cdot)$, P and Q some distributions, we define f -divergence:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

- ▶ Lower bound can be written:

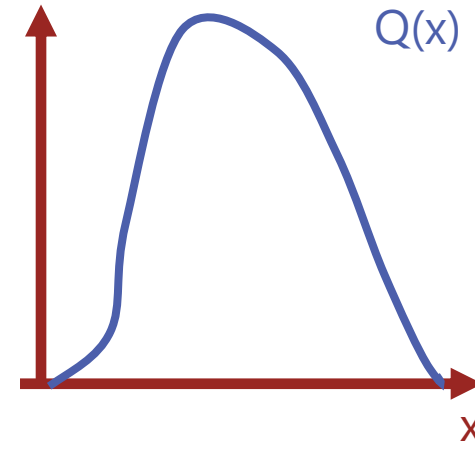
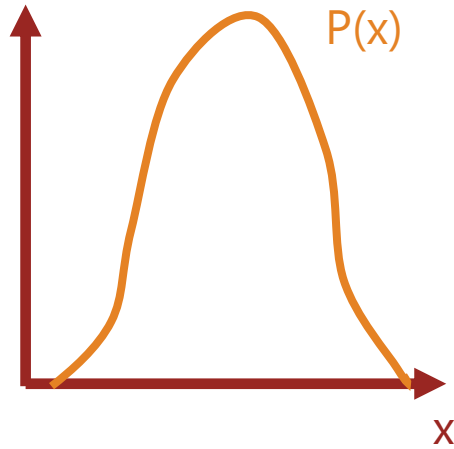
$$D_f(P||Q) \geq \max_{T(x)} \mathbb{E}_{x \sim P} T(x) - \mathbb{E}_{x \sim Q} f^*(T(x)),$$

$T(x)$ is some random function.

- ▶ The tight boundary can be estimated for each f -divergence ($T^*(x)$).
- ▶ For JS-divergence $T^*(x) = \log \frac{2p(x)}{p(x)+q(x)}$, $f^*(x) = -\log(2 - \exp(t))$.

Lower Bound for JS

$$JS(p, q) = \frac{1}{2} \left(KL(p(x) || \frac{p(x) + q_{\theta}(x)}{2}) + KL(q_{\theta}(x) || \frac{p(x) + q_{\theta}(x)}{2}) \right)$$



$$JS(P||Q) \geq \mathbb{E}_{x \sim P} \log \frac{2p(x)}{p(x) + q(x)} + \mathbb{E}_{x \sim Q} \log \frac{2q(x)}{p(x) + q(x)}$$

It would be interesting to construct something close.

Adversarial optimization



Rationale

- ▶ Need to optimize the model q_θ without the direct access to the $p(x)$.

$$\theta^* = \arg \min_{\theta} \max_{\phi} \mathbb{E}_{x \sim p, \tilde{x} \sim q_\theta} V(f_\phi(x), f_\phi(\tilde{x}))$$

- ▶ Instead of minimizing over some analytically defined divergence with parameter ϕ , one could minimize over “learned divergence”.

Generator

- ▶ G_θ is a **generator**. It should sample from a random noise:

$$z_j \sim N(0; 1);$$

$$x_j = G_\theta(z_j).$$

- ▶ Our aim is G_θ as a neural network.

- ▶ We thus have a sample:

$$\{x_j\} \sim q_\theta(x)$$

- ▶ G_θ can be defined in many ways. For example, physics generator.

Borisyak M et al. *PeerJ Computer Science* 6:e274 (2020)

Discriminator

- ▶ Add a classifying neural network, **discriminator** D_ϕ , to distinguish between the real and generated samples.
- ▶ Optimize:

$$\max_{\phi} (\mathbb{E}_{x \sim p(x)} \log(D_\phi(x)) + \mathbb{E}_{x \sim q_\theta(x)} \log(1 - D_\phi(x)))$$



Real samples



Generated samples

G+D recap

We can now put together generator and discriminator.

› objective of discriminator:

$$\max_{\phi} (\mathbb{E}_{x \sim p(x)} \log(D_{\phi}(x)) + \mathbb{E}_{x \sim q_{\theta}(x)} \log(1 - D_{\phi}(x)))$$

› objective of generator:

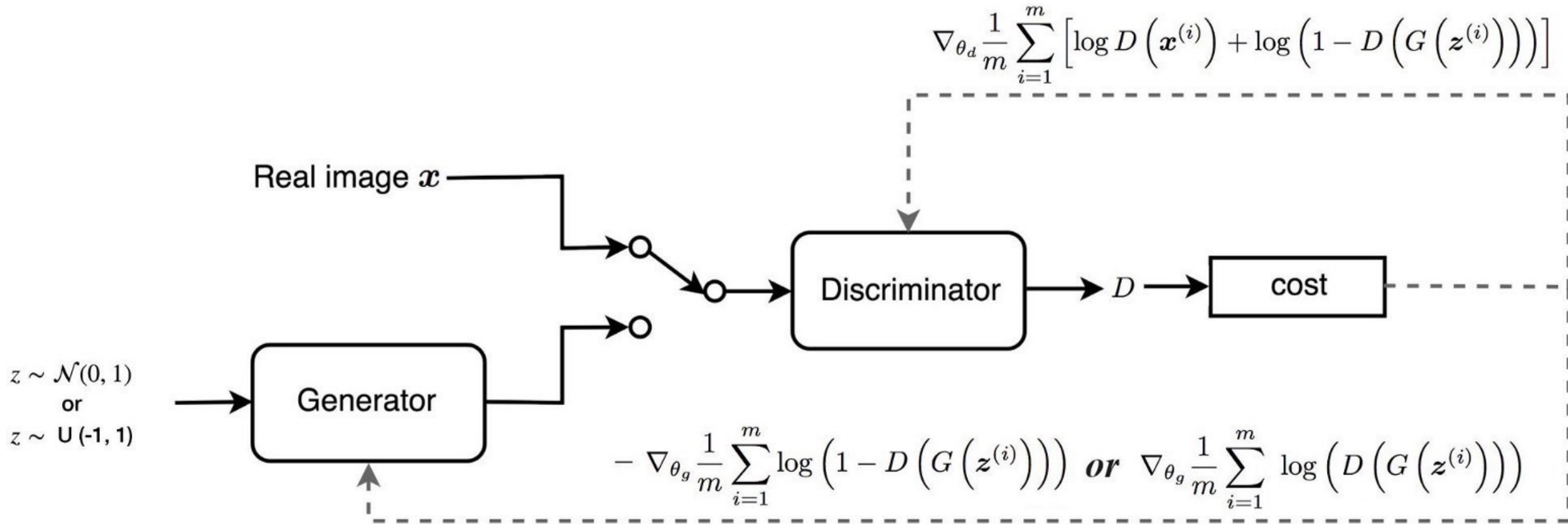
$$\min_{\phi} \mathbb{E}_{z \sim N(0;1)} \log(1 - D_{\phi}(G_{\theta}(z)))$$

We thus defined a minimax game:

$$\min_{\theta} \max_{\phi} \mathbb{E}_{x \sim p, \tilde{x} \sim q_{\theta}} V(f_{\phi}(x), f_{\phi}(\tilde{x})).$$

In exactly the way we wanted.

Training at a Glance



For D and G defined as neural networks, we can use backpropagation.

Optimal Solution

- › For a given generator, the optimal discriminator is:

$$D_{\phi}^*(G) = \frac{p(x)}{p(x) + q_{\theta}(x)}.$$

- › Incorporating that into the minimax game to yield virtual training criterion:

$$\begin{aligned} C(G) &= \max_D V(G, D) = \\ &= \mathbb{E}_{x \sim p(x)} \log(D_{\phi}^*(x)) + \mathbb{E}_{x \sim q_{\theta}(x)} \log(1 - D_{\phi}^*(x)) = \\ &= \mathbb{E}_{x \sim P} \log \frac{p(x)}{p(x) + q(x)} + \mathbb{E}_{x \sim q_{\theta}(x)} \log \frac{q(x)}{p(x) + q(x)} \end{aligned}$$

Lower Bound Reminder

- ▶ In case of ideal discriminator:

$$C(G) = \mathbb{E}_{x \sim P} \log \frac{p(x)}{p(x) + q(x)} + \mathbb{E}_{x \sim Q} \log \frac{q(x)}{p(x) + q(x)}$$

- ▶ This can be compared to variational bound:

$$JS(P||Q) \geq \mathbb{E}_{x \sim p(x)} \log \frac{2p(x)}{p(x)+q(x)} + \mathbb{E}_{x \sim q(x)} \log \frac{2q(x)}{p(x)+q(x)}$$

- ▶ Difference is only in $\log 4$

Optimal Solution

- › In an optimal case $p = q_\theta$, we have $C(G) = -\log(4)$.
- › We thus can write out:

$$C(G) = -\log(4) + \frac{1}{2}KL(p(x) || \frac{p(x) + q_\theta(x)}{2}) + \frac{1}{2}KL(q_\theta(x) || \frac{p(x) + q_\theta(x)}{2}).$$

- › In other words, we effectively optimize Jensen-Shannon divergence:

$$C(G) = -\log(4) + JS(p(x) || q_\theta(x)).$$

- › Reminder: we did it without access to $p(x)$.

GAN algorithm

1. Sample data mini-batch $(x_1, \dots, x_m \sim D)$.
2. Sample generator mini-batch $(z_1, \dots, z_m \sim q_\theta)$.
3. Use SGD to obtain new weights of generator:

$$\nabla_\theta V(G_\theta, D_\phi) = \frac{1}{m} \sum_{i=1}^m \log(1 - D_\phi(G_\theta(z_i))).$$

4. Use SGD to obtain new weights of discriminator:

$$\nabla_\phi V(G_\theta, D_\phi) = \frac{1}{m} \sum_{i=1}^m (\log D_\phi(x_i) + \log(1 - D_\phi(G_\theta(z_i)))) .$$

5. Repeat with several epochs.

GAN results



Figure 2: Visualization of samples from the model. Rightmost column shows the nearest training example of the neighboring sample, in order to demonstrate that the model has not memorized the training set. Samples are fair random draws, not cherry-picked. Unlike most other visualizations of deep generative models, these images show actual samples from the model distributions, not conditional means given samples of hidden units. Moreover, these samples are uncorrelated because the sampling process does not depend on Markov chain mixing. a) MNIST b) TFD c) CIFAR-10 (fully connected model) d) CIFAR-10 (convolutional discriminator and “deconvolutional” generator)

I. Goodfellow, et al. Generative Adversarial Networks, NIPS 2014

GAN First Paper Disclaimer

While we make no claim that these samples are better than samples generated by existing methods, we believe that these samples are at least competitive with the better generative models in the literature and highlight the potential of the adversarial framework.

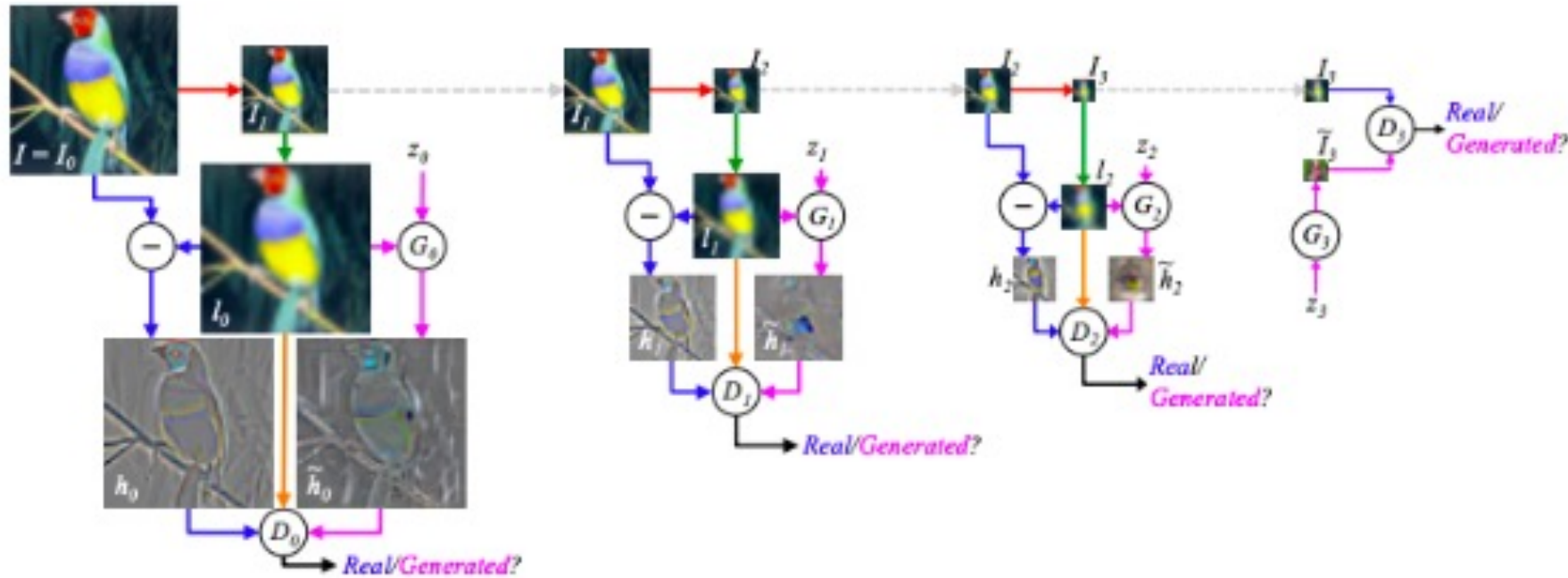
I. Goodfellow, Generative Adversarial Networks, NIPS 2014

Enhancing GAN



Unsupervised Feature Learning

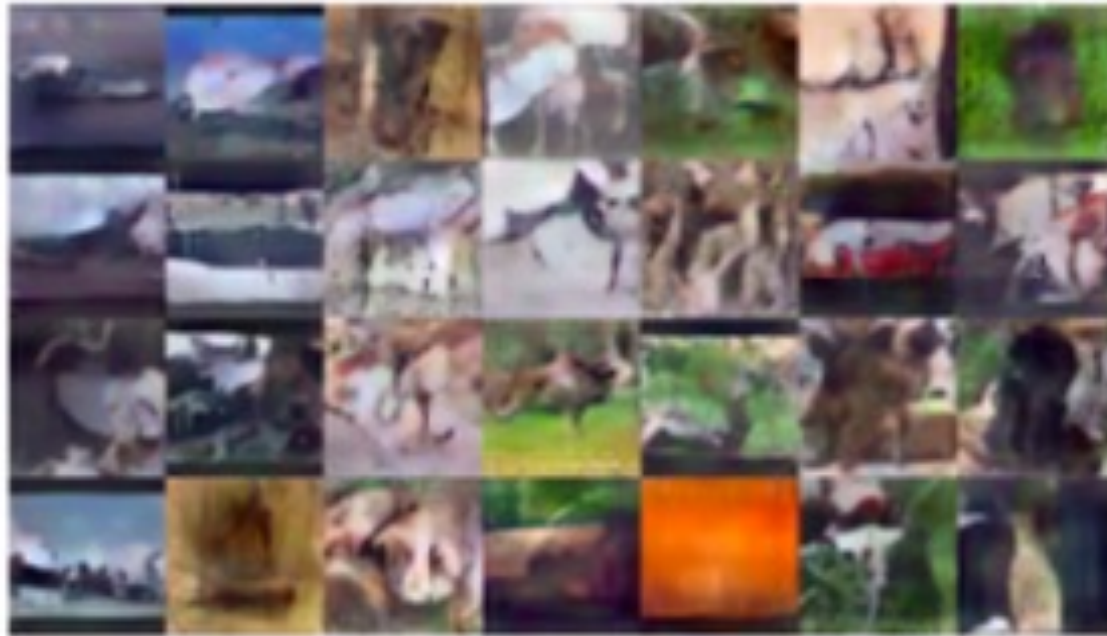
We need to decrease the size of images to make a faster convergence.
Let us make a Laplacian pyramid of images.



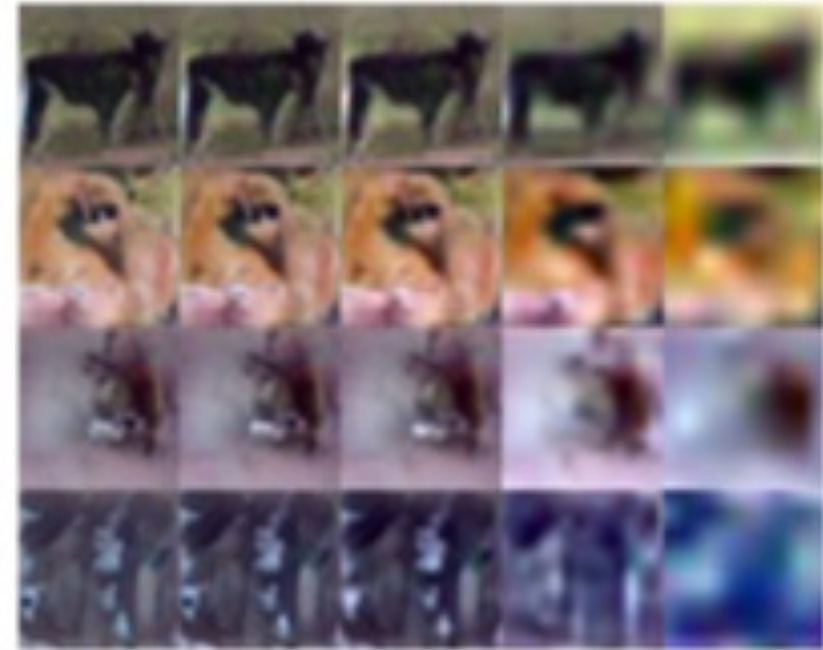
The representation is learned gradually.

E Denton et al. Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

LAPGAN: results



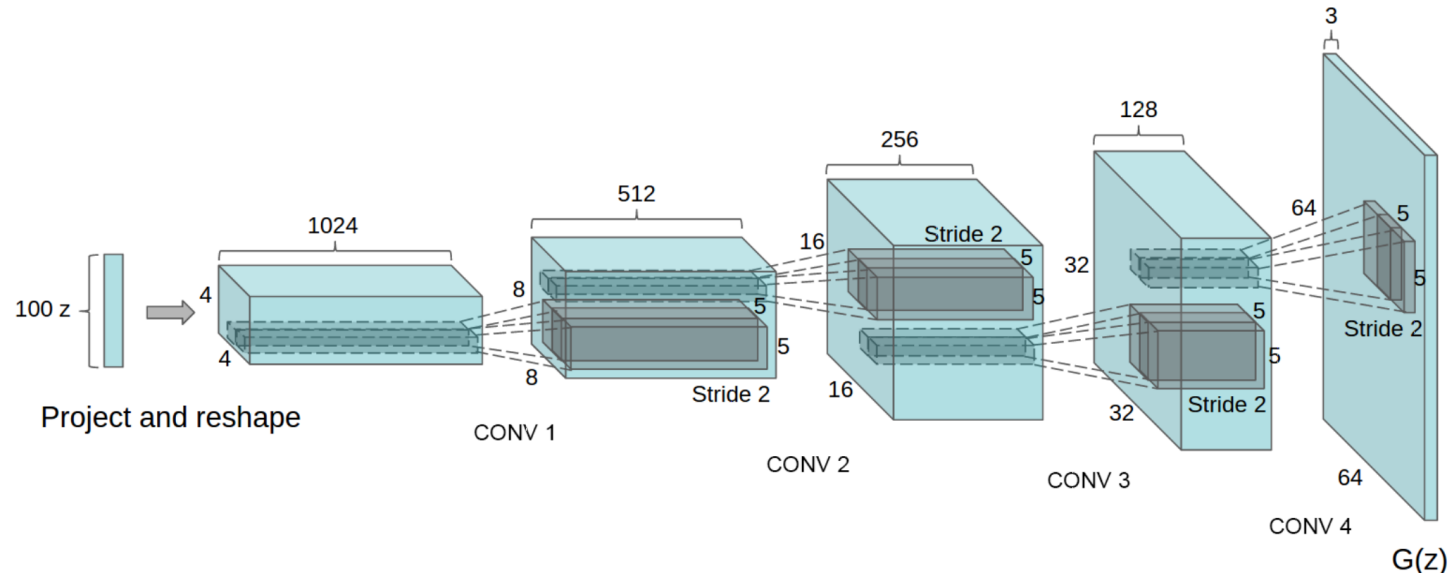
(a)



(b)

Figure 4: STL samples: (a) Random 96x96 samples from our LAPGAN model. (b) Coarse-to-fine generation chain.

Convolutional Layers are Here to Help



- ▶ pooling layers \rightarrow convolution layers.
- ▶ Use batchnorm.
- ▶ No fully connected hidden layers.
- ▶ ReLU activation in generator.
- ▶ LeakyReLU activation in the discriminator for all layers.

A. Radford et al. Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, ICLR 2016

DCGAN: results

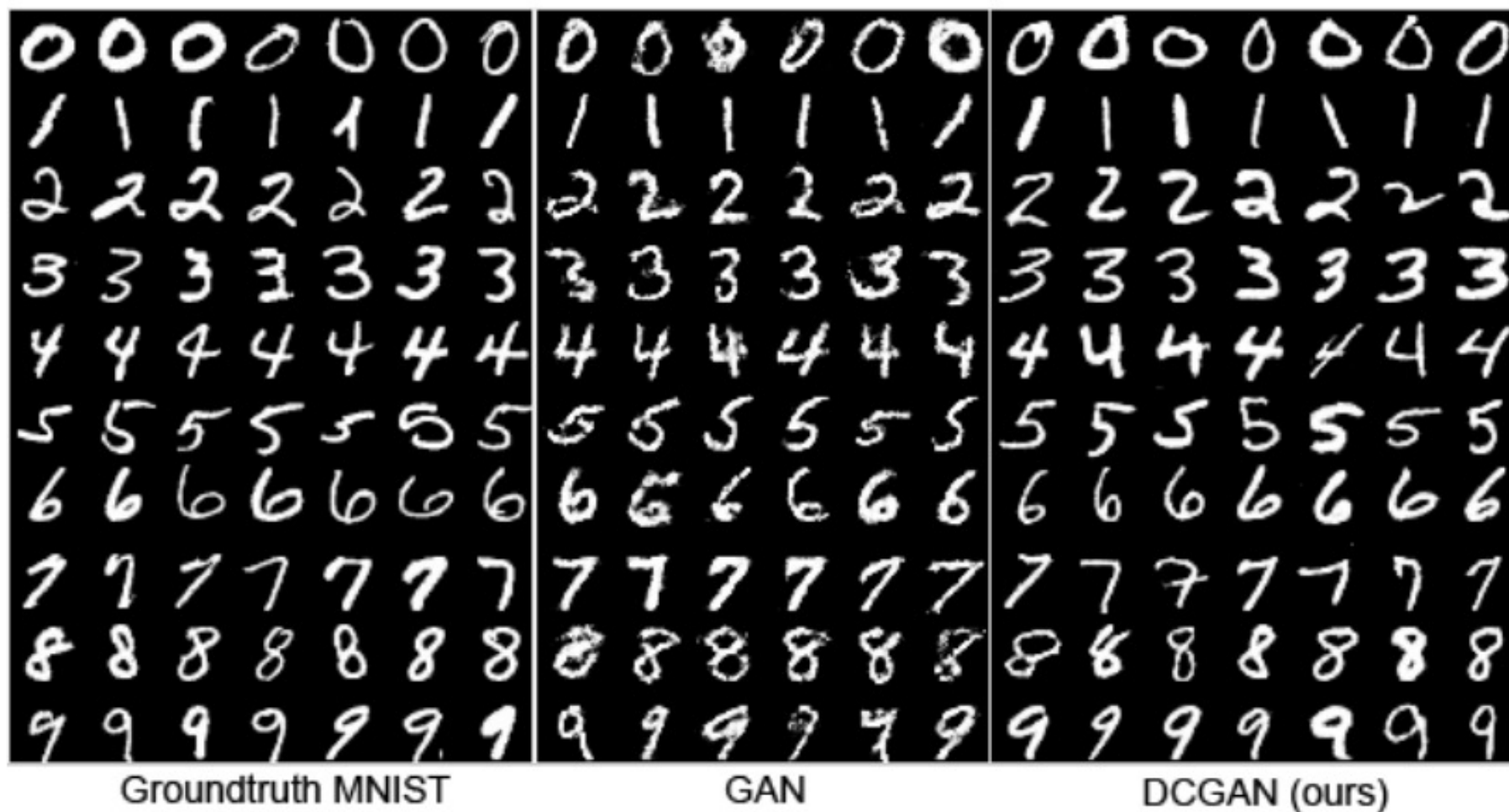


Figure 9: Side-by-side illustration of (from left-to-right) the MNIST dataset, generations from a baseline GAN, and generations from our DCGAN .

Walking in the Latent Space

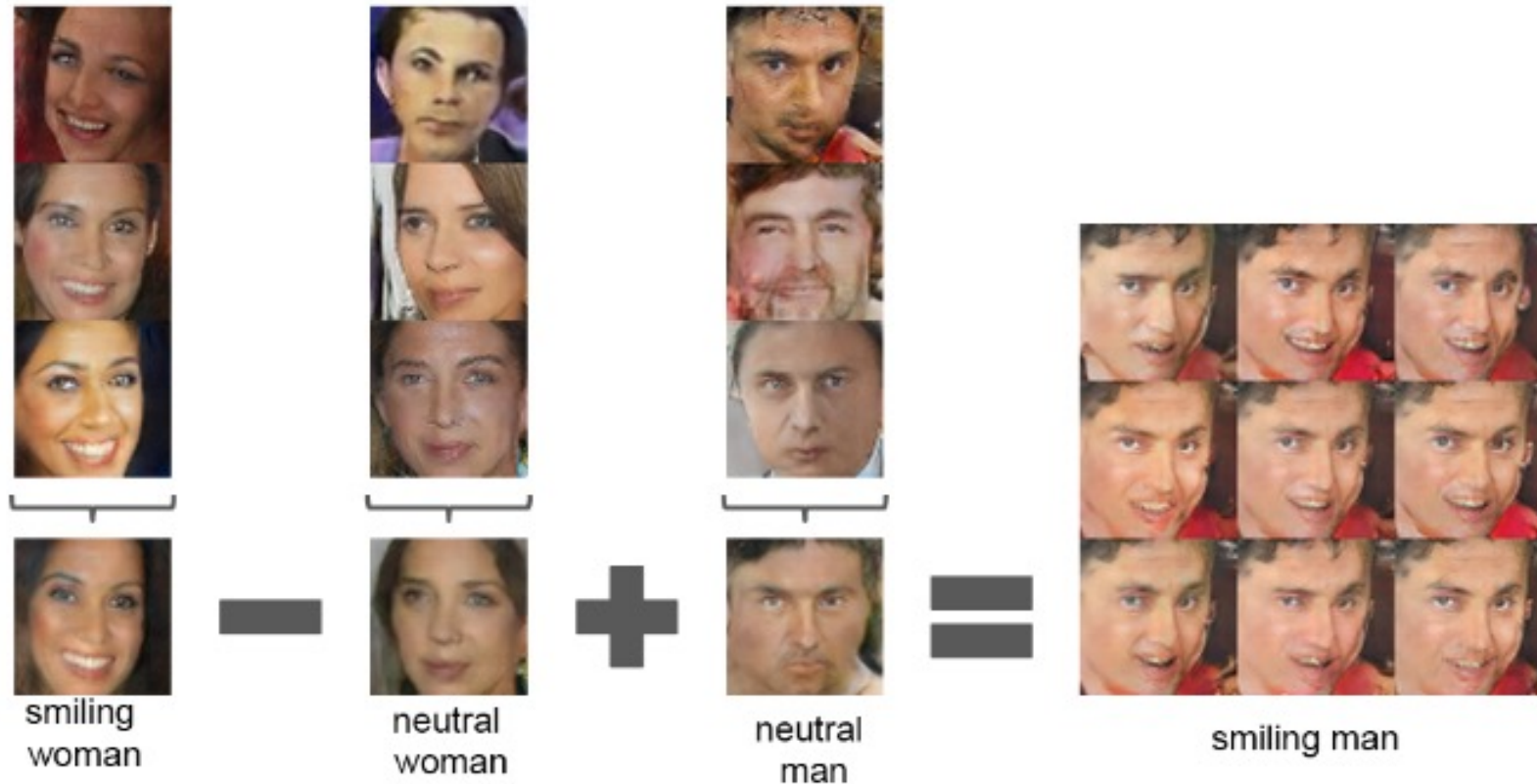


TV



Window

Arithmetic in the Latent Space

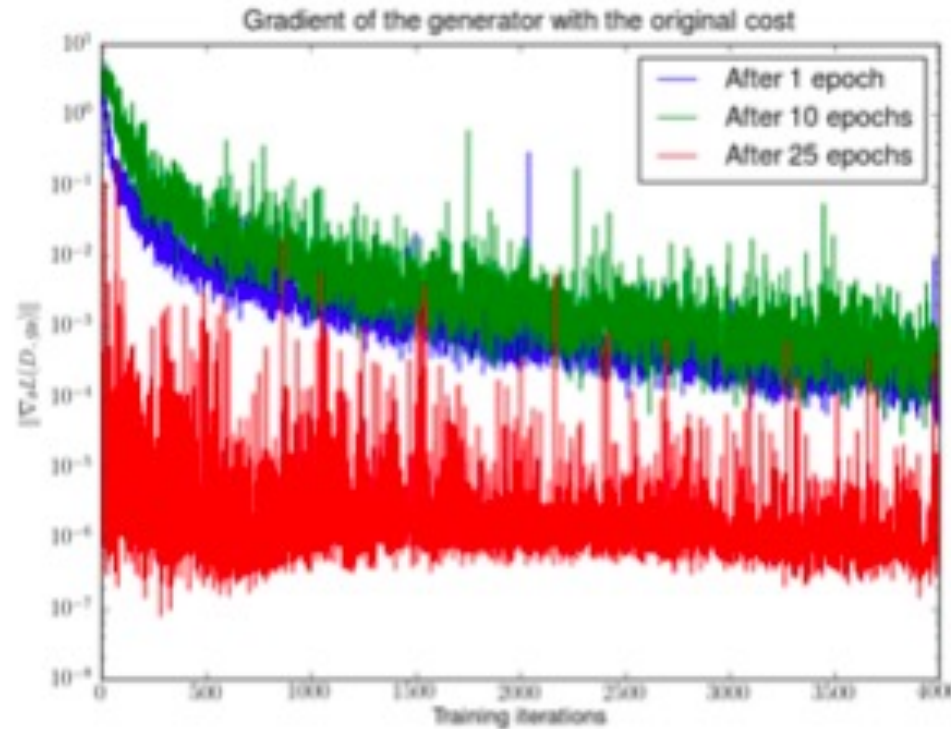


GAN problems



Game Approach Problems

- › Discriminator must be optimal on every step of convergence.
- › This is not true, you should not overtrain discriminator.
- › Loss-function can be quite noisy.

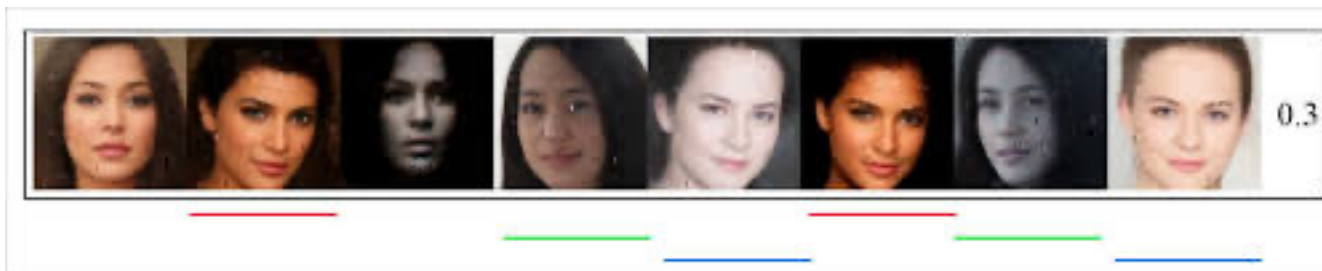


Martin Arjovsky, Towards Principled Methods for Training Generative Adversarial Networks , ICLR17

Mode Collapse

- GANs choose to generate a small number of modes due to a defect in the training procedure, rather than due to the divergence they aim to minimize.

I. Goodfellow NIPS 2016 Tutorial: Generative Adversarial Network



10k steps

20k steps



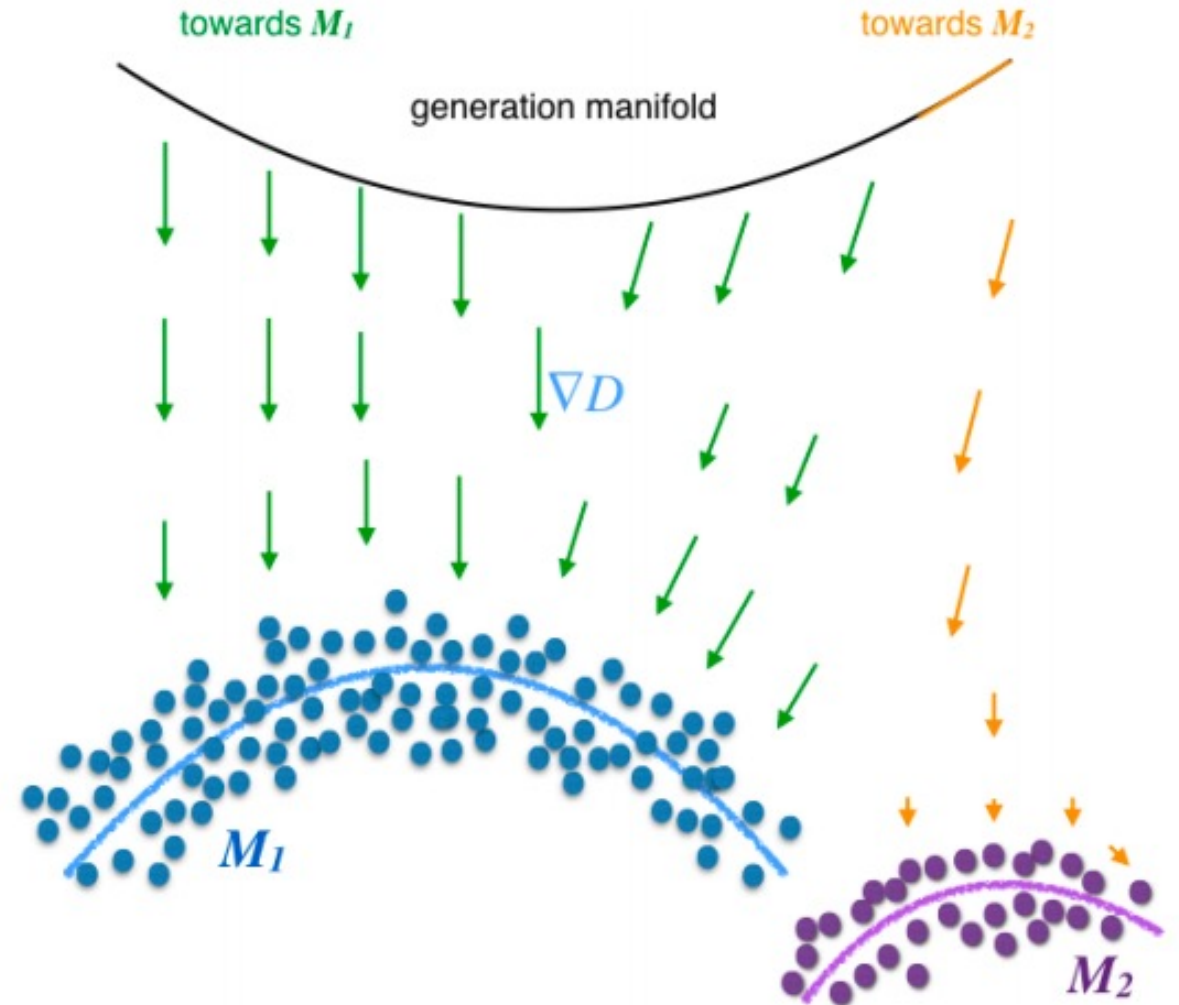
50K steps

100k steps

Luke Metz et al Unrolled Generative Adversarial Networks ICLR 2017

Mode Collapse

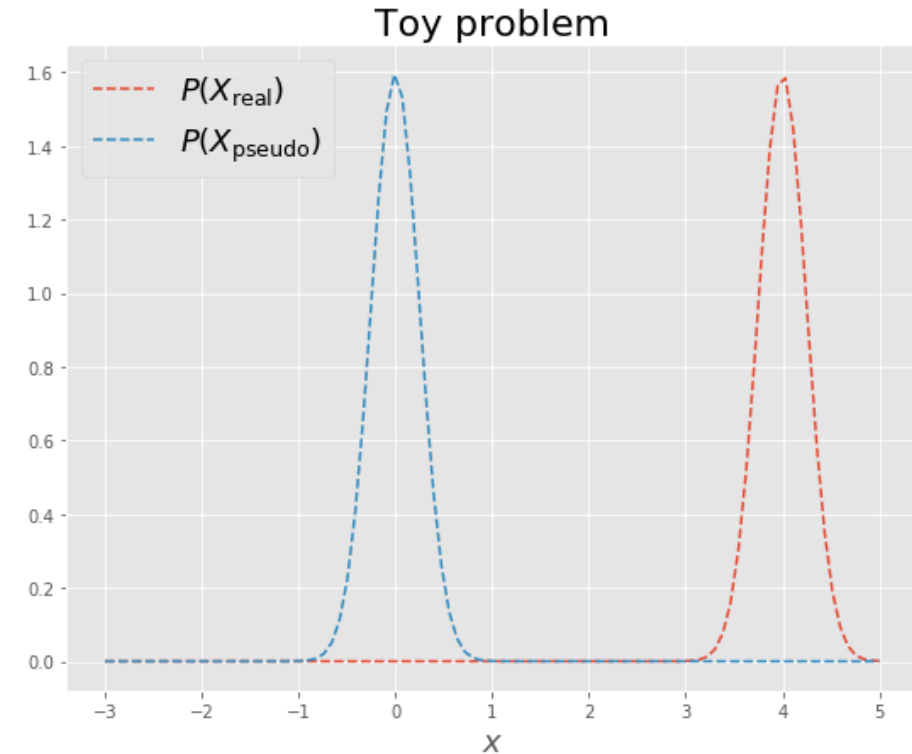
- ▶ For fixed D :
 - G tends to converge to a point x^* that fools D the most.
 - In extreme cases, G becomes independent on z .
 - Gradient on z diminishes.
- ▶ When D restarts:
 - Easily finds this x^* .
 - Pushes G to the next point x^{**} .



Vanishing Gradients

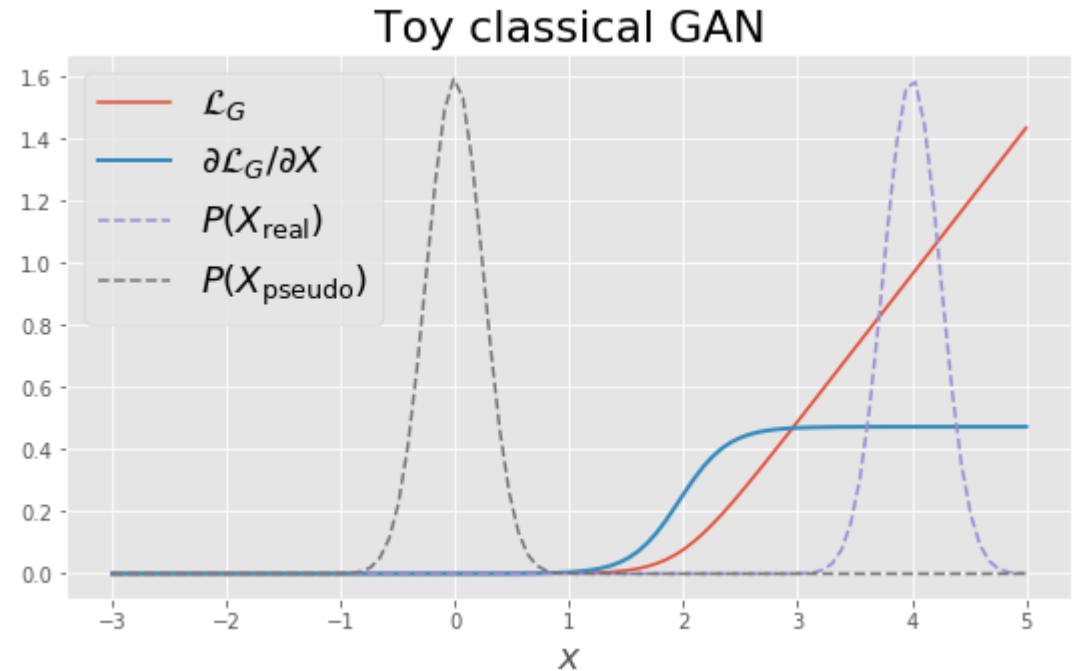
- ▶ For disjoint support of real and generated data
- ▶ An ideal discriminator can perfectly tell the real and generated data apart:

$$D(G(z)) \approx 0$$



Vanishing Gradients

- ▶ $L_G = -\log D(G(z))$
- ▶ $dD(x)/dx \approx 0$ for generated x
- ▶ $dL_G(x)/dx \approx 0$ for generated x
- ▶ Generator can't train!
- ▶ Need to start closer (how?)
- ▶ Problem is further enhanced due to noisy estimate from data.



Summary so Far

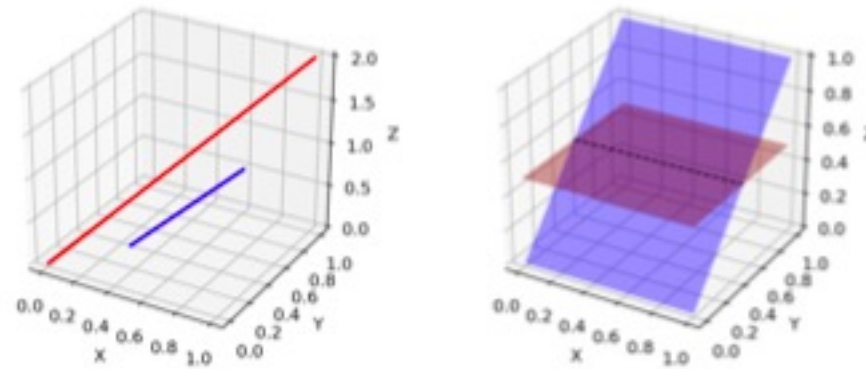
- ▶ Pros:
 - Can utilize power of back-prop.
 - No explicit intractable integral.
 - No MCMC needed.
- ▶ Cons:
 - Unclear stopping criteria.
 - No explicit representation of $g_{\theta}(x)$.
 - Hard to train.
 - No evaluation metric so hard to compare with other models.
 - Easy to get trapped in local optima that memorize training data.
 - Hard to invert generative model to get back latent z from generated x .

GAN ways out



Diminishing Gradients

- ▶ We have seen already that signal data is located on manifold.
- ▶ GAN case is in fact more complicated, as we need a discriminator that distinguishes two supports.
- ▶ This is way too easy, if supports are disjoint.



Diminishing Gradients: Noisy Supports

- ▶ Let's make the problem harder: introduce random noise $\varepsilon \sim N(0; \sigma^2 I)$:

$$\mathbb{P}_{x+\varepsilon(x)} = \mathbb{E}_{y \sim P(x)} \mathbb{P}_{\varepsilon}(x - y).$$

- ▶ This will make noisy supports, that makes it difficult for discriminator.



Martin Arjovsky, Towards Principled Methods for Training Generative Adversarial Networks , ICLR17

Feature Matching

Change the objective of the generator:

$$||\mathbb{E}_{x \sim p(x)} f(x) - \mathbb{E}_{z \sim p_z(z)} f(G(z))||^2$$

Here $f(x)$ can be any property we need (including the output of another network).

Danger of overtrain to match known tests!



Historical averaging

- › average with previous parameter values:

$$||\theta - \frac{1}{t} \sum_{i=1}^t \theta[i]||^2$$

- › this allows to create a fake agent that plays the game.
- › and solves the problems only in low dimensions.

Salimans et al. Improved Techniques for Training GANs, NIPS16

Look into the Future: unrolled GANs

- › What if we can look into the future of system?
- › We could avoid local optima and optimize better.
- › Algorithm:
 - › At each step we train discriminator 5-10 steps ahead.
 - › We DO NOT introduce it to the system.
 - › We show the possible future moves to generator and update it accordingly.

Unrolled GAN: results

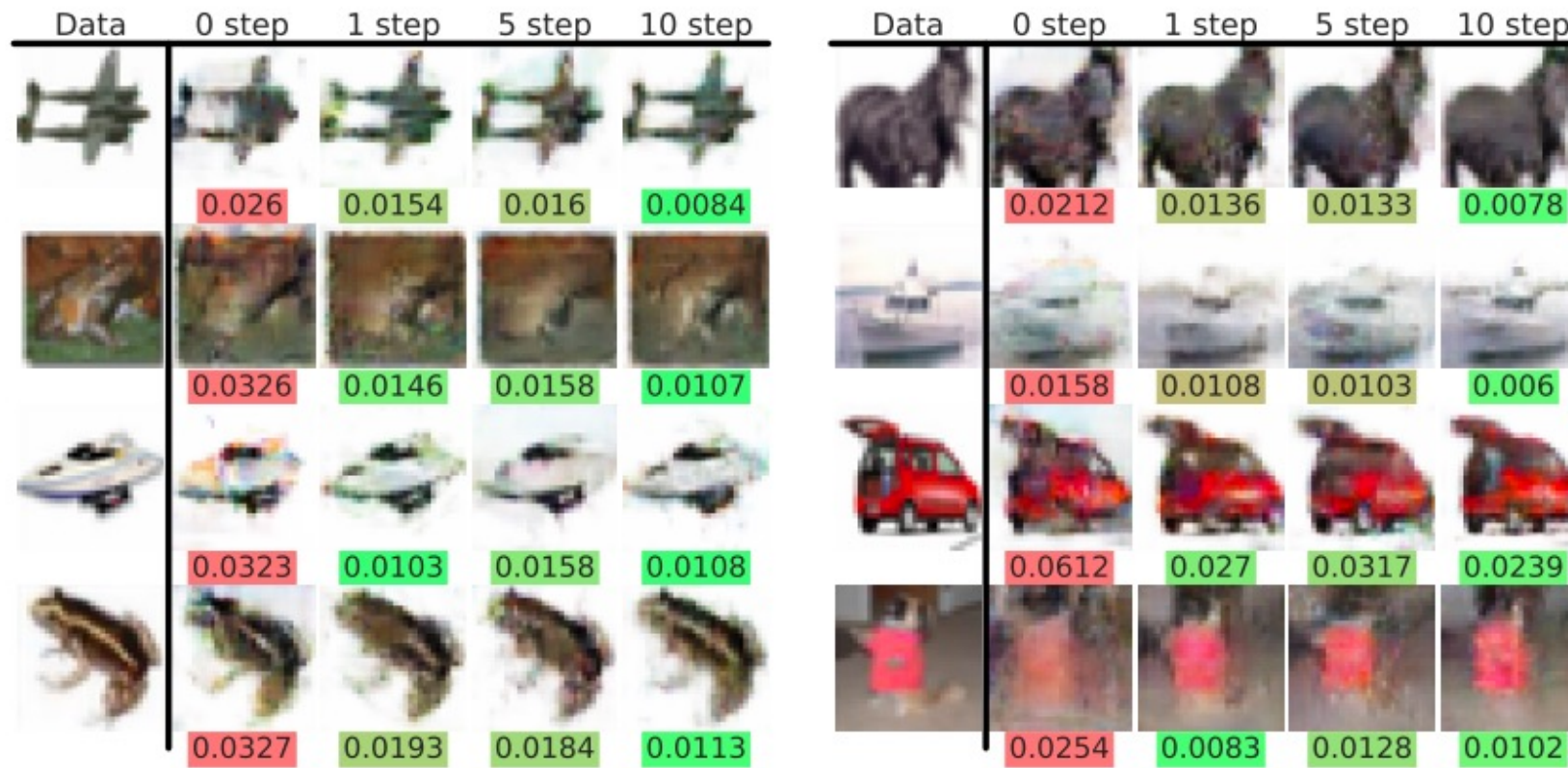


Figure 5: Training set images are more accurately reconstructed using GANs trained with unrolling than by a standard (0 step) GAN, likely due to mode dropping by the standard GAN. Raw data is on the left, and the optimized images to reach this target follow for 0, 1, 5, and 10 unrolling steps. The reconstruction MSE is listed below each sample. A random 1280 images were selected from the training set, and corresponding best reconstructions for each model were found via optimization. Shown here are the eight images with the largest absolute fractional difference between GANs trained with 0 and 10 unrolling steps.

f -GANs



Reminder: Variational Lower Bound

- ▶ For convex $f(\cdot)$, P and Q some distributions, we define f -divergence:

$$D_f(P||Q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx.$$

- ▶ This is bounded:

$$D_f(P||Q) \geq \max_{T(x)} \mathbb{E}_{x \sim P} T(x) - \mathbb{E}_{x \sim Q} f^*(T(x)),$$

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	$\int q(x) \log \frac{q(x)}{p(x)} dx$	$-\log u$	$-\frac{q(x)}{p(x)}$
Pearson χ^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	$\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx$	$-(u+1) \log \frac{1+u}{2} + u \log u$	$\log \frac{2p(x)}{p(x)+q(x)}$

Variational Divergence Minimization

$$D_f(P||Q) \geq \max_{T(x)} \mathbb{E}_{x \sim P} T(x) - \mathbb{E}_{x \sim Q} f^*(T(x)),$$

- ▶ Work in GAN paradigm:
 - generator $x \sim Q: x = G_\theta(z)$;
 - test function $T(x)$.

$$\min_{\theta} \max_{\omega} F(\omega, \theta) = \mathbb{E}_{x \sim P} T_{\omega}(x) - \mathbb{E}_{x \sim G_{\theta}(z)} f^*(T_{\omega}(x))$$

- ▶ To have wider range of functions:

$$T_{\omega}(x) = g_f(V_{\omega}(x)),$$

here $g_f: \mathbb{R} \rightarrow \text{dom}_{f^*}$ is output activation function for f -divergence used

S. Nowozin et al. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization

Output activation function

$$F(\omega, \theta) = \mathbb{E}_{x \sim P} g_f(V_\omega(x)) - \mathbb{E}_{x \sim G_\theta(z)} f^*(g_f(V_\omega(x)))$$

choice of output activation function is somewhat arbitrary.

Name	Output activation g_f
Kullback-Leibler (KL)	v
Reverse KL	$-\exp(-v)$
Pearson χ^2	v
Squared Hellinger	$1 - \exp(-v)$
Jensen-Shannon	$\log(2) - \log(1 + \exp(-v))$
GAN	$-\log(1 + \exp(-v))$

Example: GAN objective

$$F(\omega, \theta) = \mathbb{E}_{x \sim P} g_f(V_\omega(x)) - \mathbb{E}_{x \sim G_\theta(z)} f^*(g_f(V_\omega(x)))$$



$$\begin{aligned} g_{GAN} &= -\log(1 + \exp(-v)) \\ f^*(t) &= -\log(1 - \exp(t)) \end{aligned}$$

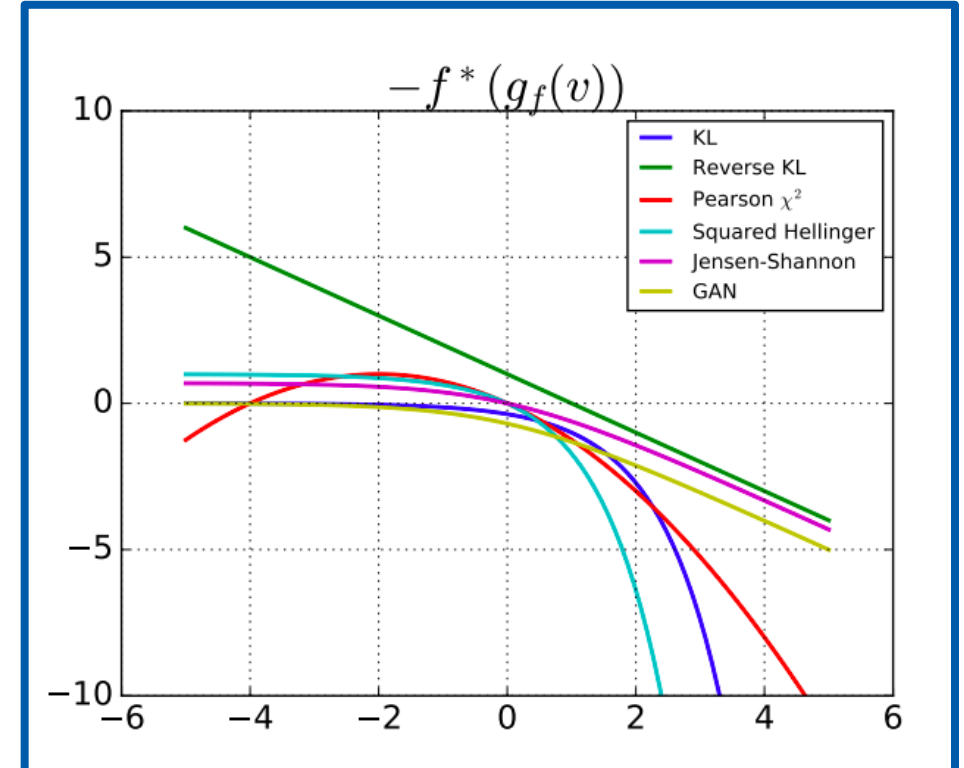
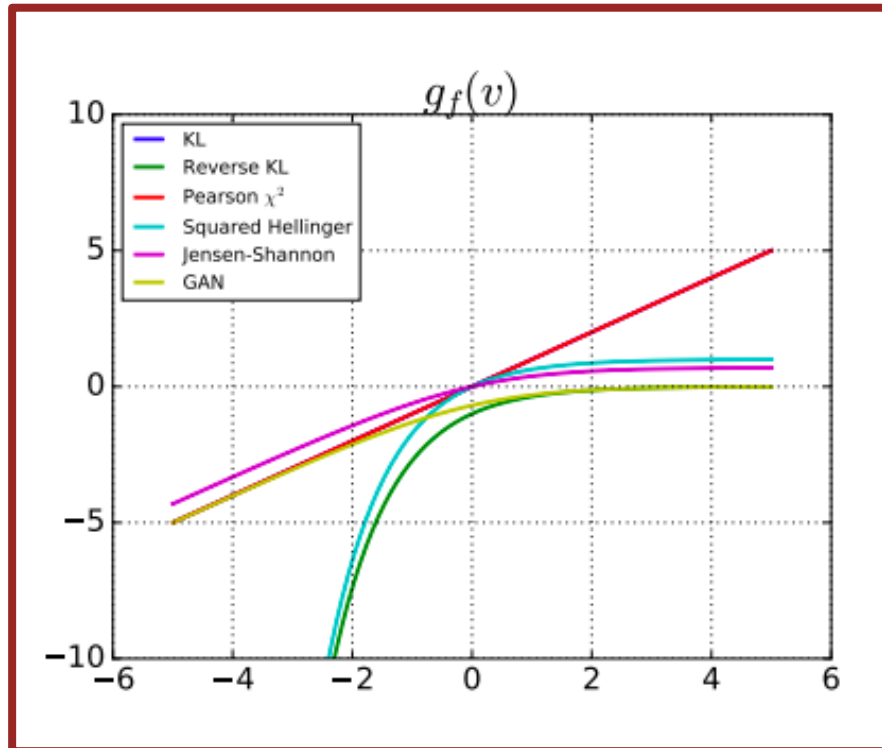
$$F(\omega, \theta) = \mathbb{E}_{x \sim P} \log D_\omega(x) - \mathbb{E}_{x \sim G_\theta(z)} \log(1 - D_\omega(x)),$$

for the last nonlinearity in the discriminator taken as the sigmoid

$$D_\omega(x) = 1/(1 + e^{-V_\omega(x)})$$

Variational Divergence Minimization

$$\min_{\theta} \max_{\omega} F(\omega, \theta) = \mathbb{E}_{x \sim P} \underline{g_f(V_{\omega}(x))} - \mathbb{E}_{x \sim G_{\theta}(z)} \underline{f^*(g_f(V_{\omega}(x)))}$$



f -GAN results

Training divergence	KDE $\langle LL \rangle$ (nats)	\pm SEM
Kullback-Leibler	416	5.62
Reverse Kullback-Leibler	319	8.36
Pearson χ^2	429	5.53
Neyman χ^2	300	8.33
Squared Hellinger	-708	18.1
Jeffrey	-2101	29.9
Jensen-Shannon	367	8.19
GAN	305	8.97
Variational Autoencoder [18]	445	5.36
KDE MNIST train (60k)	502	5.99

Table 4: Kernel Density Estimation evaluation on the MNIST test data set. Each KDE model is build from 16,384 samples from the learned generative model. We report the mean log-likelihood on the MNIST test set ($n = 10,000$) and the standard error of the mean. The KDE MNIST result is using 60,000 MNIST training images to fit a single KDE model.

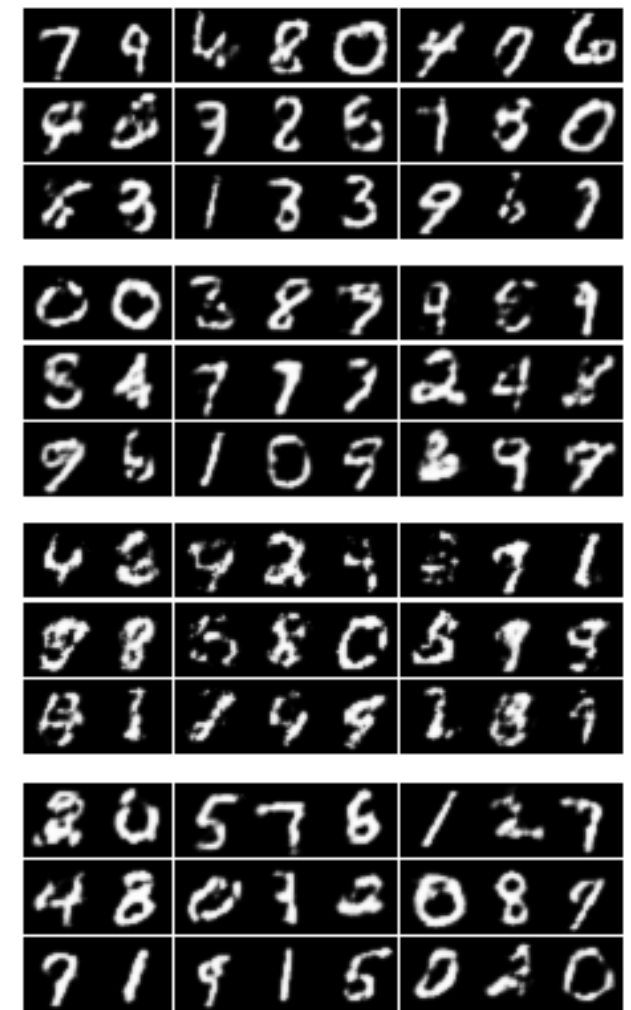


Figure 2: MNIST model samples trained using KL, reverse KL, Hellinger, Jensen from top to bottom.

f -GAN Discussion

- ▶ Using f -GAN approach, one can estimate any f -divergence.
- ▶ Construction has some freedom in choice of function.
- ▶ Using different f -divergence leads to very different learning dynamics.
- ▶ Does not solve mode collapse problem.
- ▶ We need a better way to train GANs.

Conclusions: GANs

- ▶ use Generator-Discriminator game to estimate the distance from generated distribution to the true one.
- ▶ produce sharp images.
- ▶ reconstruct implicit model of target PDF.