Unsupervised Learning

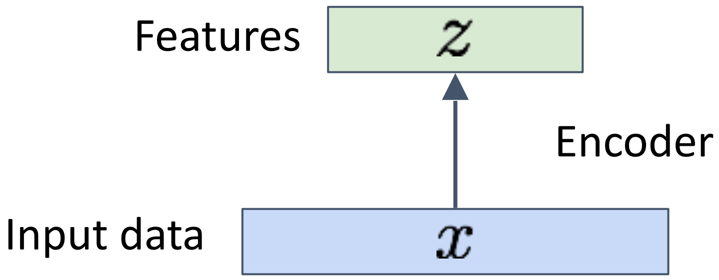
- There is no direct ground truth for the quantity of interest

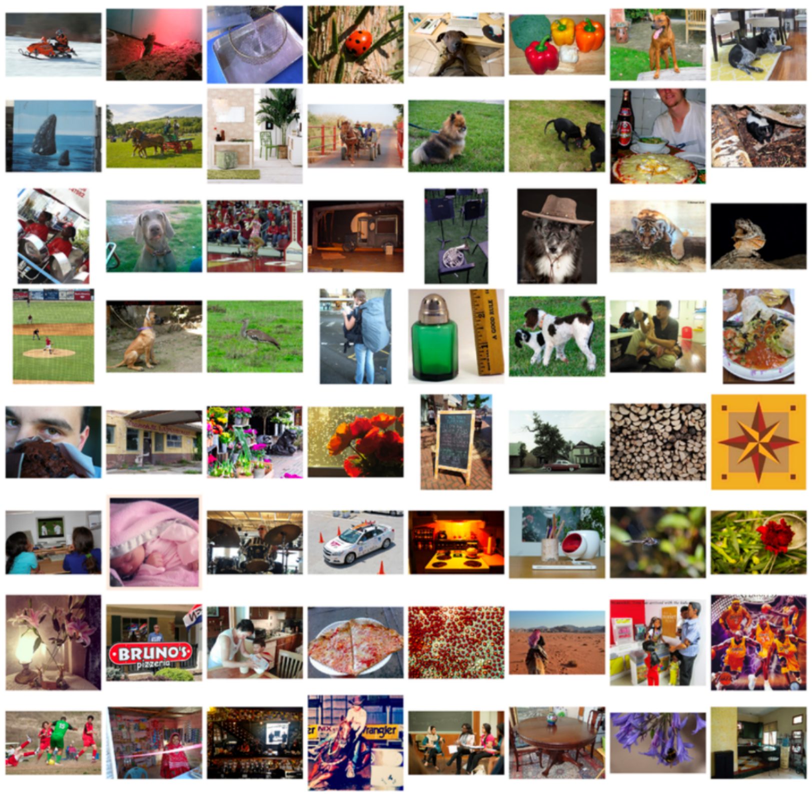
- Autoencoders
- Variational Autoencoders (VAEs)
- Generative Adversarial Networks (GANs)

Autoencoders

Goal: Meaningful features that capture the main factors of variation in the dataset

- These are good for classification, clustering, exploration, generation, …
- We have no ground truth for them



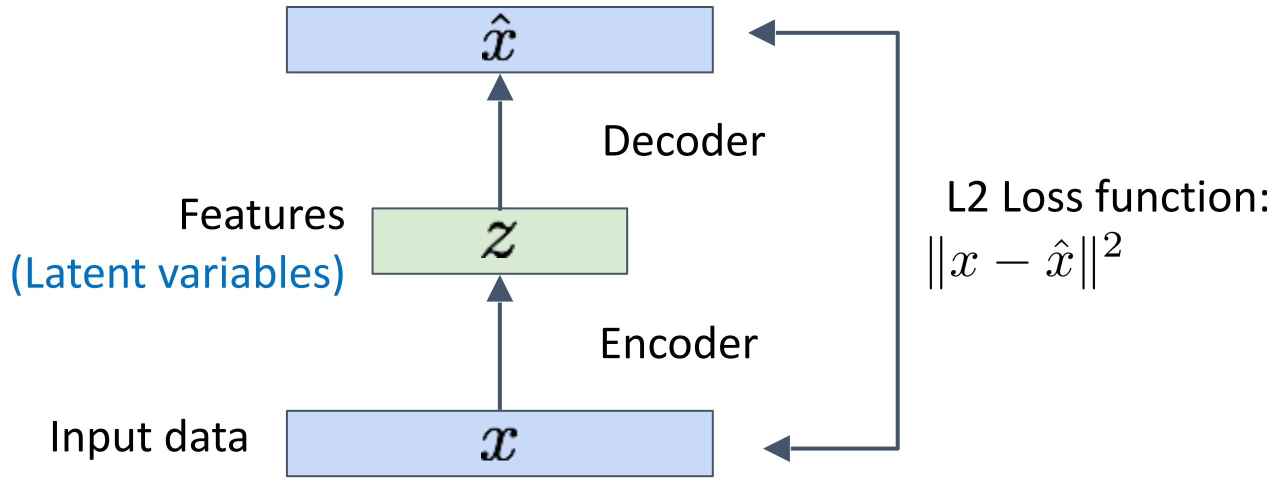


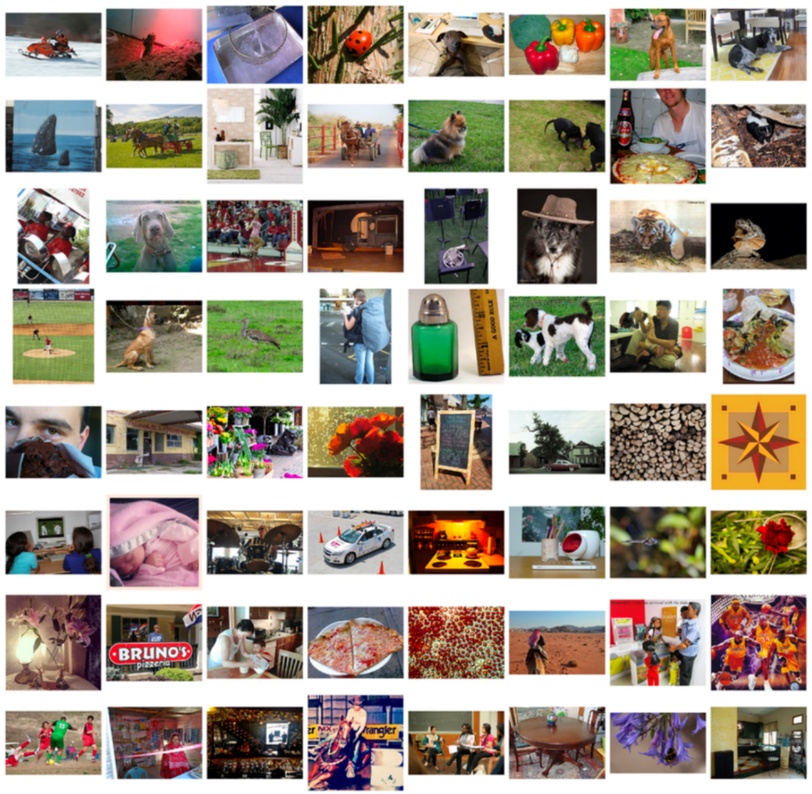
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Autoencoders

Goal: Meaningful features that capture the main factors of variation

Features that can be used to reconstruct the image





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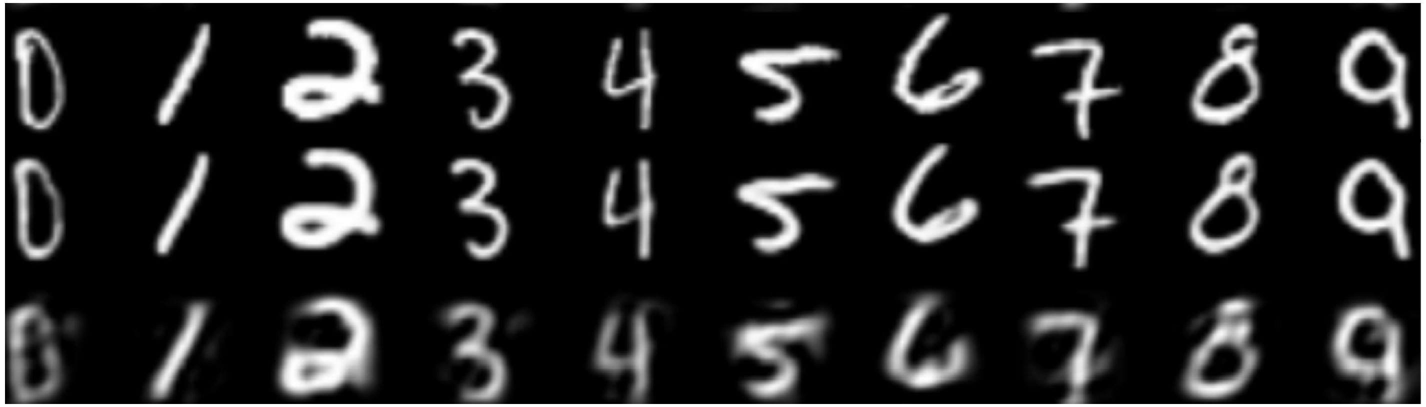
Autoencoders

Linear Transformation for Encoder and Decoder give result close to PCA

Deeper networks give better reconstructions, since basis can be non-linear



Original

Autoencoder

PCA

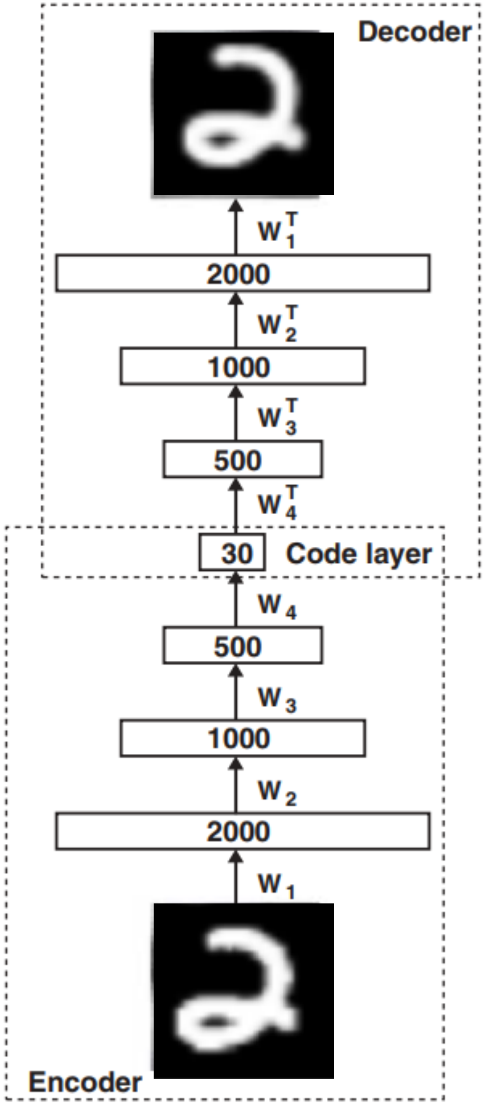


Image Credit: Reducing the Dimensionality of Data with Neural Networks, . Hinton and Salakhutdinov

Example: Document Word Prob. → 2D Code

PCA-based

Autoencoder

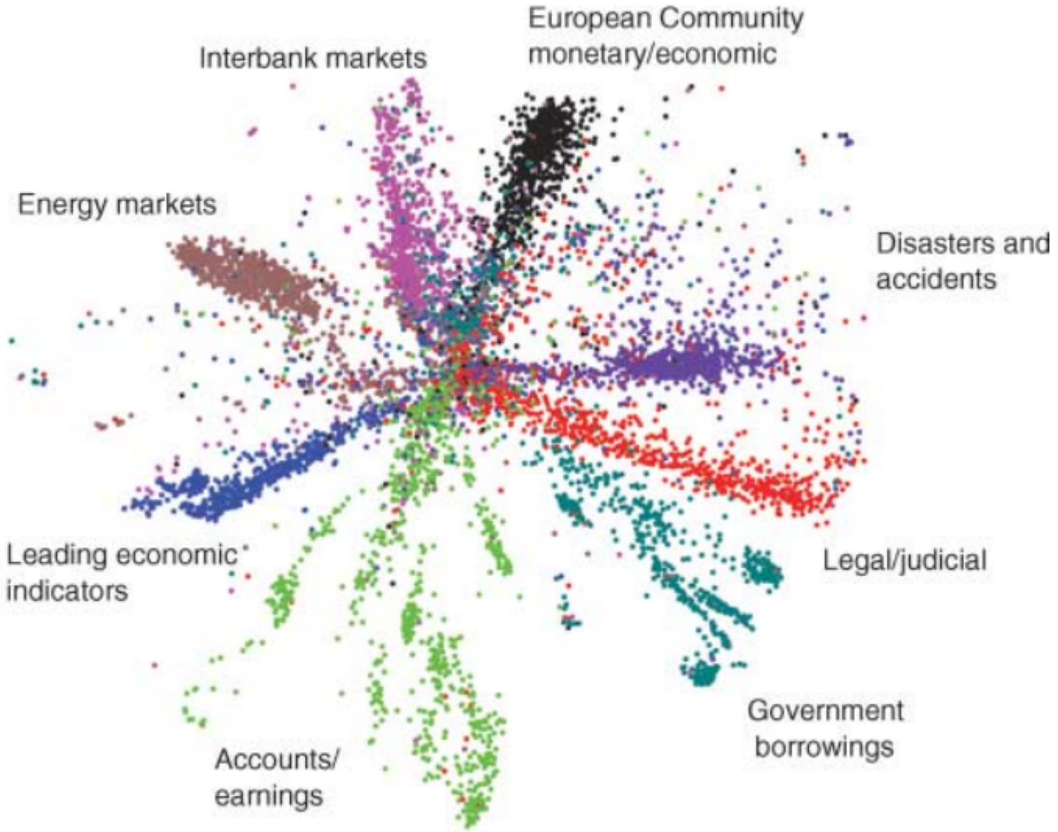
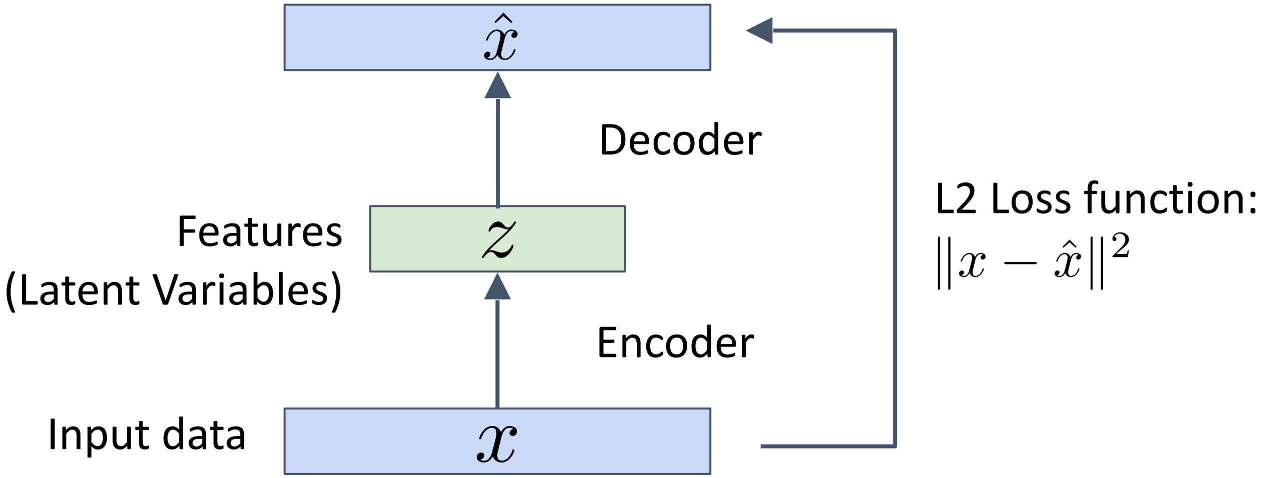


Image Credit: Reducing the Dimensionality of Data with Neural Networks, Hinton and Salakhutdinov

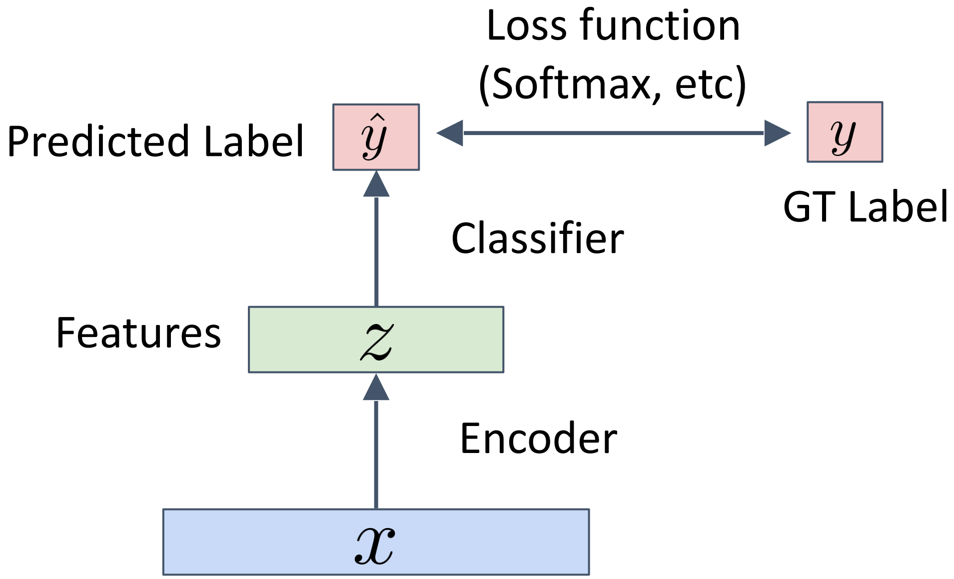
Example: Semi-Supervised Classification

- Many images, but few ground truth labels

start unsupervised
train autoencoder on many images



supervised fine-tuning
train classification network on labeled images



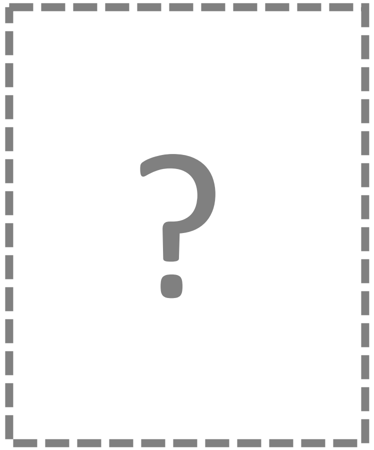
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Autoencoder

Generative Models

- Assumption: the dataset are samples from an unknown distribution
- Goal: create a new sample from $p_{\text{data}}(x)$ that is not in the dataset

Dataset



Generated

Image credit: *Progressive Growing of GANs for Improved Quality, Stability, and Variation*, Karras et al.

Generative Models

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Dataset

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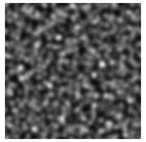
Image credit: *Progressive Growing of GANs for Improved Quality, Stability, and Variation*, Karras et al.

Generative Models

$$\boxed{p_\theta(x)} \approx p_{\text{data}}(x)$$

Generator with
parameters θ



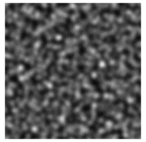
$$\boxed{p(z)}$$

known and
easy to sample from

Generative Models

$$p_\theta(x) \approx p_{\text{data}}(x)$$

Generator with parameters θ



$$p(z)$$

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How to measure similarity of $p_\theta(x)$ and $p_{\text{data}}(x)$?

1) Likelihood of data in $p_\theta(x)$

Variational Autoencoders (VAEs)

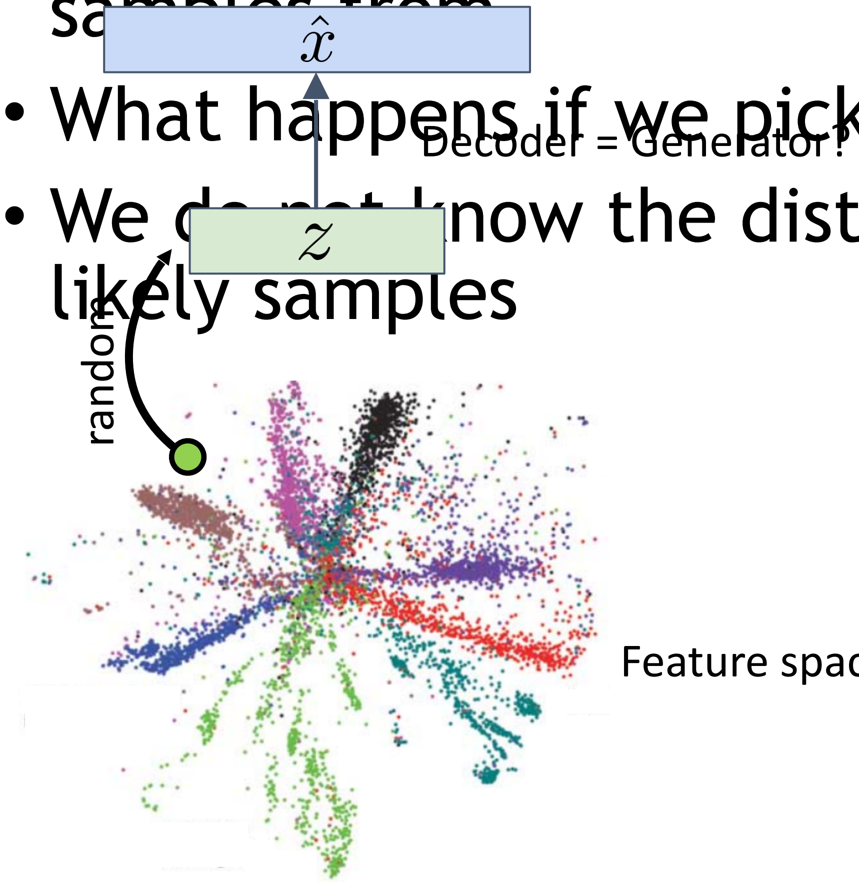
2) Adversarial game:

Discriminator distinguishes $p_\theta(x)$ and $p_{\text{data}}(x)$ vs *Generator* makes it hard to distinguish

Generative Adversarial Networks (GANs)

Autoencoders as Generative Models?

- A trained decoder transforms some features z to approximate samples from $p_{\text{data}}(x)$
- What happens if we pick a random z?
- We do not know the distribution $p(z)$ of features that decode to likely samples



Feature space / latent space

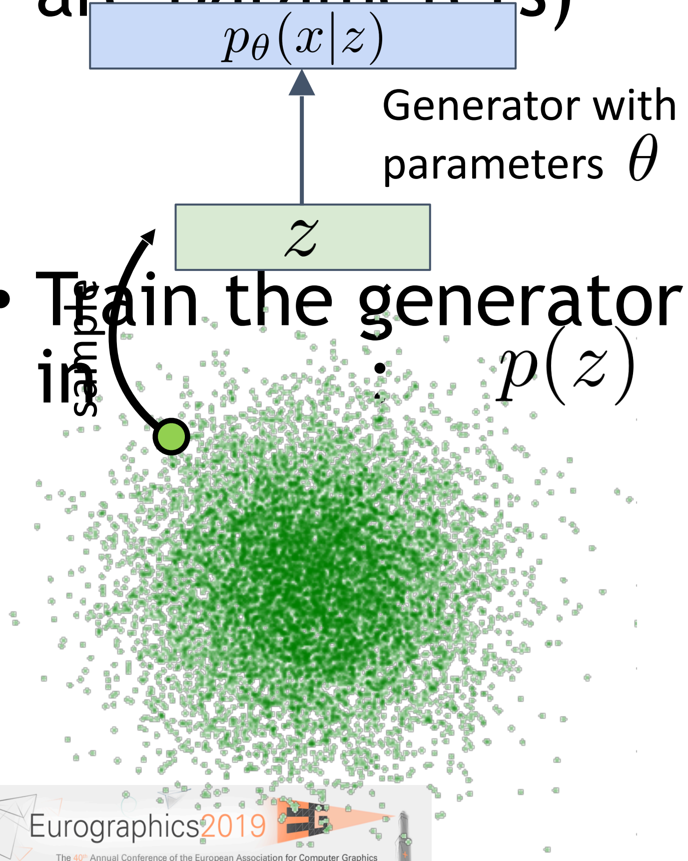
Image Credit: *Reducing the Dimensionality of Data with Neural Networks*, Hinton and Salakhutdinov

Variational Autoencoders (VAEs)

- Pick a parametric distribution for features
- The generator maps to an image distribution $p(z)$ (where are parameters)

$p(z)$

$p_\theta(x)$ θ



$$p_\theta(x) = \int p_\theta(x|z)\; p(z)\; dz$$

- Train the generator to maximize the likelihood of the data in : $p(z)$

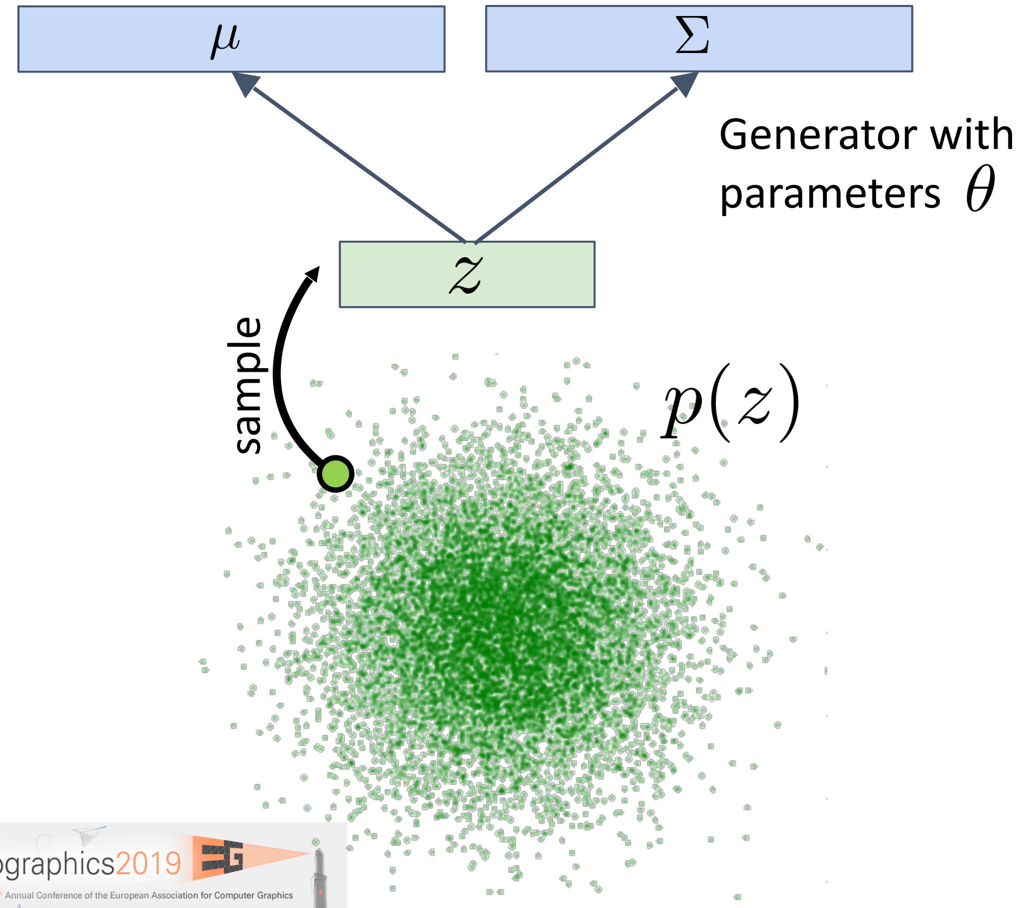
$p_\theta(x)$

$$\max_\theta \sum_{x_i \in \text{data}} \log p_\theta(x_i)$$

Outputting a Distribution

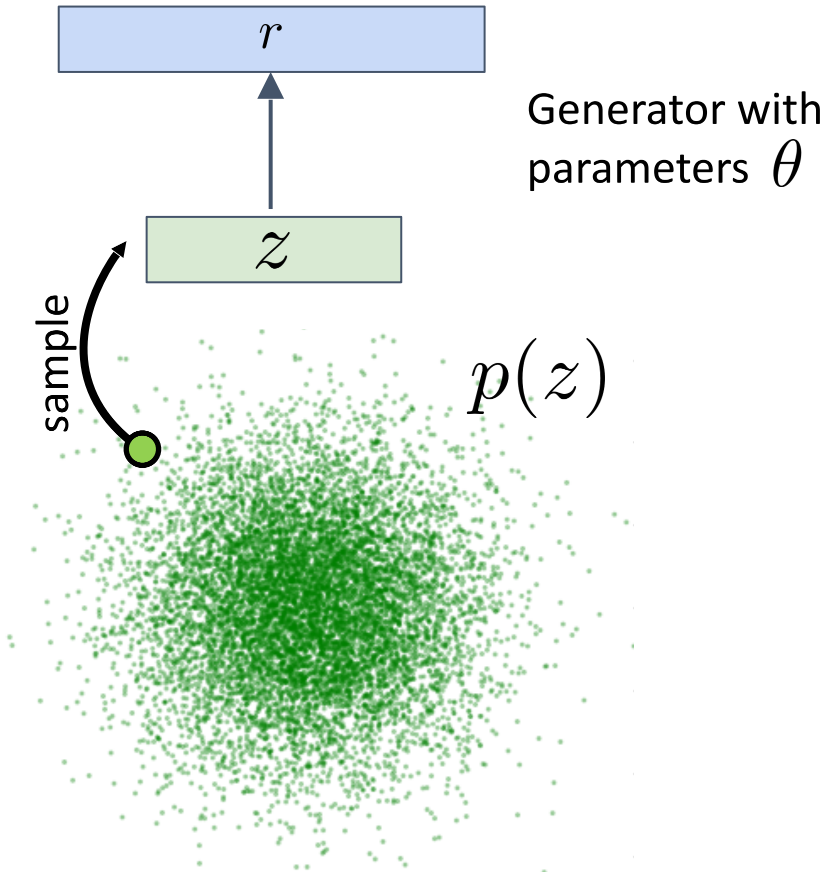
Normal distribution

$$p_\theta(x|z) = N(x; \mu(z), \Sigma(z))$$



Bernoulli distribution

$$p_\theta(x|z) = Bern(x; r(z))$$



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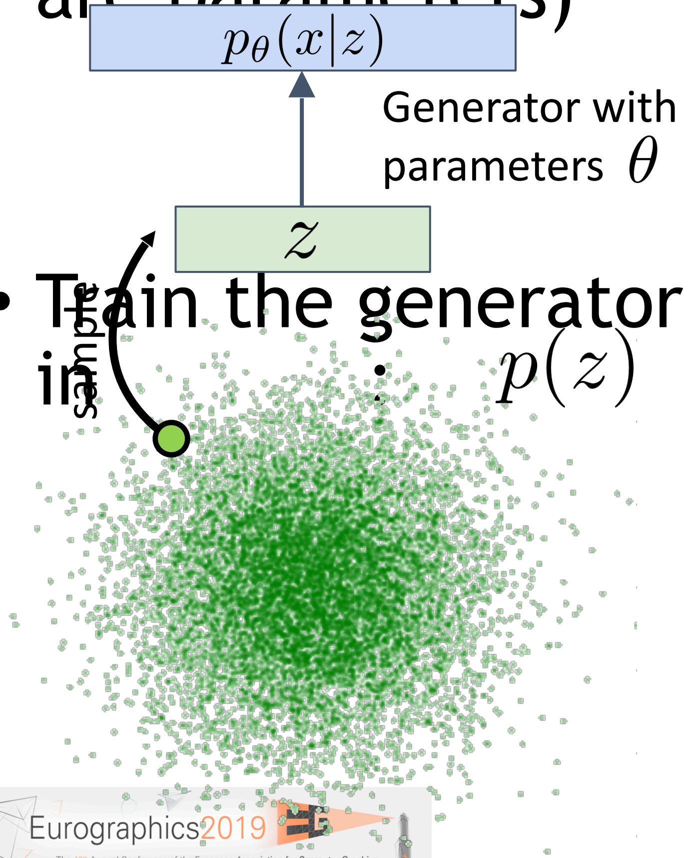


$p(z)$

$p_\theta(x)$ θ

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

- Train the generator to maximize the likelihood of the data in :

$p_\theta(x)$

$$\max_\theta \sum_{x_i \in \mathrm{data}} \log p_\theta(x_i)$$

Variational Autoencoders (VAEs): Naïve Sampling (Monte-Carlo)

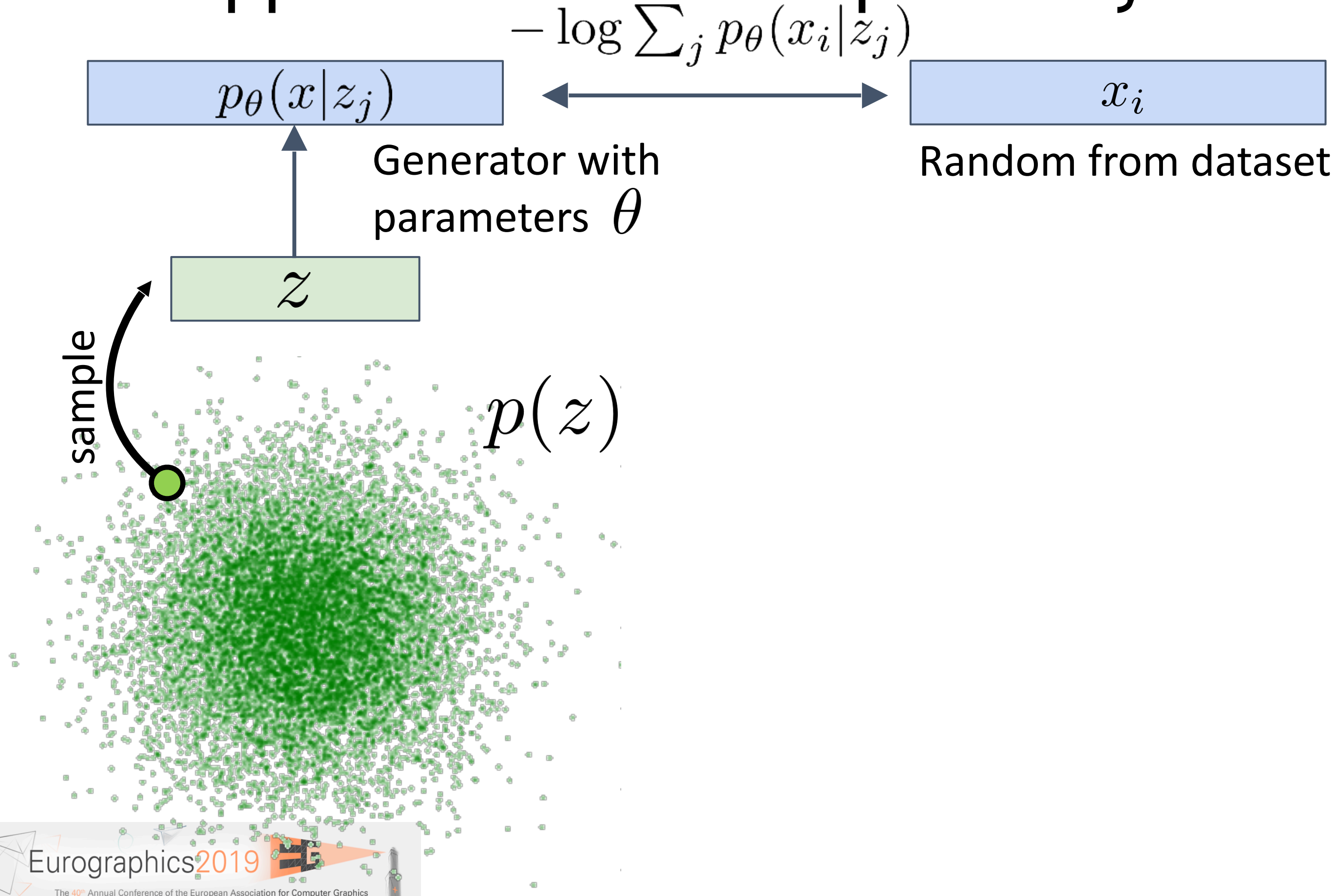
- Approximate Integral with Monte-Carlo in each iteration
- SGD approximates the sum over data
- Maximum likelihood of data in generated distribution:

$$\theta^* = \arg\max_\theta \sum_{x_i \in \text{data}} \log \int p_\theta(x_i|z)\; p(z)\; dz$$

$$\theta^* \approx \arg\max_\theta \mathbb{E}_{x_i \sim p_{\text{data}}(x)} \log \mathbb{E}_{z \sim p(z)}\; p_\theta(x_i|z)$$

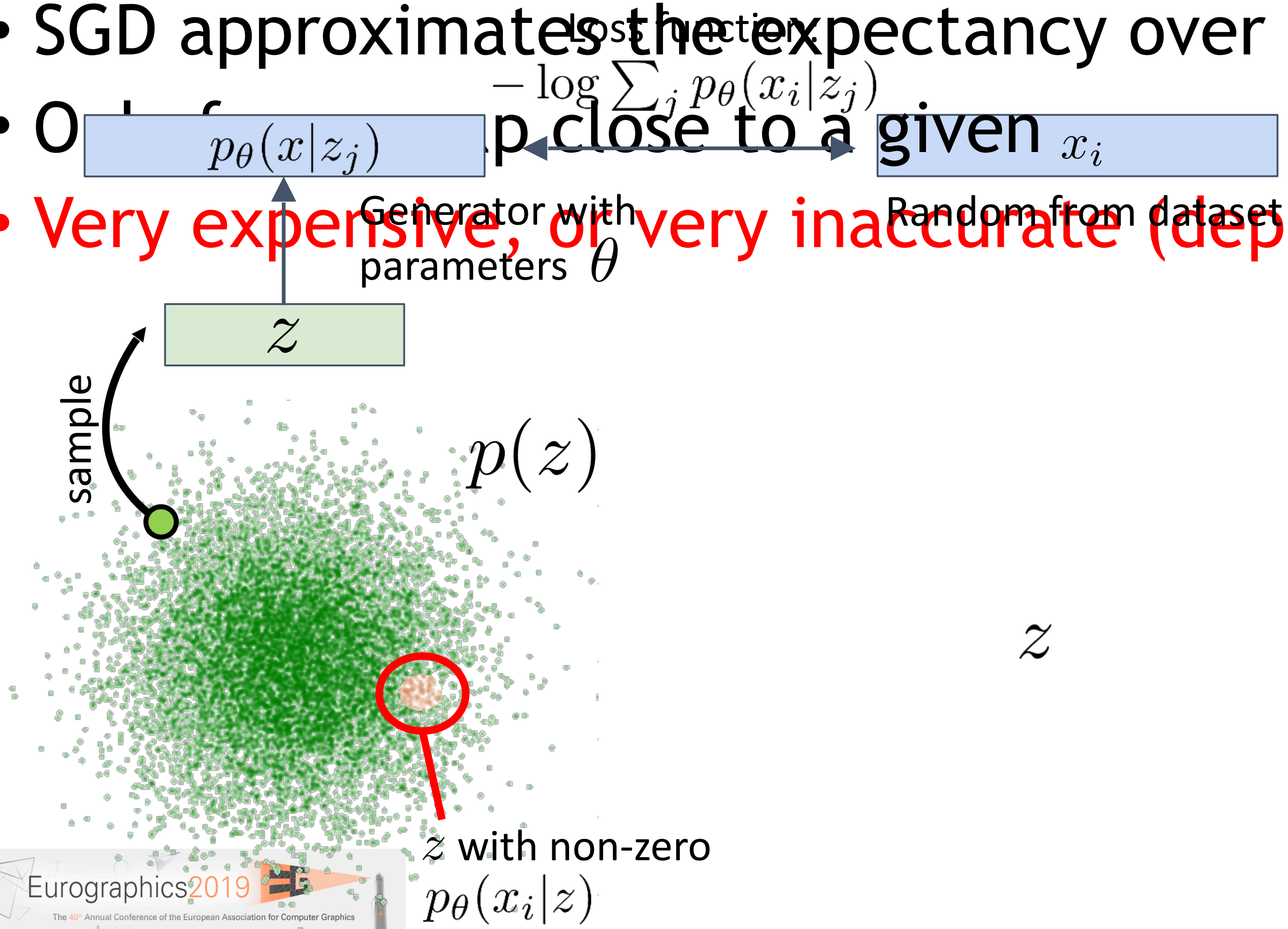
Variational Autoencoders (VAEs):
Naïve Sampling (Monte-Carlo)

- Approximate Integral with Monte-Carlo in each iteration
- SGD approximates the expectancy over data



Variational Autoencoders (VAEs): Naïve Sampling (Monte-Carlo)

- Approximate Integral with Monte-Carlo in each iteration
- SGD approximates the expectancy over data
- O … p close to a given
- Very expensive, or very inaccurate (depending on sample count)



z x_i

Variational Autoencoders (VAEs): The Encoder

- During training, another network can learn a distribution of good z for a given x_i
- $q_\phi(z|x_i)$ should be much smaller than $p(z)$
- A single sample is good enough

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

Loss function:
$-\log p_\theta(x_i|z)$

$p_\theta(x|z)$

Generator with parameters θ

z

sample

$q_\phi(z|x_i)$

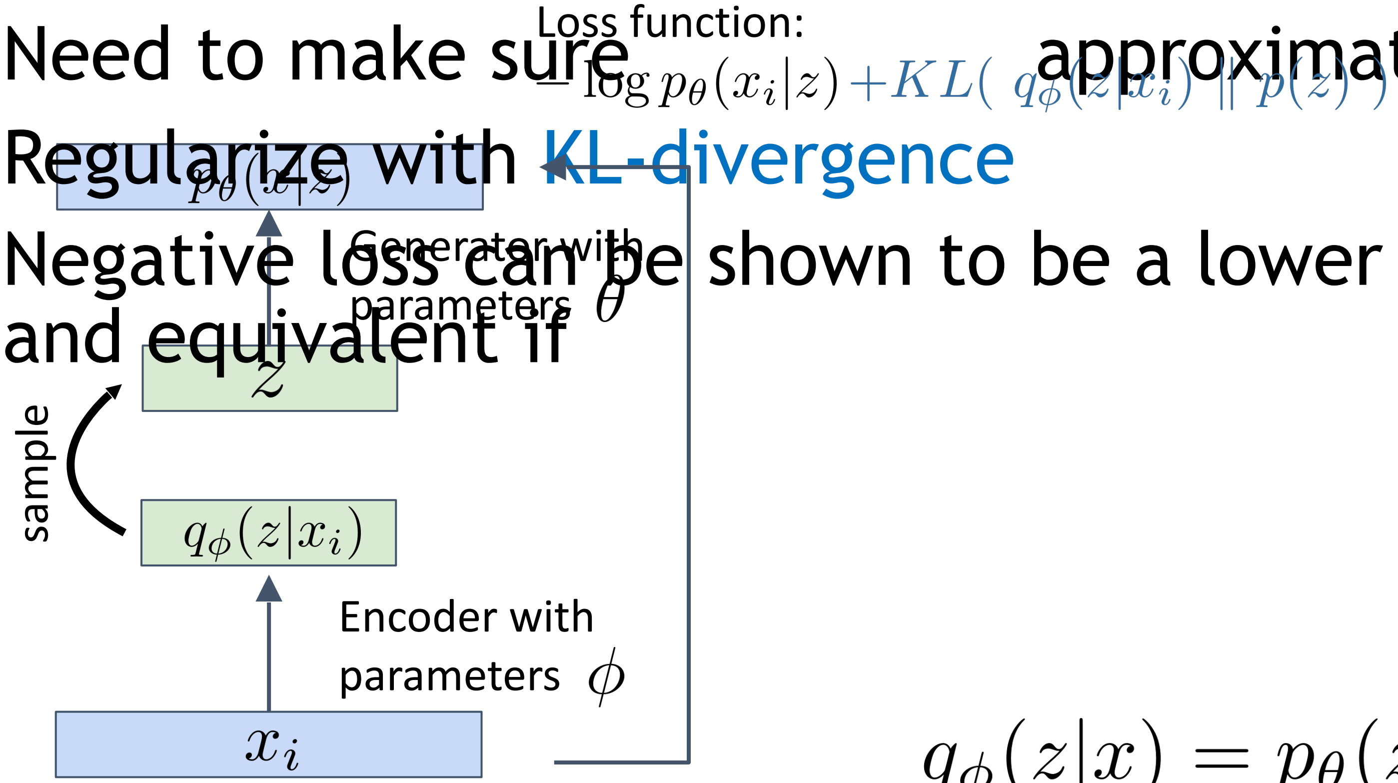
Encoder with parameters ϕ

x_i

Variational Autoencoders (VAEs): The Encoder

- Can we still easily sample a new z ?
- Need to make sure $q_\phi(z|x_i)$ approximates $p(z)$
- Regularize with KL-divergence
- Negative loss can be shown to be a lower bound for the likelihood, and equivalent if

$$q_\phi(z|x) = p_\theta(z|x)$$

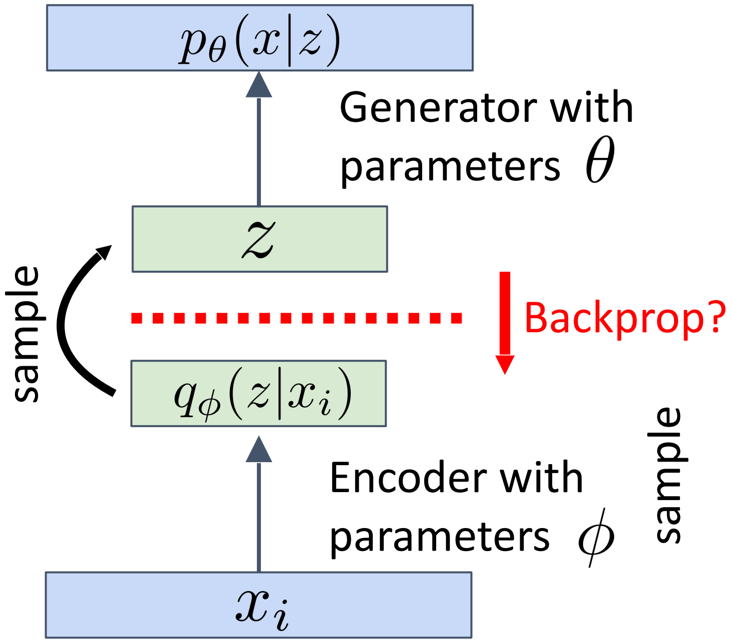


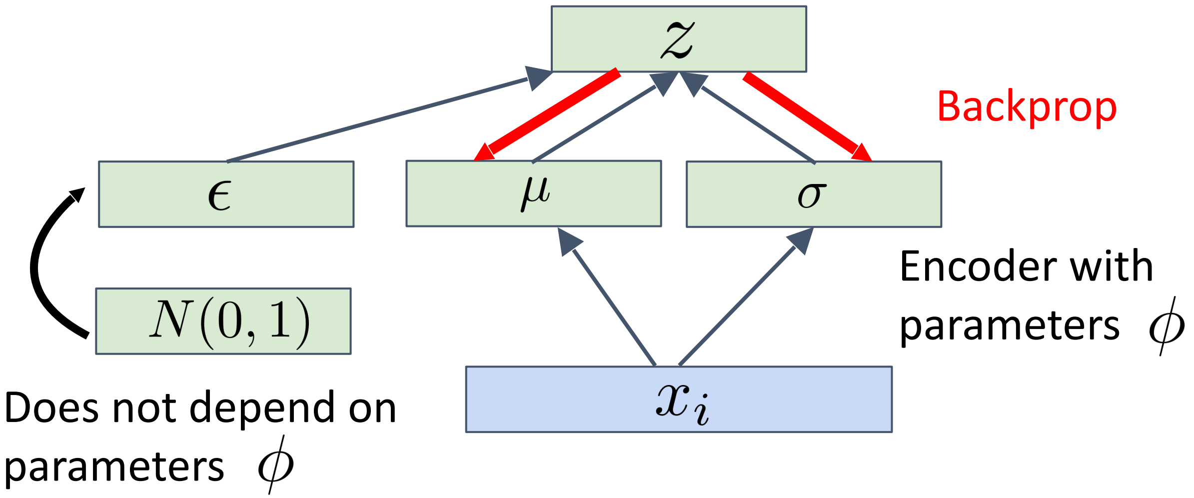
Reparameterization Trick

Example when $q_\phi(z|x_i) = N(z; \mu(x_i), \sigma(x_i))$

$z = \sigma + \mu \cdot \epsilon$, where $\epsilon \sim N(0,1)$

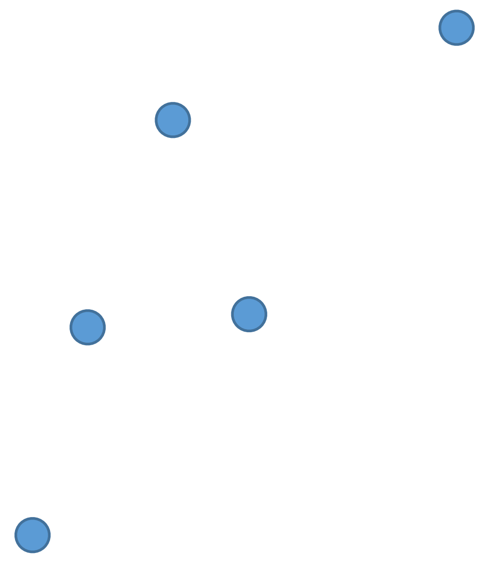
$$\frac{\partial z}{\partial \phi} = \frac{\partial \mu}{\partial \phi} + \frac{\partial \sigma}{\partial \phi} \cdot \epsilon$$



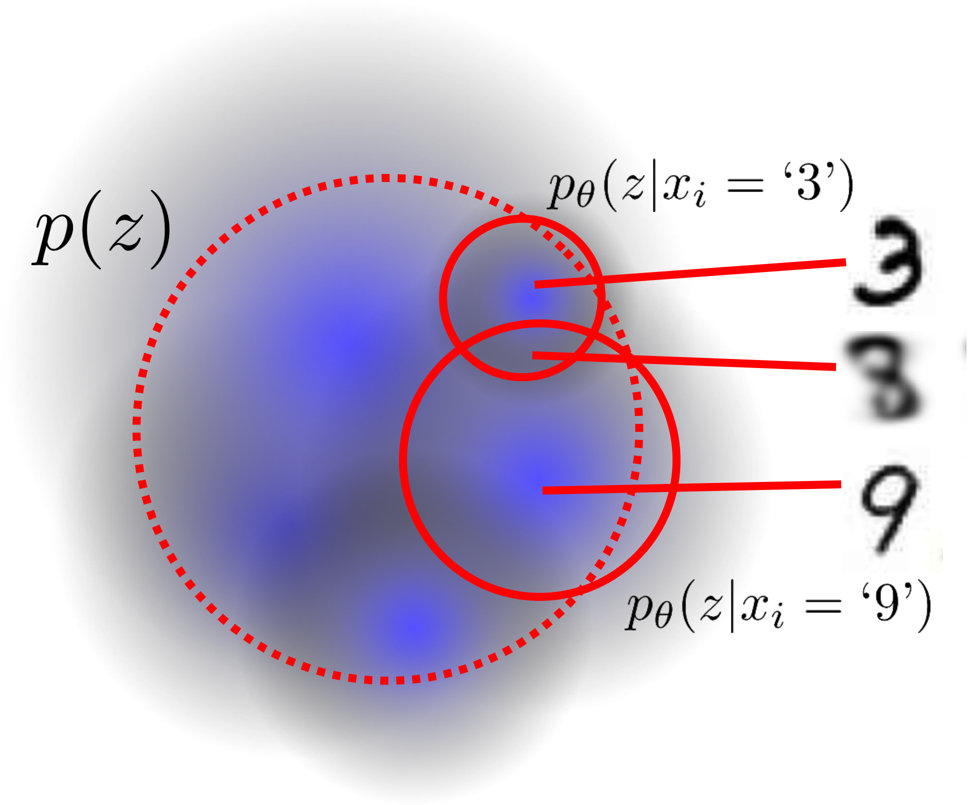


Feature Space of Autoencoders vs. VAEs

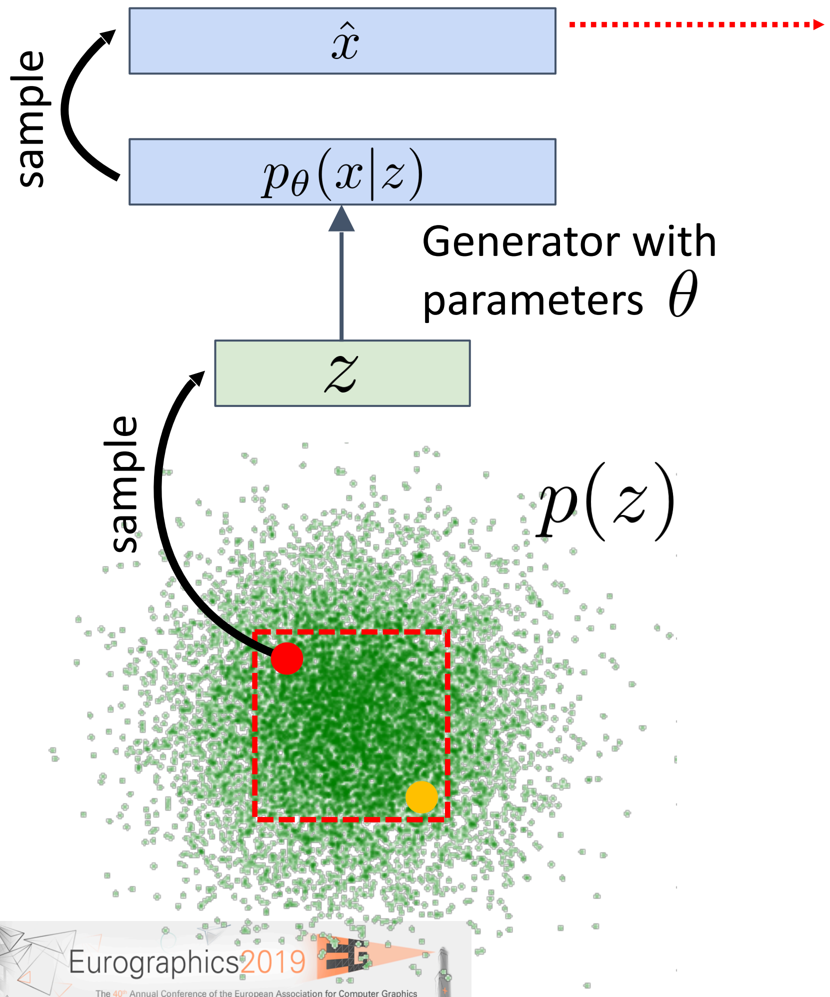
Autoencoder



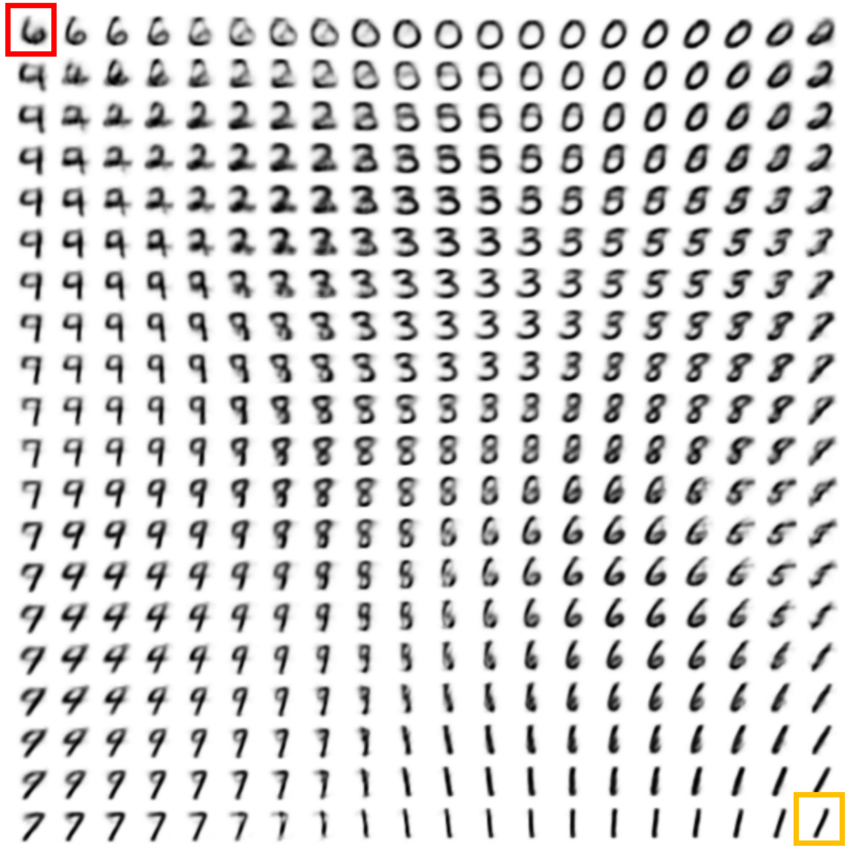
VAE



Generating Data



MNIST



Frey Faces

Image Credit: *Auto-Encoding Variational Bayes*, Kingma and Welling

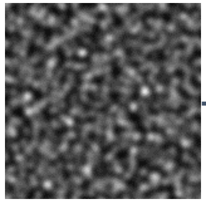
VAE on MNIST

https://www.siarez.com/projects/variational-autoencoder

Variational Autoencoder

geometry.cs.ucl.ac.uk/creativeai

Generative Adversarial Networks



from dataset

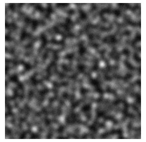
Player 1: generator
Scores if discriminator can't distinguish output from real image

Player 2: discriminator → real/fake
Scores if it can distinguish between real and fake

Generative Models

$p_\theta(x) \approx p_{\text{data}}(x)$

Generator with parameters θ



$p(z)$

known and
easy to sample from

How to measure similarity of $p_\theta(x)$ and $p_{\text{data}}(x)$?

1) Likelihood of data in $p_\theta(x)$

Variational Autoencoders (VAEs)

2) Adversarial game:

Discriminator distinguishes $p_\theta(x)$ and $p_{\text{data}}(x)$

vs

Generator makes it hard to distinguish

Generative Adversarial Networks (GANs)

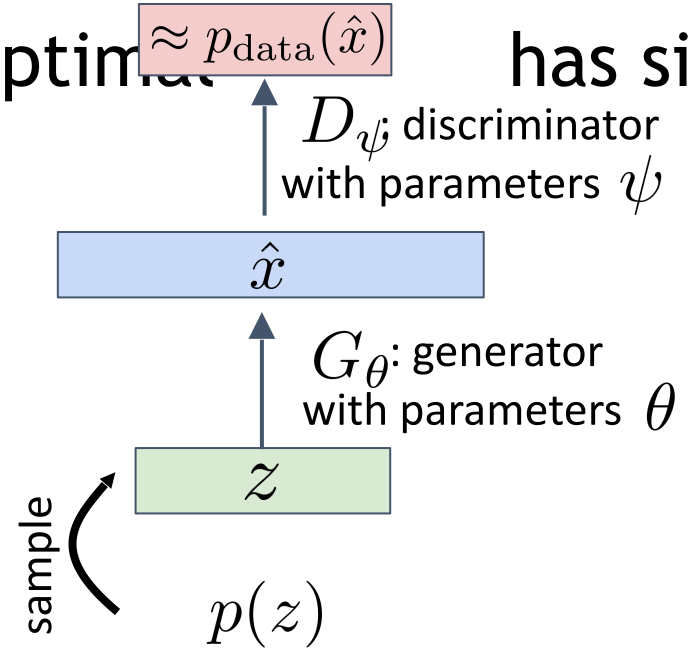
Why Adversarial?

- If discriminator approximates :
- at maximum of has lowest loss
- Optimal has single mode at , small variance

$p_{\mathrm{data}}(x)$

x^* $p_{\mathrm{data}}(x)$

$p_\theta(x)$ x^*



$D_\psi \approx p_{\mathrm{data}}(\hat{x})$

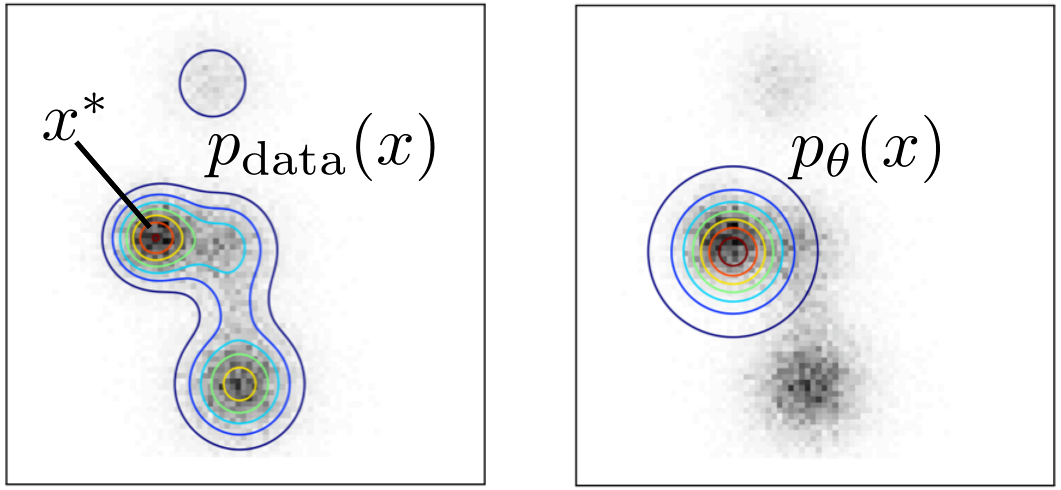
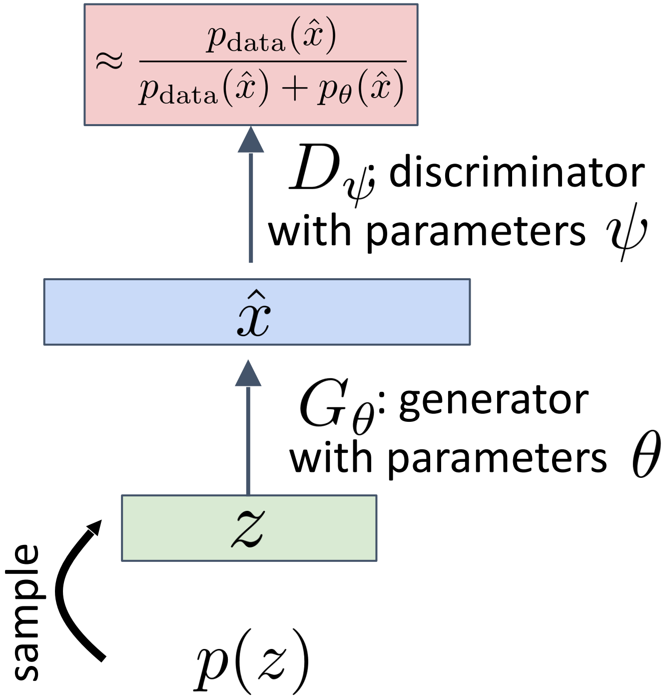


Image Credit: *How (not) to Train your Generative Model: Scheduled Sampling, Likelihood, Adversary?*, Ferenc Huszár

Why Adversarial?

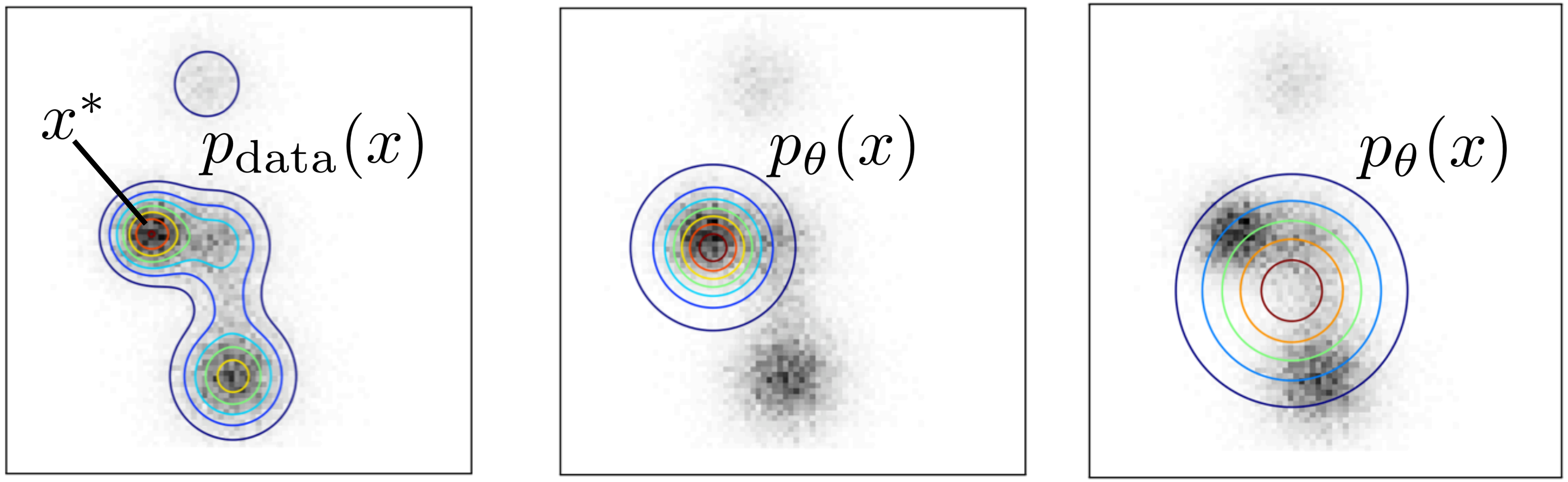
- For GANs, the discriminator instead approximates:



$$\frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_\theta(x)}$$

depends on the generator

$D_\psi \approx p_{\text{data}}(\hat{x})$ $\quad$ $D_\psi \approx \frac{p_{\text{data}}(x)}{p_{\text{data}}(x)+p_\theta(x)}$



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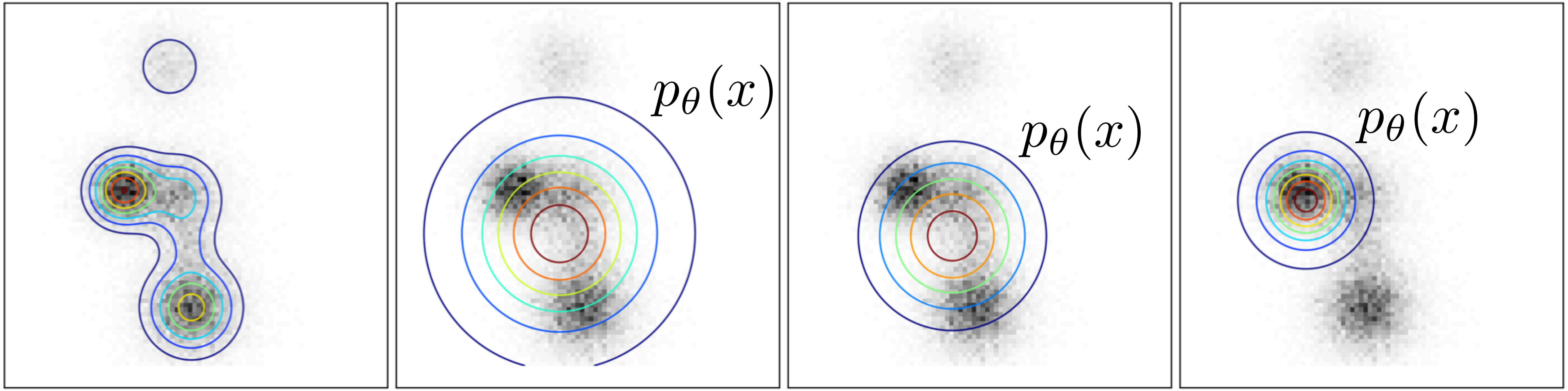
Why Adversarial?



$p_{\text{data}}(x)$

VAEs:
Maximize likelihood of **data samples** in $p_\theta(x)$

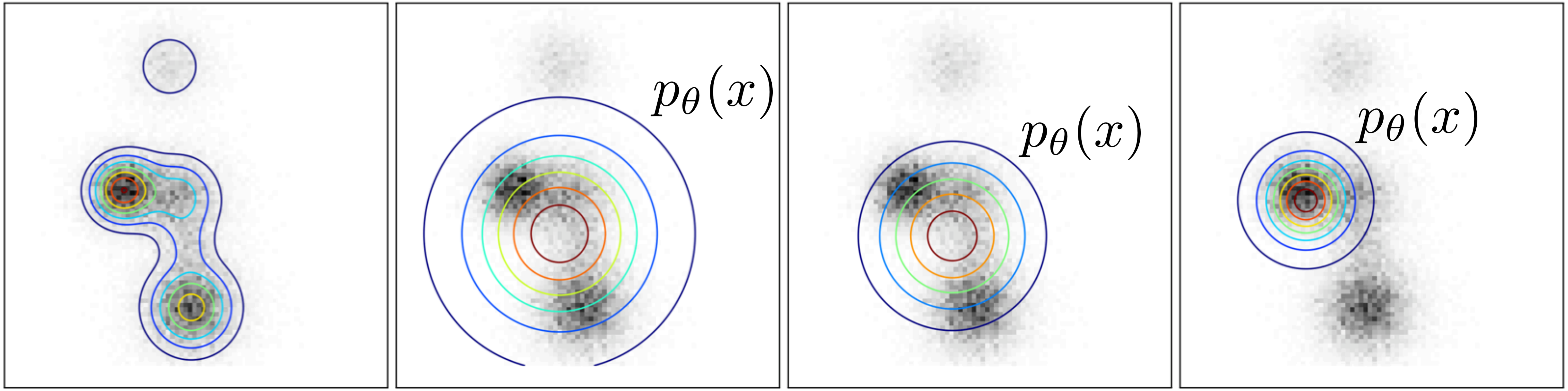
GANs:
Adversarial game

Maximize likelihood of **generator samples** in approximate $p_{\text{data}}(x)$

Image Credit: *How (not) to Train your Generative Model: Scheduled Sampling, Likelihood, Adversary?*, Ferenc Huszár

Why Adversarial?

$\approx KL(p_{\text{data}} \parallel p_\theta)$ $\approx JS(p_{\text{data}} \parallel p_\theta)$ $\approx KL(p_\theta \parallel p_{\text{data}})$



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Adversarial game

Maximize likelihood of **generator samples** in approximate $p_{\text{data}}(x)$

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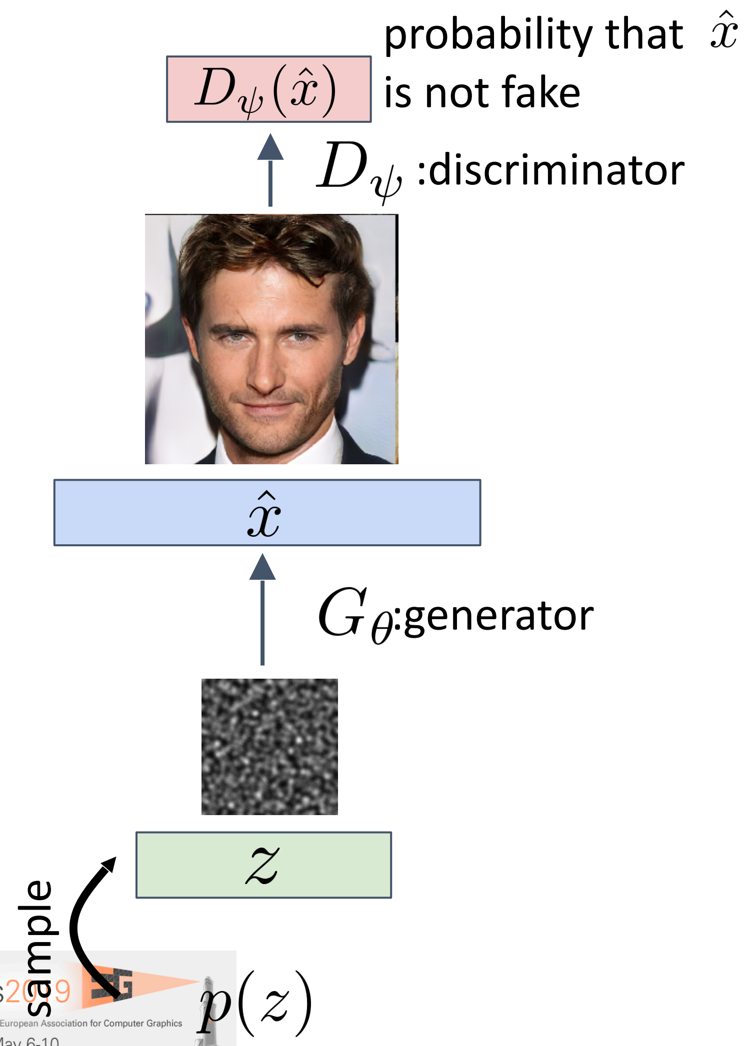
GAN Objective



fake/real classification loss (BCE):

$$L(\theta, \psi) = -0.5\, \mathbb{E}_{x \sim p_{\mathrm{data}}} \log D_\psi(x) - 0.5\, \mathbb{E}_{x \sim p_\theta} \log(1 - D_\psi(x))$$

Discriminator objective:

$$\min_\psi L(\theta, \psi)$$

Generator objective:

$$\max_\theta L(\theta, \psi)$$

Non-saturating Heuristic

$$L(\theta, \psi) = -0.5\ \mathbb{E}_{x \sim p_{\text{data}}} \log D_\psi(x) \\ -0.5\ \mathbb{E}_{x \sim p_\theta} \log(1 - D_\psi(x))$$

Generator loss is negative binary cross-entropy:

$$L_G(\theta, \psi) = 0.5\ \mathbb{E}_{x \sim p_\theta} \log(1 - D_\psi(x))$$ poor convergence

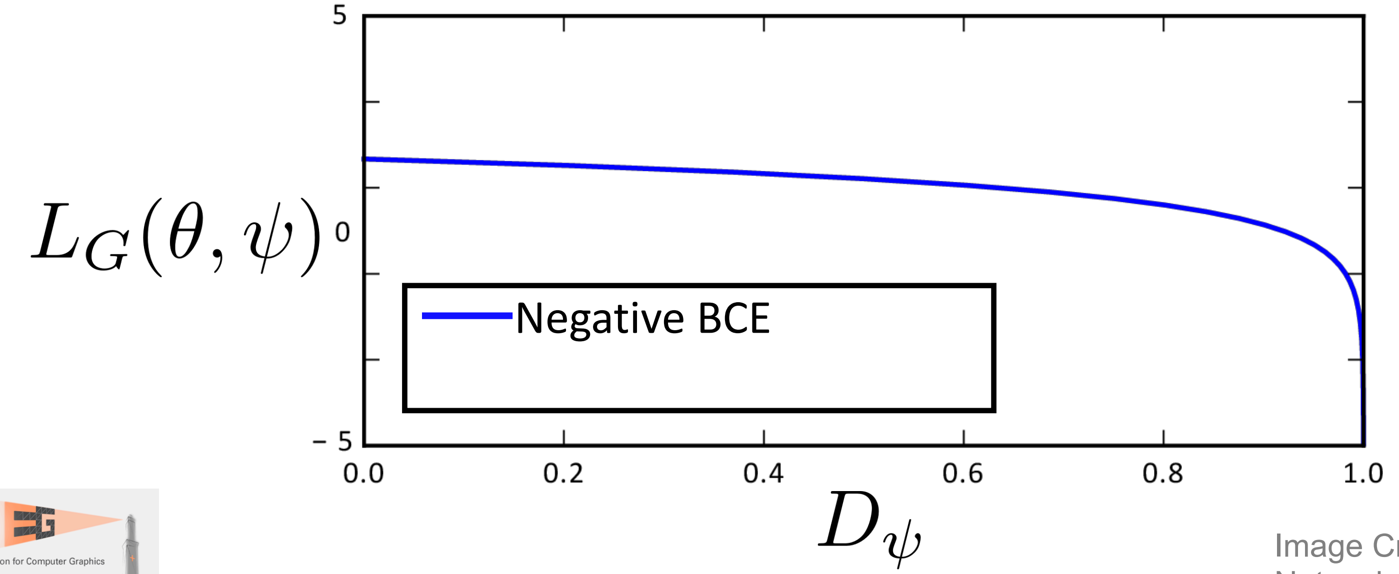


Image Credit: NIPS 2016 Tutorial: Generative Adversarial Networks, Ian Goodfellow

Non-saturating Heuristic

Generator loss is negative binary cross-entropy:

$$L_G(\theta, \psi) = 0.5\ \mathbb{E}_{x \sim p_\theta}\ \log(1 - D_\psi(x))$$ poor convergence

Flip target class instead of flipping the sign for generator loss:

$$L_G(\theta, \psi) = -0.5\ \mathbb{E}_{x \sim p_\theta}\ \log D_\psi(x)$$ good convergence – like BCE

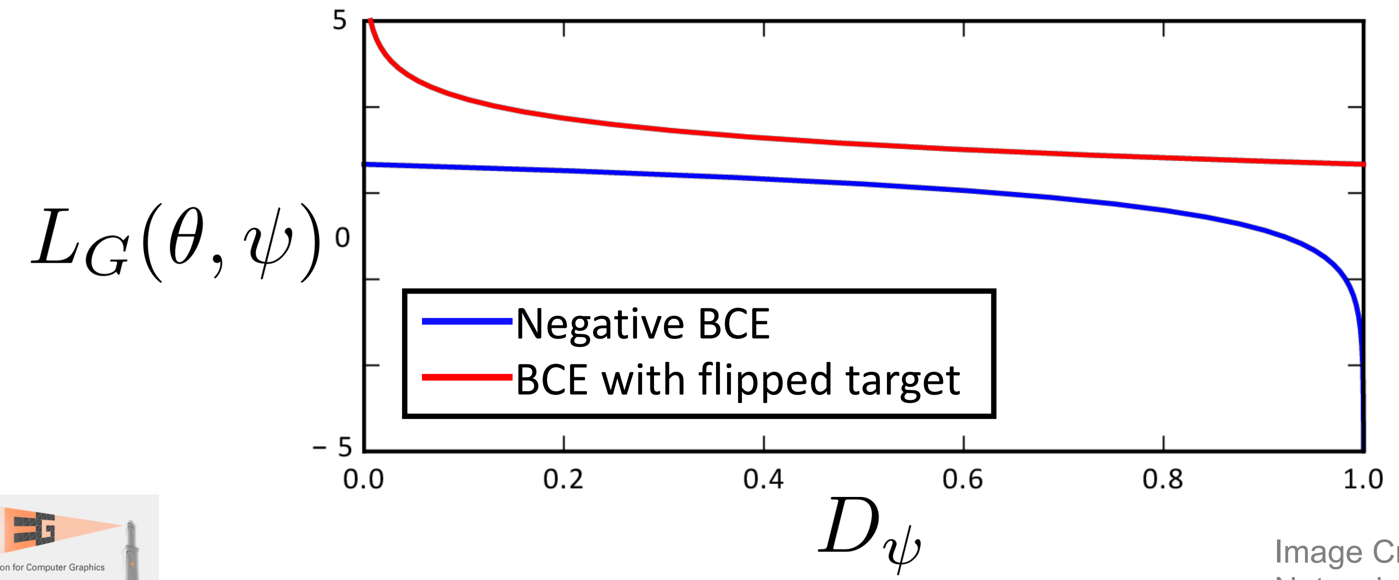


Image Credit: NIPS 2016 Tutorial: Generative Adversarial Networks, Ian Goodfellow

GAN Training

Generator training

Loss:

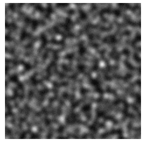
$$L_G(\theta, \psi) = -\log D_\psi(\hat{x})$$

$D_\psi(\hat{x})$

D_ψ :discriminator

$\hat{x}$

G_θ:generator



z

sample

$p(z)$

Discriminator training

Loss:

$$L_D(\theta, \psi) = -0.5 \log(1 - D_\psi(\hat{x})) - 0.5 \log D_\psi(x_i)$$

$D_\psi(\hat{x})$ $D_\psi(x_i)$

D_ψ :discriminator

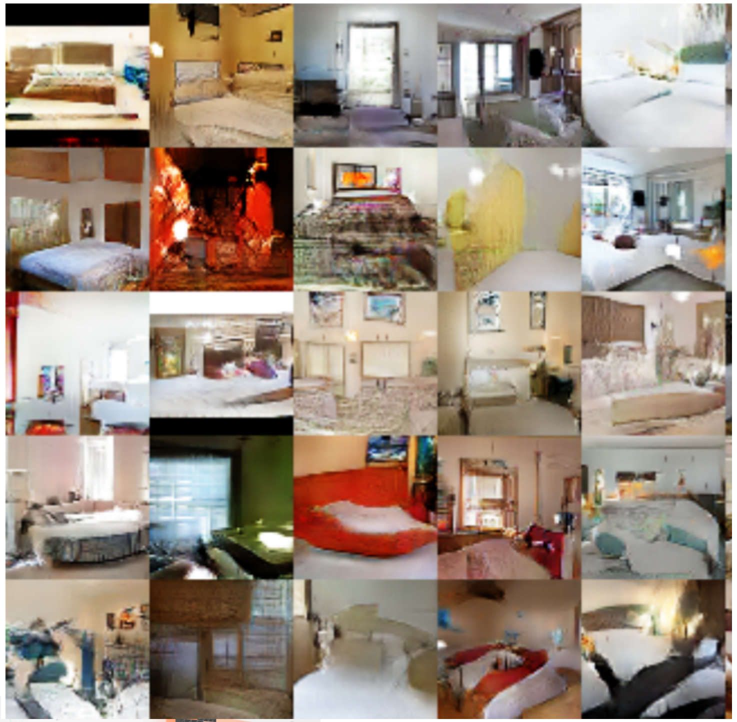
$\hat{x}$ x_i

from dataset

Interleave in each training step

DCGAN

- First paper to successfully use CNNs with GANs
- Due to using novel components (at that time) like batch norm., ReLUs, etc.



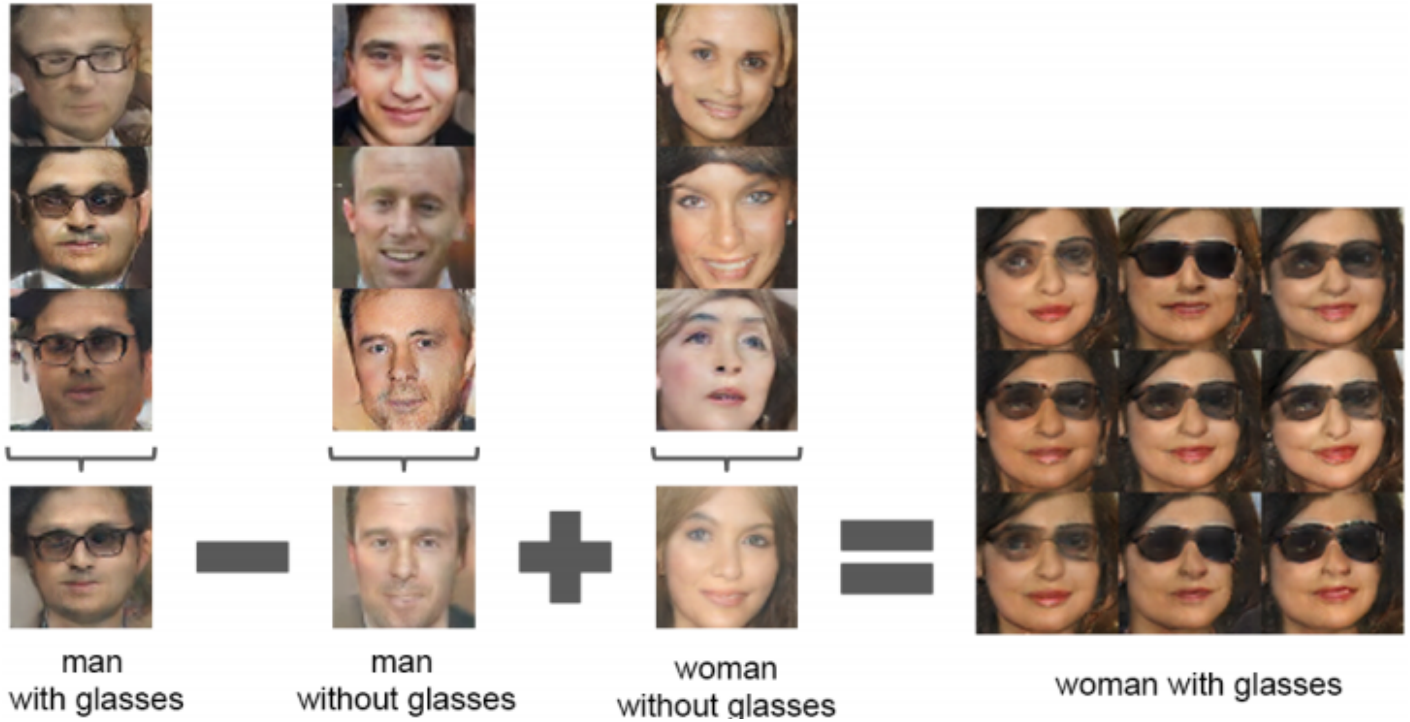


Image Credit: *Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks*, Radford et al.

Generative Adversarial Network

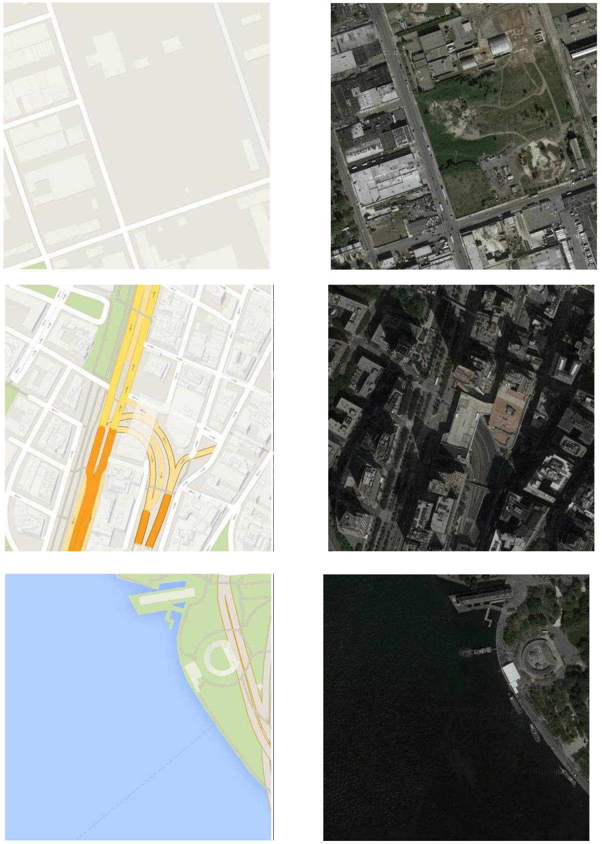
geometry.cs.ucl.ac.uk/creativeai

Conditional GANs (CGANs)

- ≈ learn a mapping between images from example pairs
- Approximate sampling from a conditional distribution $p_{\text{data}}(x \mid c)$

c x

c x



c x

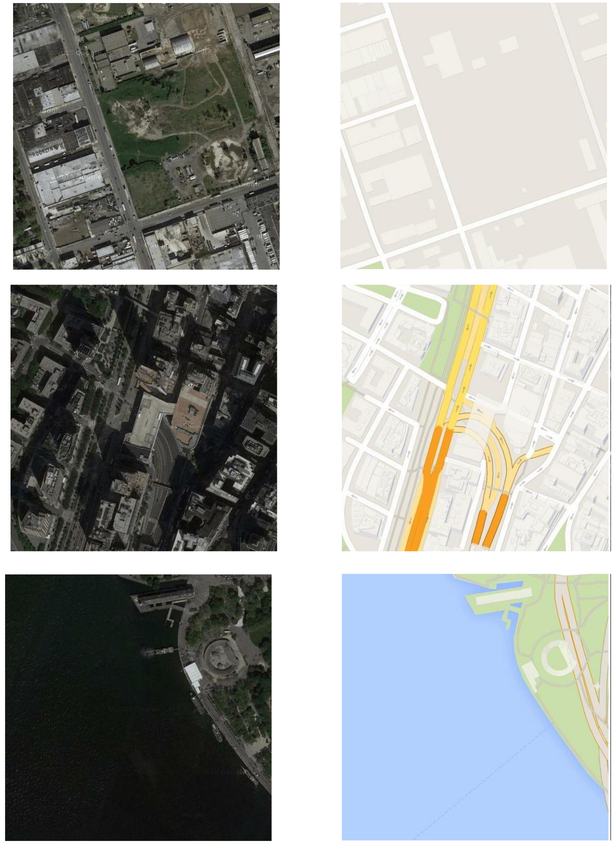


Image Credit: *Image-to-Image Translation with Conditional Adversarial Nets*, Isola et al.

Conditional GANs

Loss:
$$L_G(\theta, \psi) = -\log D_\psi(\hat{x}, c)$$

Loss:
$$L_D(\theta, \psi) = -0.5 \log(1 - D_\psi(\hat{x}, c)) - 0.5 \log D_\psi(x_i, c)$$

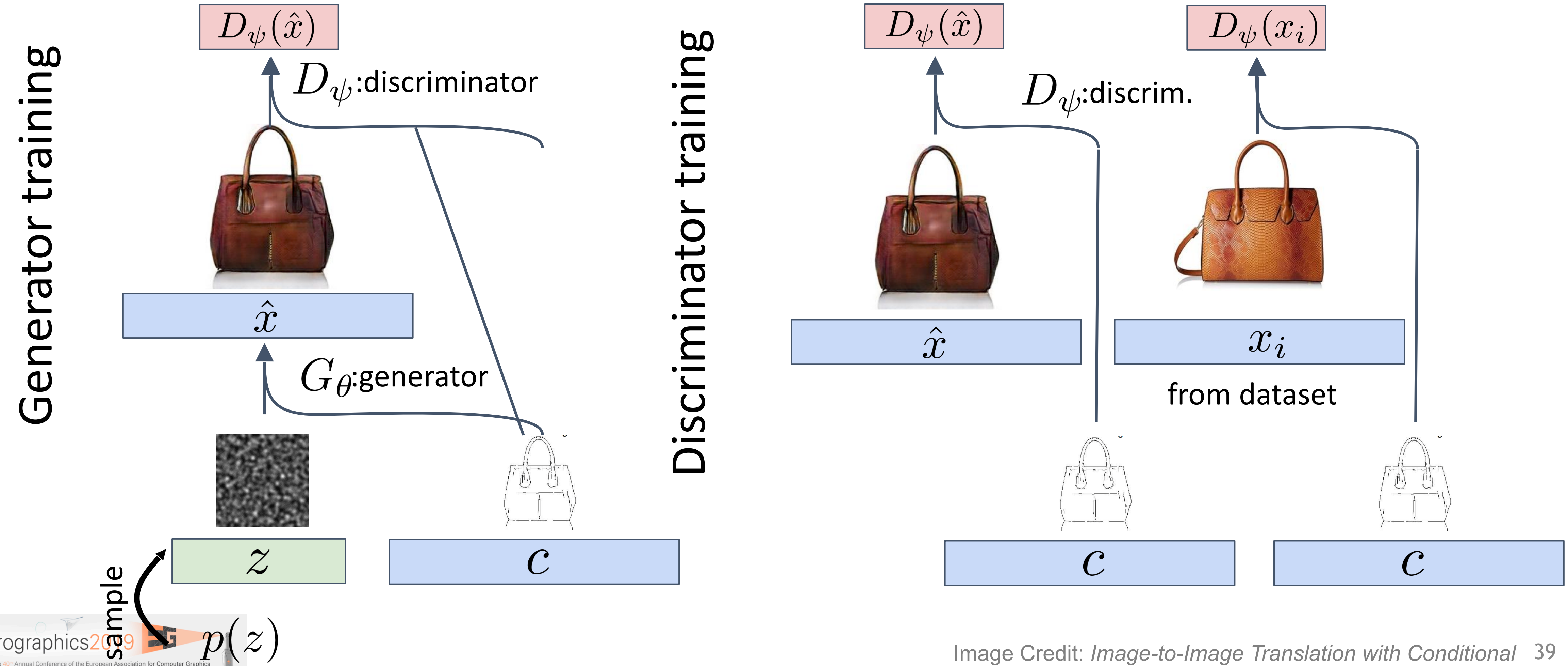


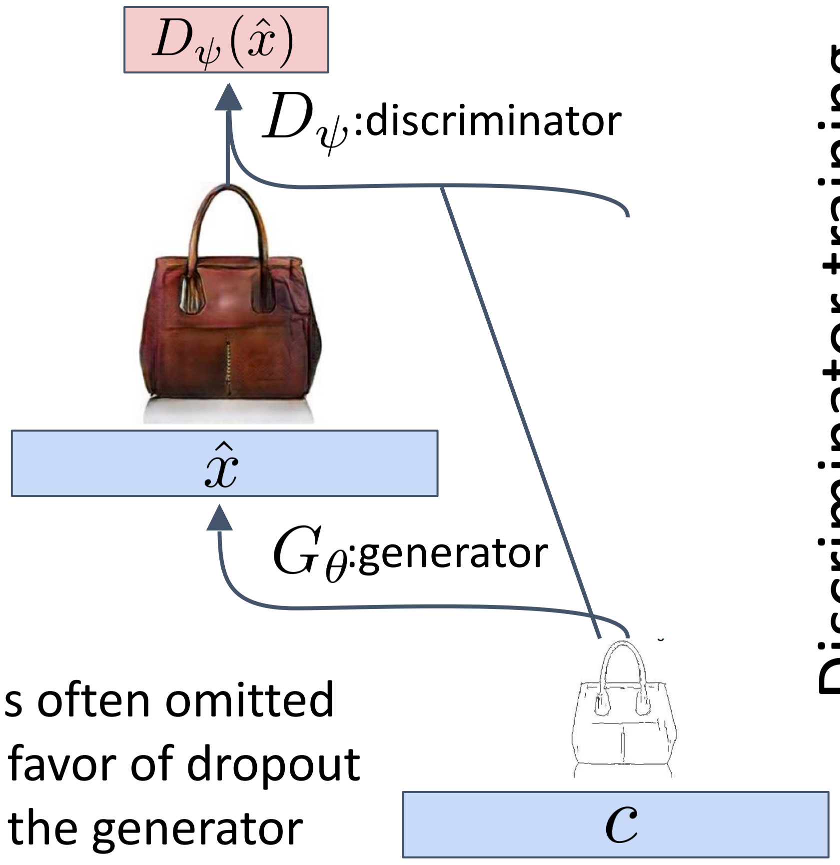
Image Credit: *Image-to-Image Translation with Conditional Adversarial Nets*, Isola et al.

Conditional GANs: Low Variation per Condition

Generator training

Loss:

$$L_G(\theta, \psi) = -\log D_\psi(\hat{x}, c)$$

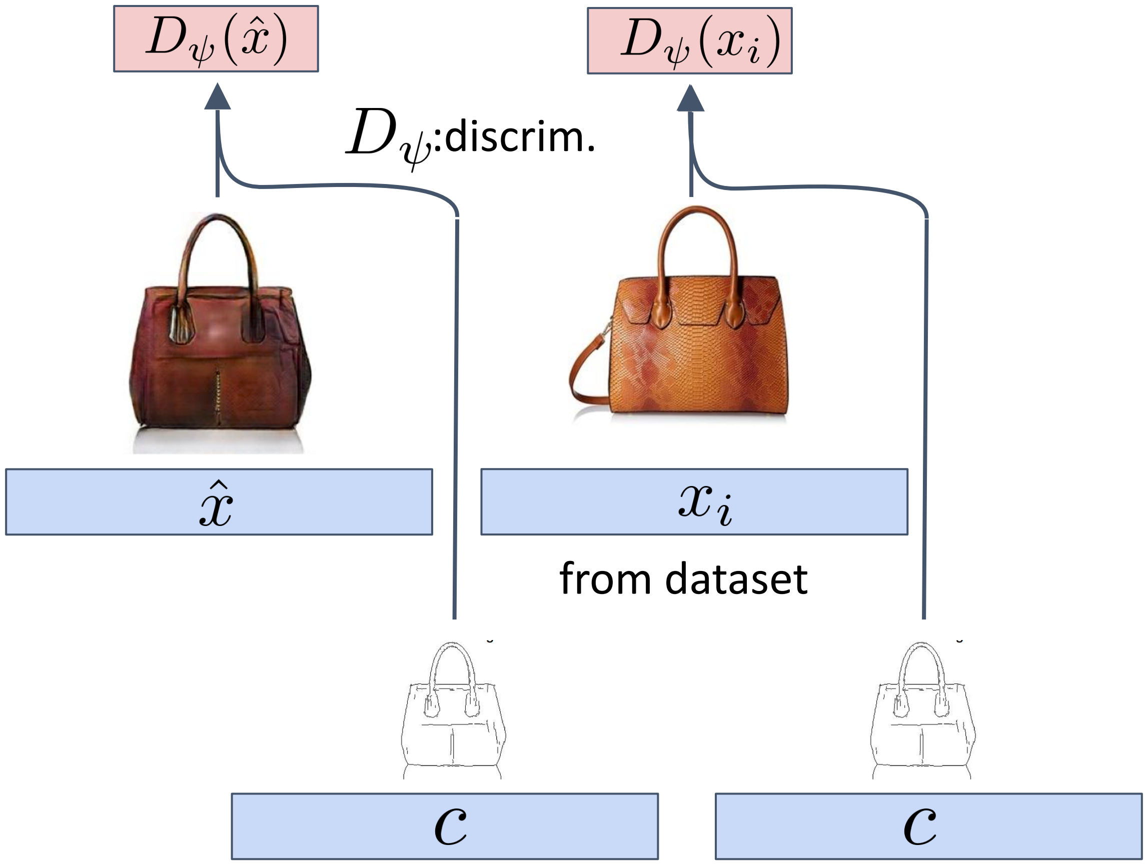


z is often omitted
in favor of dropout
in the generator

Discriminator training

Loss:

$$L_D(\theta, \psi) = -0.5\log(1 - D_\psi(\hat{x}, c)) - 0.5\log D_\psi(x_i, c)$$



CGAN

https://affinelayer.com/pixsrv/index.html

Unstable Training

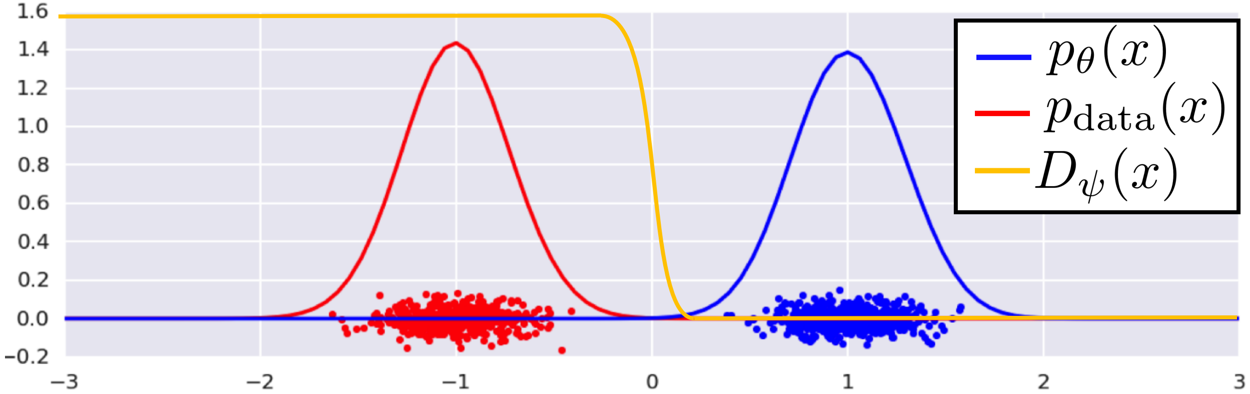
GAN training can be unstable

Three current research problems (may be related):

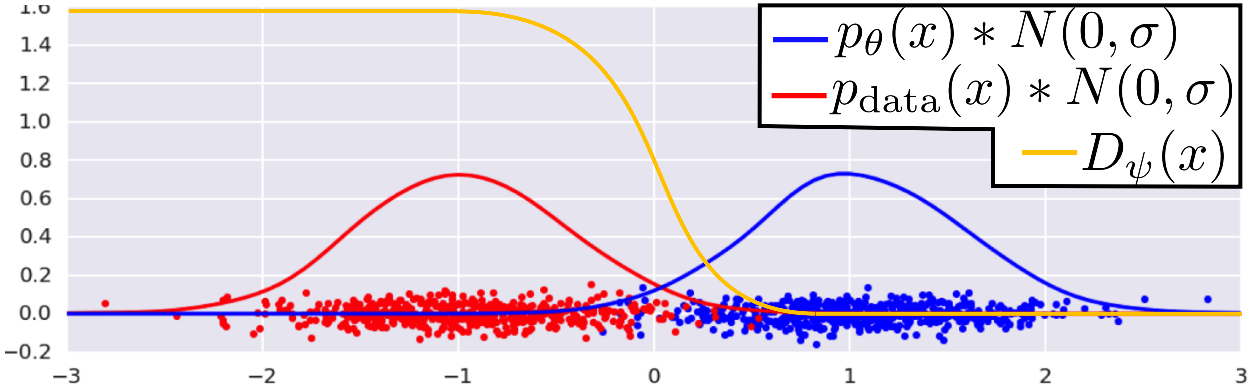
- Reaching a Nash equilibrium (the gradient for both L_G and L_D is 0)
- p_θ and p_{data} initially don't overlap
- Mode Collapse

Generator and Data Distribution Don't Overlap

Standard



Instance noise: adding noise to generated and real images



Roth et al. suggest an analytic convolution with a gaussian:

Stabilizing Training of Generative Adversarial Networks through Regularization, Roth et al. 2017

Wasserstein GANs: EMD as distance between p_θ and p_{data}

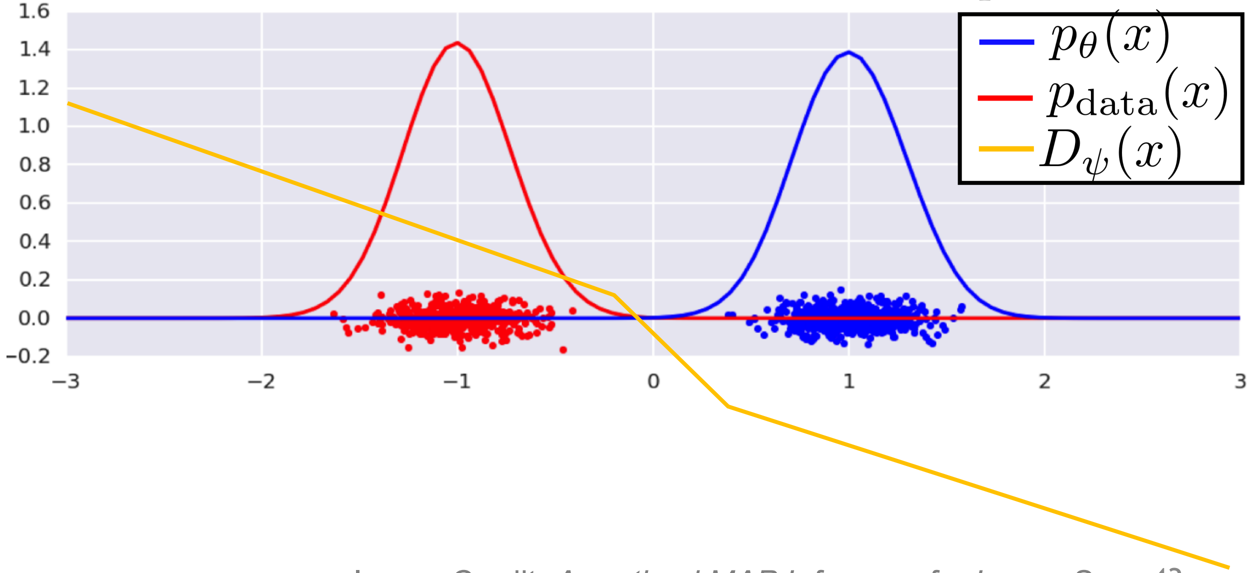
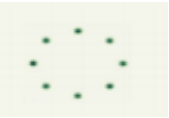


Image Credit: *Amortised MAP Inference for Image Super-resolution*, Sønderby et al.

Mode Collapse

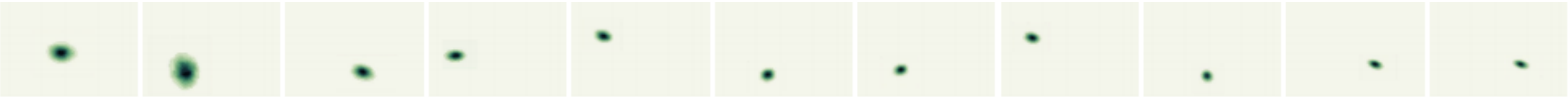
Optimal $D_\psi(x)$: $\dfrac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_\theta(x)}$

p_θ only covers one or a few modes of p_{data}



p_{data}

0 5000 10000 15000 20000 25000 30000 35000 40000 45000 50000



p_θ after n training steps

Image Credit: *Wasserstein GAN*, Arjovsky et al.
Unrolled Generative Adversarial Networks, Metz et al.

Mode Collapse

Solution attempts:

- Minibatch comparisons: Discriminator can compare instances in a minibatch (*Improved Techniques for Training GANs*, Salimans et al.)
- Unrolled GANs: Take k steps with the discriminator in each iteration, and backpropagate through all of them to update the generator

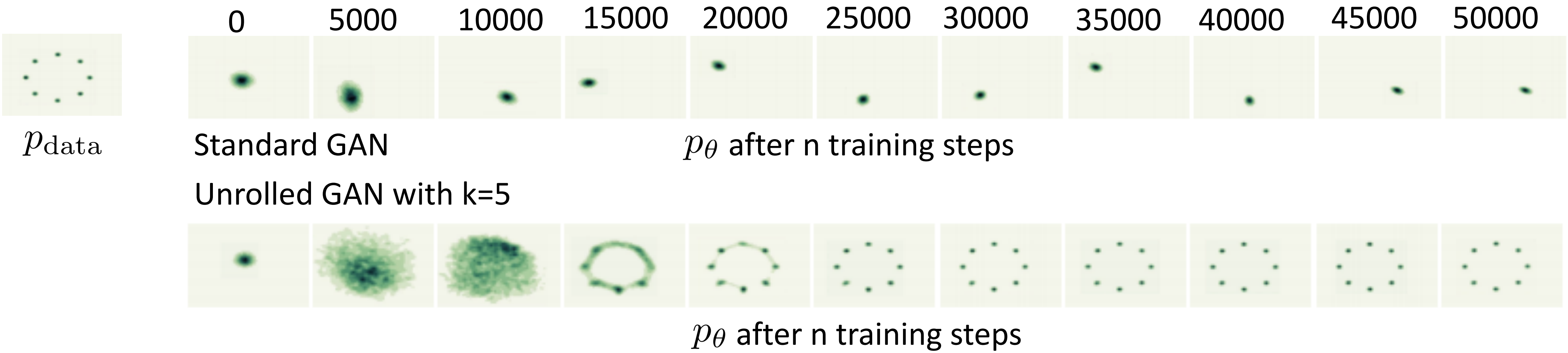


Image Credit: *Wasserstein GAN*, Arjovsky et al.
Unrolled Generative Adversarial Networks, Metz et al.

Summary

- Autoencoders
  - Can infer useful latent representation for a dataset
  - Bad generators
- VAEs
  - Can infer a useful latent representation for a dataset
  - Better generators due to latent space regularization
  - Lower quality reconstructions and generated samples (usually blurry)
- GANs
  - Can not find a latent representation for a given sample (no encoder)
  - Usually better generators than VAEs
  - Currently unstable training (active research)