

# Deep Generative Models: GANs and VAE

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AMLAB, Universiteit van Amsterdam

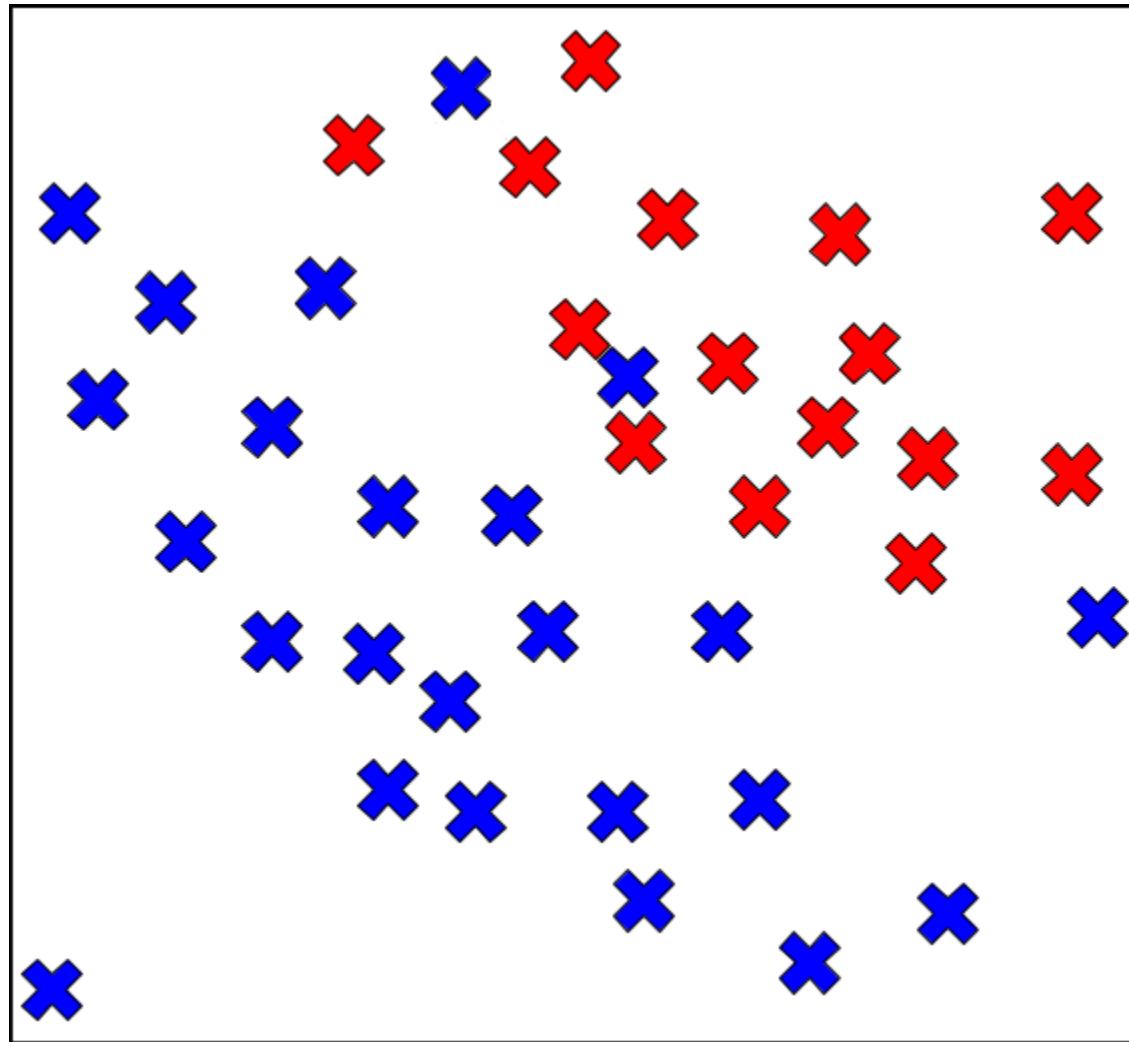
Split, Croatia 2017



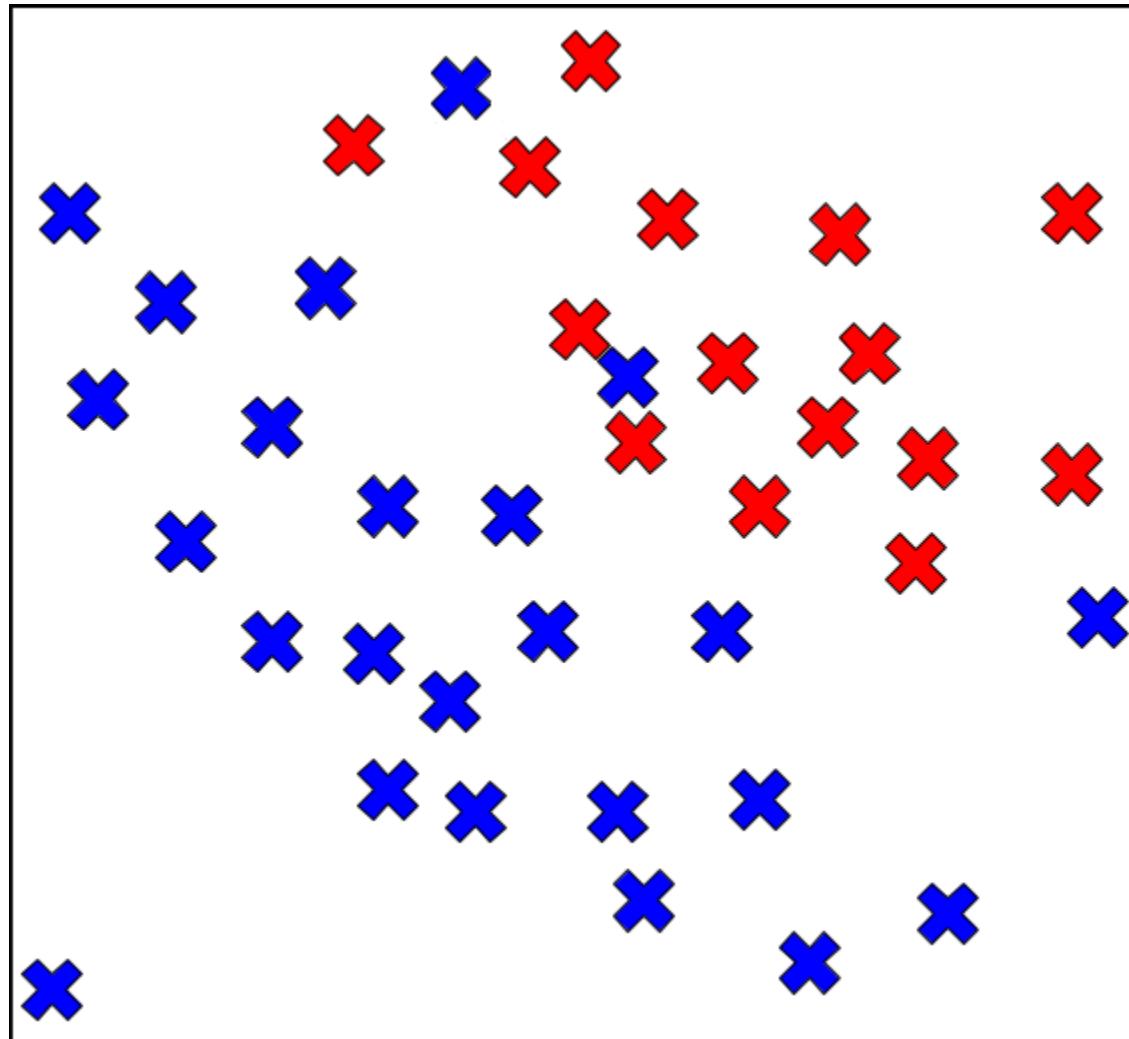
UNIVERSITY OF AMSTERDAM

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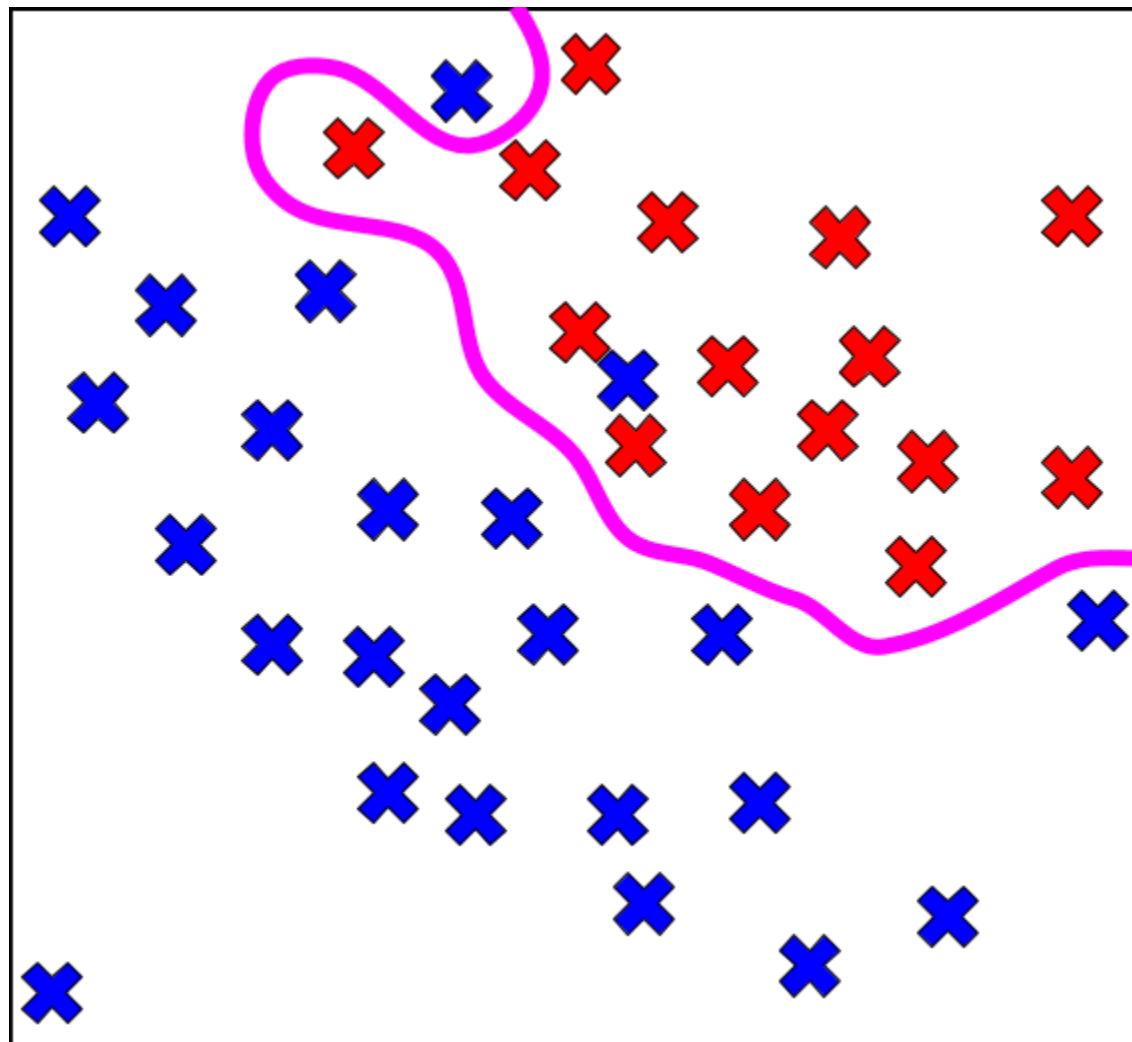


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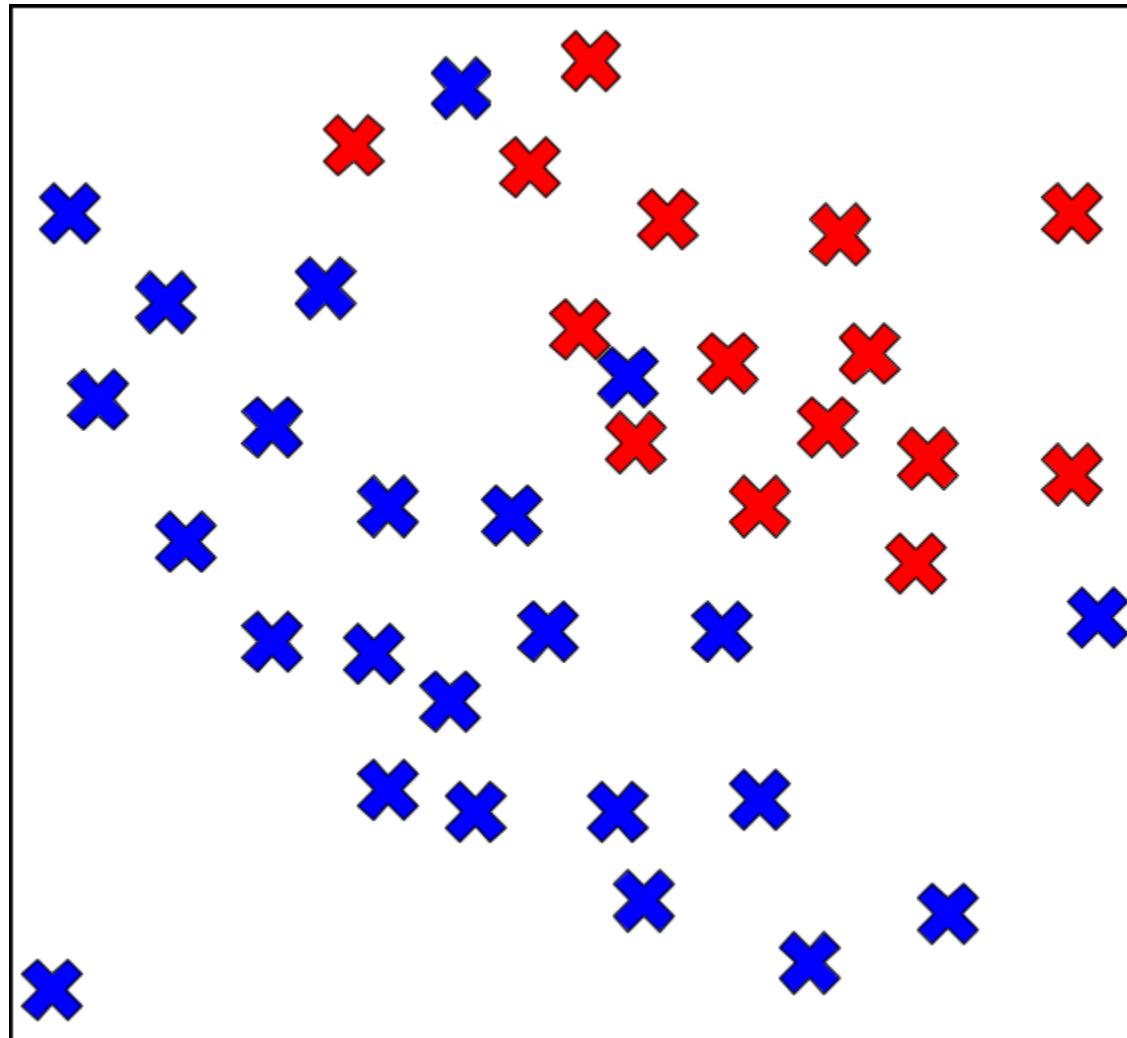
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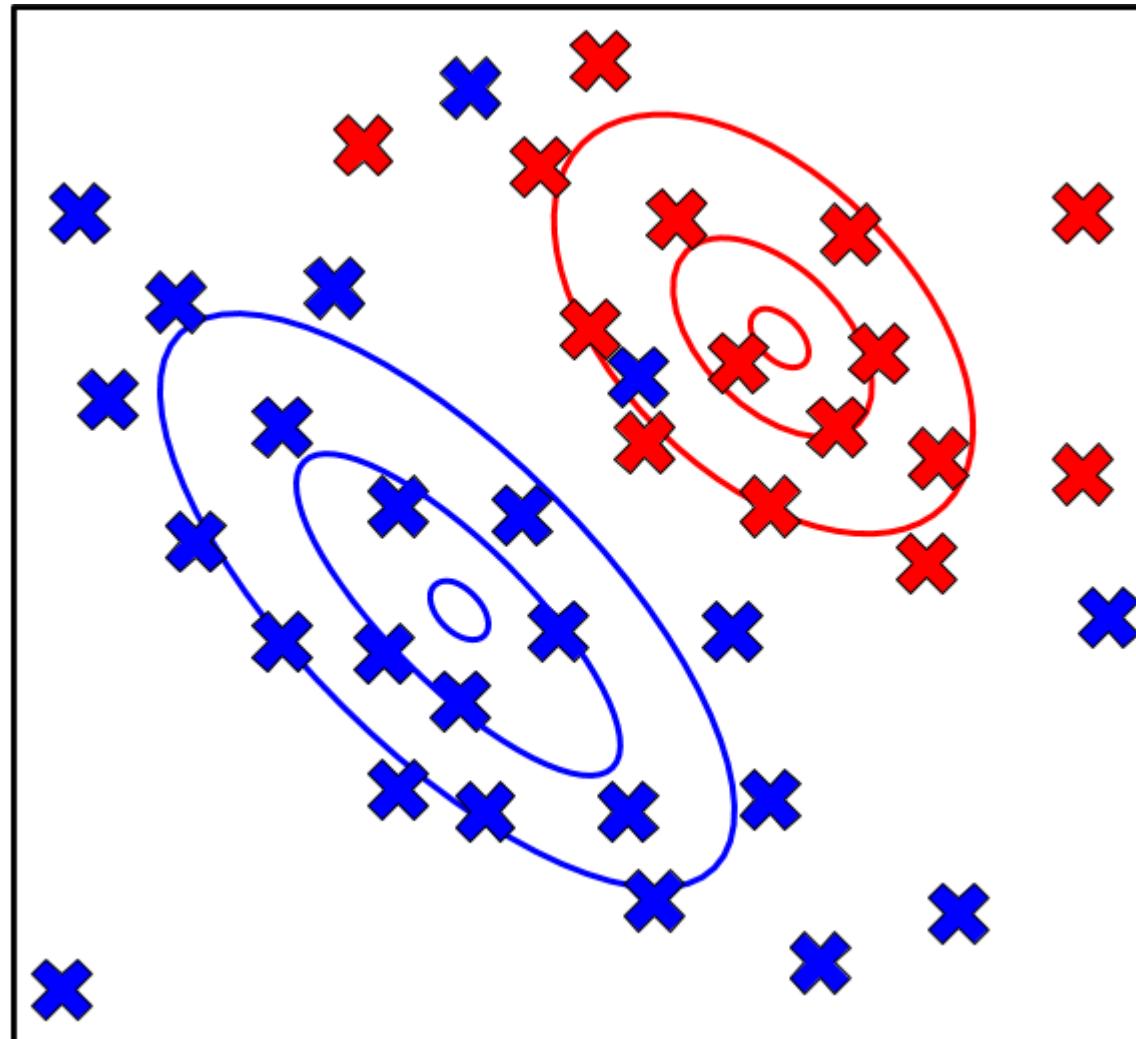
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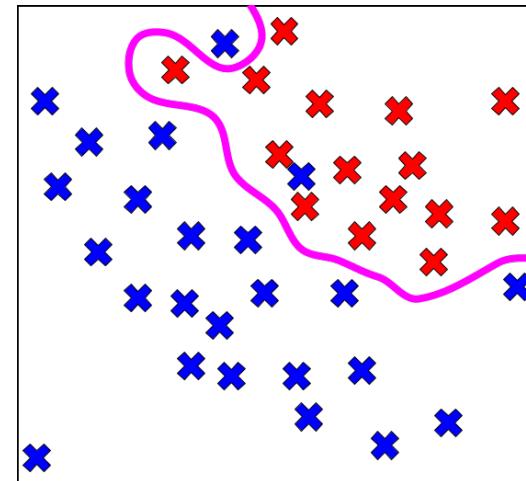
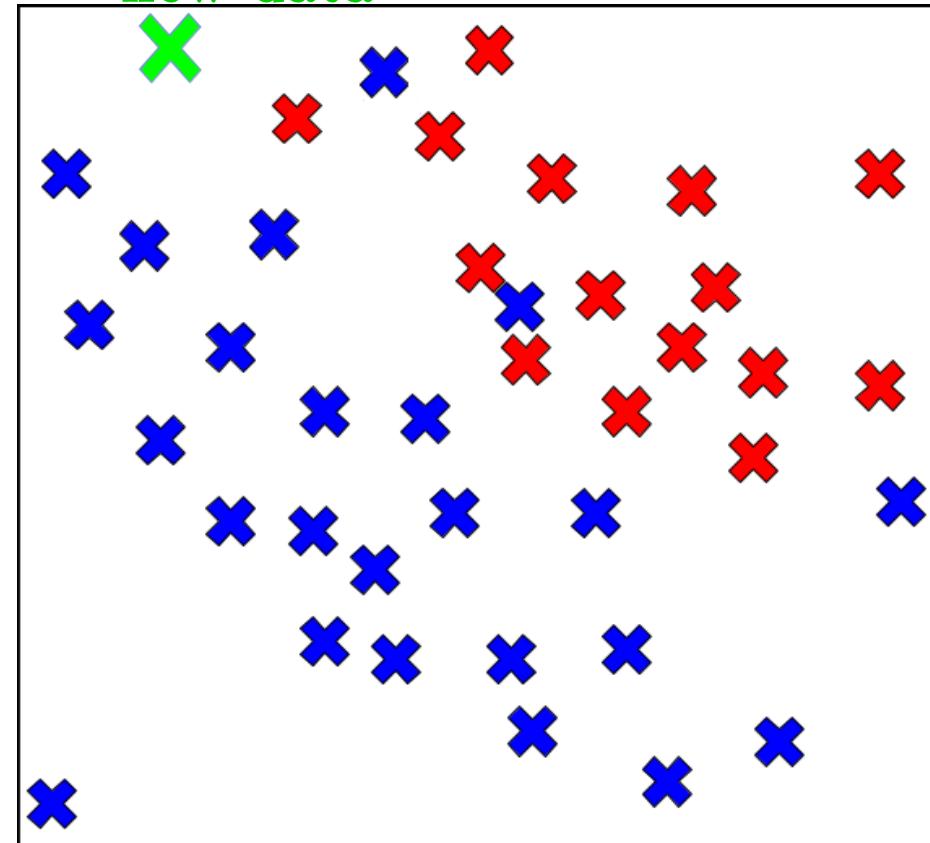
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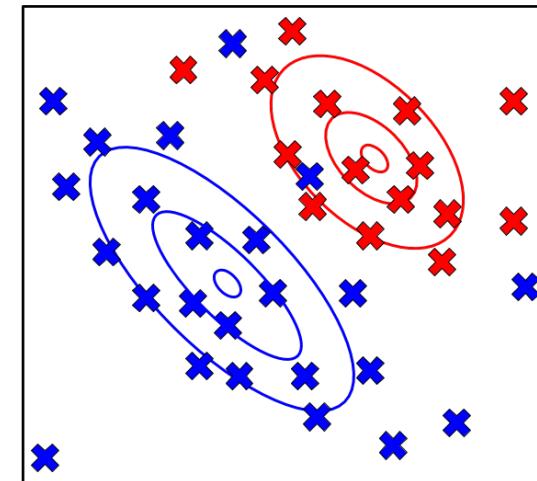
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new data



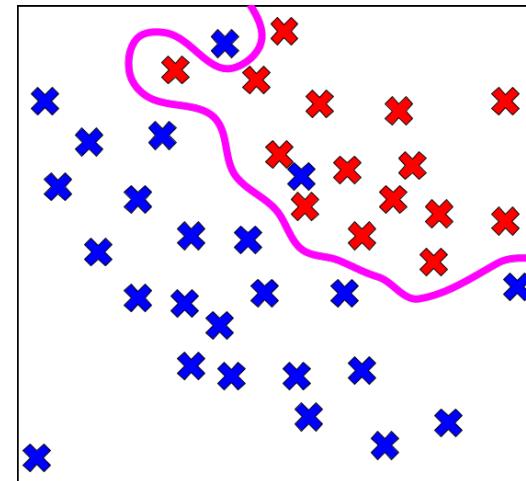
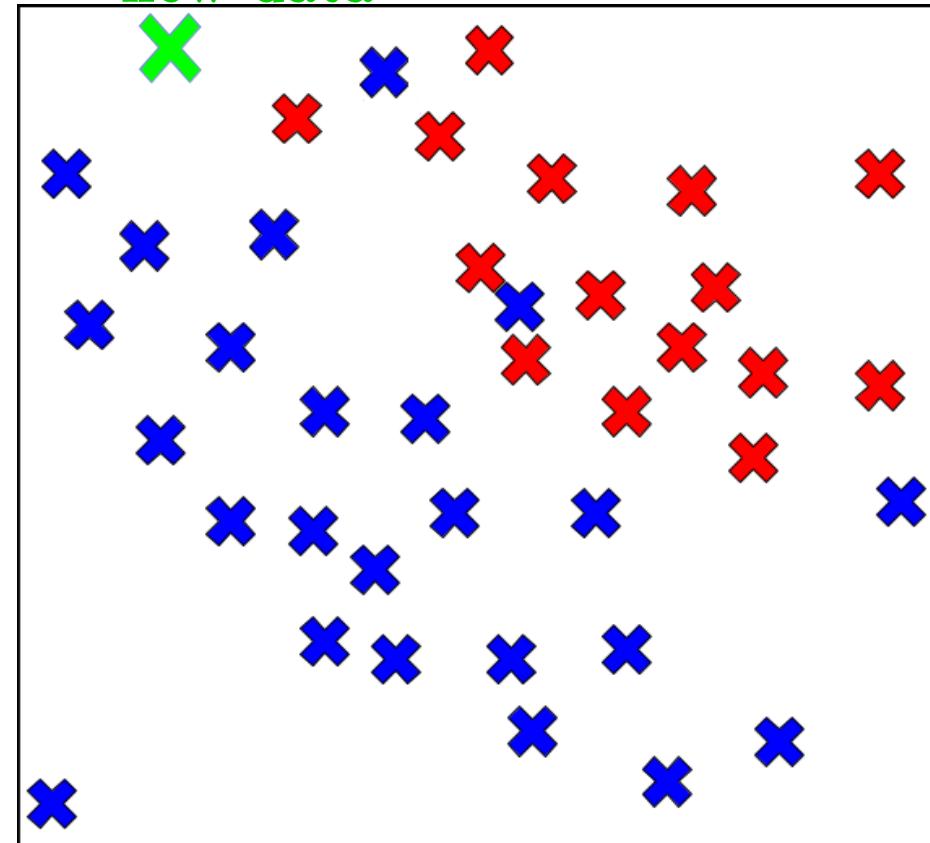
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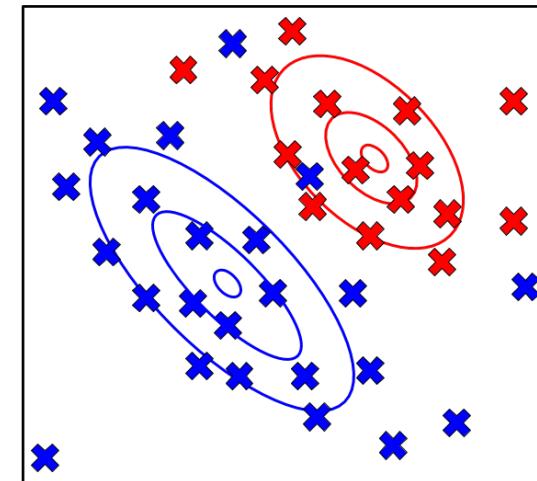
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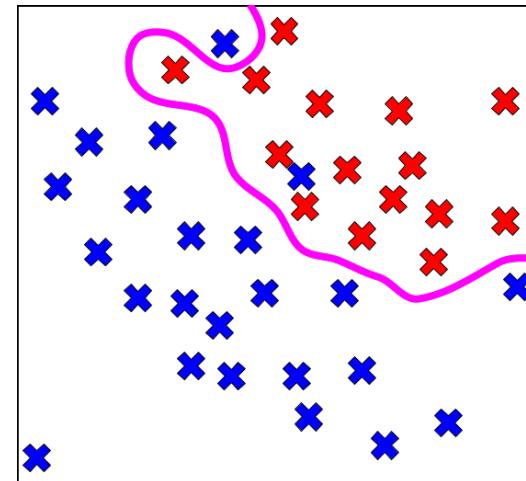
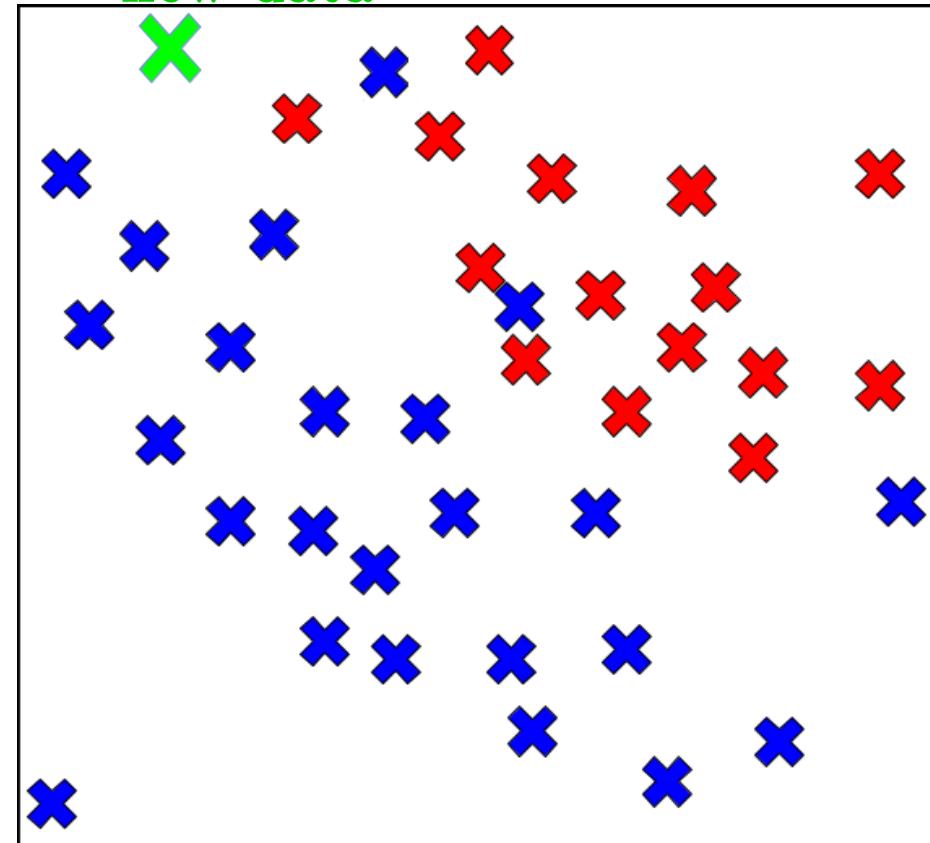


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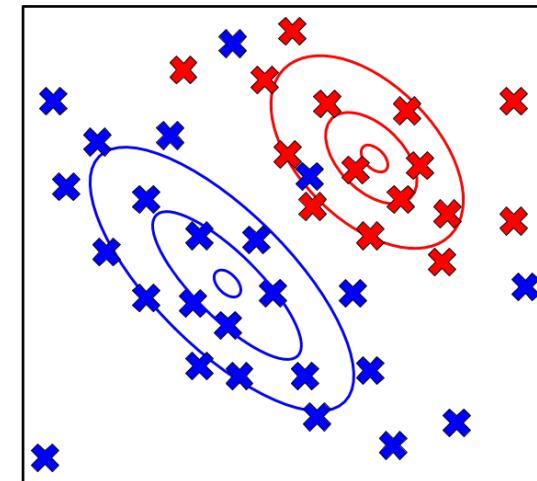
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of the **blue** label.  
=  
**Highly probable  
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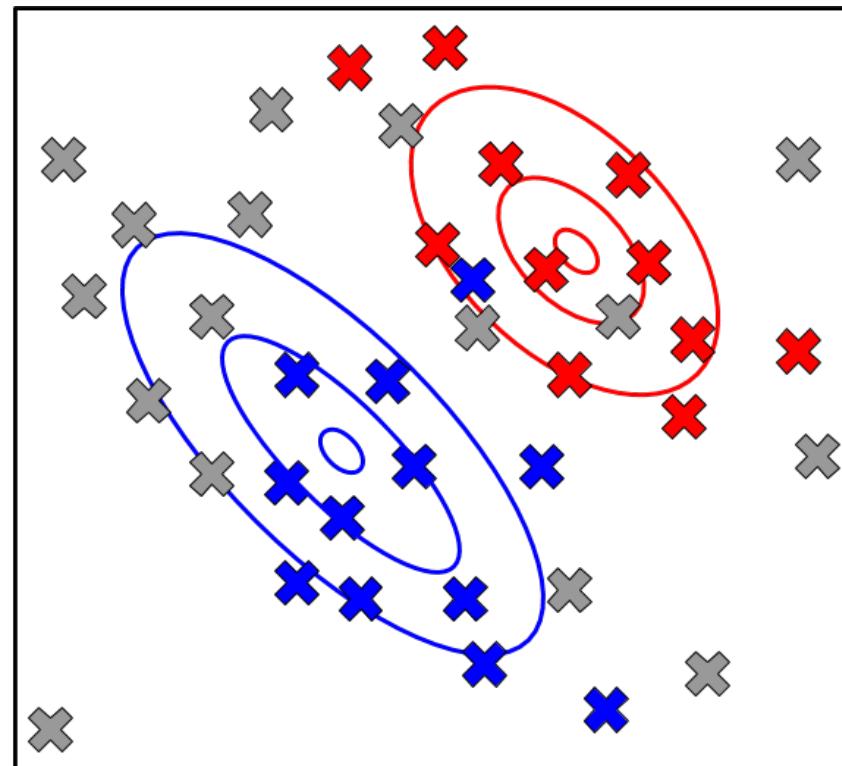
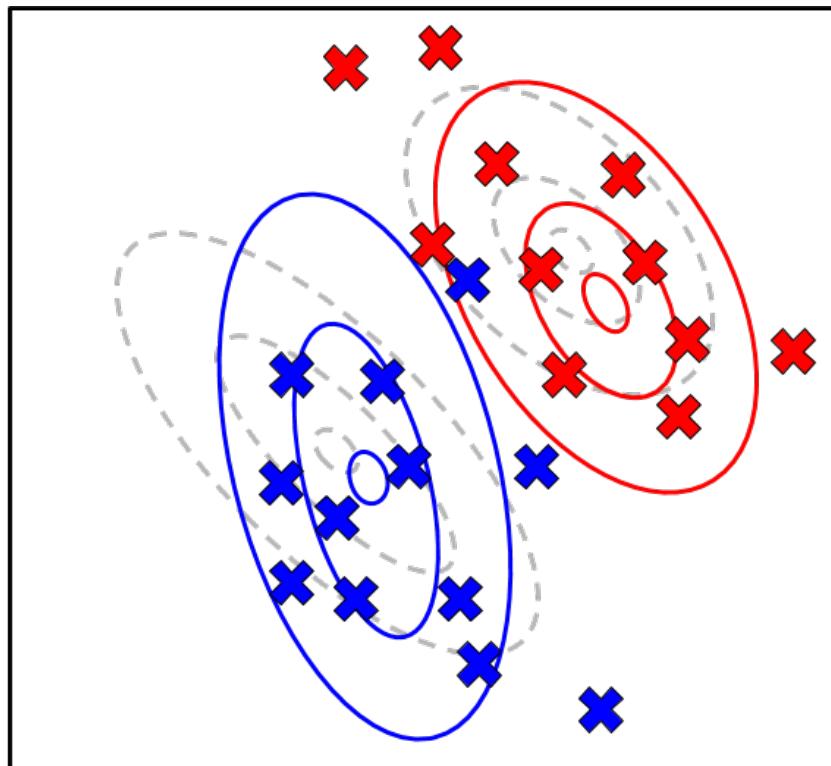
High probability  
of the **blue** label.  
x  
Low probability  
of the **object**.  
=  
**Uncertain  
decision!**

# Generative Modeling

- Providing decision is not enough. *How to evaluate uncertainty? Distribution of  $y$  is only a part of the story.*
- Generalization problem. *Without knowing the distribution of  $\mathbf{x}$  how we can generalize to new data?*
- Understanding the problem is crucial (“**What I cannot create, I do not understand**”, Richard P. Feynman). *Properly modeling data is essential to make better decisions.*

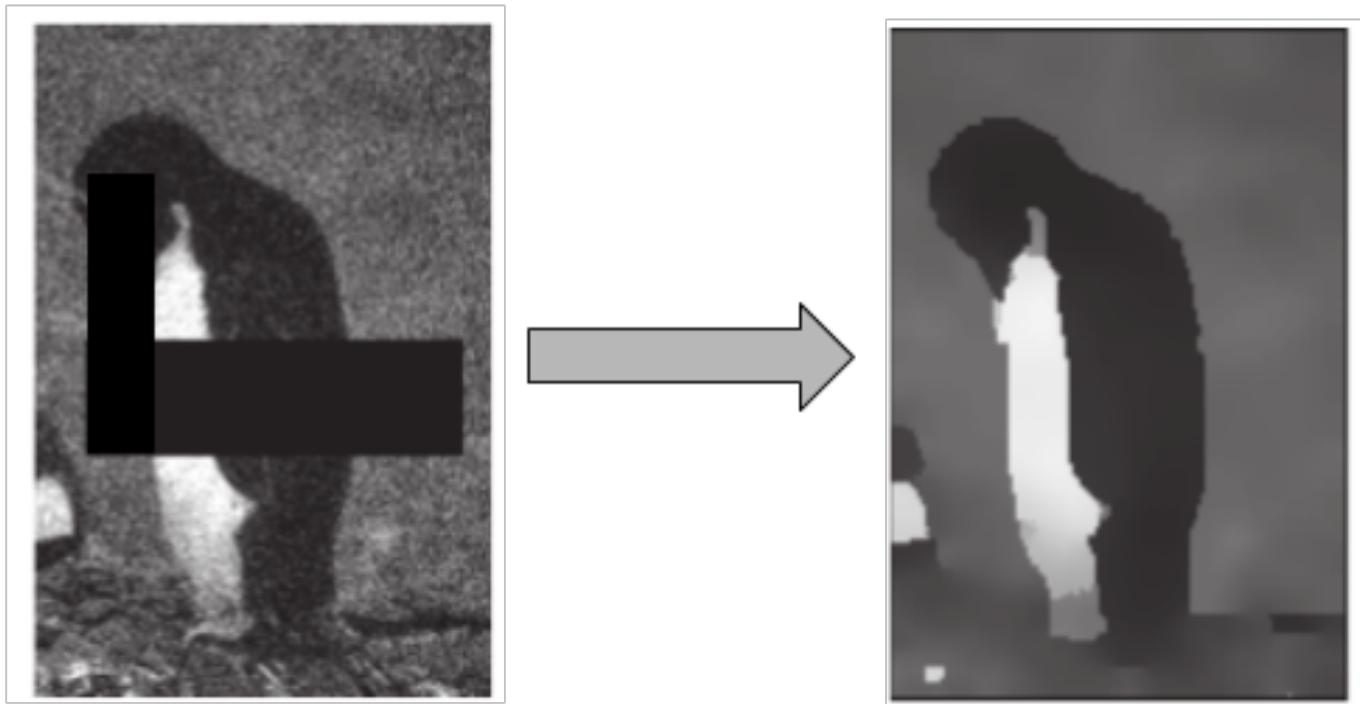
# Generative Modeling

- Semi-supervised learning.  
*Use unlabeled data to train a better classifier.*



# Generative Modeling

- Handling missing or distorted data.  
*Reconstruct and/or denoise data.*

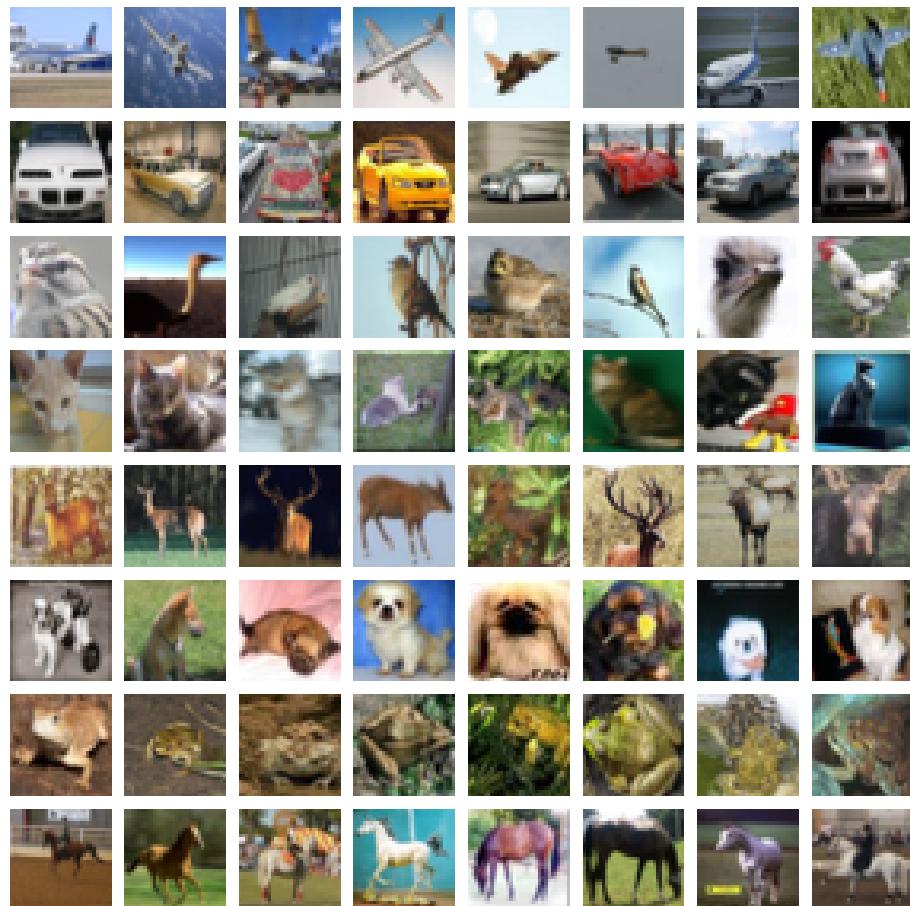


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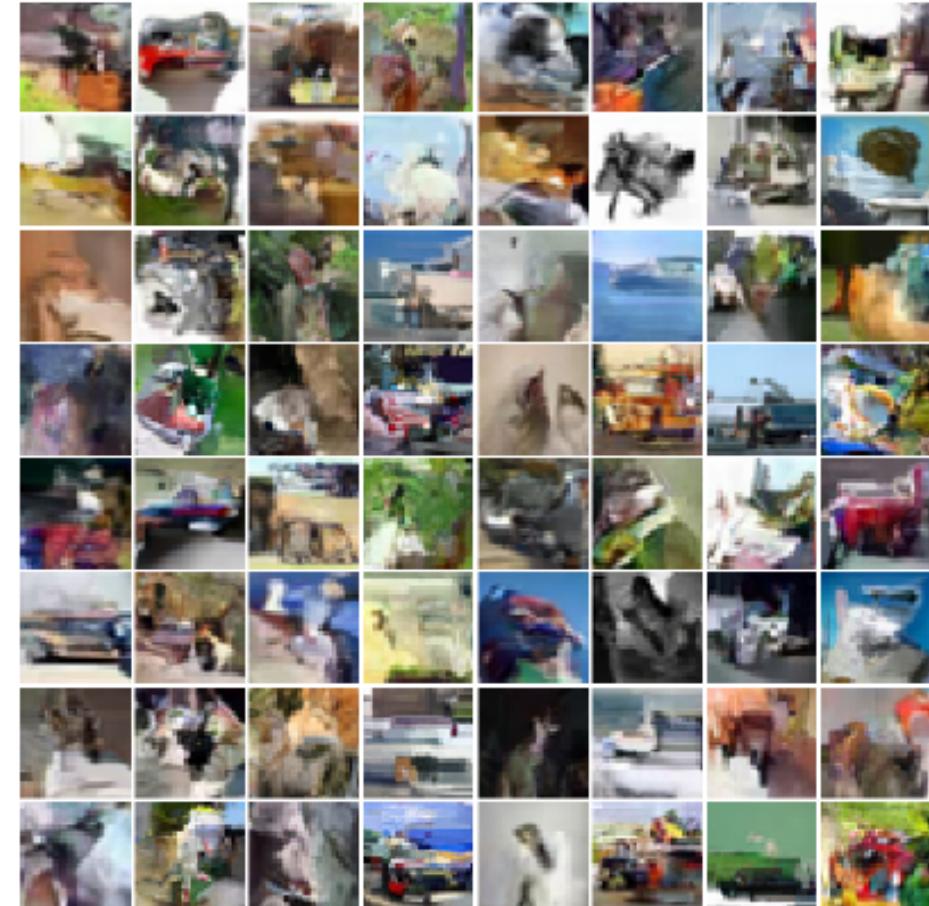
penguin!

# Generative Modeling

## Image generation



Real



Generated

# Generative Modeling

## Sequence generation

---

*he had been unable to conceal the fact that there was a logical explanation for his inability to alter the fact that they were supposed to be on the other side of the house .*

---

*with a variety of pots strewn scattered across the vast expanse of the high ceiling , a vase of colorful flowers adorned the tops of the rose petals littered the floor and littered the floor .*

---

*atop the circular dais perched atop the gleaming marble columns began to emerge from atop the stone dais, perched atop the dais .*

---

Generated

# How to formulate a generative model?

Modeling in high-dimensional space is difficult.



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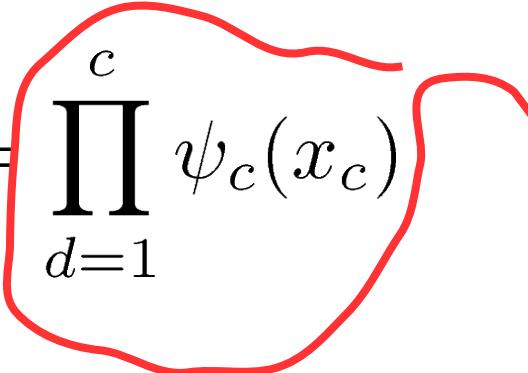
# How to formulate a generative model?

Modeling in high-dimensional space is difficult.  
→ modeling all dependencies among pixels.

$$p(x) = \prod_{d=1}^c \psi_c(x_c)$$

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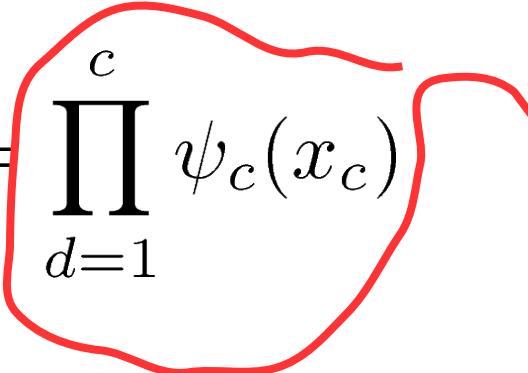
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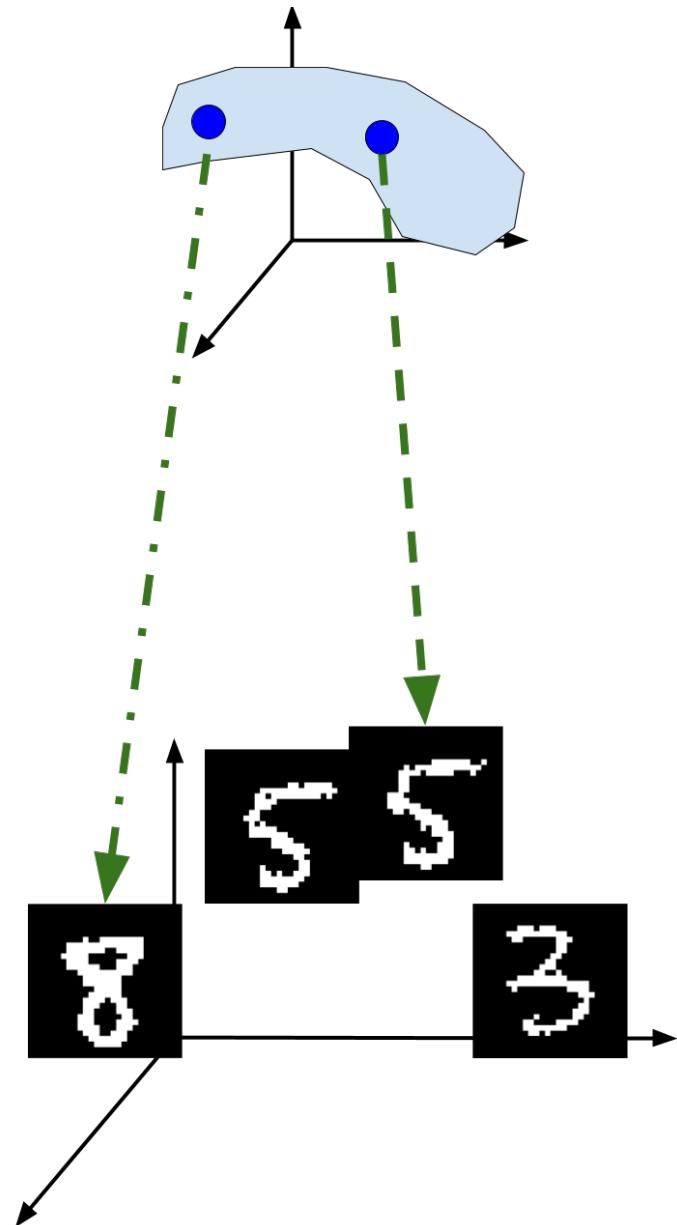
very inefficient!

A possible **solution**? → **Latent variable models**

# Latent Variable Models

- Latent variable model:

$$p(\mathbf{x}) = \int p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z}) d\mathbf{z}$$



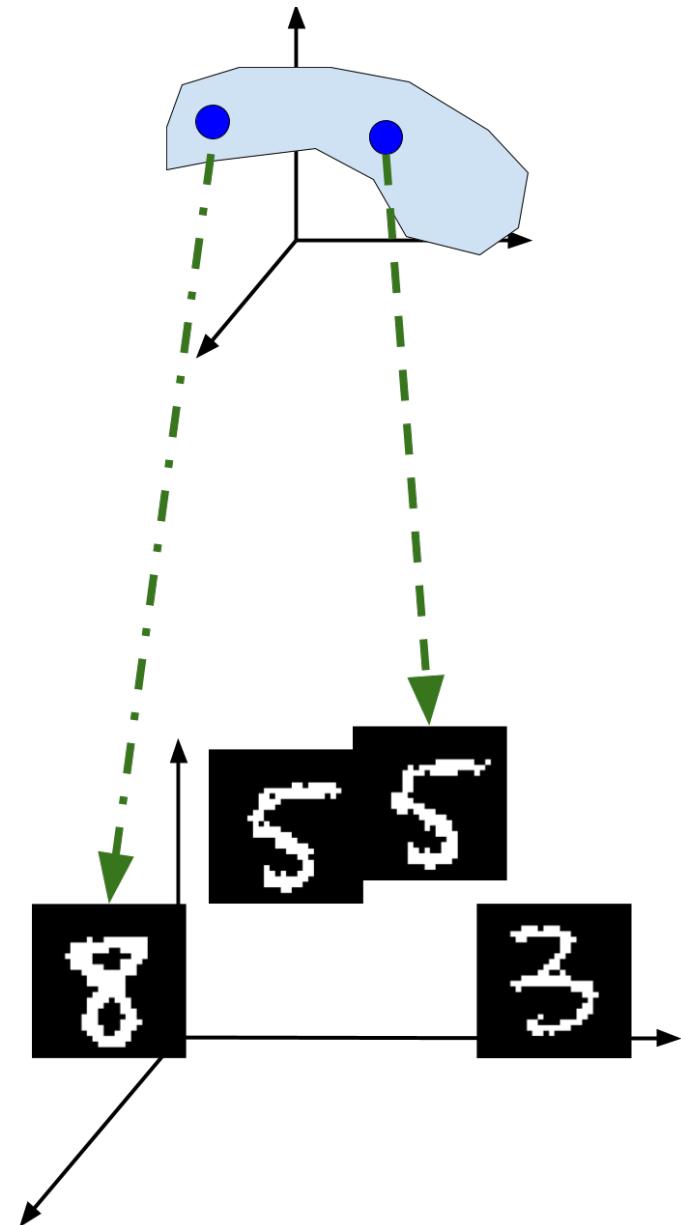
# Latent Variable Models

- Latent variable model:

$$p(\mathbf{x}) = \int p_{\theta}(\mathbf{x}|\mathbf{z}) \underbrace{p_{\lambda}(\mathbf{z})}_{\text{First sample } \mathbf{z}.} d\mathbf{z}$$

First sample  $\mathbf{z}$ .

Second, sample  $\mathbf{x}$  for given  $\mathbf{z}$ .



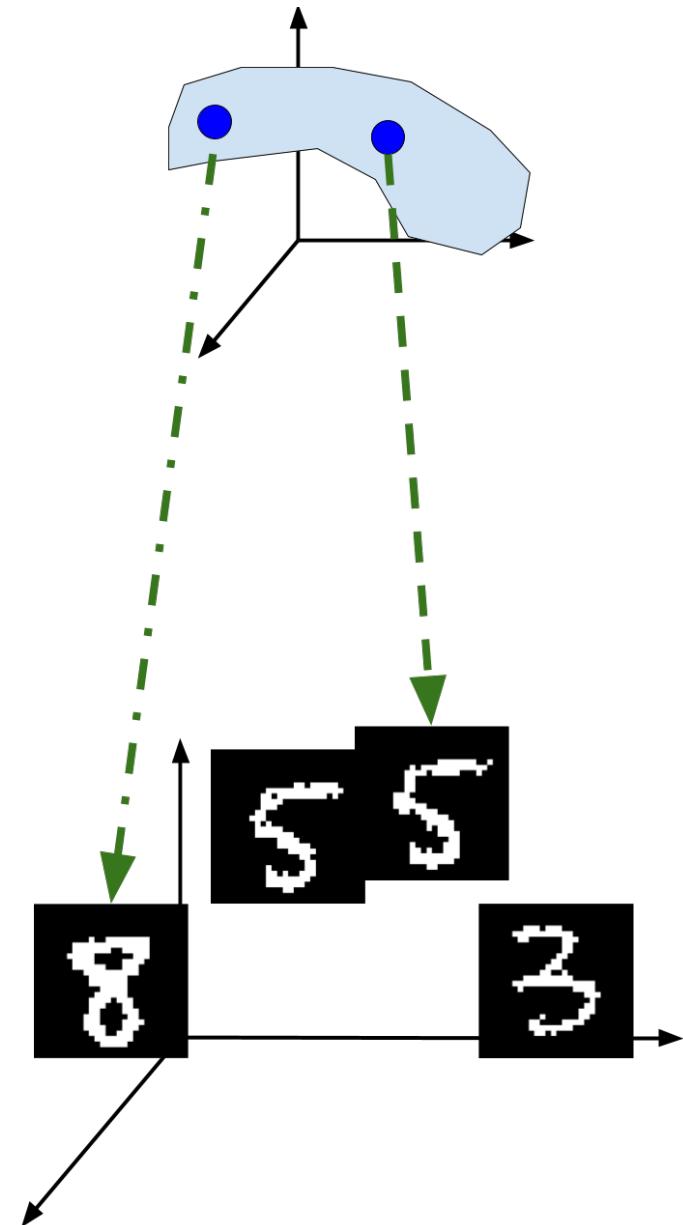
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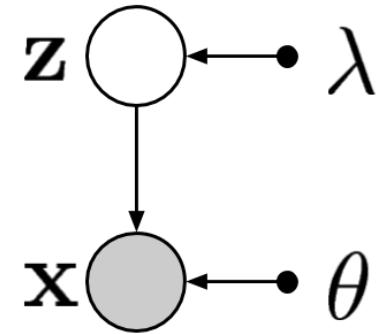
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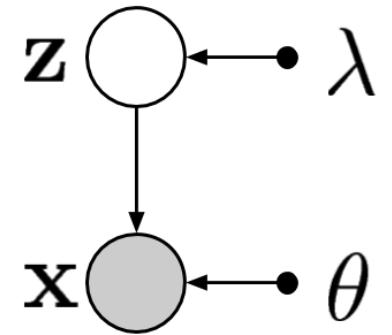


- If  $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{Wz} + \mathbf{b}, \Psi)$  and  $p_{\lambda}(\mathbf{z}) = \mathcal{N}(\mu_0, \Sigma_0)$  , then → **Factor Analysis**.
- What if we take a non-linear transformation of  $\mathbf{z}$ ?  
→ *an infinite mixture of Gaussians*.

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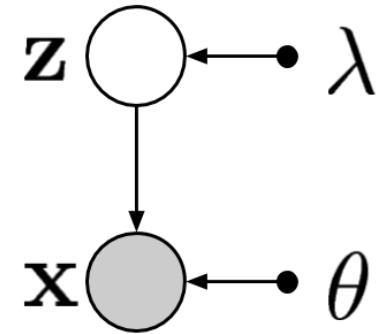
Convenient but limiting!

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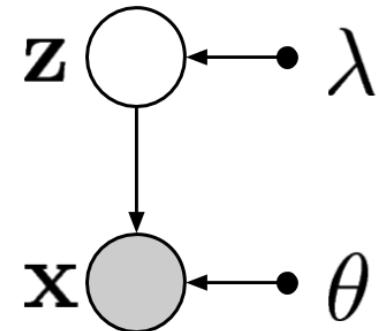


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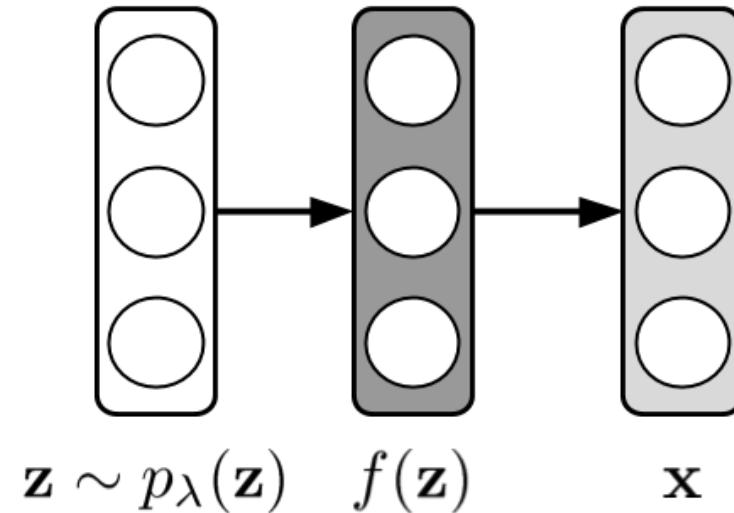
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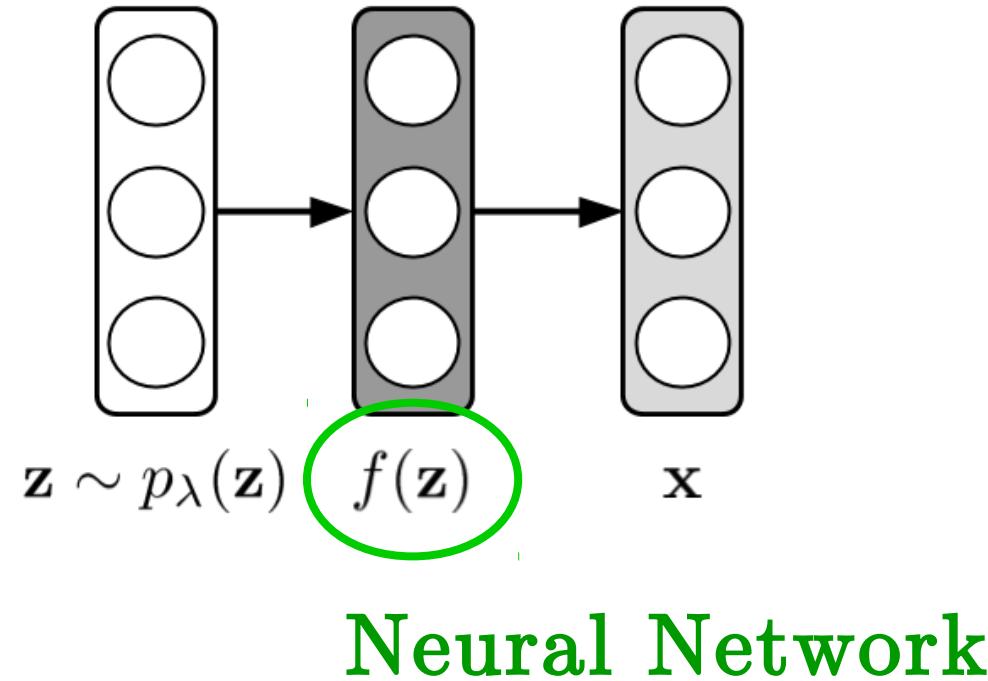
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Neural network

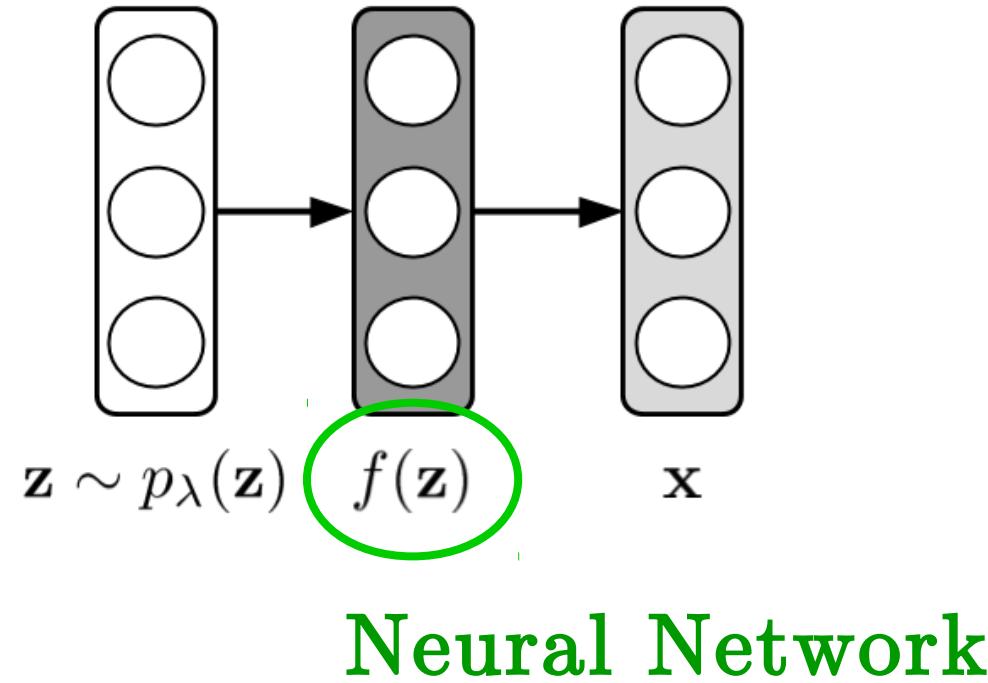
# Deep Generative Models (DGM): Density Network



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How to train this model?!

# DGM: Density Network

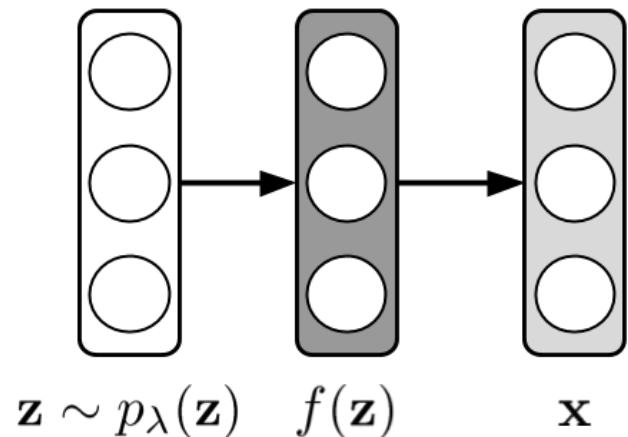
- MC approximation:

$$\log p(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z}) d\mathbf{z}$$

$$\approx \log \frac{1}{S} \sum_{s=1}^S \exp \left( \log p_{\theta}(\mathbf{x}|\mathbf{z}_s) \right)$$

where:

$$\mathbf{z}_s \sim p_{\lambda}(\mathbf{z})$$



# DGM: Density Network

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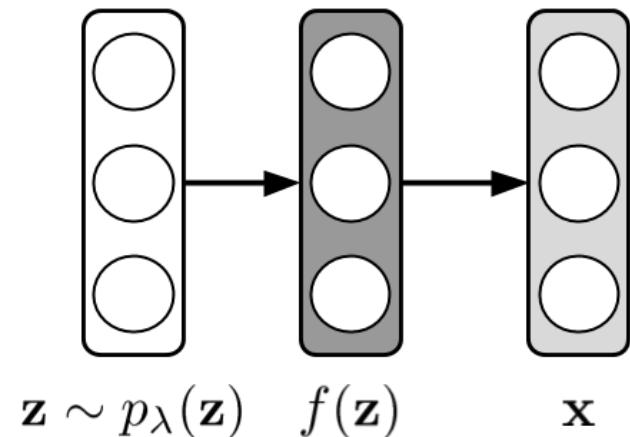
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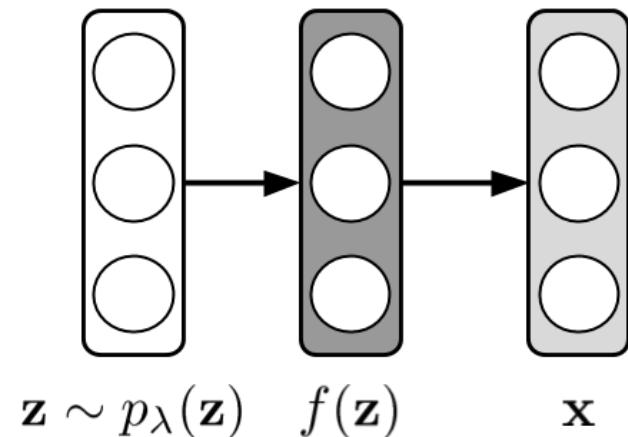
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**It scales badly in high  
dimensional cases!**



# DGM: Density Network

## PROS

Log-likelihood approach

Easy sampling

Training using gradient-based methods

## CONS

Requires explicit models

Fails in high dim. cases

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Training using **gradient-based methods**

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Fails in **high dim.** cases

Can we do better?

# DGM: Generative Adversarial Nets

Let image two agents:

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Let image two agents:



A **fraud**

# DGM: Generative Adversarial Nets

Let image two agents:



A fraud



An art expert

# DGM: Generative Adversarial Nets

Let image two agents:



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... and a real artist



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The fraud aims  
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The fraud aims to copy the real artist and cheat the art expert.



The expert assesses a painting and gives her opinion.

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Let image two agents:



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The expert assesses a painting and gives her opinion.

An art expert

The fraud learns and tries to fool the expert.

# DGM: Generative Adversarial Nets

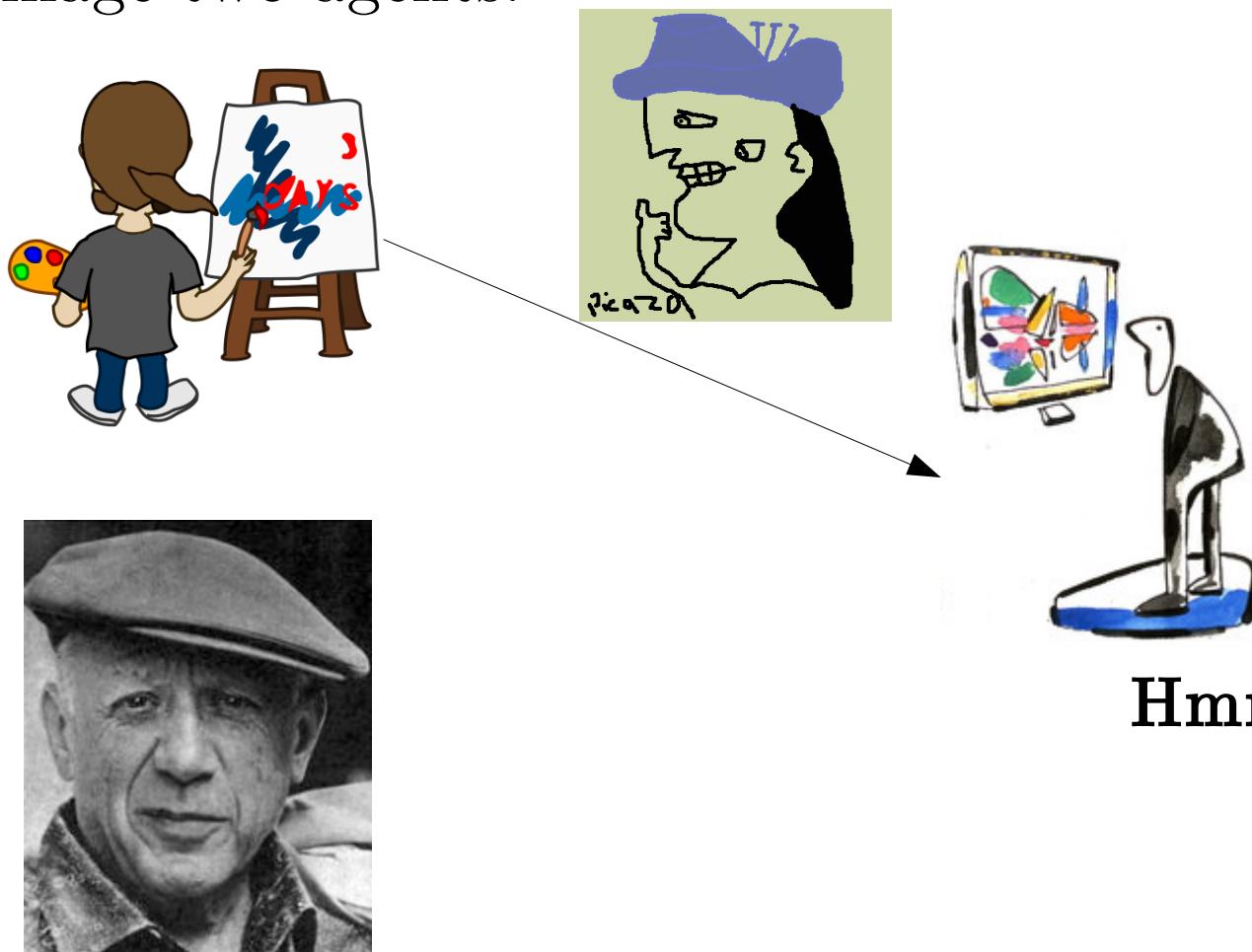
Let image two agents:



Hmmm... fake!

# DGM: Generative Adversarial Nets

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Hmmm... Pablo!

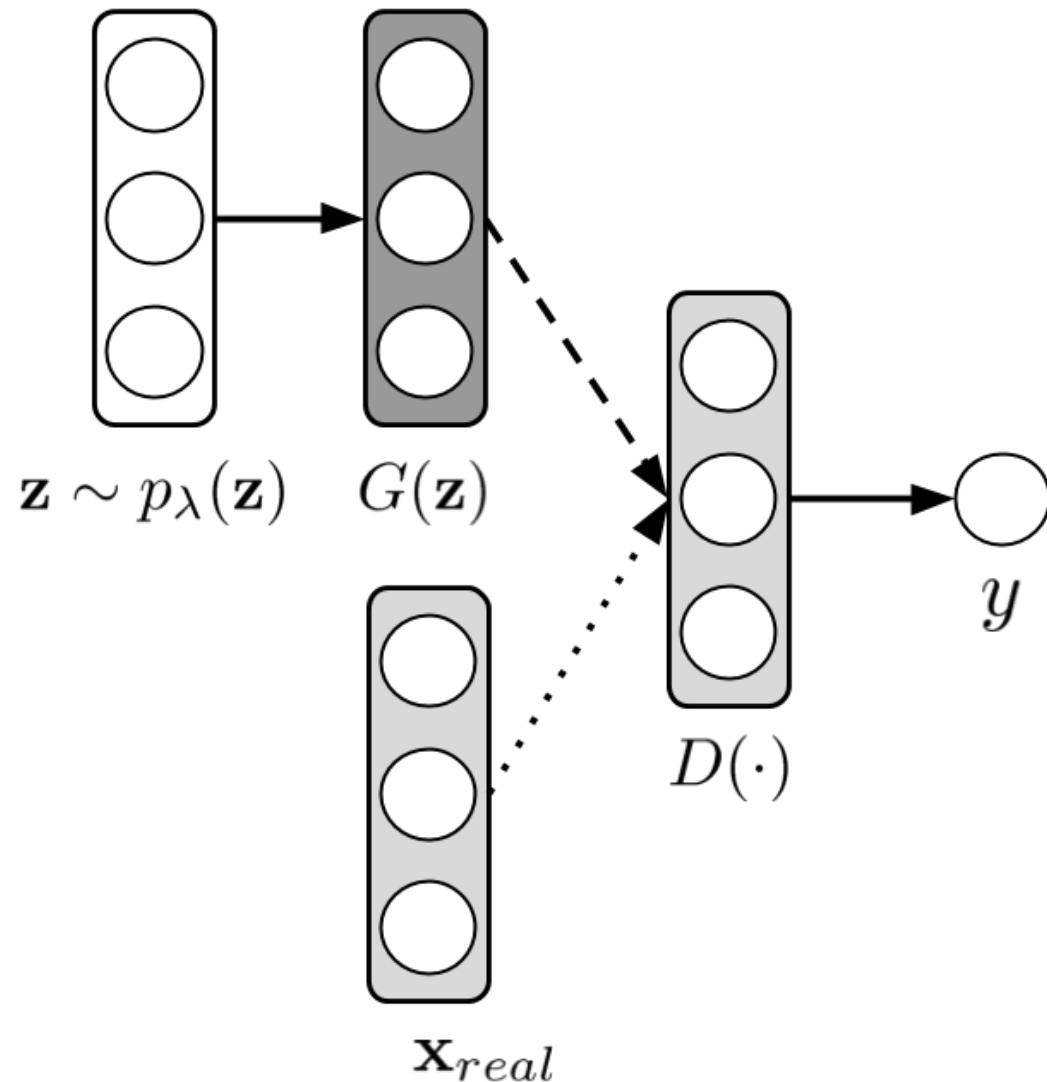
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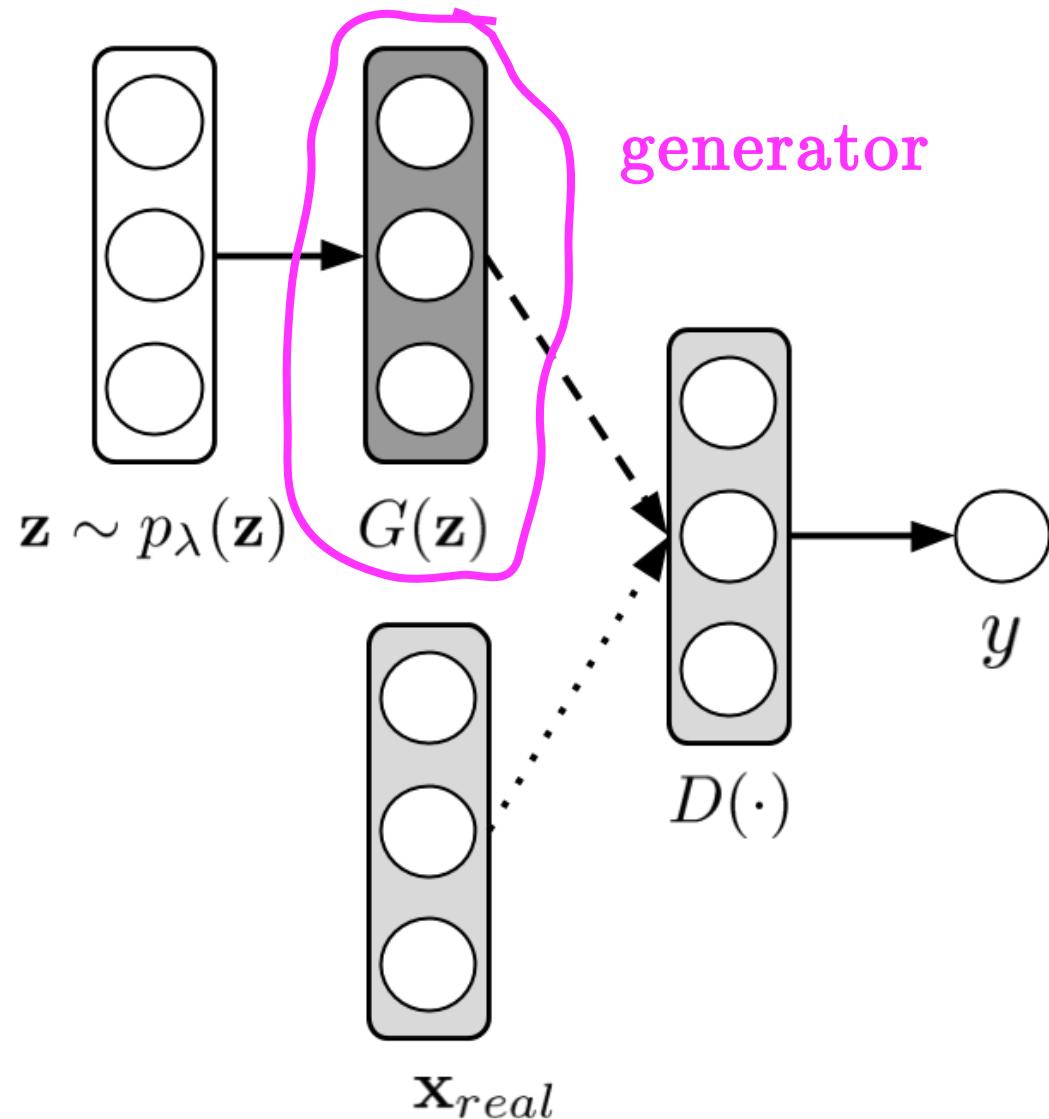


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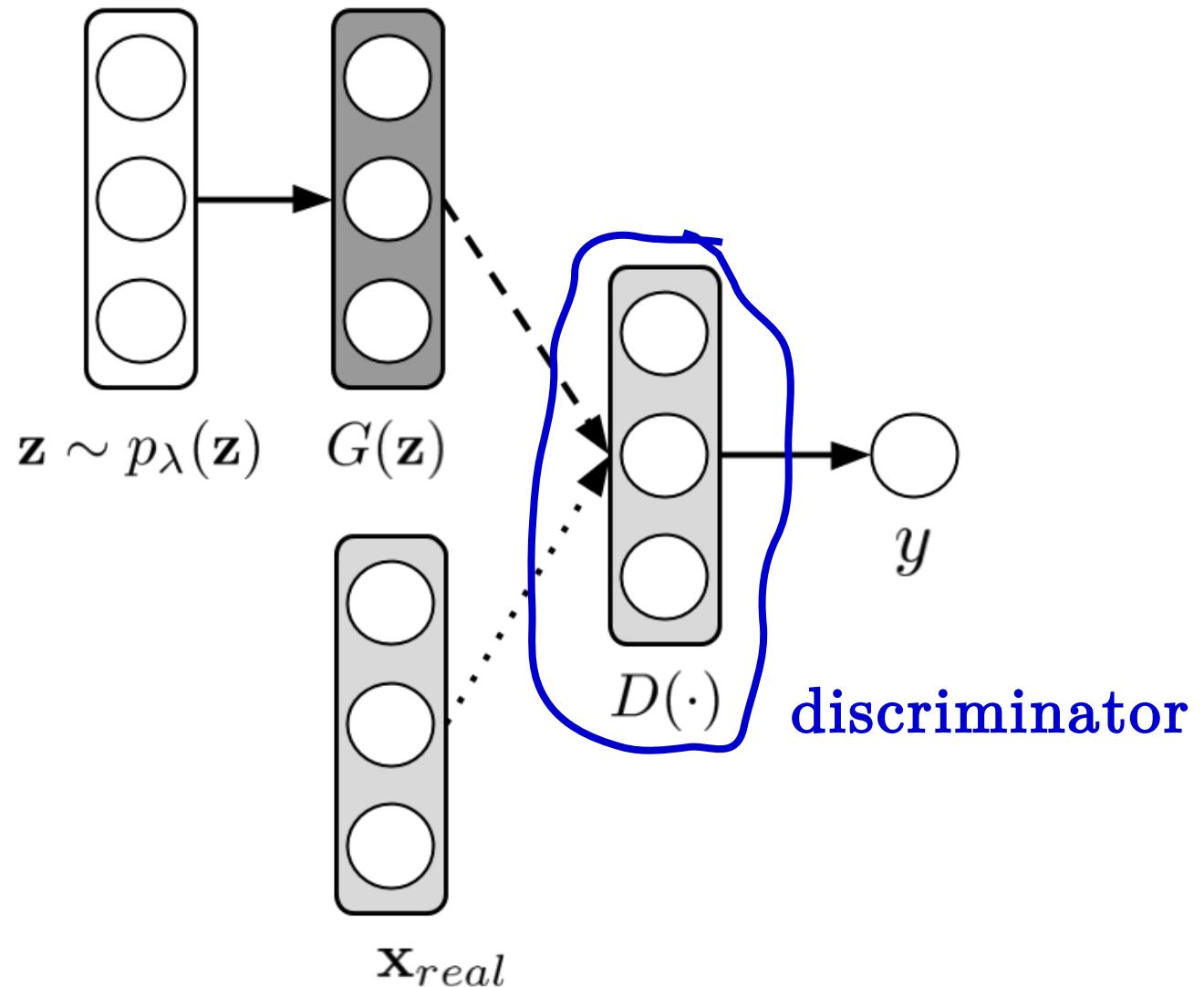
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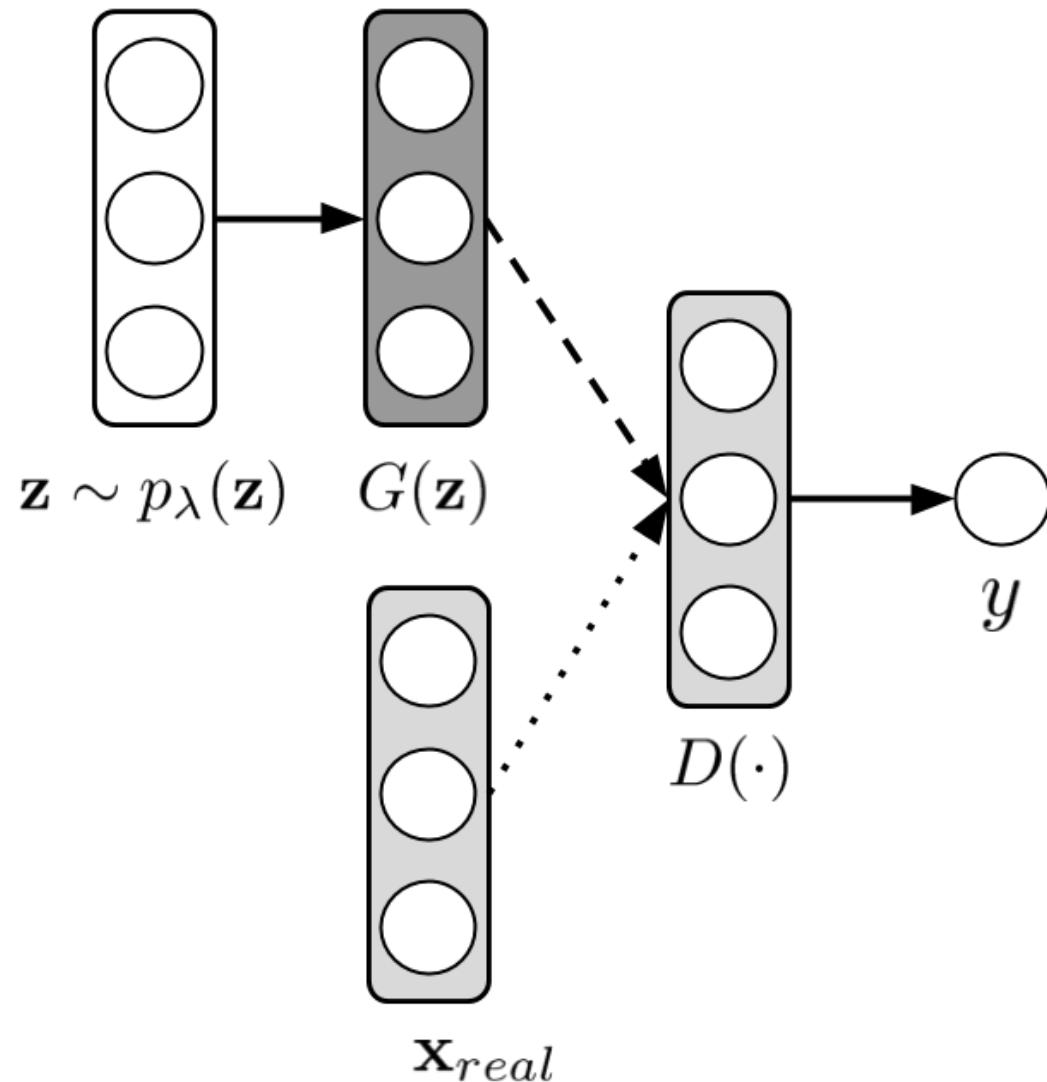


# DGM: Generative Adversarial Nets



# DGM: Generative Adversarial Nets

1. Sample  $\mathbf{z}$ .
2. Generate  $G(\mathbf{z})$ .
3. Discriminate whether given image is **real** or **fake**.



# DGM: Generative Adversarial Nets

Formally, the problem is the following:

$$\min_G \max_D \mathbb{E}_{\mathbf{x} \sim p_{real}} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\log(1 - D(G(\mathbf{z})))]$$

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Minimize wrt. generator

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Maximize wrt. discriminator

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Once we converge, we can generate images that are almost **indistinguishable** from real images.

# DGM: Generative Adversarial Nets

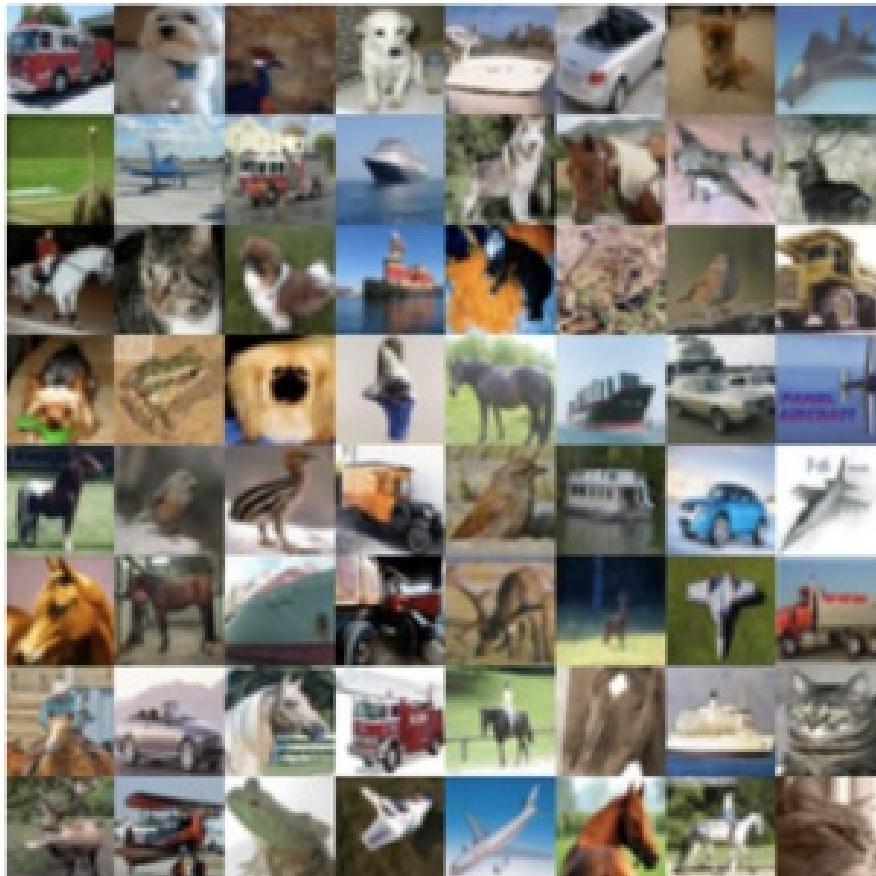
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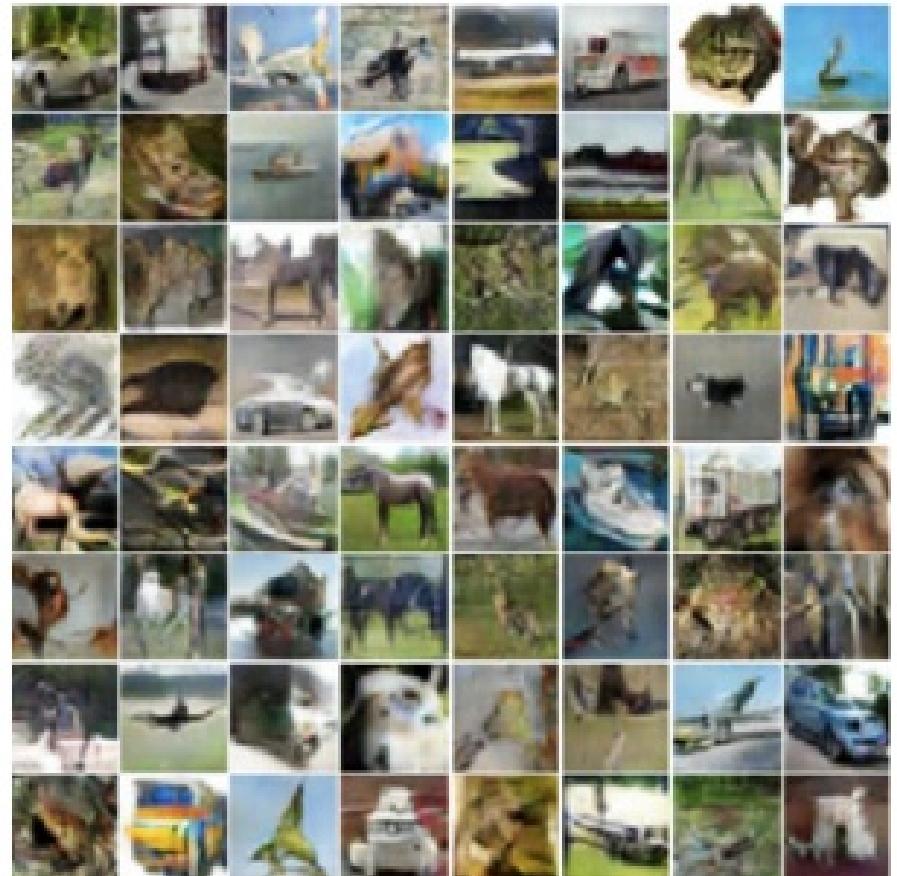
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**BUT training is very unstable...**

# DGM: Generative Adversarial Nets



## Training Data



## Samples

# DGM: GANs

## PROS

Allows **implicit** models

Easy **sampling**

Training using **gradient-based methods**

Works in **high dim.** cases

## CONS

**Unstable** training

**Does not** correspond to likelihood solution

No clear way for **quantitative assessment**

**Missing mode** problem

# DGM: Wasserstein GAN

We can consider an earth-mover distance to formulate GAN-like optimization problem as follows:

$$\min_G \max_{D \in \mathcal{W}} \mathbb{E}_{\mathbf{x} \sim p_{real}} [D(\mathbf{x})] - \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [D(G(\mathbf{z}))]$$

where the discriminator is a 1-Lipshitz function.

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It means we need to **clip** weights of the discriminator,  
*i.e.*,

`clip(weights, -c, c).`

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where the discriminator is a 1-Lipshitz function.

Wasserstein GAN **stabilizes training** (but other problems **remain**).

# DGM: More GANs (selected)

## Deep convolutional generative adversarial networks

Radford, A., Metz, L., & Chintala, S. (2015). Unsupervised representation learning with deep convolutional generative adversarial networks. arXiv preprint arXiv:1511.06434.

## Auxiliary classifier GANs

Odena, A., Olah, C., & Shlens, J. (2016). Conditional image synthesis with auxiliary classifier gans. arXiv preprint arXiv:1610.09585.

## From optimal transport to generative modeling: the VEGAN cookbook

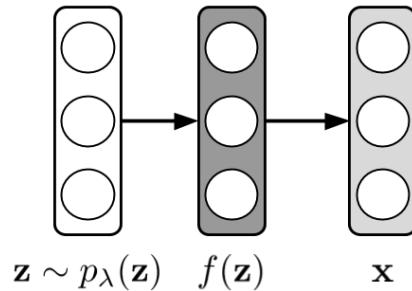
Bousquet, O., Gelly, S., Tolstikhin, I., Simon-Gabriel, C. J., & Schoelkopf, B. (2017). From optimal transport to generative modeling: the VEGAN cookbook. arXiv preprint arXiv:1705.07642.

## Bidirectional Generative Adversarial Networks

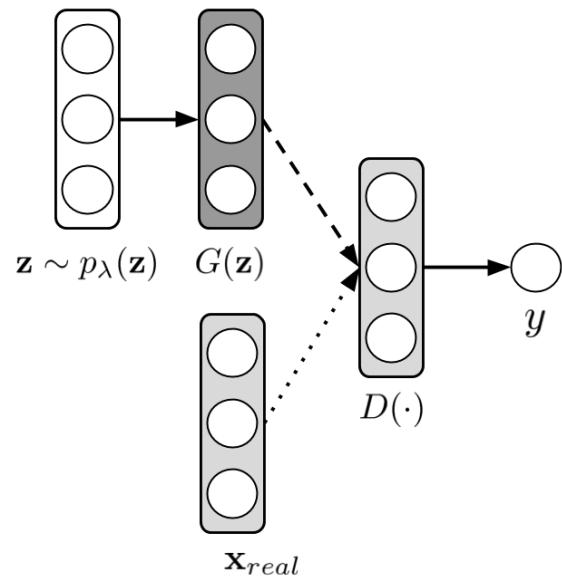
Donahue, J., Krähenbühl, P., & Darrell, T. (2016). Adversarial feature learning. arXiv preprint arXiv:1605.09782.

# Questions?

# DGM: so far we have

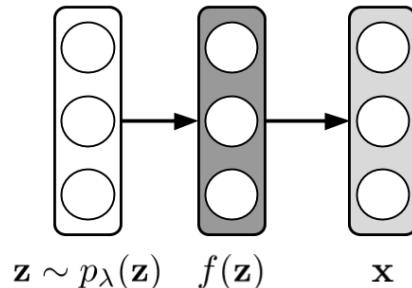


Density Network

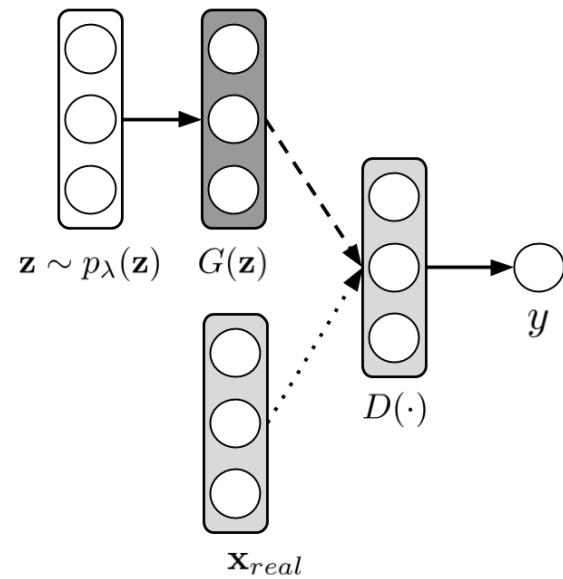


Generative Adversarial Net

# DGM: so far we have



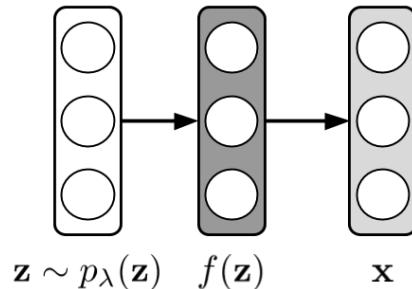
Density Network



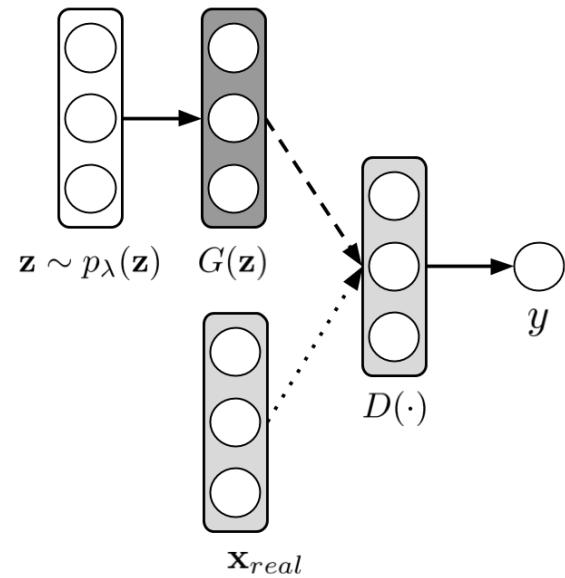
Generative Adversarial Net

Works only for low dim. cases...  
Inefficient training...

# DGM: so far we have



Density Network

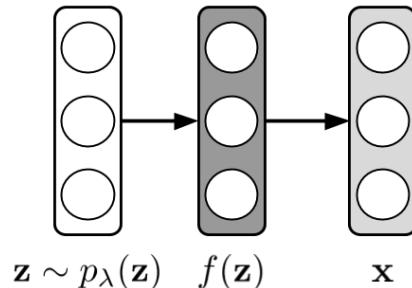


Generative Adversarial Net

Works only for low dim. cases...  
Inefficient training...

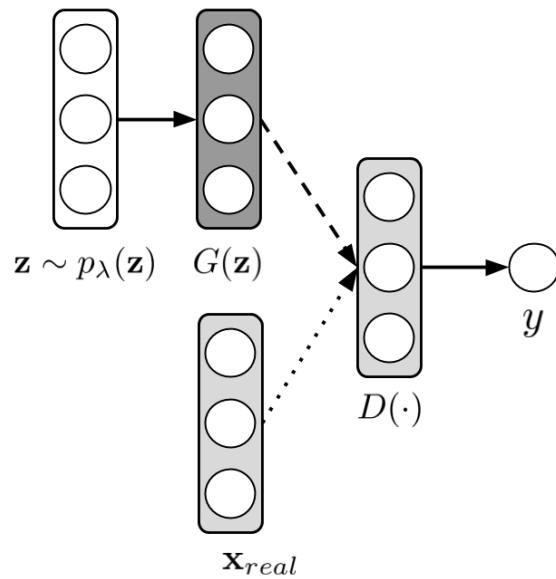
Works for high dim. cases!

# DGM: so far we have



Density Network

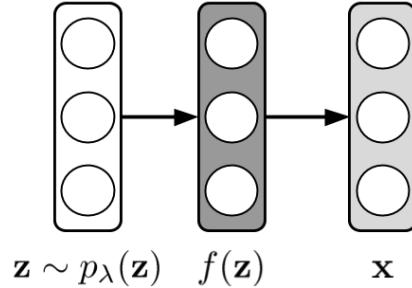
Works only for low dim. cases...  
Inefficient training...



Generative Adversarial Net

Works for high dim. cases!  
Doesn't train a distribution...  
Unstable training...

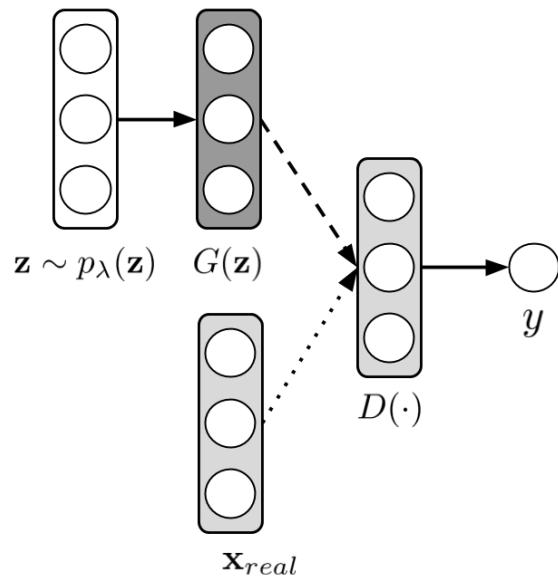
# DGM: so far we have



Density Network

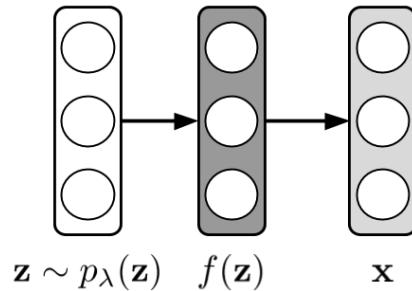
QUESTION

Can we stick to the log-likelihood approach  
but with a simple training procedure?

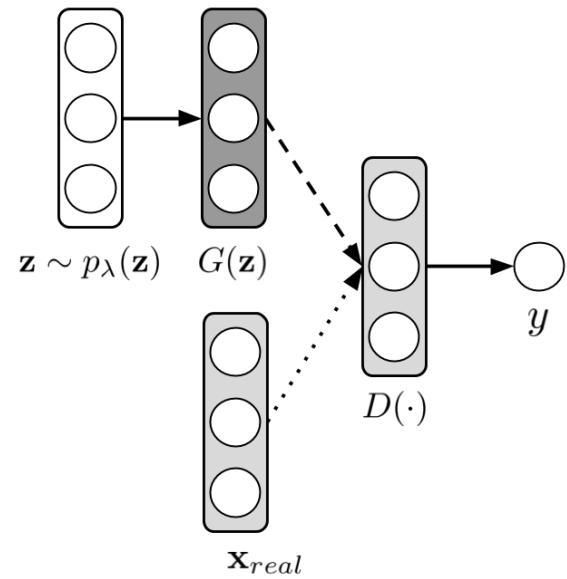


Generative Adversarial Net

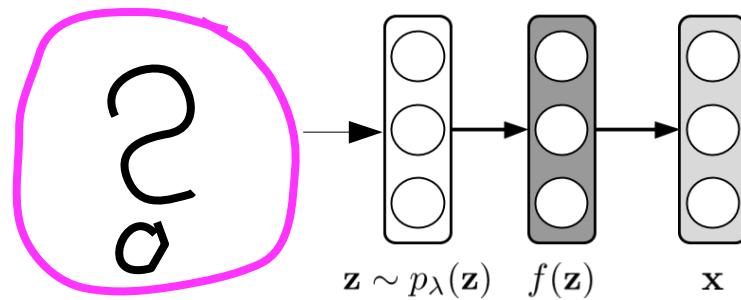
# DGM: so far we have



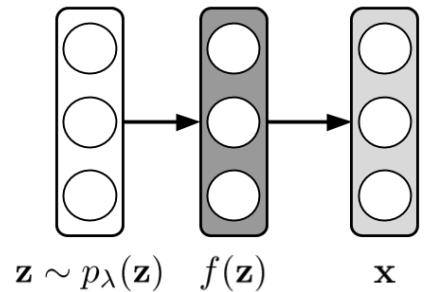
Density Network



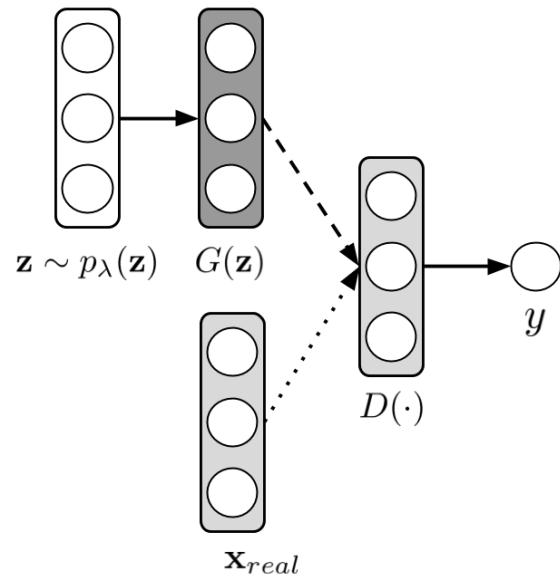
Generative Adversarial Net



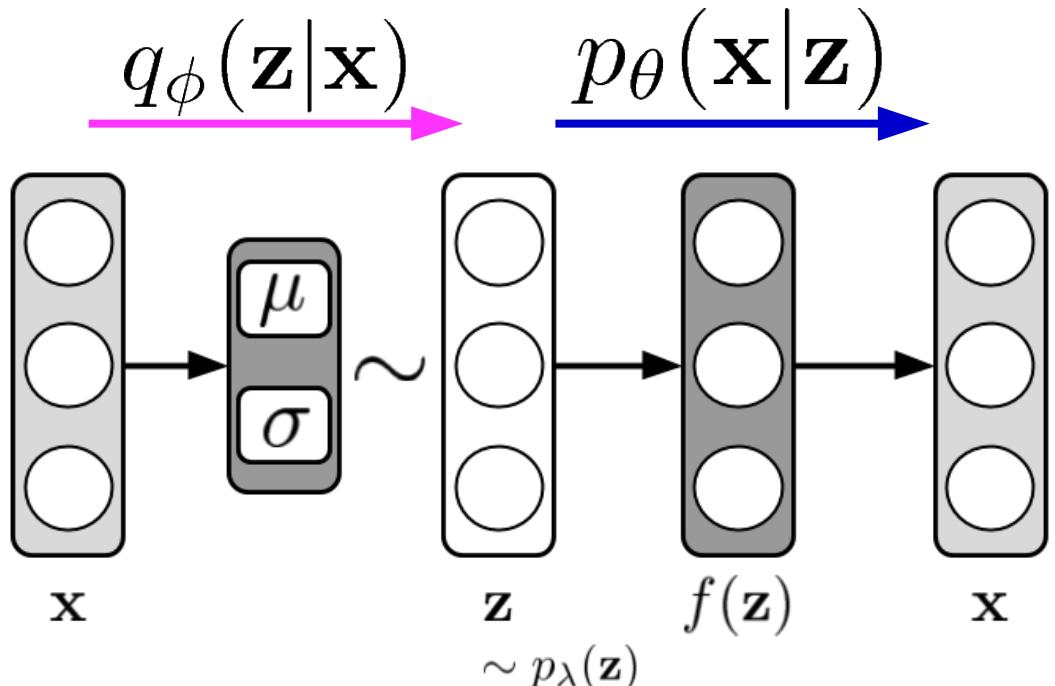
# DGM: Variational Auto-Encoder



Density Network

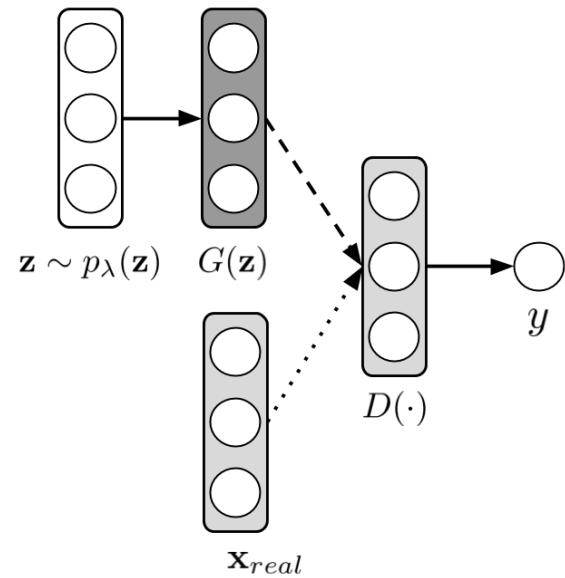
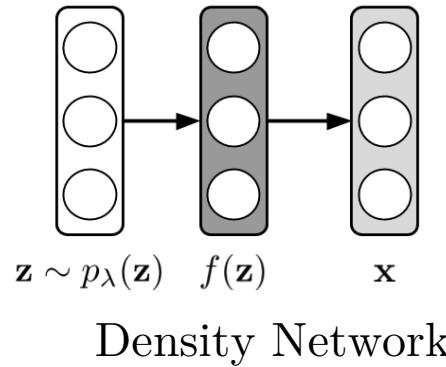


Generative Adversarial Net

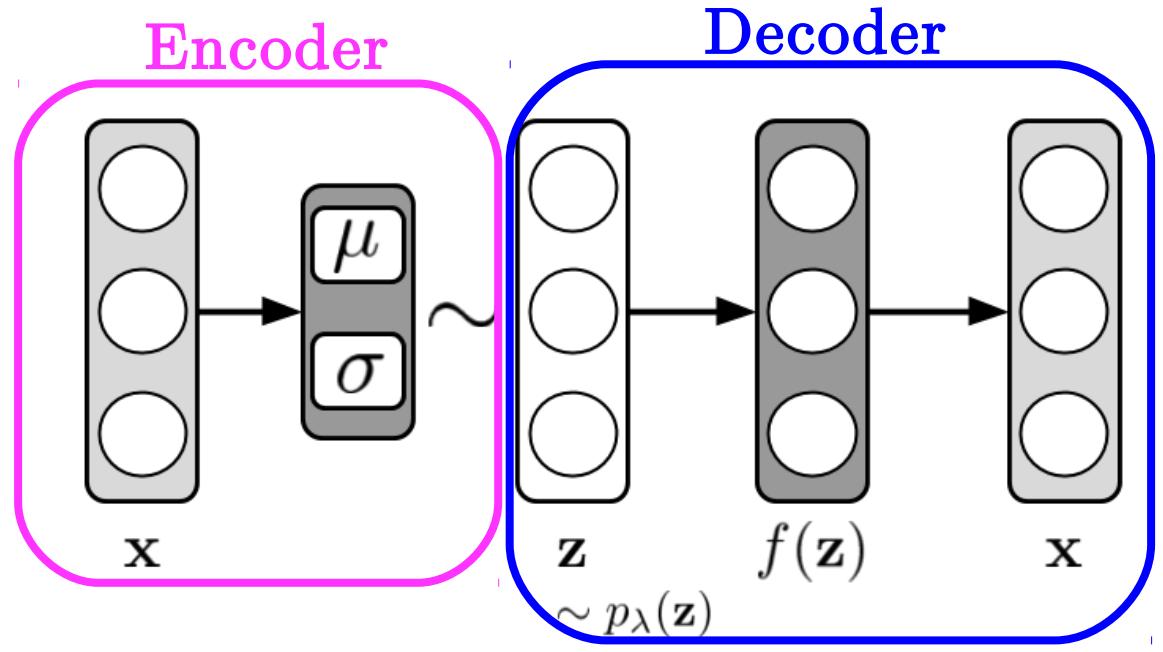


Variational Auto-Encoder

# DGM: Variational Auto-Encoder



Generative Adversarial Net



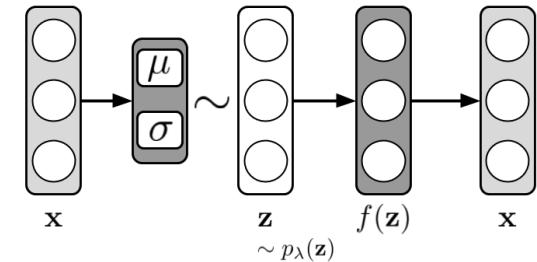
# DGM: Variational Auto-Encoder

$$\log p(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z}) \ dz$$

$$= \log \int \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \ p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z}) \ dz$$

$$\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \ \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \ dz$$

$$= \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}|\mathbf{z})] - \text{KL}[q_{\phi}(\mathbf{z}|\mathbf{x}) || p_{\lambda}(\mathbf{z})]$$



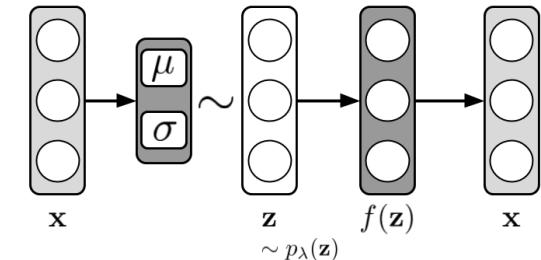
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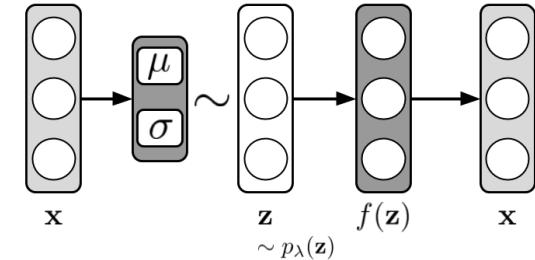
$$\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \ \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \ dz$$

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# DGM: Variational Auto-Encoder

$$\begin{aligned}
 \log p(\mathbf{x}) &= \log \int p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z}) \ d\mathbf{z} \\
 &= \log \int \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \ p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z}) \ d\mathbf{z} \\
 &\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \ \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z}) \ p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \ d\mathbf{z} \\
 &= \underbrace{\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction error}} - \underbrace{\text{KL}[q_{\phi}(\mathbf{z}|\mathbf{x}) || p_{\lambda}(\mathbf{z})]}_{\text{Regularization}}
 \end{aligned}$$



# DGM: Variational Auto-Encoder

Our objective is the evidence lower bound.

$$\log p(\mathbf{x}) \geq \mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \text{KL}[q_\phi(\mathbf{z}|\mathbf{x}) || p_\lambda(\mathbf{z})]$$

We can approximate it using MC sample.

$$\mathcal{L}(\mathbf{x}) \approx \frac{1}{S} \sum_{s=1}^S [\log p_\theta(\mathbf{x}|\mathbf{z}_s) - \log q_\phi(\mathbf{z}_s|\mathbf{x}) + \log p_\lambda(\mathbf{z}_s)]$$

# DGM: Variational Auto-Encoder

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How to properly calculate gradients (*i.e.*, train the model)?

# DGM: Variational Auto-Encoder

$$\mathcal{L}(\mathbf{x}) \approx \frac{1}{S} \sum_{s=1}^S [\log p_\theta(\mathbf{x}|\mathbf{z}_s) - \log q_\phi(\mathbf{z}_s|\mathbf{x}) + \log p_\lambda(\mathbf{z}_s)]$$

**PROBLEM:** calculating gradient wrt parameters of the variational posterior (*i.e.*, sampling process).

# DGM: Variational Auto-Encoder

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**PROBLEM:** calculating gradient wrt parameters of the variational posterior (*i.e.*, sampling process).

**SOLUTION:** use a non-centered parameterization (a.k.a. *reparameterization trick*).

$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\sigma}^2)$$

$$\mathbf{z}_s = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$$

# DGM: Variational Auto-Encoder

$$\mathcal{L}(\mathbf{x}) \approx \frac{1}{S} \sum_{s=1}^S [\log p_\theta(\mathbf{x}|\mathbf{z}_s) - \log q_\phi(\mathbf{z}_s|\mathbf{x}) + \log p_\lambda(\mathbf{z}_s)]$$

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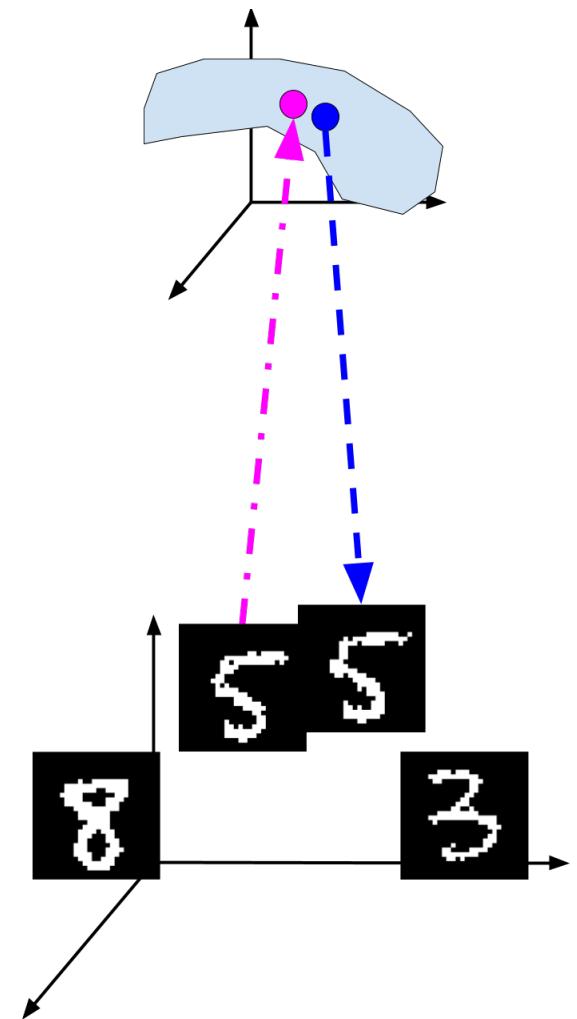
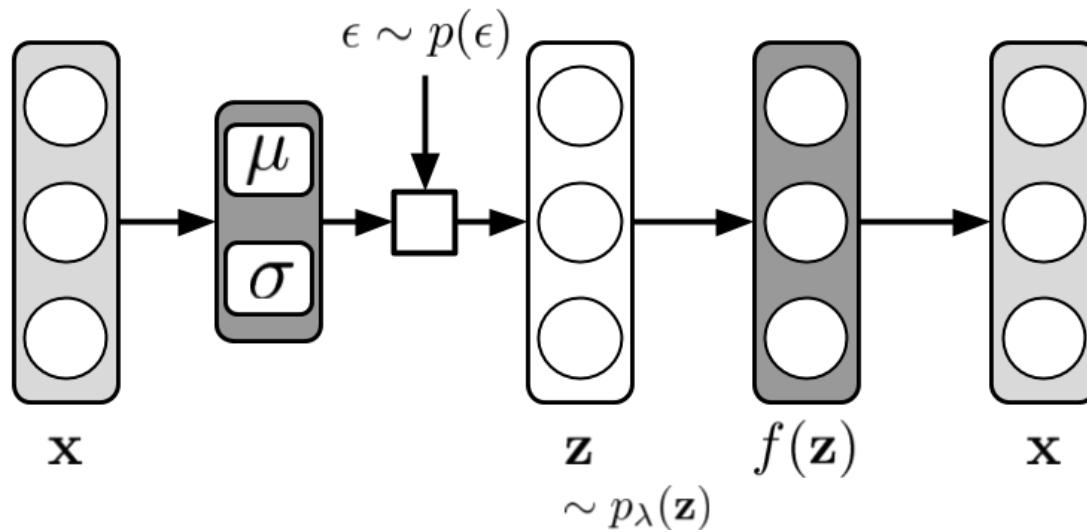
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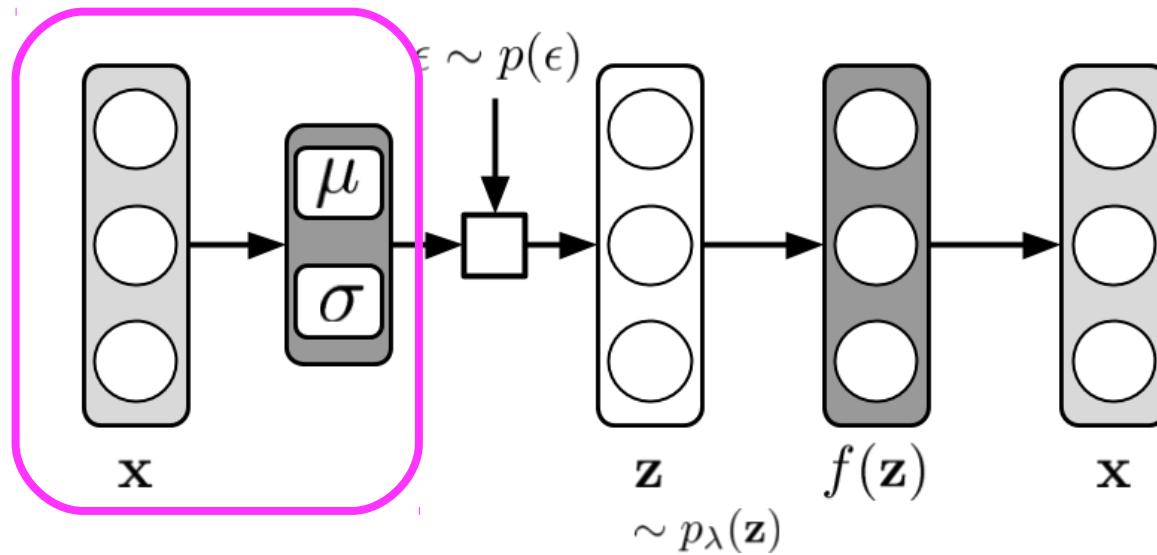
$$\mathbf{z}_s = \boxed{\boldsymbol{\mu}} + \boxed{\boldsymbol{\sigma}} \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$$

Output of a neural network

# DGM: Variational Auto-Encoder

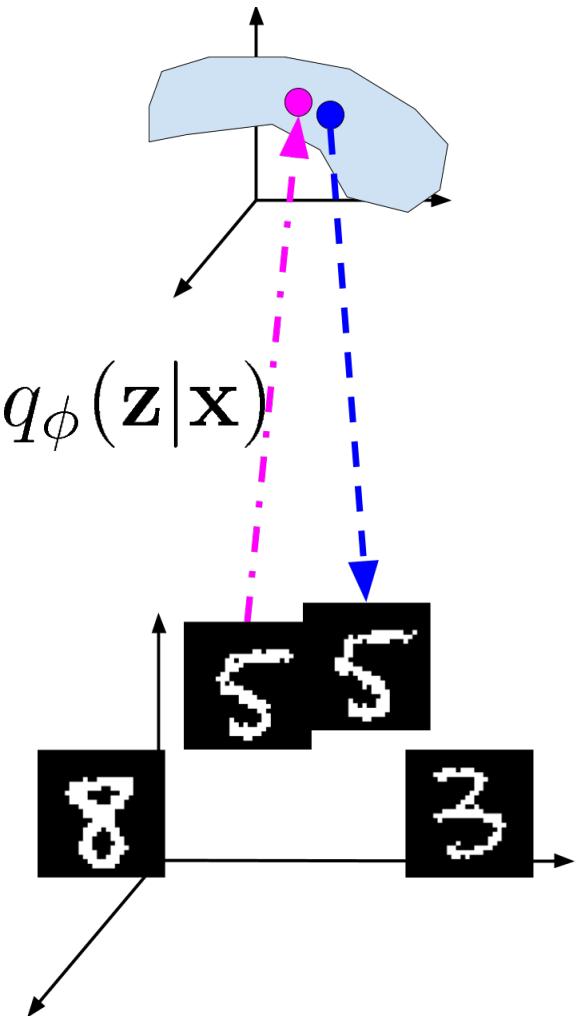


# DGM: Variational Auto-Encoder

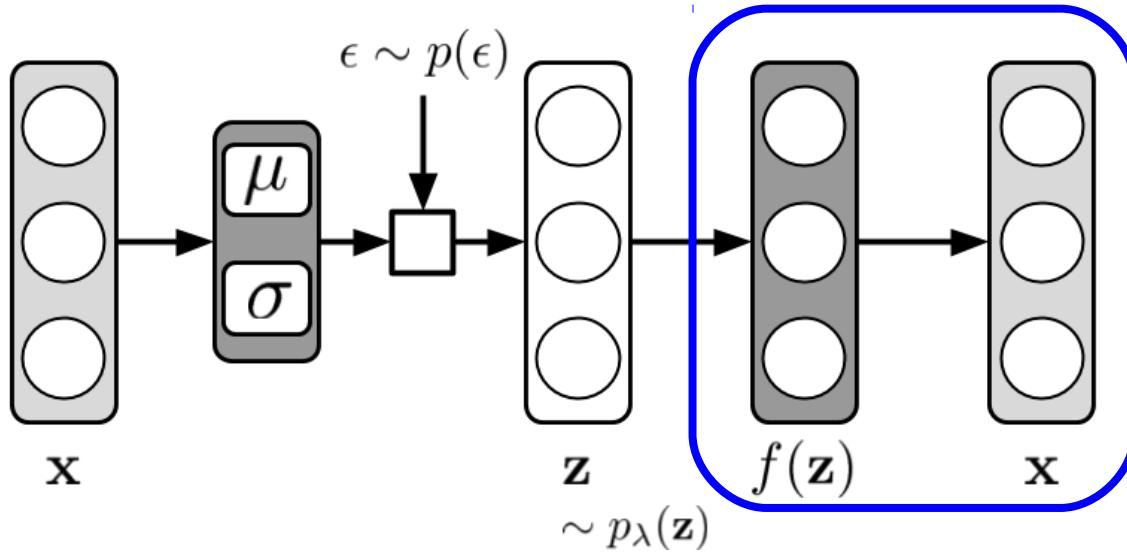


A **deep neural net** that outputs parameters of the variational posterior (**encoder**):

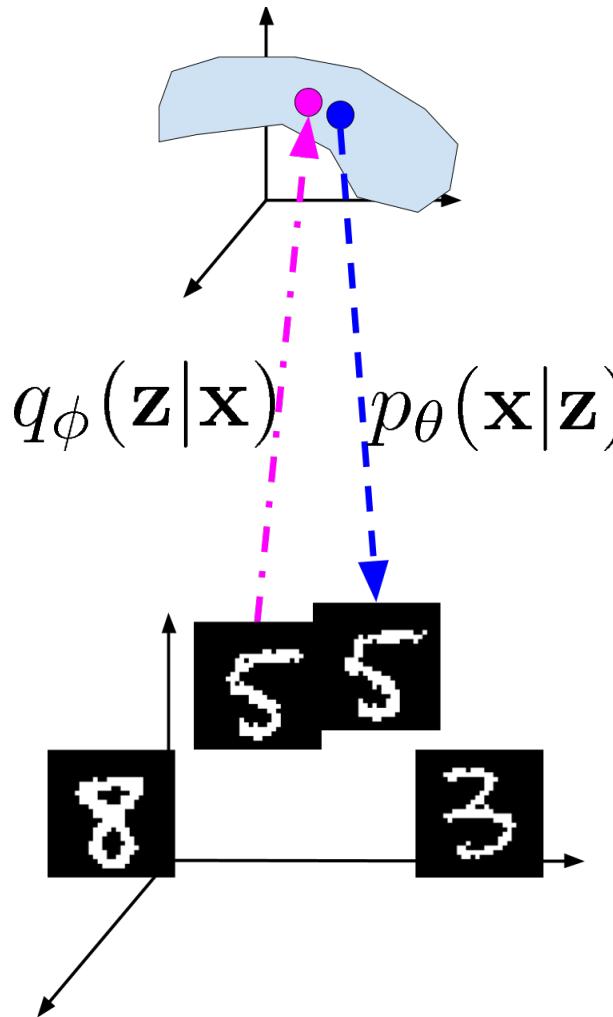
$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z} | \underline{\mu}(\mathbf{x}), \text{diag}\{\underline{\sigma^2}(\mathbf{x})\})$$



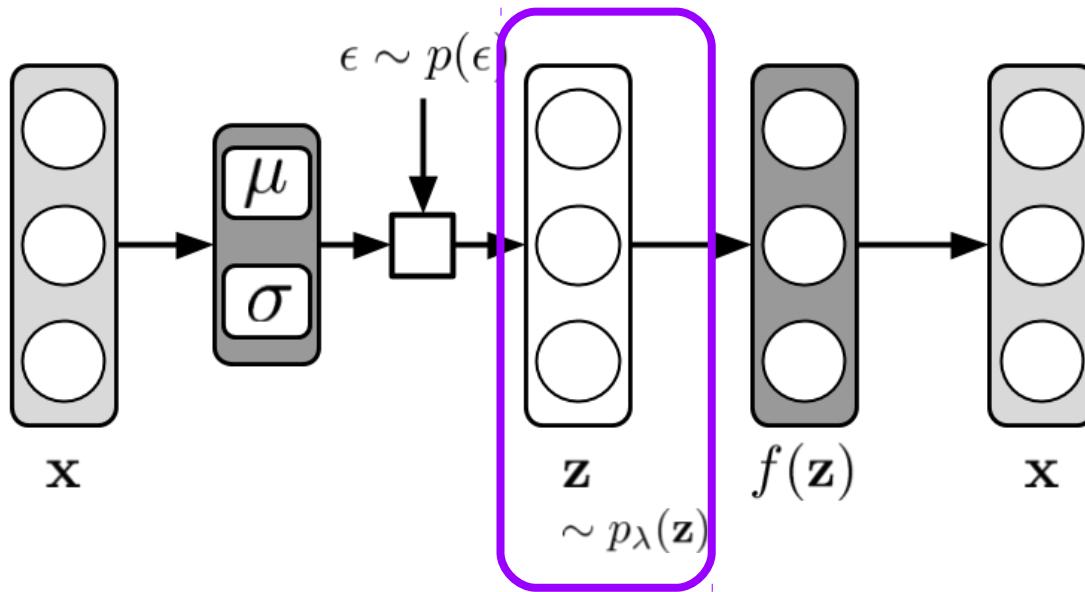
# DGM: Variational Auto-Encoder



A **deep neural net** that outputs parameters of the generator (**decoder**), e.g., a normal distribution or Bernoulli distribution.

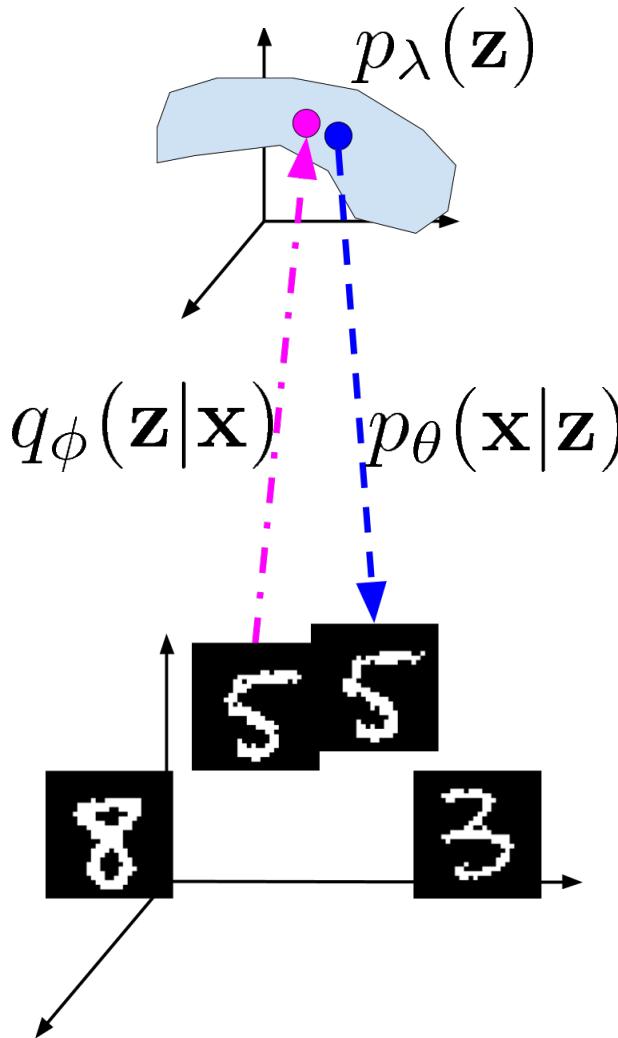


# DGM: Variational Auto-Encoder



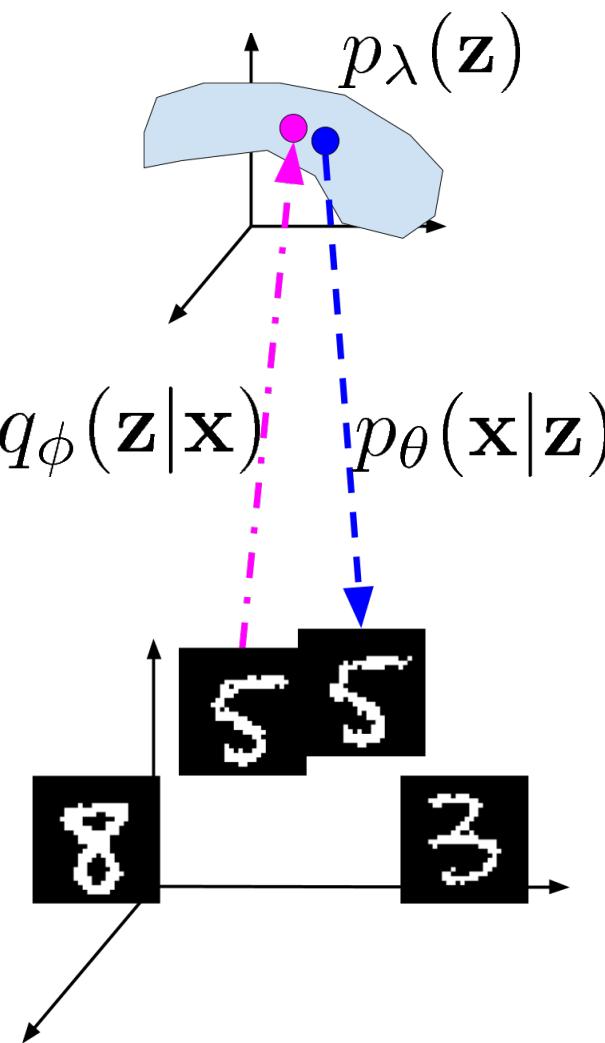
A **prior** that **regularizes** the encoder and takes part in the **generative process**.

$$p_\lambda(z) = \mathcal{N}(z|0, \mathbf{I})$$



# DGM: Variational Auto-Encoder

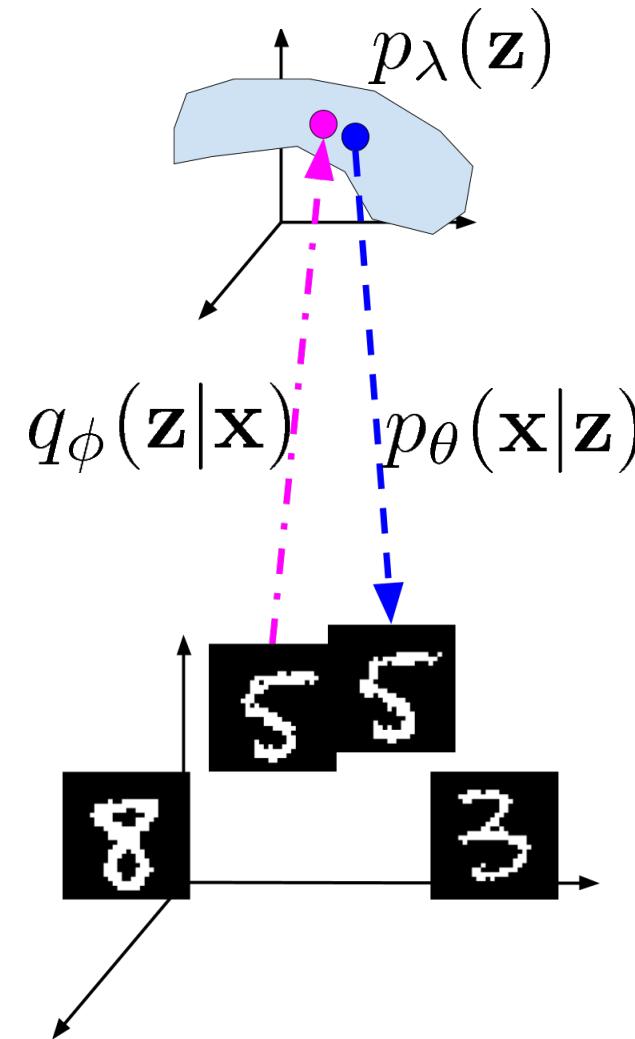
$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z})$$



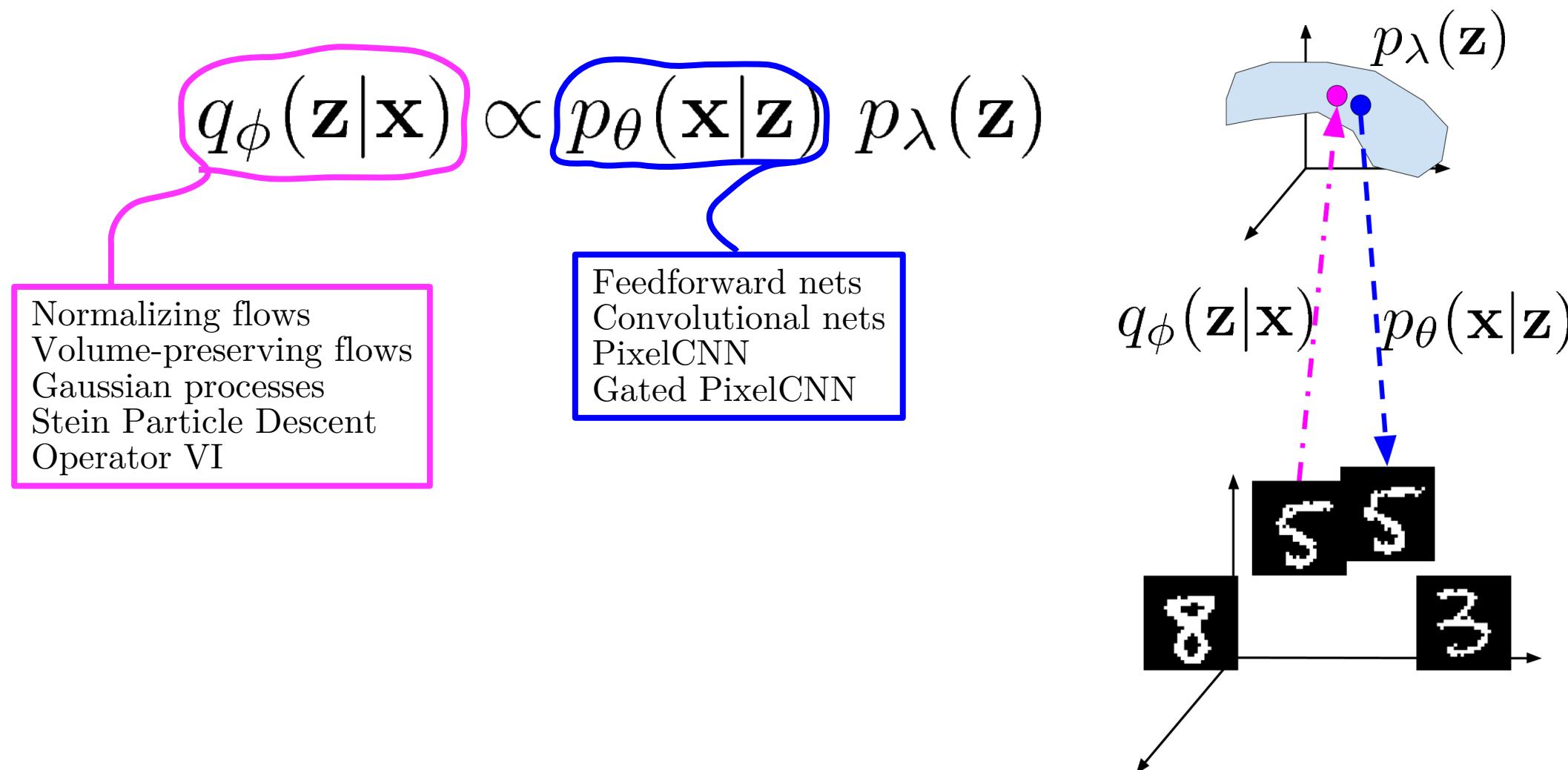
# DGM: Variational Auto-Encoder

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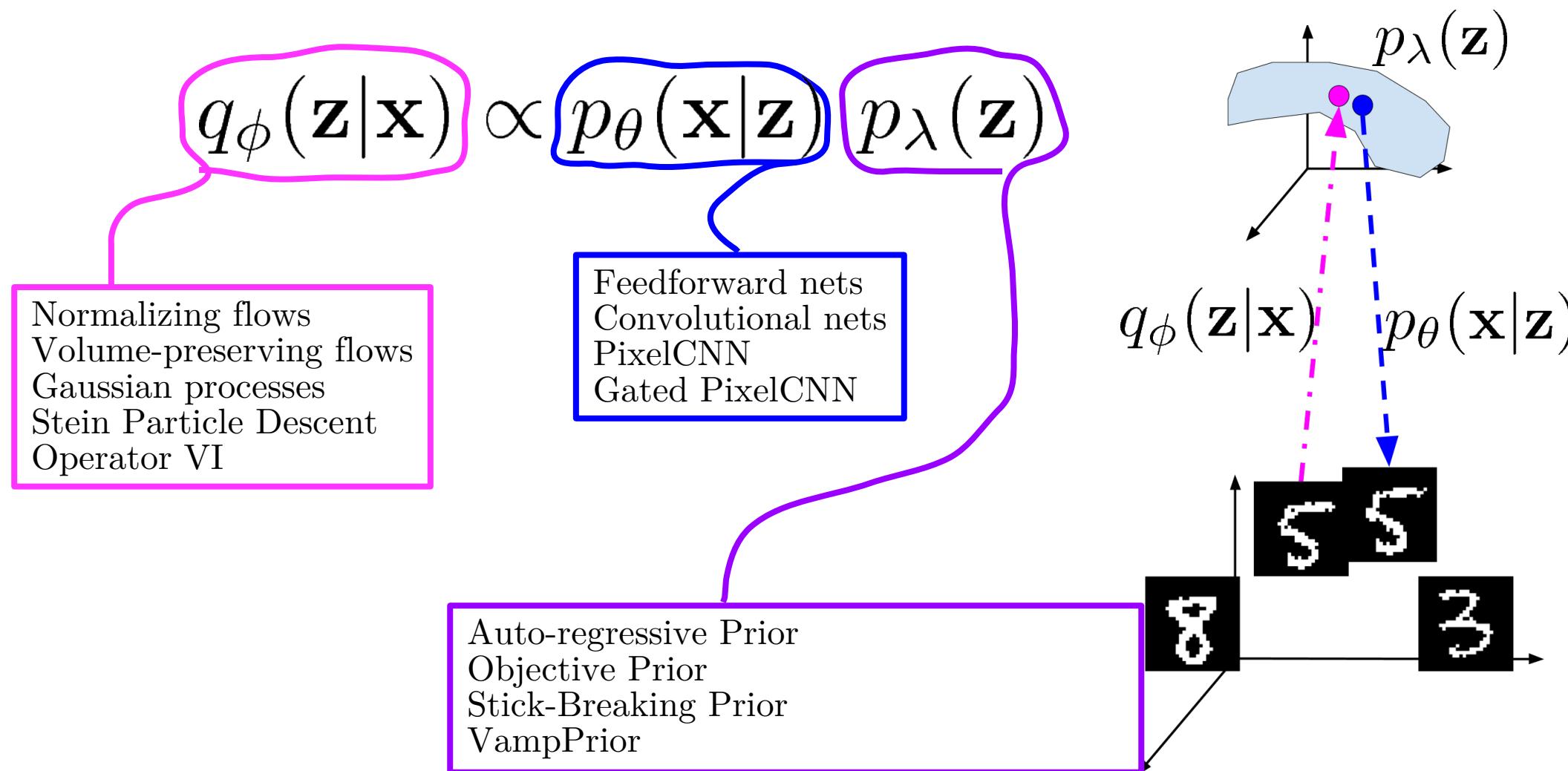
Feedforward nets  
Convolutional nets  
PixelCNN  
Gated PixelCNN



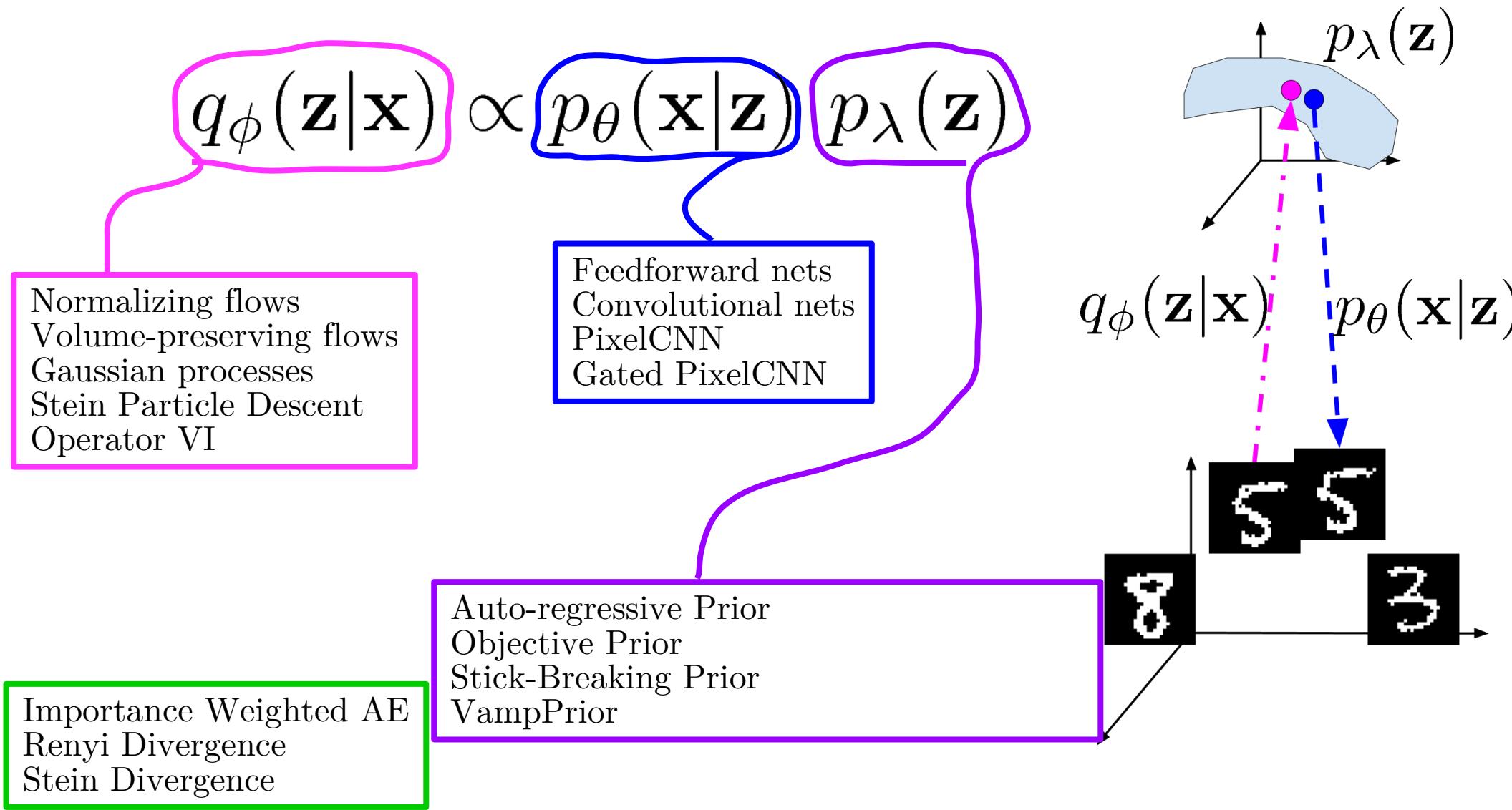
# DGM: Variational Auto-Encoder



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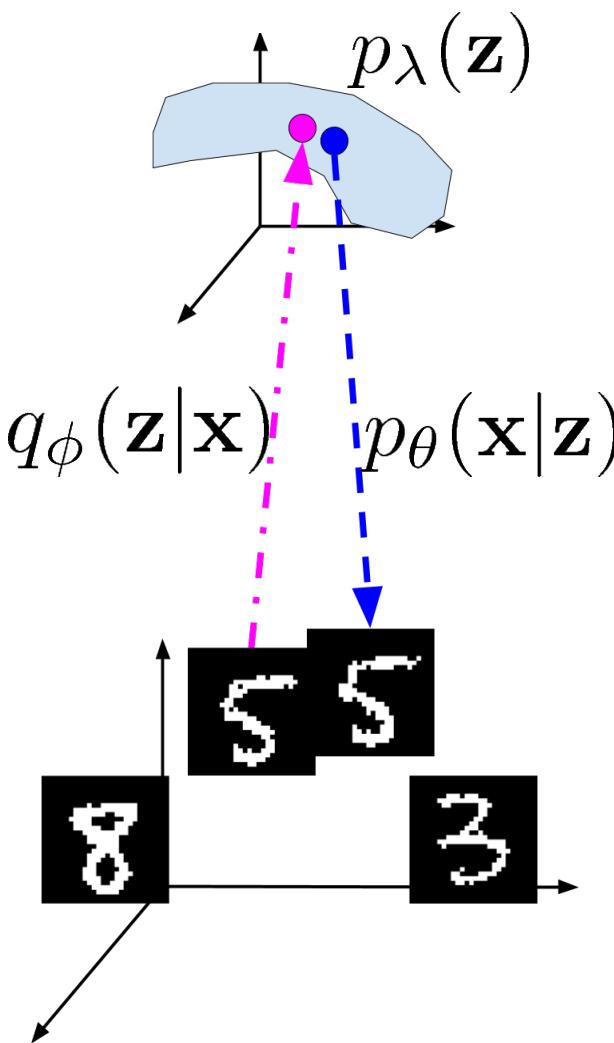


# DGM: Variational Auto-Encoder



# Improving the posterior

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z})$$



# Normalizing flows

- Diagonal posterior – **insufficient** and **inflexible**.
- How to get more flexible posterior?  
→ apply a series of  $T$  invertible transformations  
 $\mathbf{f}^{(t)}$  to  $\mathbf{z}^{(0)} \sim q(\mathbf{z}|\mathbf{x})$ .
- New objective:

$$\ln p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}^{(0)}|\mathbf{x})} \left[ \ln p(\mathbf{x}|\mathbf{z}^{(T)}) + \sum_{t=1}^T \ln \left| \det \frac{\partial \mathbf{f}^{(t)}}{\partial \mathbf{z}^{(t-1)}} \right| \right] - \text{KL}(q(\mathbf{z}^{(0)}|\mathbf{x}) || p(\mathbf{z}^{(T)})).$$

# Normalizing flows

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- New objective:

$$\ln p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}^{(0)}|\mathbf{x})} \left[ \ln p(\mathbf{x}|\mathbf{z}^{(T)}) \right]$$

$$q(\mathbf{z}^{(T)}|\mathbf{x}) = q(\mathbf{z}^{(0)}|\mathbf{x}) \prod_{t=1}^T \left| \det \frac{\partial f^{(t)}}{\partial \mathbf{z}^{(t-1)}} \right|^{-1}$$

# Normalizing flows

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# Normalizing flows

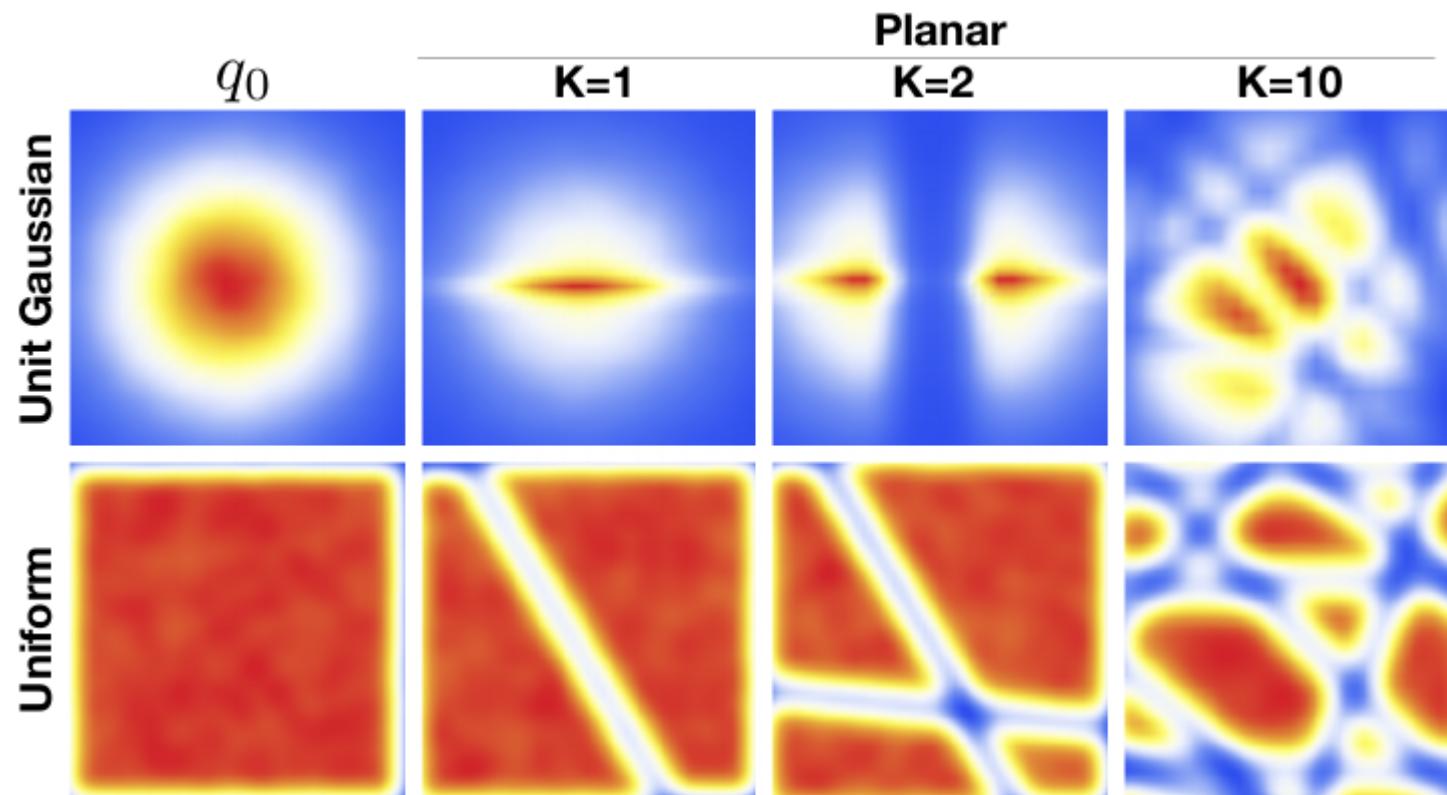
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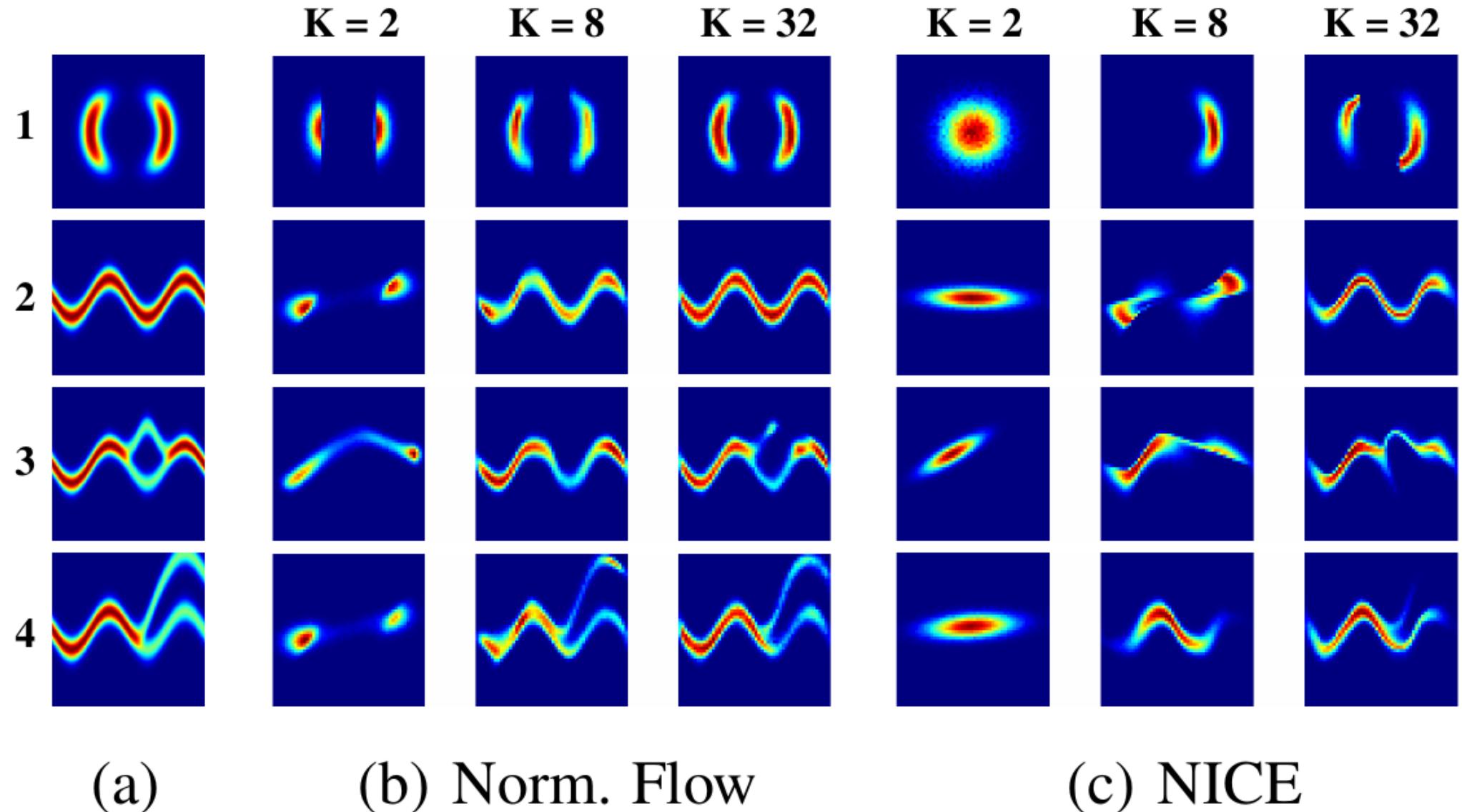
Jacobian-determinant: (i) general normalizing flow ( $|\det J|$  is *easy* to compute)

(ii) volume-preserving flow, i.e.,  $|\det J|=1$

# Normalizing Flow



# Normalizing Flow



# Extensions of normalizing flows

- How to obtain more **flexible** posterior and preserve  $|\det \mathbf{J}|=1$ ?
  - using *orthogonal matrices* → **Householder flow**

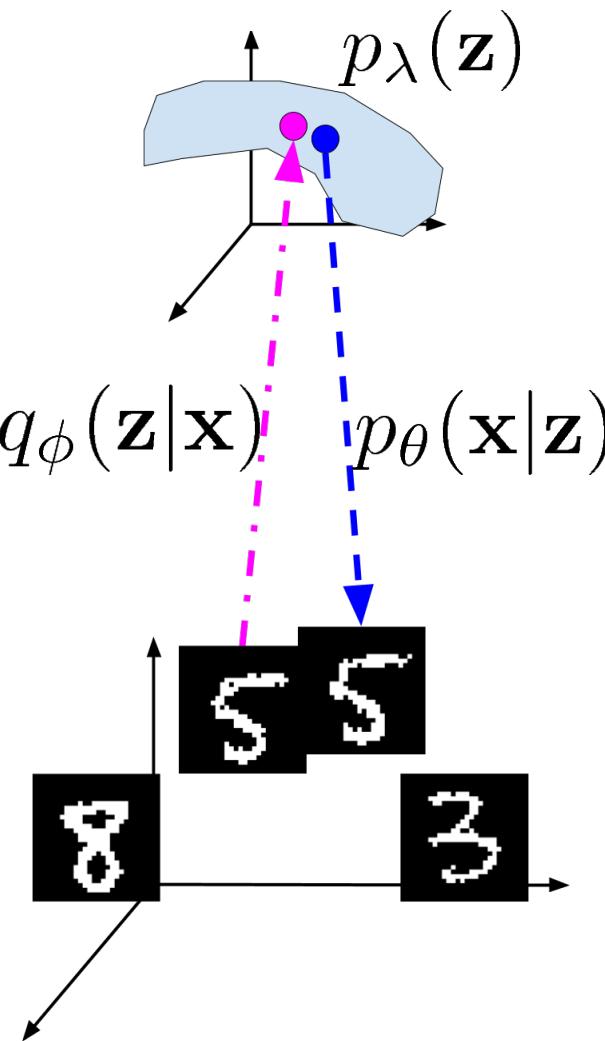
Tomczak, J. M., & Welling, M. (2016). Improving Variational Inference with Householder Flow. arXiv preprint arXiv:1611.09630. NIPS Workshop on Bayesian Deep Learning 2016

- **General** normalizing flow:
  - using *autoregressive model* → **Inverse Autoregressive Flow**

Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., & Welling, M. (2016). Improving Variational Inference with Inverse Autoregressive Flow. NIPS 2016

# Improving the decoder

$$q_\phi(\mathbf{z}|\mathbf{x}) \propto p_\theta(\mathbf{x}|\mathbf{z}) p_\lambda(\mathbf{z})$$

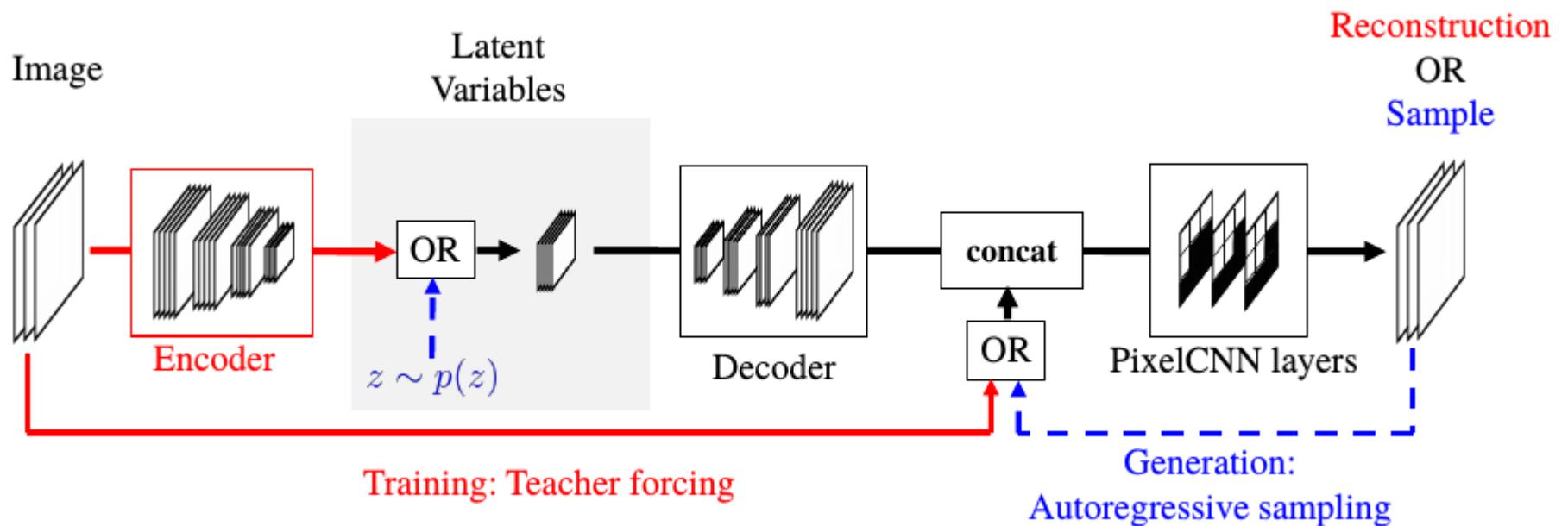


# Improving the decoder

- Dependency only on  $\mathbf{z}$  – **missing correlations**.
- How to get more flexible decoderposterior?  
→ apply **autoregressive model**

$$p(\mathbf{x}|\mathbf{z}) = p(x_1|\mathbf{z}) \prod_{d=2}^D p(x_d|x_1, \dots, x_{d-1}, \mathbf{z})$$

# PixelVAE (PixelCNN + VAE)



# PixelVAE (PixelCNN + VAE)

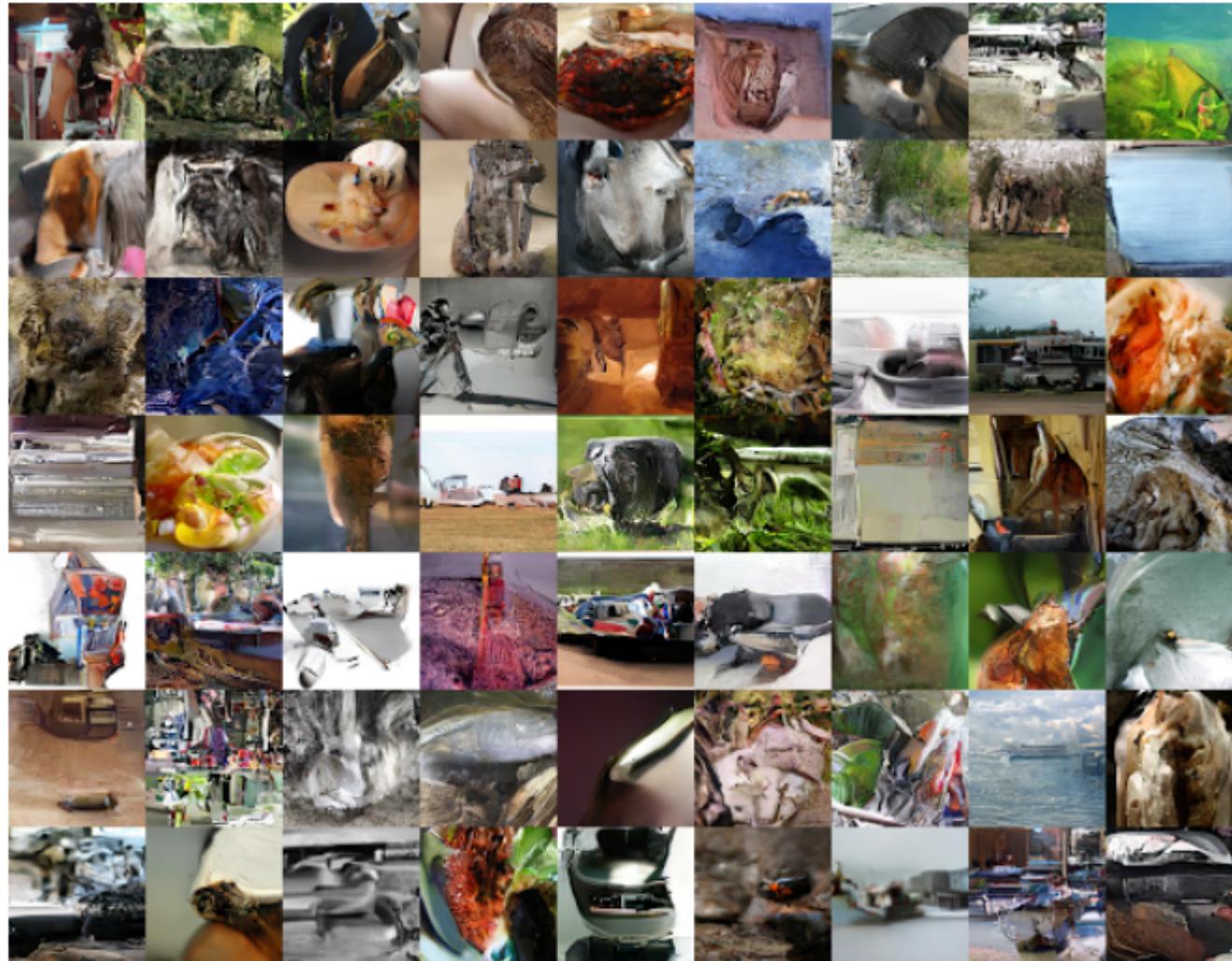
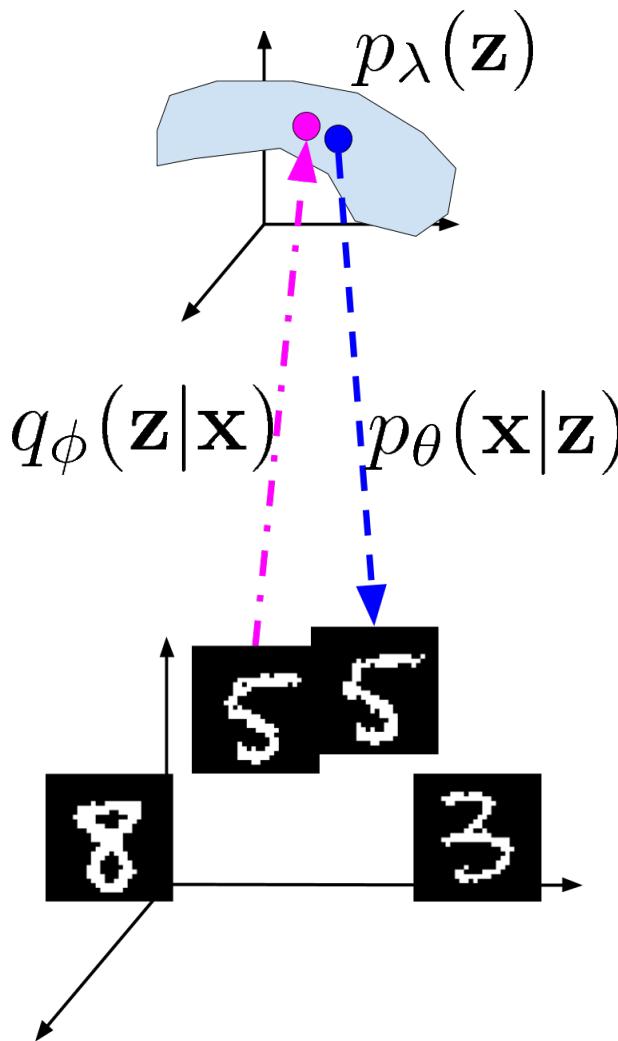


Figure 6: Samples from hierarchical PixelVAE on the 64x64 ImageNet dataset.

# Improving the prior

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\lambda}(\mathbf{z})$$



# Improving the prior

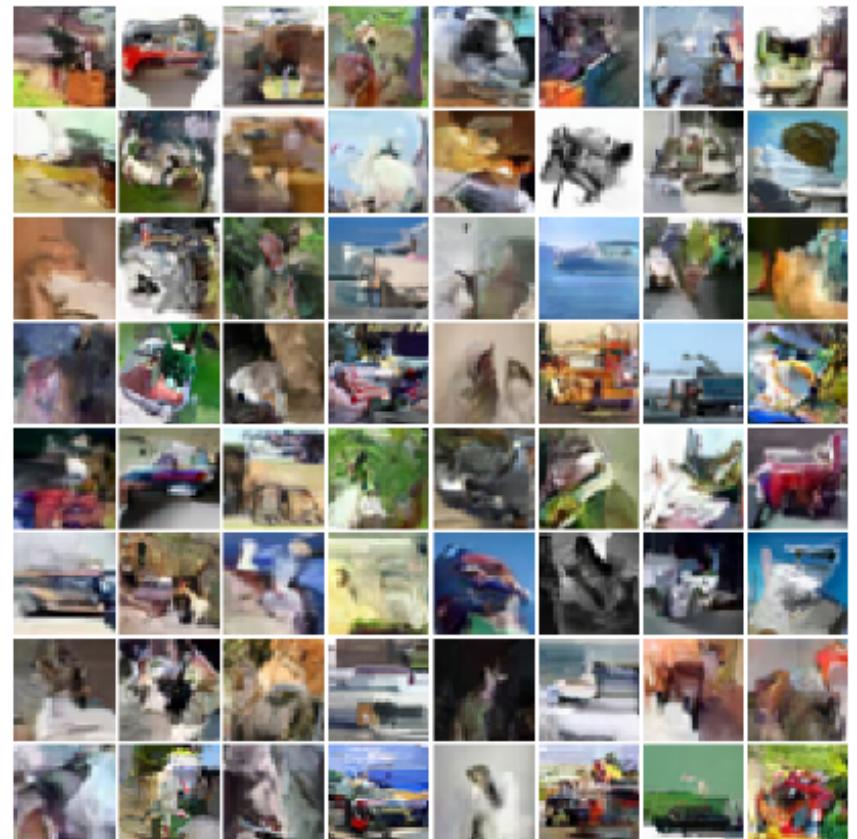
- Standard normal prior – **unimodal, too restrictive.**
- How to get more flexible prior?  
→ apply **autoregressive prior**

Chen, X., Kingma, D. P., Salimans, T., Duan, Y., Dhariwal, P., Schulman, J., ... & Abbeel, P. (2016). Variational lossy autoencoder. arXiv preprint arXiv:1611.02731.

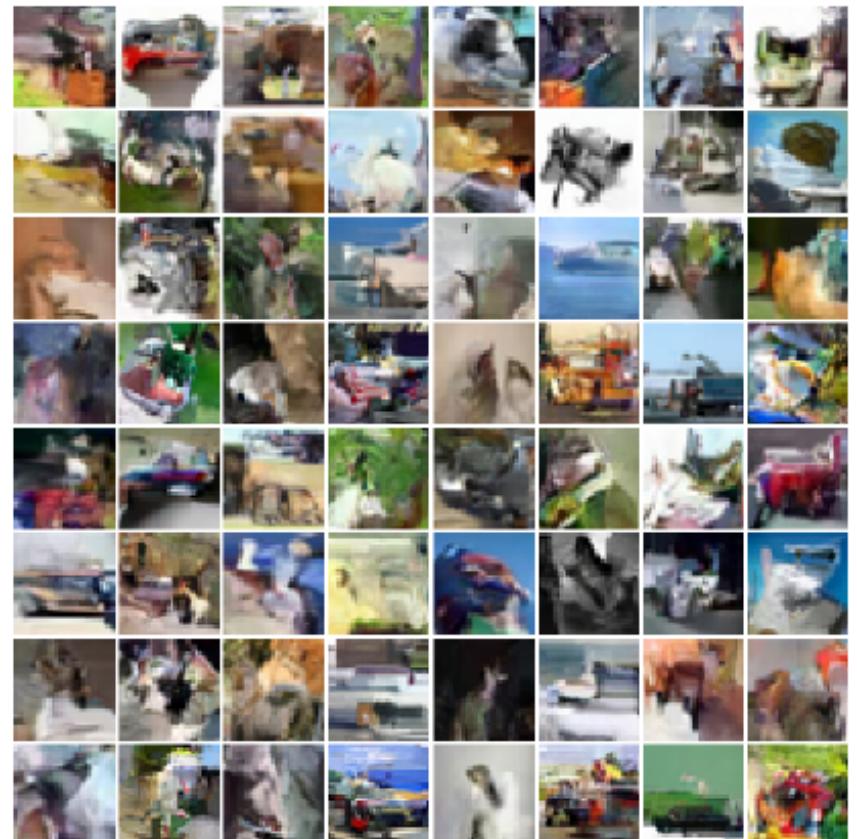
→ apply **variational mixture of posteriors (VampPrior)**

Tomczak, J. M., & Welling, M. (2017). VAE with a VampPrior. arXiv preprint arXiv:1705.07120.

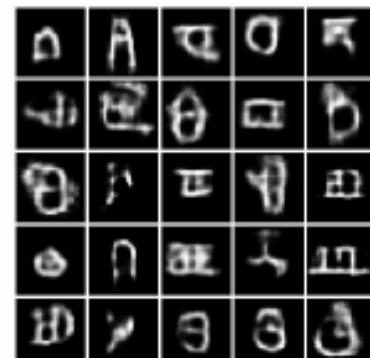
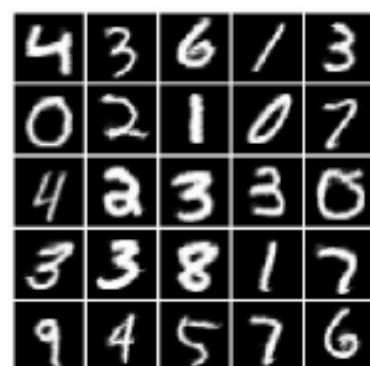
# Autoregressive prior



# Autoregressive prior



# VampPrior



(a) real data

(b) VAE

(c) HVAE + VampPrior

(d) convHVAE + VampPrior

# Some extensions and applications of VAE

- Semi-supervised learning with VAE.

Kingma, D. P., Mohamed, S., Rezende, D. J., & Welling, M. (2014). *Semi-supervised learning with deep generative models*. NIPS

- VAE for sequences.

Bowman, S. R., Vilnis, L., Vinyals, O., Dai, A. M., Jozefowicz, R., & Bengio, S. (2015). *Generating sentences from a continuous space*. arXiv preprint arXiv:1511.06349.

Chung, J., Kastner, K., Dinh, L., Goel, K., Courville, A. C., & Bengio, Y. (2015). *A recurrent latent variable model for sequential data*. NIPS

- More powerful decoders (using PixelCNN).

Gulrajani, I., Kumar, K., Ahmed, F., Taiga, A. A., Visin, F., Vazquez, D., & Courville, A. (2016). *PixelVAE: A latent variable model for natural images*. arXiv preprint arXiv:1611.05013.

Chen, X., Kingma, D. P., Salimans, T., Duan, Y., Dhariwal, P., Schulman, J., ... & Abbeel, P. (2016). *Variational lossy autoencoder*. arXiv preprint arXiv:1611.02731.

# Some extensions and applications of VAE

- Applications: graph data

Kipf, T. N., & Welling, M. (2016). *Variational Graph Auto-Encoders*. arXiv preprint arXiv:1611.07308. NIPS Workshop

Berg, R. V. D., Kipf, T. N., & Welling, M. (2017). *Graph Convolutional Matrix Completion*. arXiv preprint arXiv:1706.02263.

- Applications: drug response prediction

Rampasek, L., & Goldenberg, A. (2017). *Dr. VAE: Drug Response Variational Autoencoder*. arXiv preprint arXiv:1706.08203.

- Applications: text generation

Yang, Z., Hu, Z., Salakhutdinov, R., & Berg-Kirkpatrick, T. (2017). *Improved Variational Autoencoders for Text Modeling using Dilated Convolutions*. arXiv preprint arXiv:1702.08139.

# DGM: VAE

## PROS

Log-likelihood framework

Easy sampling

Training using gradient-based methods

Stable training

Discovers latent representation

Could be easily combined with other probabilistic frameworks

## CONS

Only explicit models

Produces blurry images(?)

1283 + 1146

*Number of citations\* of seminal papers on  
GANs and VAE.*

\*According to GoogleScholar, 26.09.2017

In order to *make better decisions*, we need a *better understanding* of *reality*.

=

generative modeling

**Web-page:**

<https://jmtomczak.github.io>

**Code on github:**

<https://github.com/jmtomczak>

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