Generative models: An introduction

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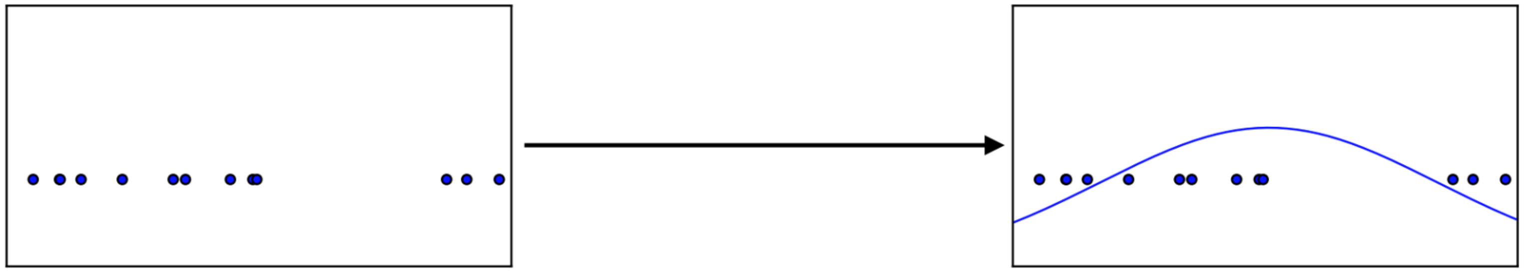
Generative models

- Training data $D = \{x_1, \ldots, x_N\} \sim p_{data}(x)$

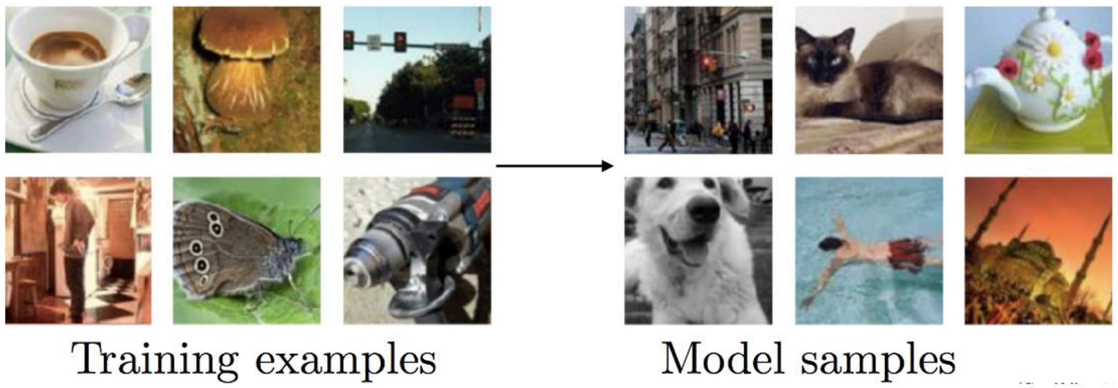
- Result: distribution $p_{model}(x) \cong p_{data}(x)$

Generative models

- $p_{model}(x)$ directly



- Generate samples from $p_{model}(x)$



Applications

- Additional training data
- Missing values
- Semi-supervised learning
- Reinforcement learning
- Multiple correct answers
- Text-to-Image Synthesis
- Learn useful embeddings
- ...

Maximum likelihood

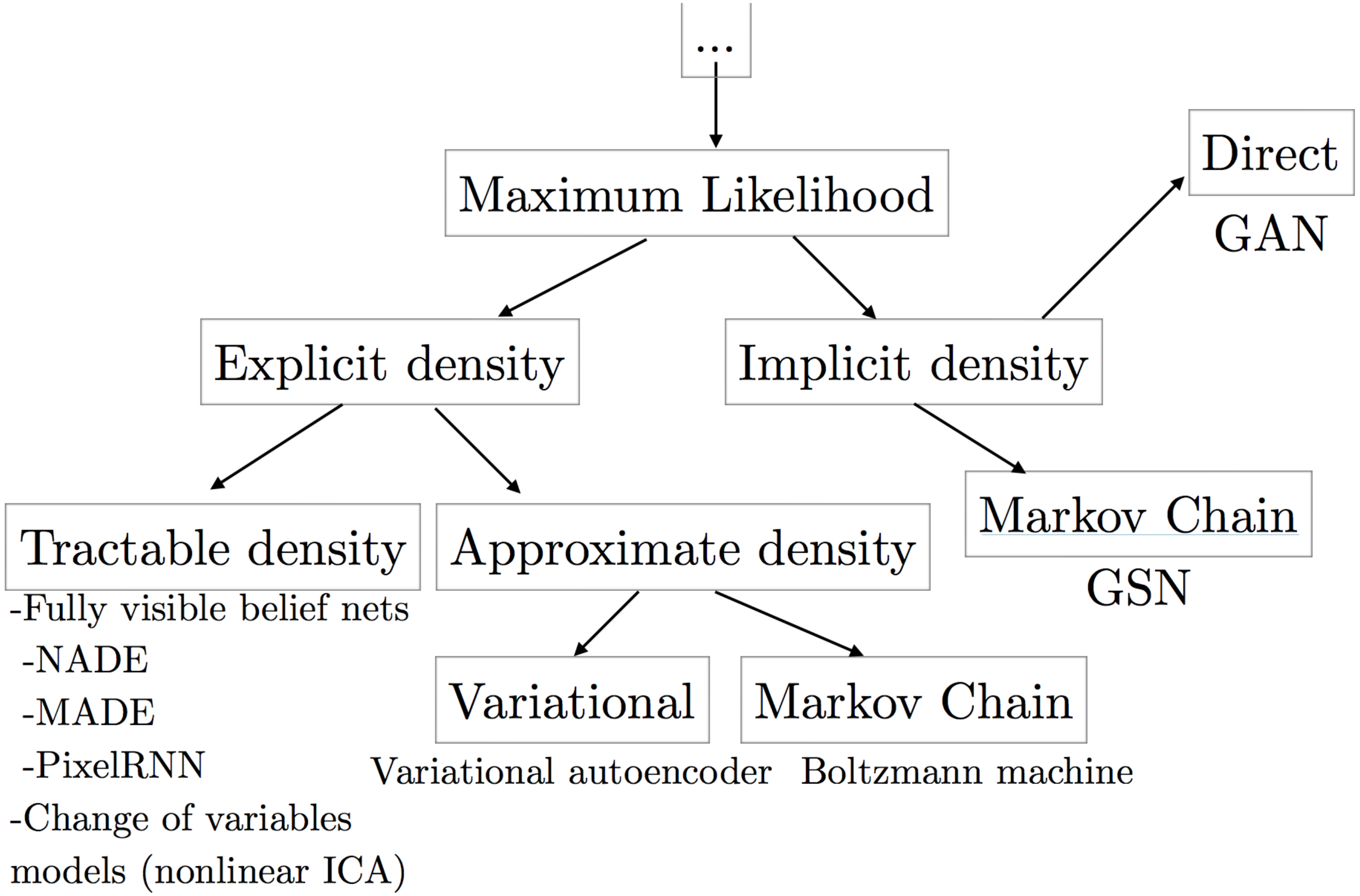
- Maximum likelihood :

$$\begin{aligned}\boldsymbol{\theta}^* &= \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{\text{model}}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right) \\ &= \arg\max_{\boldsymbol{\theta}} \log \prod_{i=1}^{m} p_{\text{model}}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right) \\ &= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{m} \log p_{\text{model}}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right).\end{aligned}$$

- Minimize Kullback-Leibler divergance:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} D_{\text{KL}}\left(p_{\text{data}}(\boldsymbol{x}) \| p_{\text{model}}(\boldsymbol{x}; \boldsymbol{\theta})\right)$$

Generative models



Explicit density

- Probability density : $p_{model}(x;\ \theta)$
- How to design $p_{model}(x;\ \theta)$?
    - Tractable density
    - Approximate density

Tractable density

- Fully visible belief networks:

$$p_{model}(x) = \prod_{i=1}^{n} p_{model}\,(x_i|x_1, \dots, x_{i-1})$$

- WaveNet, NADE, RNN, PixelRNN, PixelCNN
- Disadvantages:
  - O(n) sample generation
  - Non parallelizable sample generation
  - Generation not controlled by a latent code

Tractable density

- Nonlinear independent component analysis
- Continuous, differentiable, invertible transformation g between X i Z, $x = g(z)$:

$$p_x(x) = p_z(g^{-1}(x)) \left| \det\left(\frac{\partial g^{-1}(x)}{\partial x}\right) \right|$$

- Disadvantages:
  - Choosing transformation g
  - dim(X) = dim(Z)

Approximate density

- Deterministic approximation (variational methods)
- Lower bound:

$$\mathcal{L}(x;\, \theta) \leq log p_{model}(x;\, \theta)$$

- Computationally tractable for carefully designed lower bound
- Disadvantages:
  - gap between lower bound and true likelihood

Approximate density

- Stochastic approximation (Deep Boltzmann Machines)
- Markov chain Monte Carlo:

$$x' \sim q(x'|x)$$

- Disadvantages:
  - Slow convergence
  - Curse of dimensionality
  - Slow sample generation

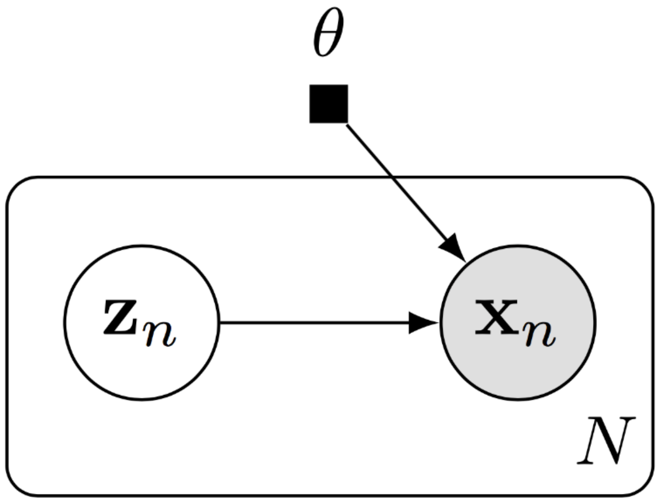
Implicit density

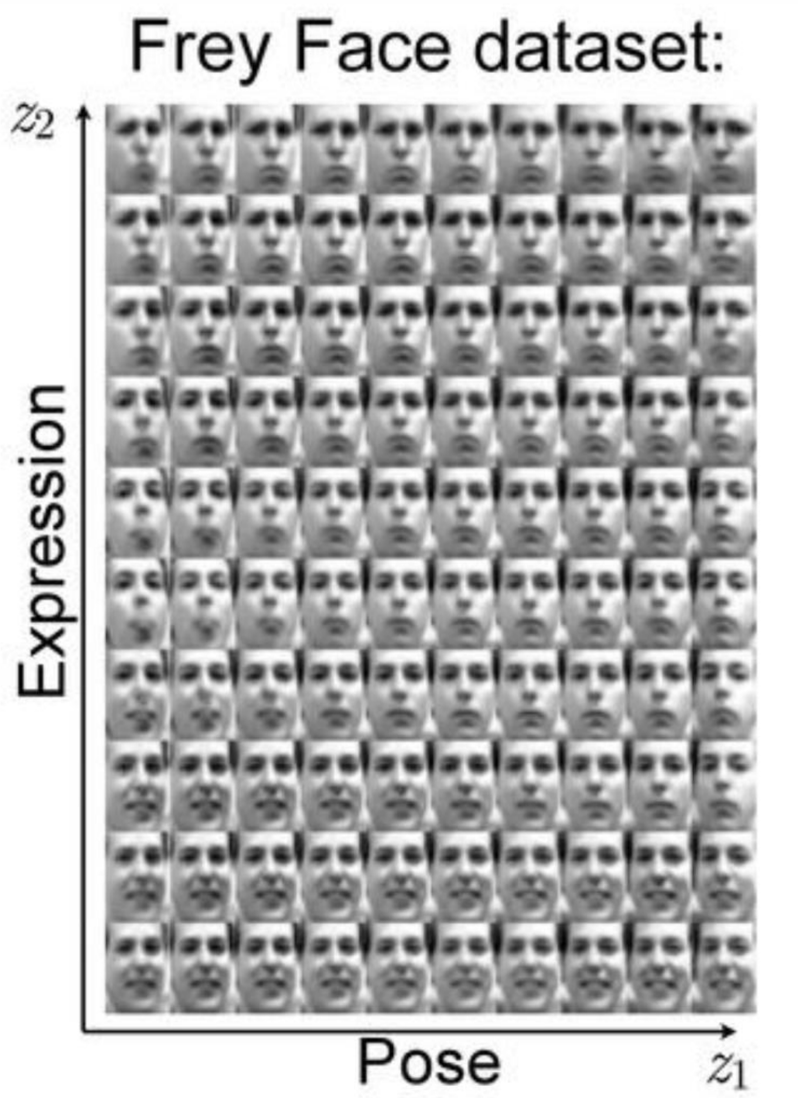
- Sample generation from $p_{model}(x;\ \theta)$
  - Markov chain
    - Generative Stochastic Network
    - Disadvantages: slow sample generation for high dimensional data
  - Sample generation in a single step
    - GAN

Models with latent variables

- x – observed variables
- z – latent variables

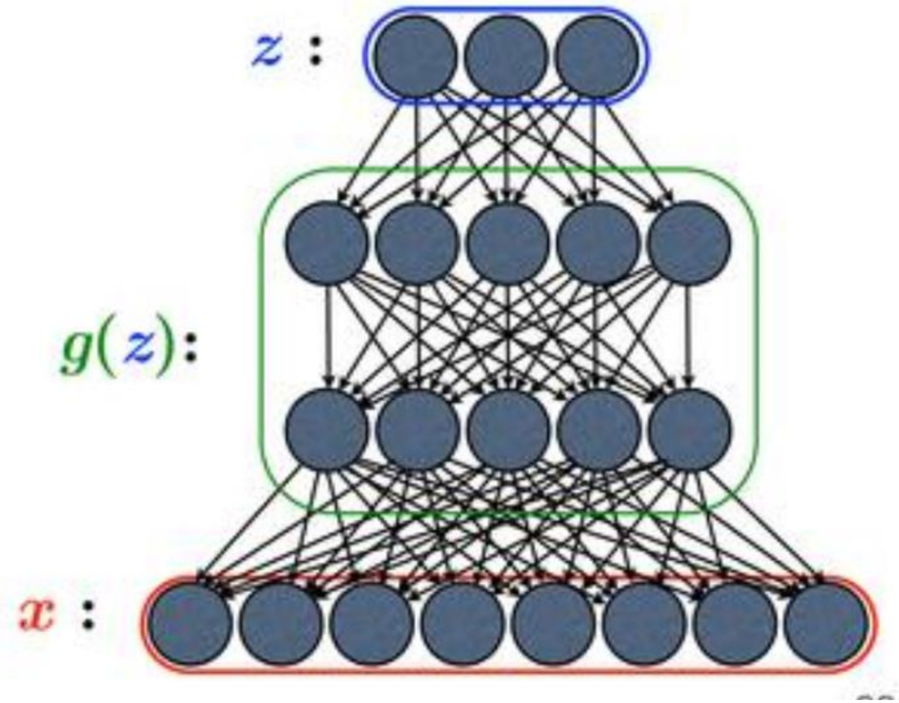
$$p_{model}(x) = \int p_{model}(x, z) dz$$





Models with latent variables

- $p(x, z;\ \theta) = p(x|z;\ \theta)p(z)$
- $p(z)$ - simple distribution
- $p(x|z;\ \theta)$ = $g(z)$ – neural network



Expectation Maximization

$$lnp(x;\ \theta) = \mathcal{L}(q;\ \theta) + KL(q||p)$$

$$\mathcal{L}(q;\ \theta) = \int_z q(z)\ln(\frac{p(x,z|\theta)}{q(z)})$$

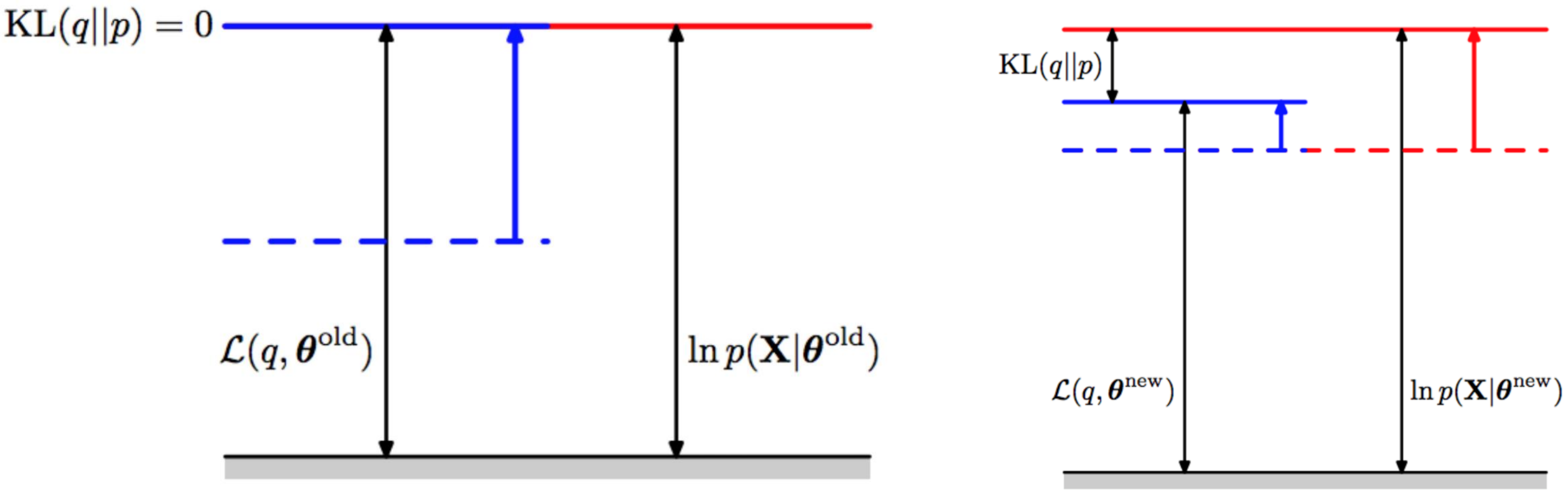
$$KL(q||p) = -\int_z q(z)\ln(\frac{p(z|x,\theta)}{q(z)})$$

$$KL(q||p) \geq 0, KL(q||p) = 0 \ \Leftrightarrow q(z) = p(z|x,\theta)$$

$\mathcal{L}(q;\ \theta) = lnp(x|\theta) - KL(q||p) \leq lnp(x|\theta)$ lower bound

Expectation Maximization

- E step: for fixed parameters θ^{old}, maximize $\mathcal{L}(q;\ \theta)$ with respect to q: $q(z) = p(z|x; \theta^{old})$
- M step: for fixed $q(z)$ maximize $\mathcal{L}(q;\ \theta)$ with respect to θ



Variational Inference

Problems:

- E step: evaluation of $p(z|x;\theta^{old})$
- M step: compute expectation with respect to $p(z|x;\theta^{old})$

Solutions:

- Stochastic approximation: Markov chain Monte Carlo
- Deterministic approximation: parametrize $q(z;\ \omega)$ i minimize $KL(q||p)$

Variational Autoencoders

- $p(x) = \int_z p(x, z;\ \theta) = \int_z p(x|z;\ \theta)p(z)$
- How to define the latent variables z?
  - $z_i \sim N(0, 1)$ independent
- How to calculate integral?
  - Sample $\{z_1, z_2, \ldots, z_N\}$ and calculate $p(x) \approx \frac{1}{N}\sum_{i=1}^{N} p(x|z_i)$
  - $q(z|x;\ \omega) \sim p(z|x; \theta)$

Variational Autoencoder

$$lnp(x;\theta) - KL(q(z|x;\omega)||p(z|x;\theta)) = \int_z q(z|x;\omega)\ln(\frac{p(x,z;\theta)}{q(z|x;\omega)})$$

$$lnp(x;\theta) - KL(q(z|x;\omega)||p(z|x;\theta)) = \int_z q(z|x;\omega)\ln(\frac{p(x|z;\theta)p(z)}{q(z|x;\omega)})$$

$$lnp(x;\theta) - KL(q(z|x;\omega)\big|\big|p(z|x;\theta)\big) = \int_z q(z|x;\omega)\ln p(x|z;\theta) + \int_z q(z|x;\omega)\ln\left(\frac{p(z)}{q(z|x;\omega)}\right)$$

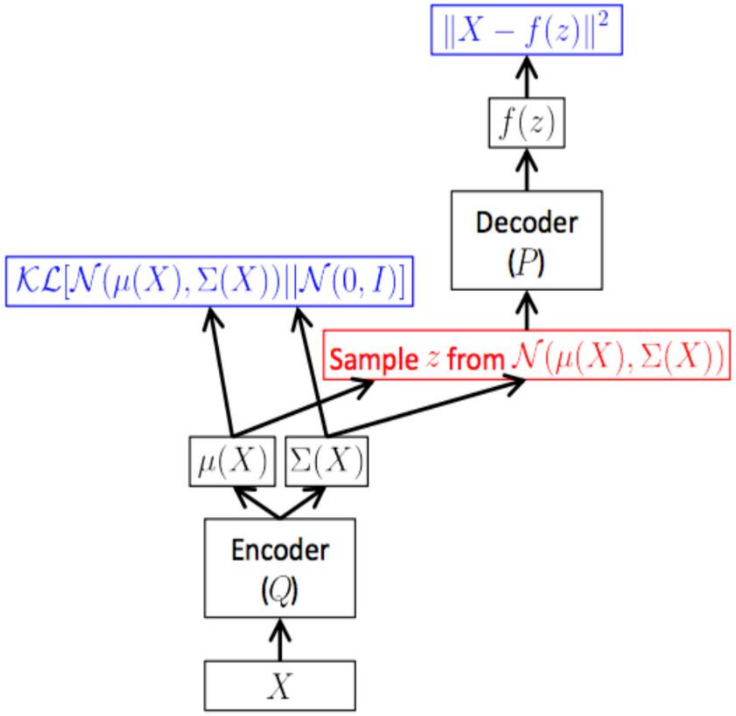
$$lnp(x;\theta) - KL(q(z|x;\omega)\big|\big|p(z|x;\theta)\big) = E_{z\sim q(Z|x;\,\omega)}[lnp(x|z;\theta)] - KL(q(z|x;\omega)|p(z))$$

$$\mathcal{L}(x;\omega,\theta) = E_{z\sim q(Z|x;\,\omega)}[lnp(x|z;\theta)] - KL(q(z|x;\omega)|p(z))$$

Stochastic gradient descent

- $q(z|x;\omega) = N(\mu(x;\omega), \Sigma(x;\omega))$, $\mu(x;\omega), \Sigma(x;\omega)$ neural network
- $KL(N(\mu(x), \Sigma(x)) || N(0,1)) = \frac{1}{2}(Tr(\Sigma(x)) + \mu^T(x)\mu(x) - k - logdet\Sigma(x))$
- $E_{z \sim q(z|x;\,\omega)}[lnp(x|z;\theta)] \cong lnp(x|z_i;\theta), z_i \sim q(z|x;\omega)$
- Maximize using stochastic gradient descent:

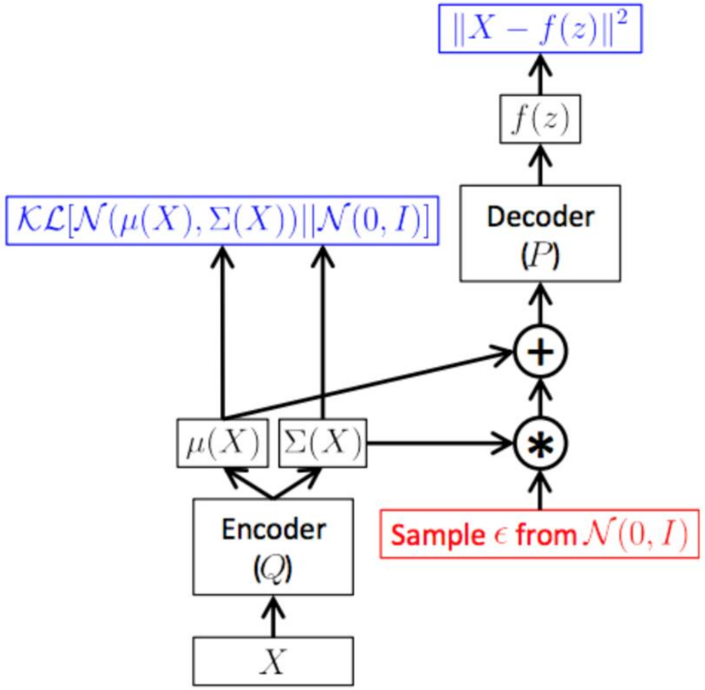
$$E_{x \sim D}[E_{z \sim q(z|x;\,\omega)}[lnp(x|z;\theta)] - KL(q(z|x;\omega)||p(z))]$$



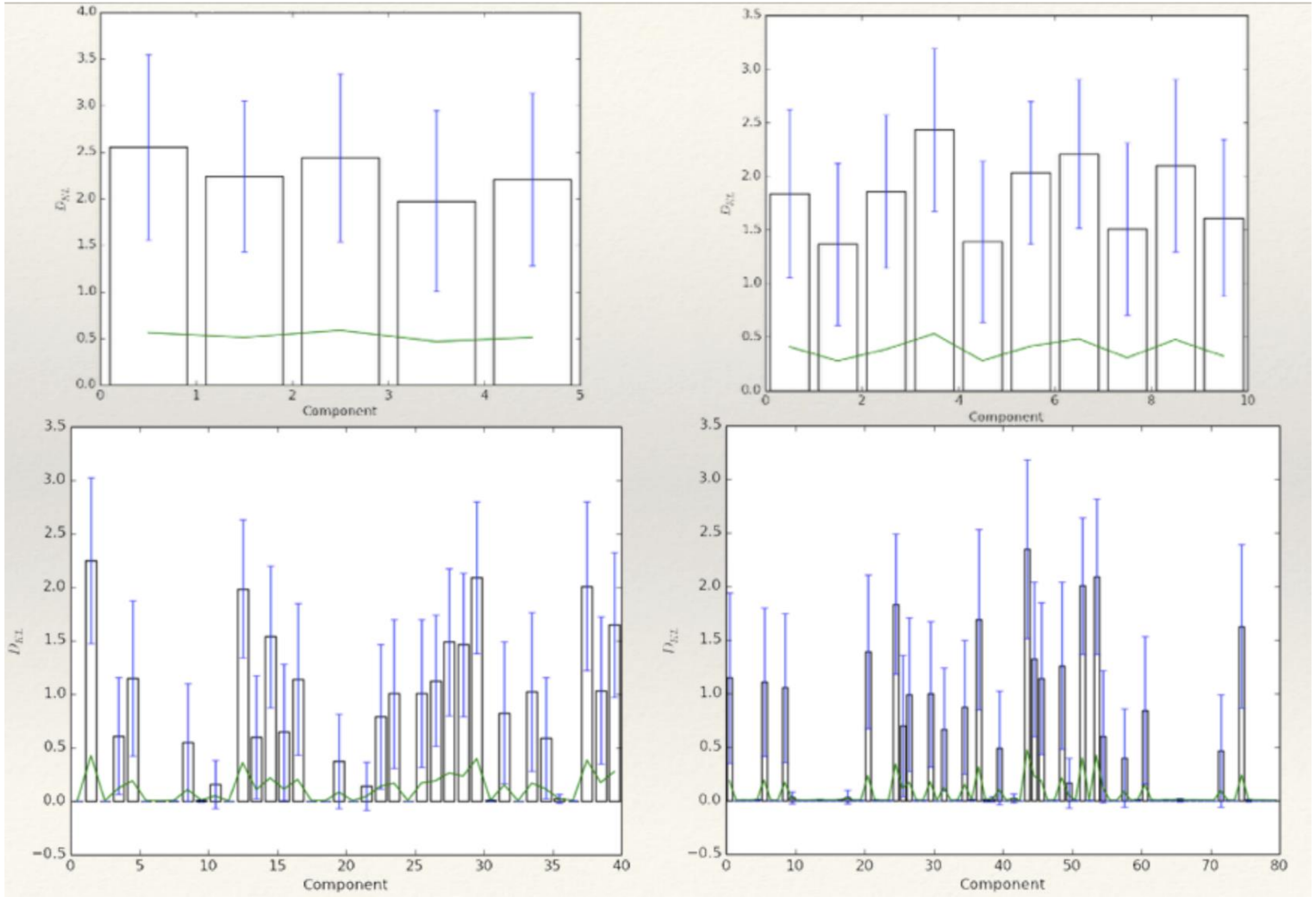
Reparameterization trick

- $q(z|x;\omega) = N(\mu_z(x), \Sigma_z(x))$
- $z = \mu_z(x) + \Sigma_z^{\frac{1}{2}}(x)\varepsilon_z, \varepsilon_z \sim N(0,1)$

$$E_{x\sim D}[E_{z\sim N(0,1)}\left[lnp\left(x\,\middle|\,z = \mu(x;\omega) + \Sigma^{\frac{1}{2}}(x;\omega) * \varepsilon\right);\theta\right)\Big] - KL(q(z|x;\omega)||p(z))]$$



Variational autoencoders - results



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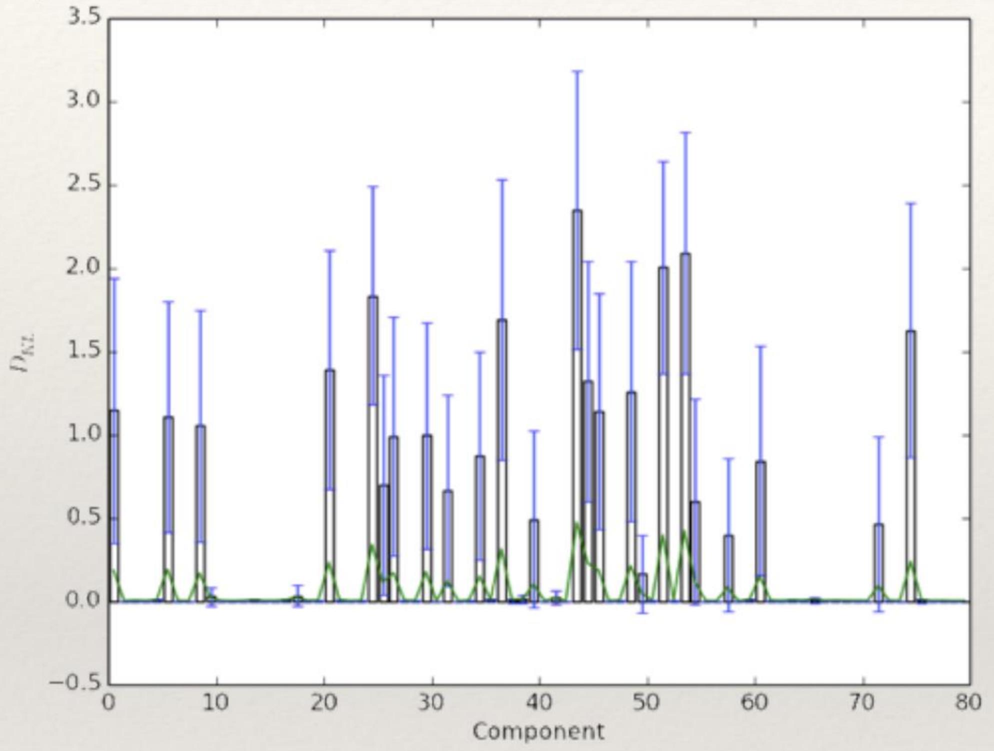
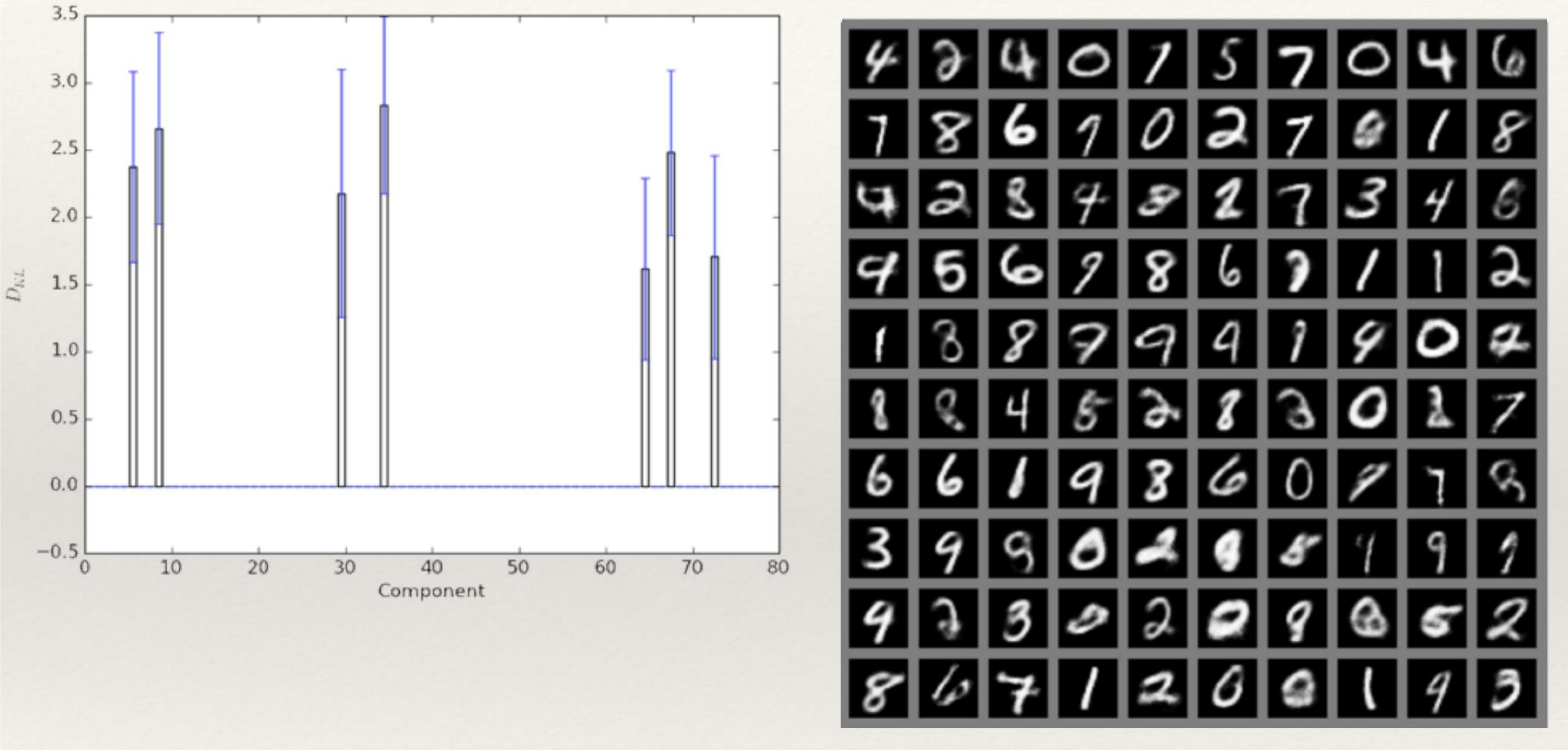


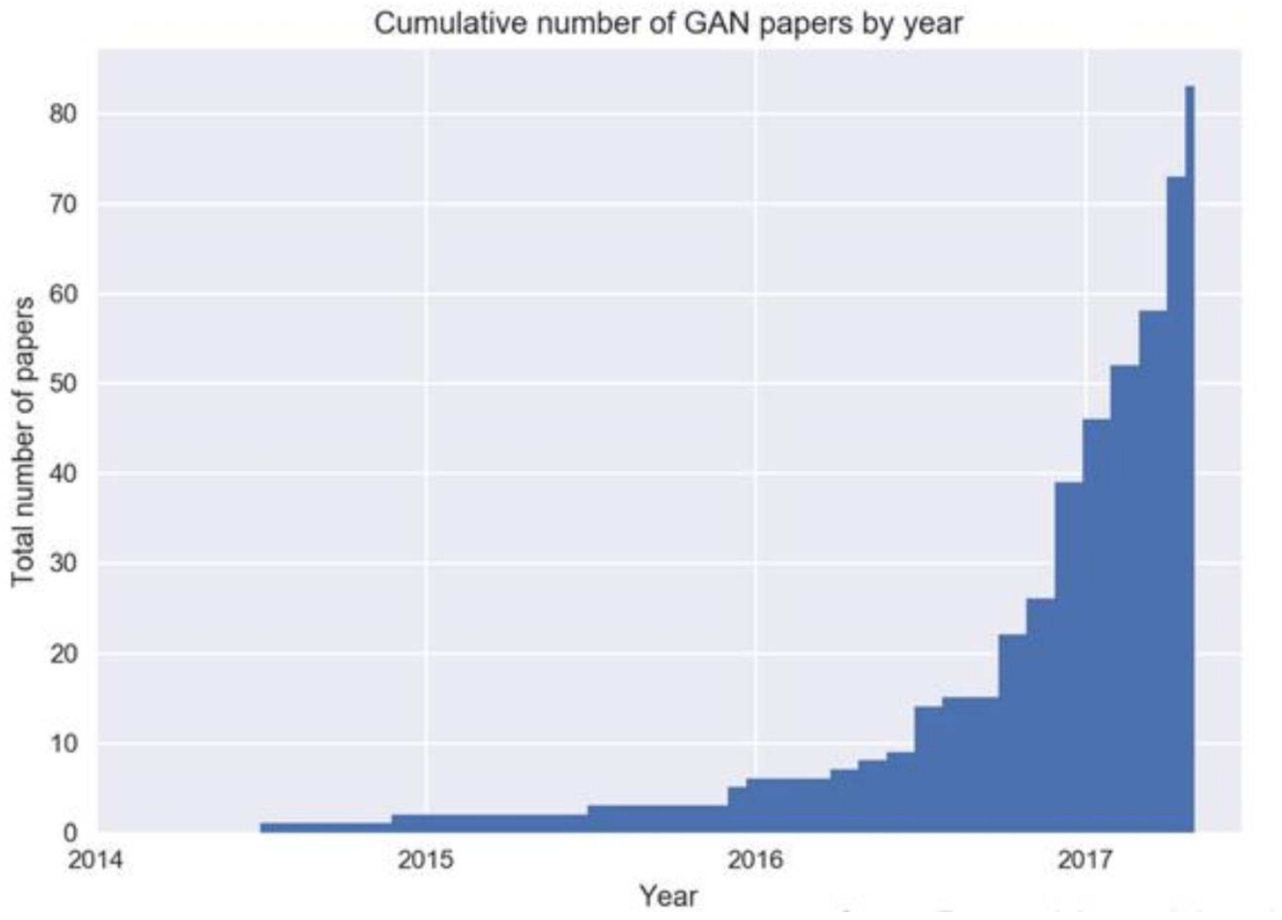
Variational autoencoders - results



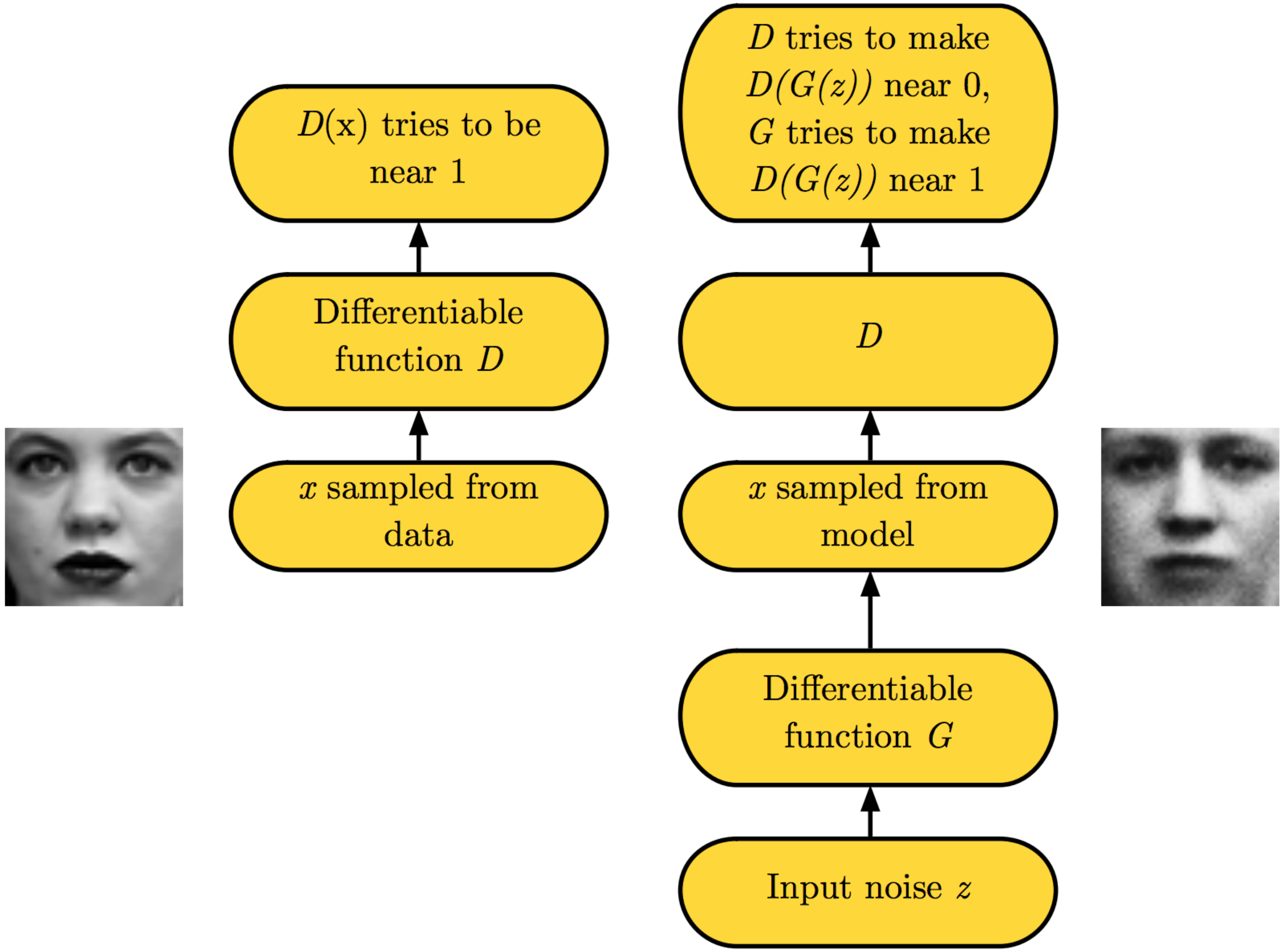
Generative Adversarial Networks

- Advantages:
  - Sample generation in a single step (does not depend on dimensionality of X)
  - Does not use Markov chain
  - Does not use lower bound
  - Generation function has very few restrictions
- Disadvantages:
  - Hard to train

Generative Adversarial Networks



GAN - architecture

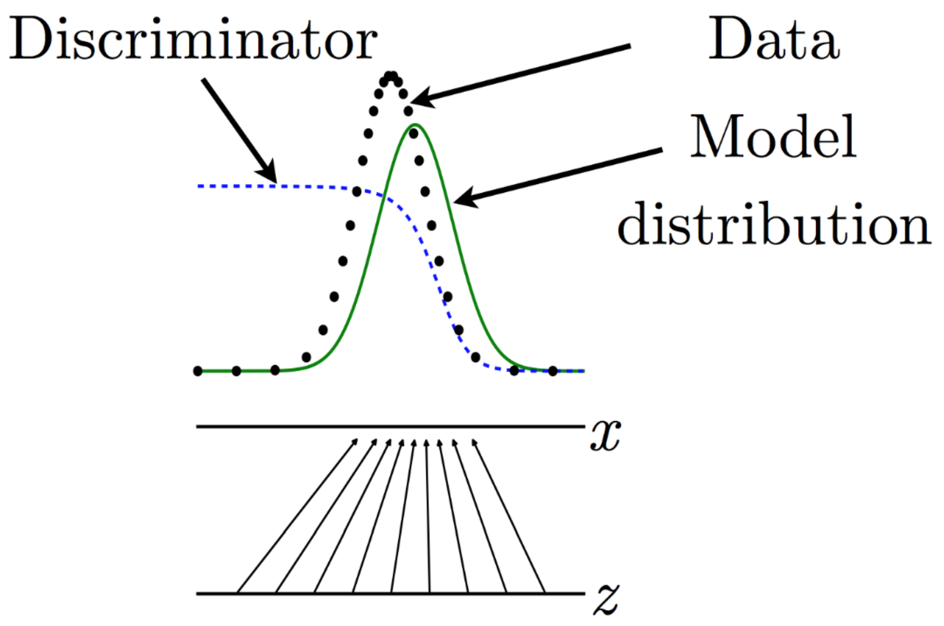


GAN - discriminator

$$J^{(D)}(\theta^{(D)}, \theta^{(G)}) = -\frac{1}{2} E_{x\sim p_{data}} log D(x) - \frac{1}{2} E_z \log(1 - D(G(z)))$$

- Optimal discriminator:

$$D^*(x) = \frac{p_{data}(x)}{p_{model}(x) + p_{data}(x)}$$



Zero-sum game

- N players
- Payoff matrix

Blue / Red	A	B	C
1	-30 30	10 -10	-20 20
2	10 -10	-20 20	20 -20

A zero-sum game

- Nash equilibrium of a game

GAN - generator

$$J^{(G)}\left(\theta^{(D)},\theta^{(G)}\right) = -J^{(D)}\left(\theta^{(D)},\theta^{(G)}\right)$$

- Minimax game:

$$V(\theta^{(D)},\theta^{(G)}) = -J^{(D)}\left(\theta^{(D)},\theta^{(G)}\right)$$

- Solution:

$$\theta^{(D)*} = argmin_{\theta^{(G)}} \max_{\theta^{(D)}} V(\theta^{(D)},\theta^{(G)})$$

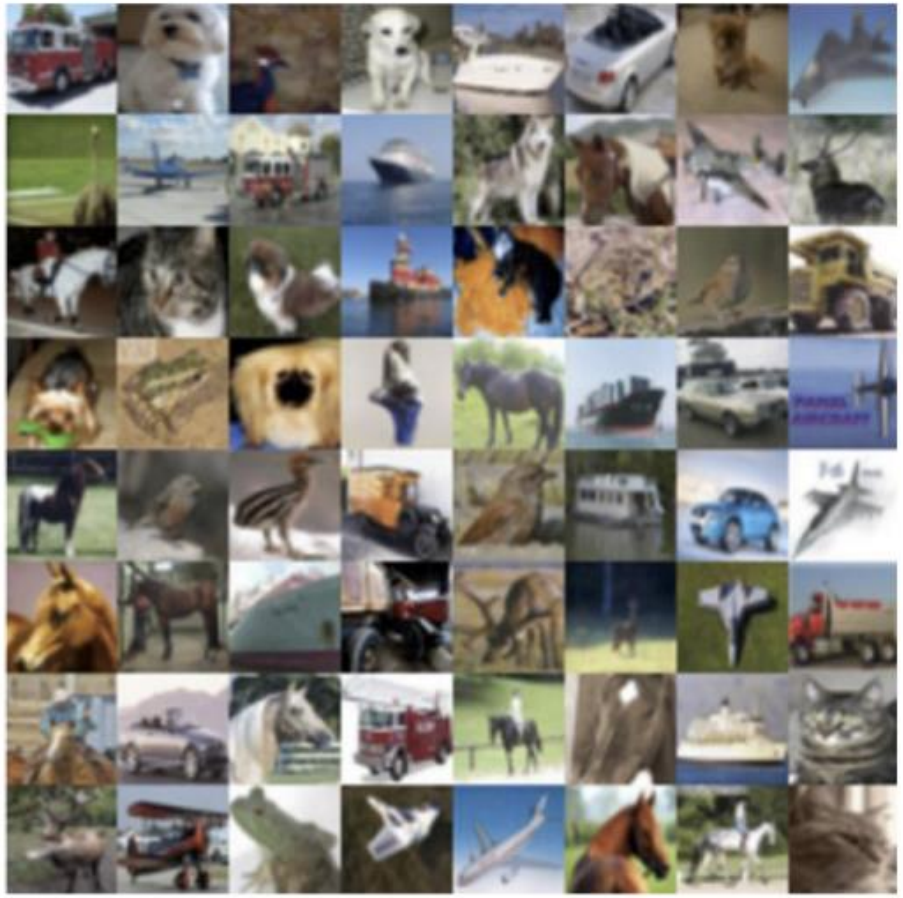
In practice:

$$J^{(G)}\left(\theta^{(D)},\theta^{(G)}\right) = -\frac{1}{2}E_z \log(D(G(z)))$$

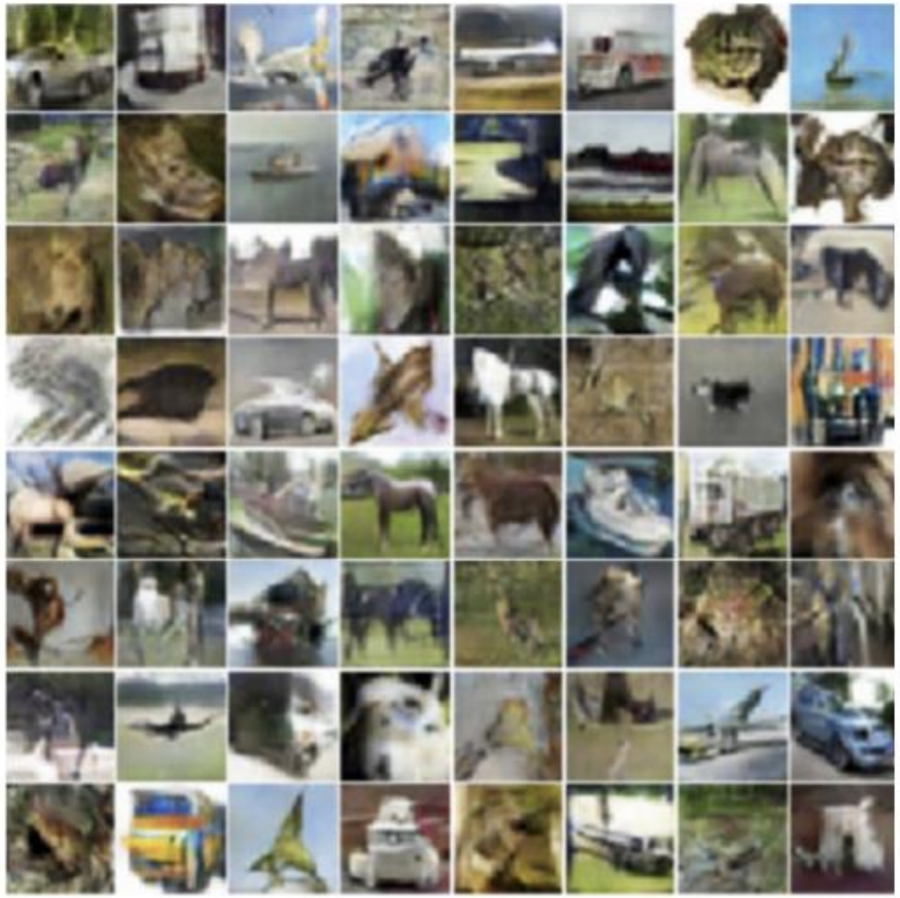
GAN - Tricks

- $x \in [-1, 1]$
- Using labels
- One-side label smoothing
- Batch normalization
- Running more steps of one player

GAN - rezultati

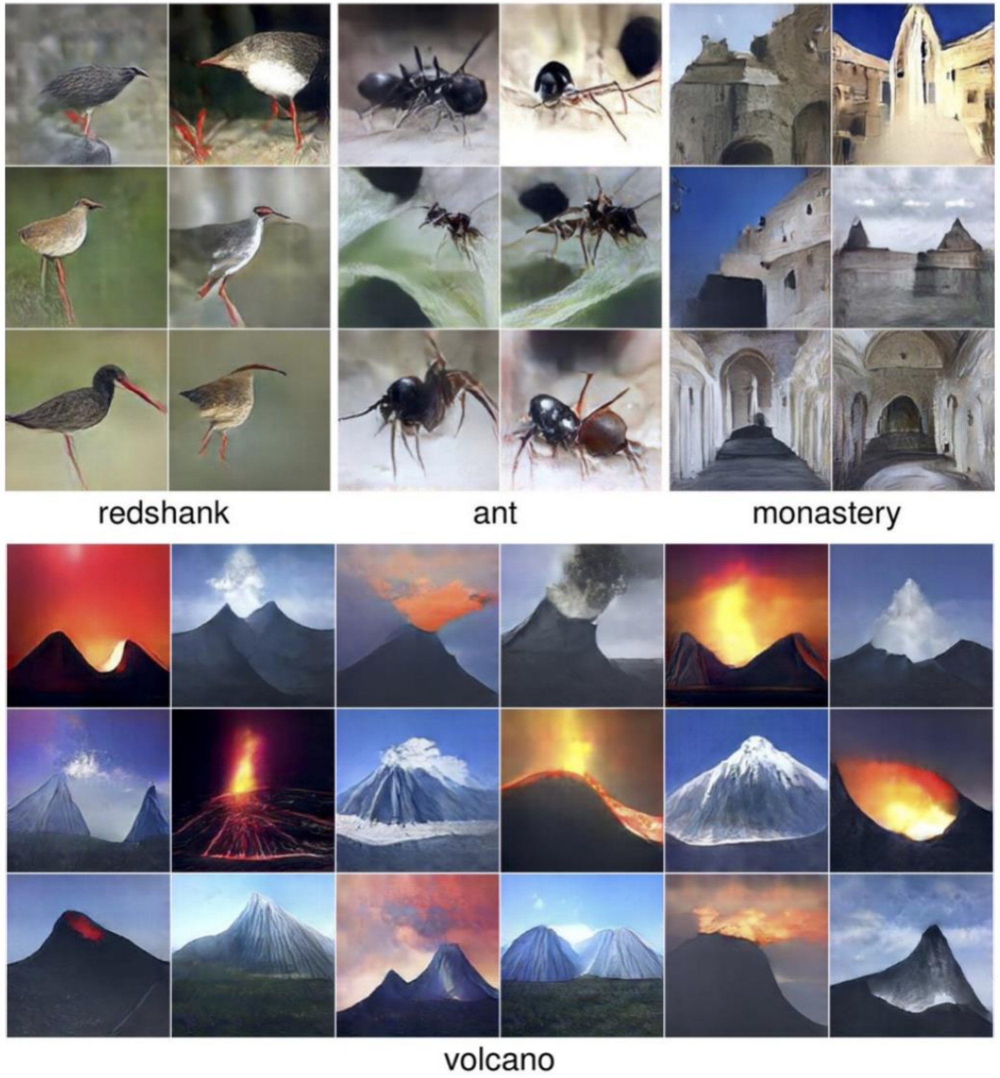


Training Data



Samples

Plug and Play Generative Networks



Summary

- Explicit density
  - Tractable density
  - Approximate density
    - Deterministic approximations
    - Stochastic approximations
- Implicit density
  - Markov chain
  - GAN

THANKS!