Introduction to Deep Learning

Lecture 7
Generative Models and GANs

Maria Vakalopoulou & Stergios Christodoulidis

MICS Laboratory

CentraleSupélec
Université Paris-Saclay

CentraleSupélec

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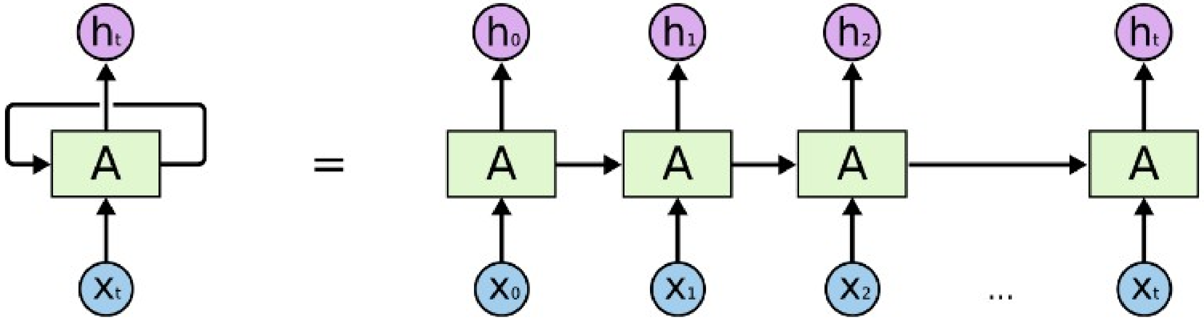
Last Lecture

Recurrent Neural Networks (RNNs)

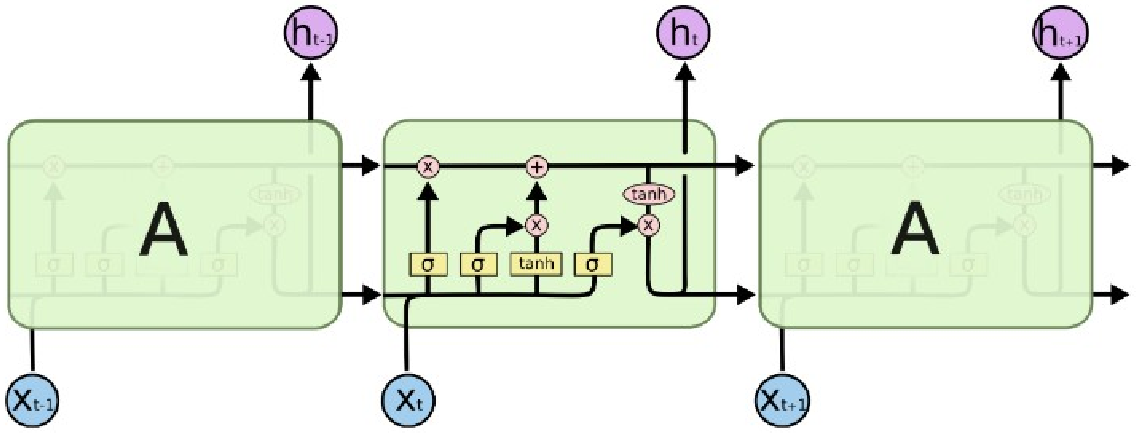
- They were first introduced in 1986.
- They are neural networks with loops in order to allow information to persist.
- These loops represent the influence of previous value on the same value at the current step.
- For a simpler representation we could unroll this RNN in time.



(http://colah.github.io/posts/2015-08-Understanding-LSTMs/)

LSTMs

- LSTMs are an RNN architecture.
- They are capable of learning long-term dependencies
- Tackling the vanishing gradient problem
- The LSTM has been found extremely successful in many applications



(http://colah.github.io/posts/2015-08-Understanding-LSTMs/)

Transformers

- A sequence-to-sequence model with an Encoder-Decoder architecture.
- Even though it is not a reccurent network, it is designed such that it can work with sequences
  - It utilizes positional encoding of the input to capture the relative positions across
  - It utilizes a self-attention mechanism ti decide which other parts of the sequence are important.
- The state-of-the-art for a lot of applications, extended to vision
  - Vision Transformers

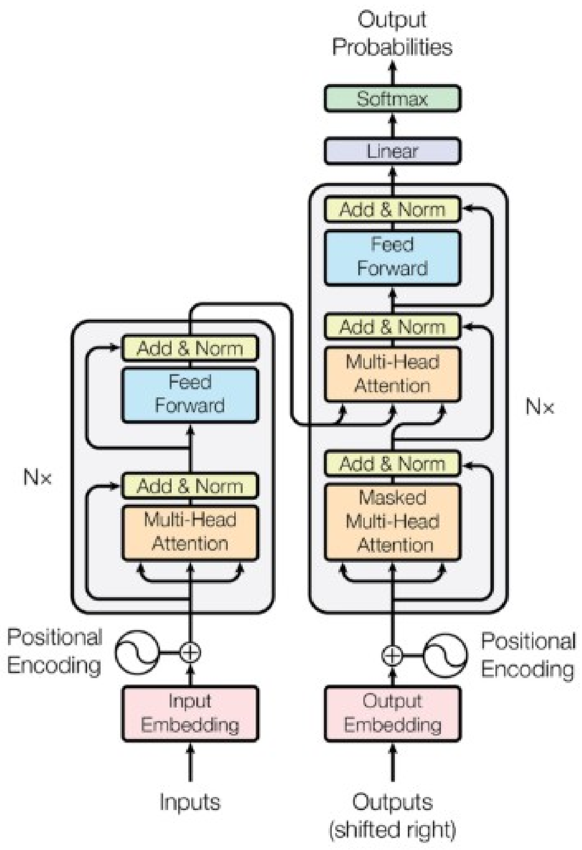
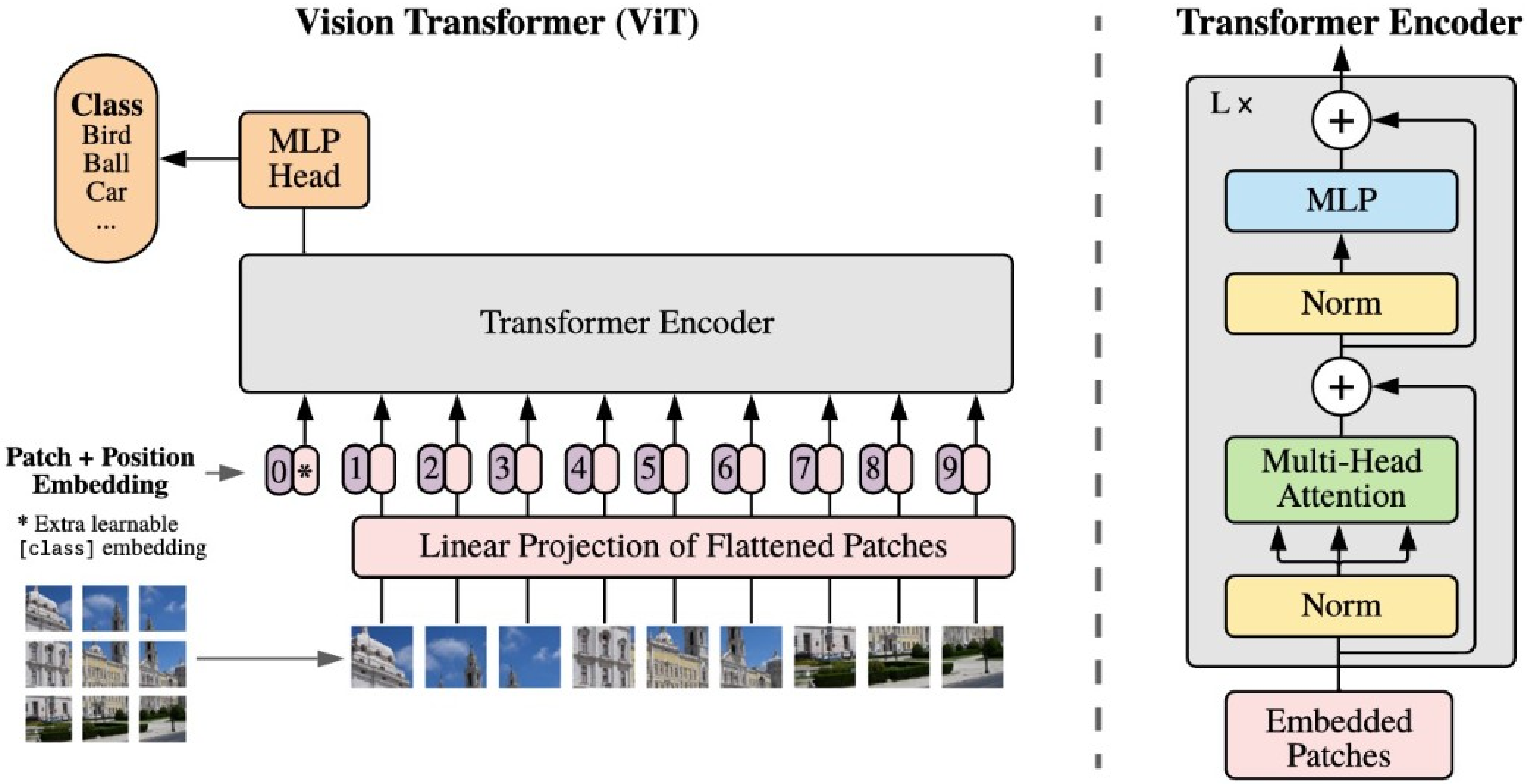


Figure 1: The Transformer - model architecture.

Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).

Vision Transformers



Dosovitskiy, Alexey, et al. "An image is worth 16x16 words: Transformers for image recognition at scale." arXiv preprint arXiv:2010.11929 (2020).

Today’s Lecture

Today’s Lecture

- Gentle intro to generative models
- Variational Autoencoders
- Generative Adversarial Networks
- Variants of Generative Adversarial Networks

Types of Learning

- Generative modelling
  - Learn the joint pdf: p(x,y)
  - Model the world → Perform tasks, e.g. use Bayes rule to classify: p(y|x)
  - Naive Bayes, Variational Autoencoders, GANs

Types of Learning

- Generative modelling
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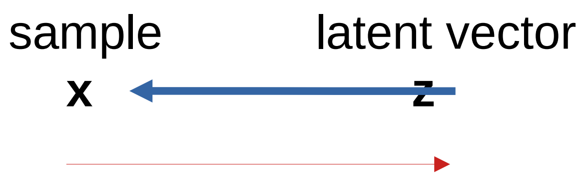
  - Model the world → Perform tasks, e.g. use Bayes rule to classify: p(y|x)
  - Naive Bayes, Variational Autoencoders, GANs
- Discriminative modelling
  - Learn the conditional pdf:
  - Task-oriented
  - E.g., Logistic Regression, SVM



Types of Learning

- What to pick?
  - V. Vapnik: “One should solve the *[classification]* problem directly and never solve a more general *[and harder]* problem as an intermediate step”
- Typically, discriminative models are selected to do **the** job
- Generative models give us more theoretical guarantees that the model is going to work as intended
  - Better generalization
  - Less overftiting
  - Better modelling of causal relationships

Applications of generative modeling?

Applications of generative modeling?

- Act as a regularizer in discriminative learning
  - Discriminative learning often too goal-oriented
  - Overfitting to the observations
- Semi-supervised learning
- Simulating “possible futures” for Reinforcement Learning
- Data-driven generation/sampling/ simulation

Applications of generative modeling?

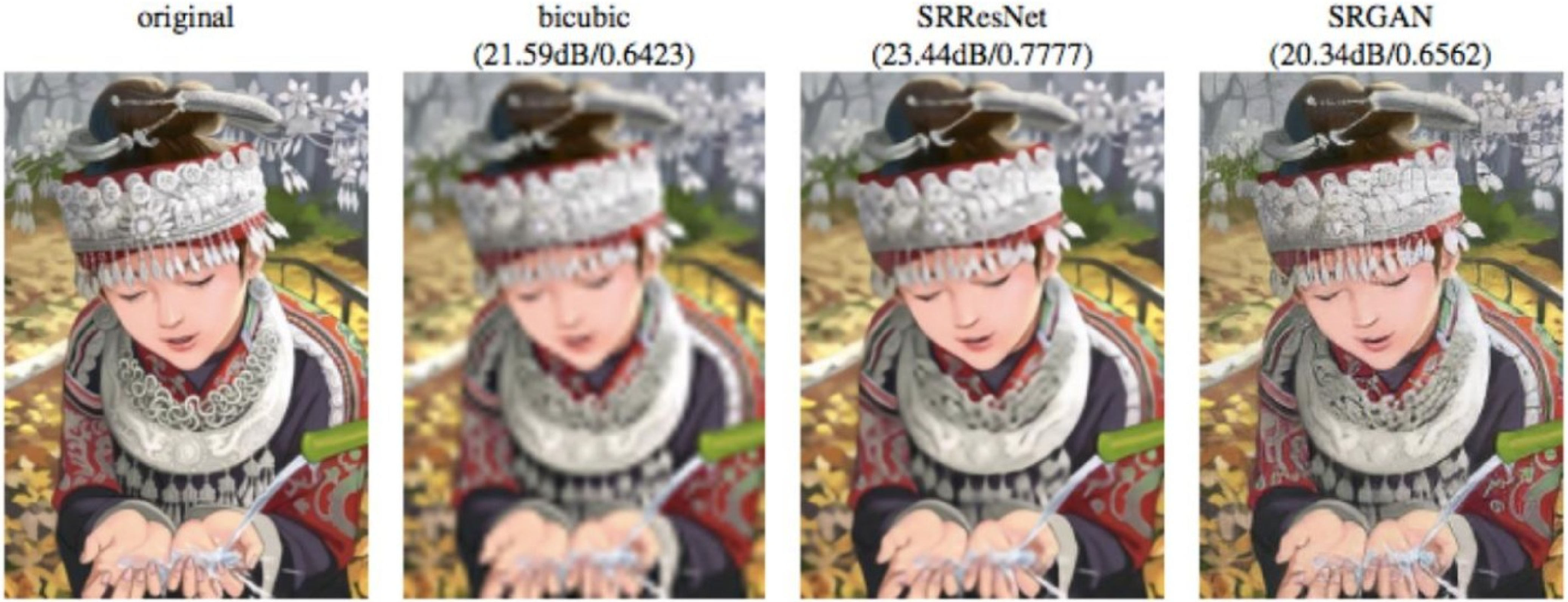
- Image Generation

(b) Generated by DCGANs (Reported in [13]).

(a) Generated by LSGANs.

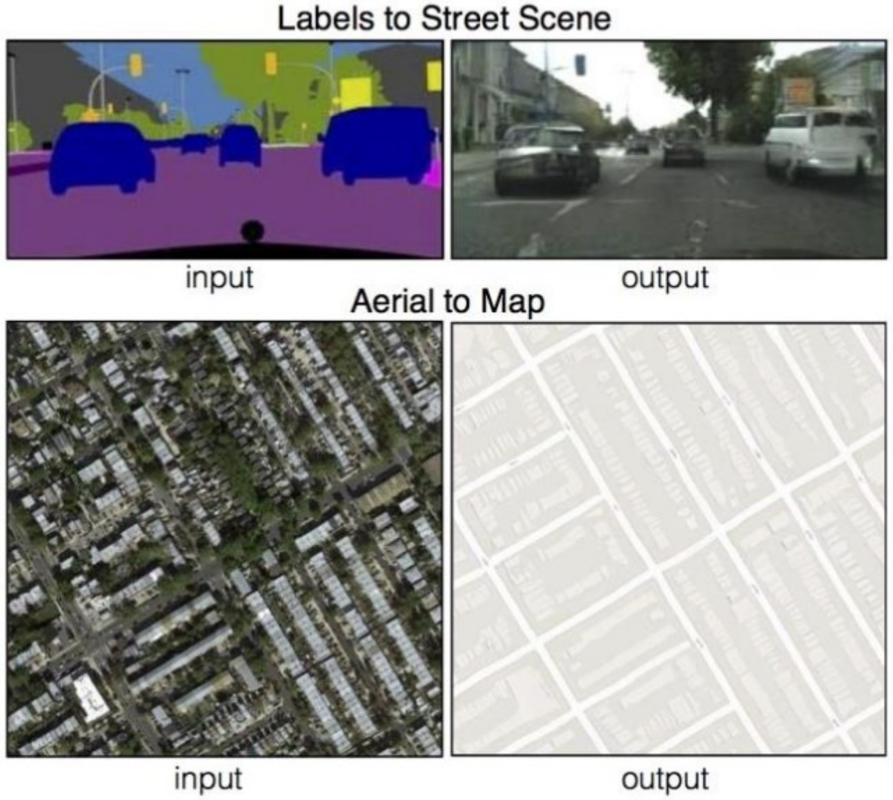
Applications of generative modeling?

- Super-resolution



Applications of generative modeling?

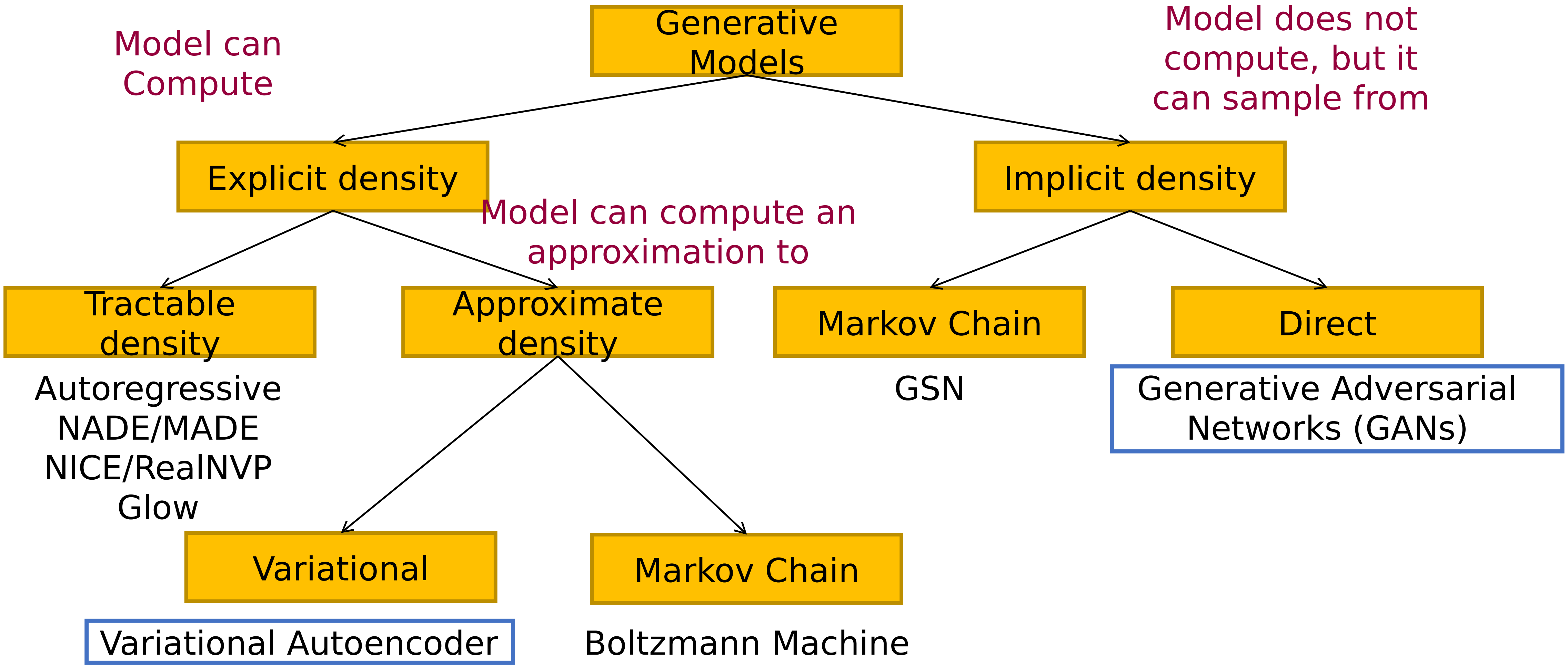
- Cross-model translation



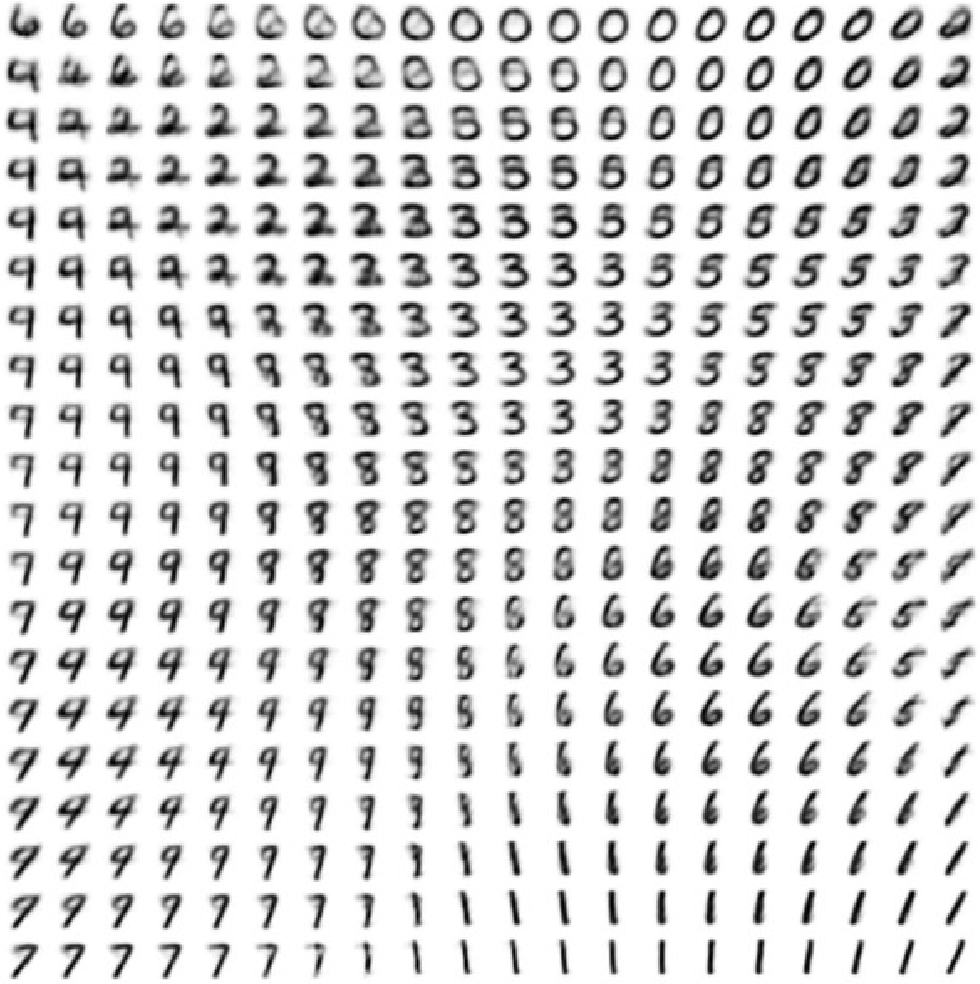
Other Applications

- M. Mustafa et al. “Cosmogan: Creating High-Fidelity Weak Lensing Covergence Maps Using Generative Adversarial Networks” in Arxiv 2017
- S. Collaboration. “Fast Simulation of Muons Produced at the ShiP Experiment Using Generative Adversarial Networks”. In Arxiv 2019
- Z. E. et al. “Deep Learning Enables Rapid Identification of Potent DDR1Kinase Inhibitors” In. Nature Biotechnology 2019
- Deep Fakes.

A map of generative models



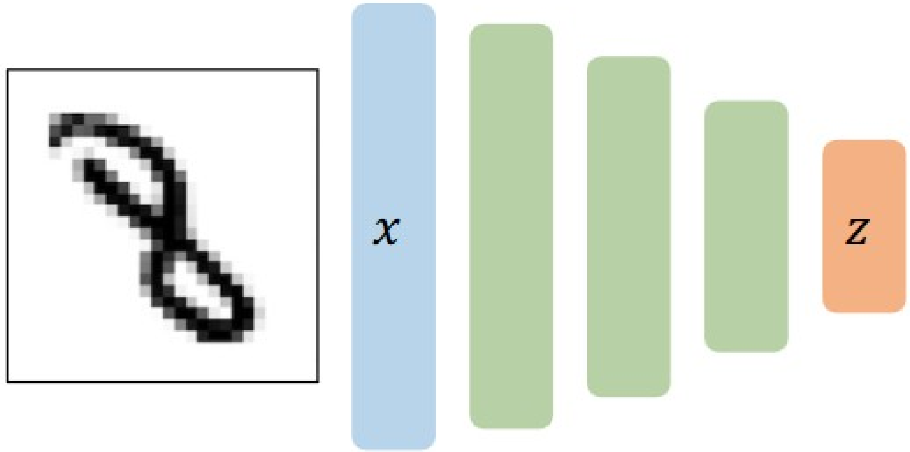
Varietional Autoencoders



Kingma, D.P. and Welling, M., 2013. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114.

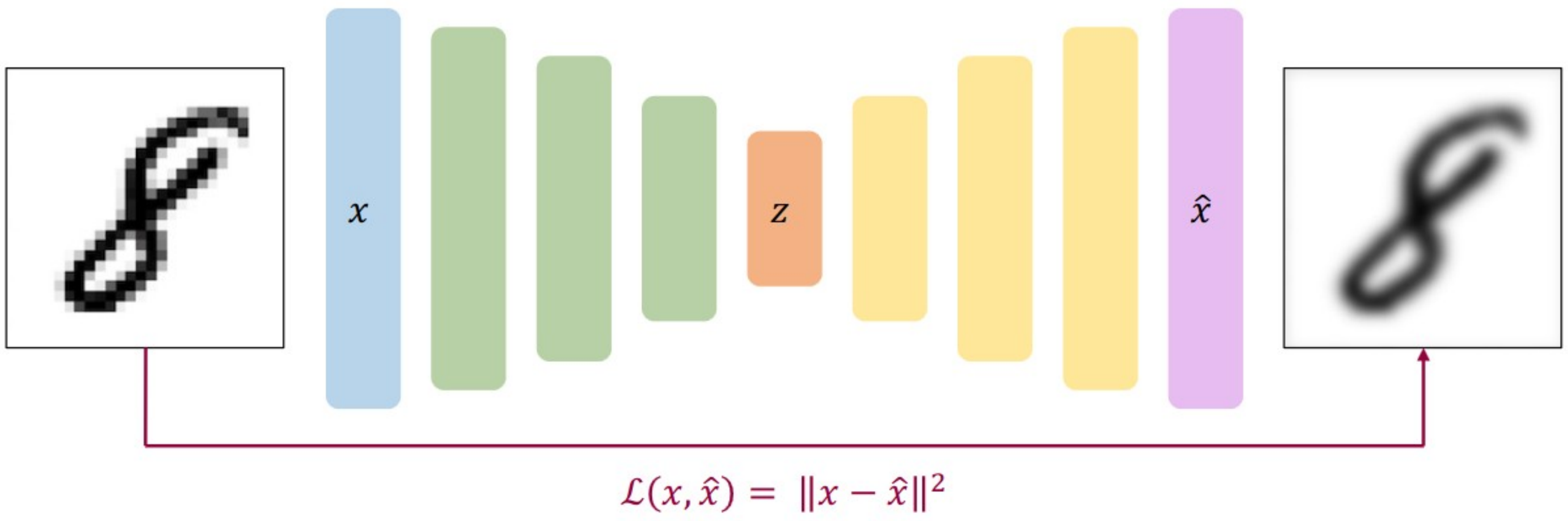
Latent Representation Models

- Latent variables are high level features:
  - In combination they generate the data
- In Latent Representation models we are interested to learn these representations
  - i.e., Figure out what these latent variables are.
  - Can we learn these in a supervised manner?



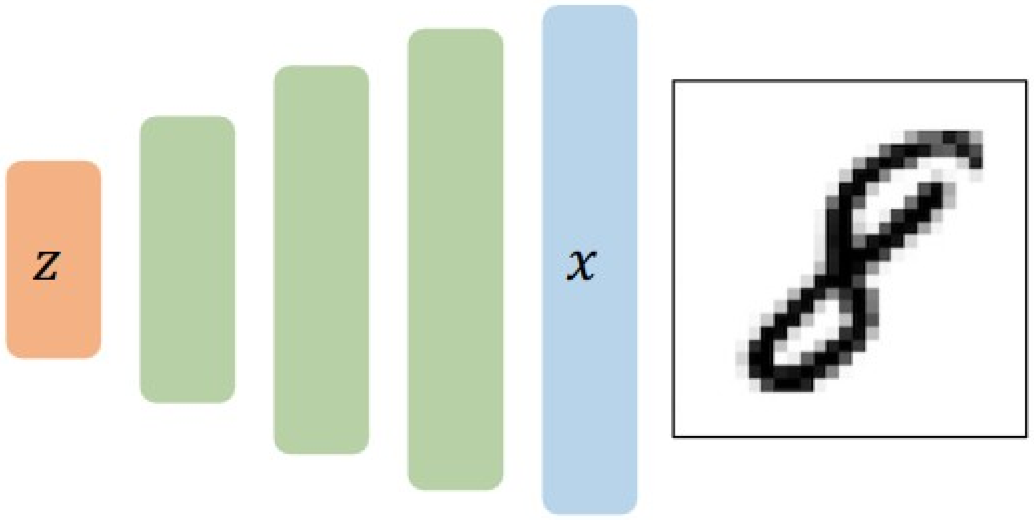
Autoencoders (AE)

- Idea: Use the latent representation to reconstruct the input data (Autoencoding == encoding itself)
  - Encoder part (Green): maps the observed data x to a latent representation z
  - Decoder part (Yellow): reconstructs the observed data using the latent representation z



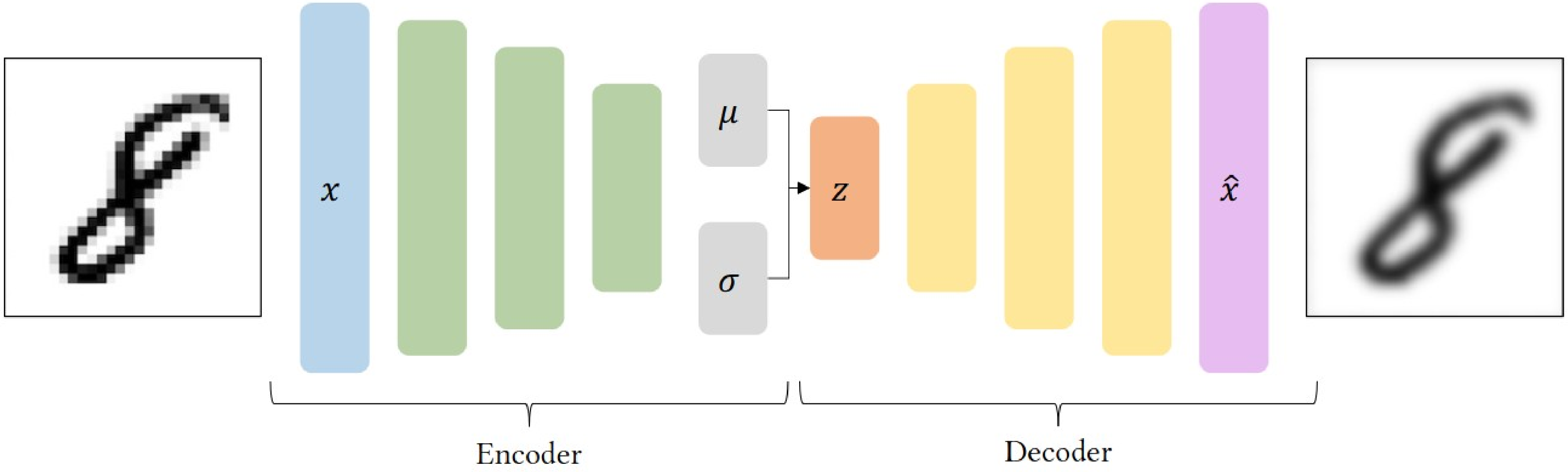
Variational Autoencoders (VAE)

- Generative spin on autoencoders
- Can we use the model to generate data?
- There is no explicit way to know how to set z



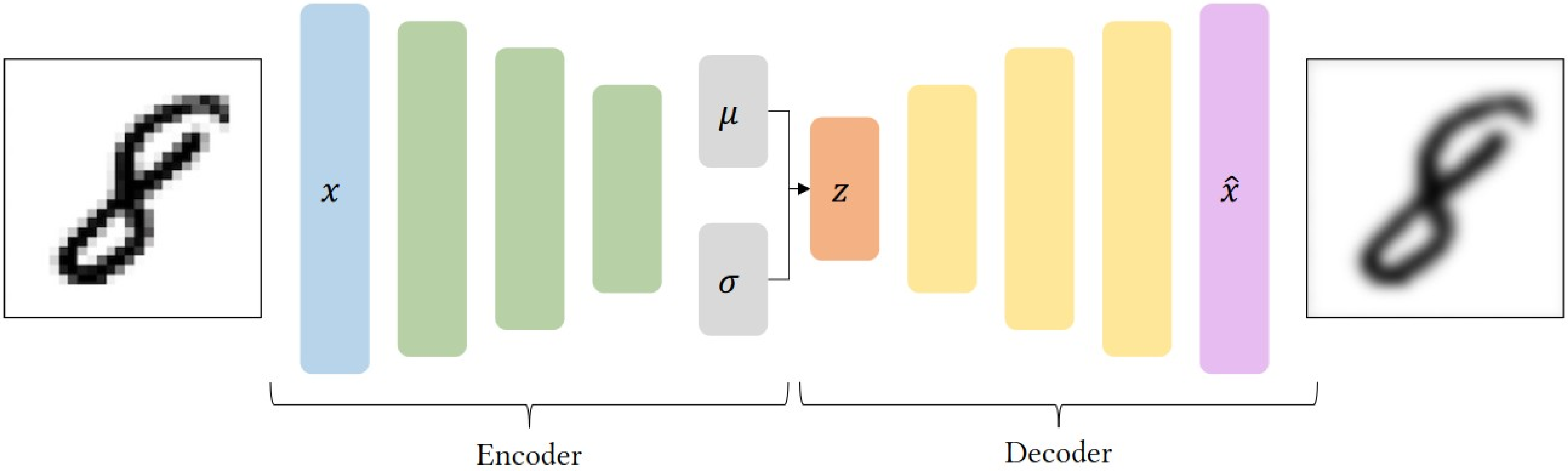
Variational Autoencoders (VAE)

- Instead of straight learning the latent representation z
- We learn the parameters of a multivariate gaussian from which we sample z
- Not deterministic any more → Stochastic sampling operation



Variational Autoencoders (VAE)

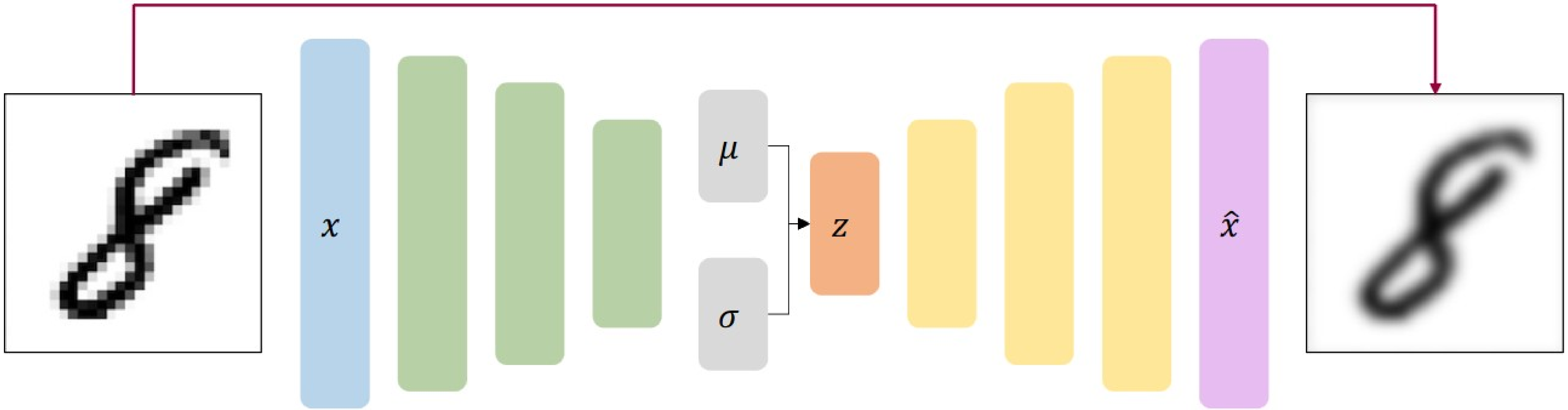
- Probabilistic twist:
  - Encoder learns $p(z|x)$
  - $\boxed{\text{Decoder learns } p(x|z)}$ Generative Model!



Variational Autoencoders (VAE)

- Reconstruction loss
  - Mean Square Error

$$\mathcal{L}(x, \hat{x}) = \|x - \hat{x}\|^2$$

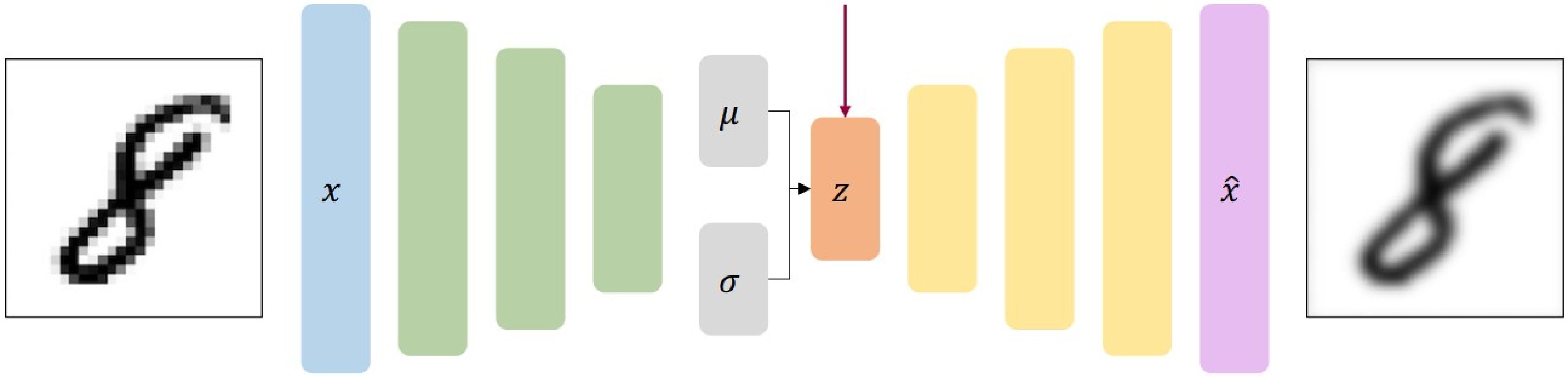


$$\mathcal{L}(x, \hat{x}) = \boxed{(reconstruction\ loss)} + (regularization\ term)$$

Variational Autoencoders (VAE)

- Regularization Term
  - KL divergence between the inferred latent distribution and a prior distribution.
  - Typically zero mean unit std normal distribution

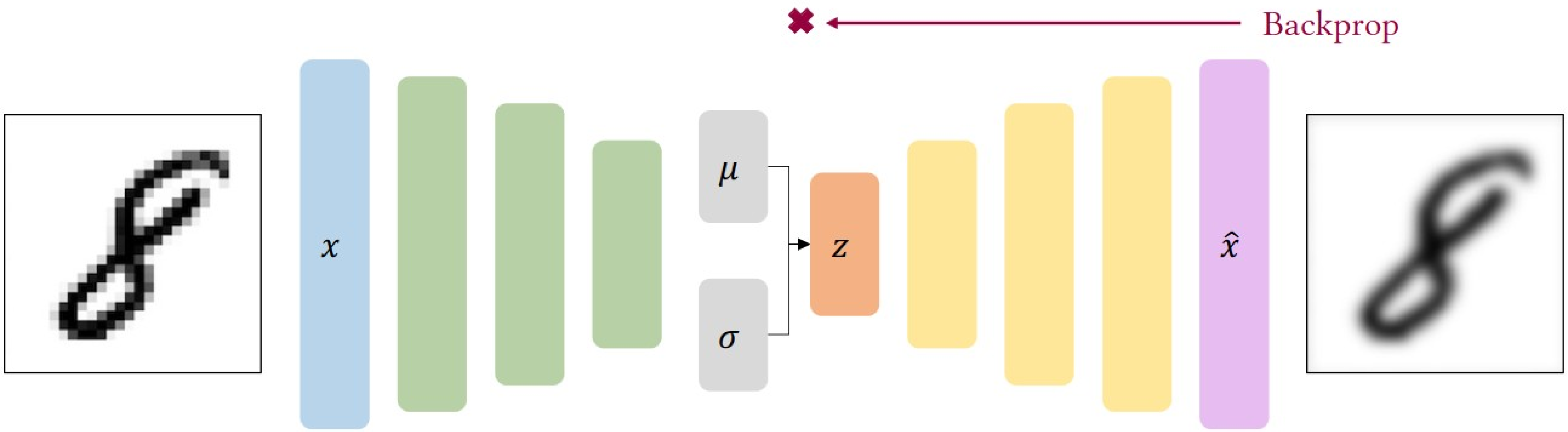
$$\mathrm{R}(z) = D_{KL}(p(z|x) \parallel \mathcal{N}(\mu = 0, \sigma = 1))$$



$$\mathcal{L}(x, \hat{x}) = (reconstruction\ loss) + \boxed{(regularization\ term)}$$

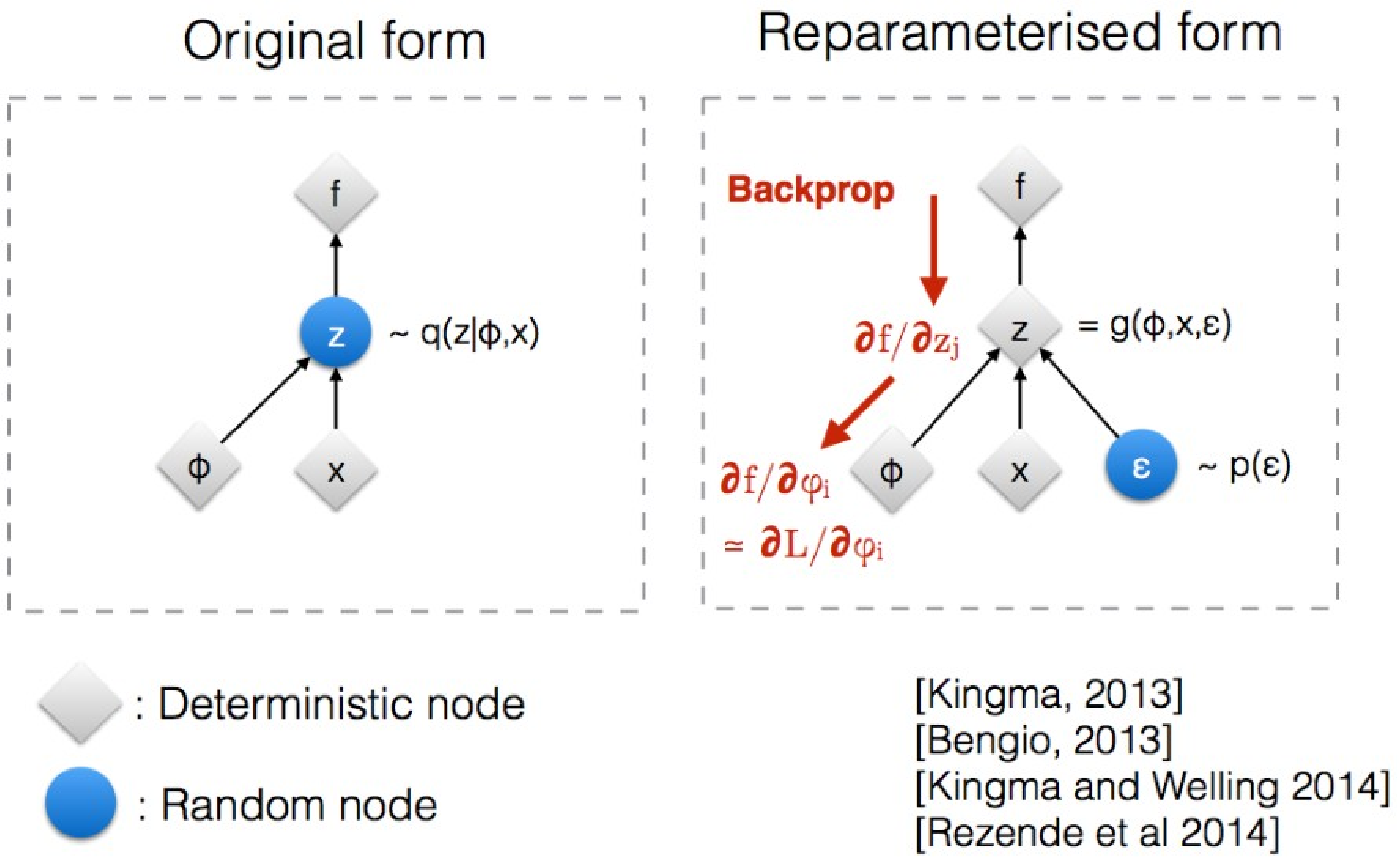
Variational Autoencoders (VAE)

- Sampling operation is not differentiable
  - How can we solve this?



$$\mathcal{L}(x, \hat{x}) = (reconstruction\ loss) + (regularization\ term)$$

Reparametrization Trick



Kingma, D.P. and Welling, M., 2013. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114.

VAE: Summary

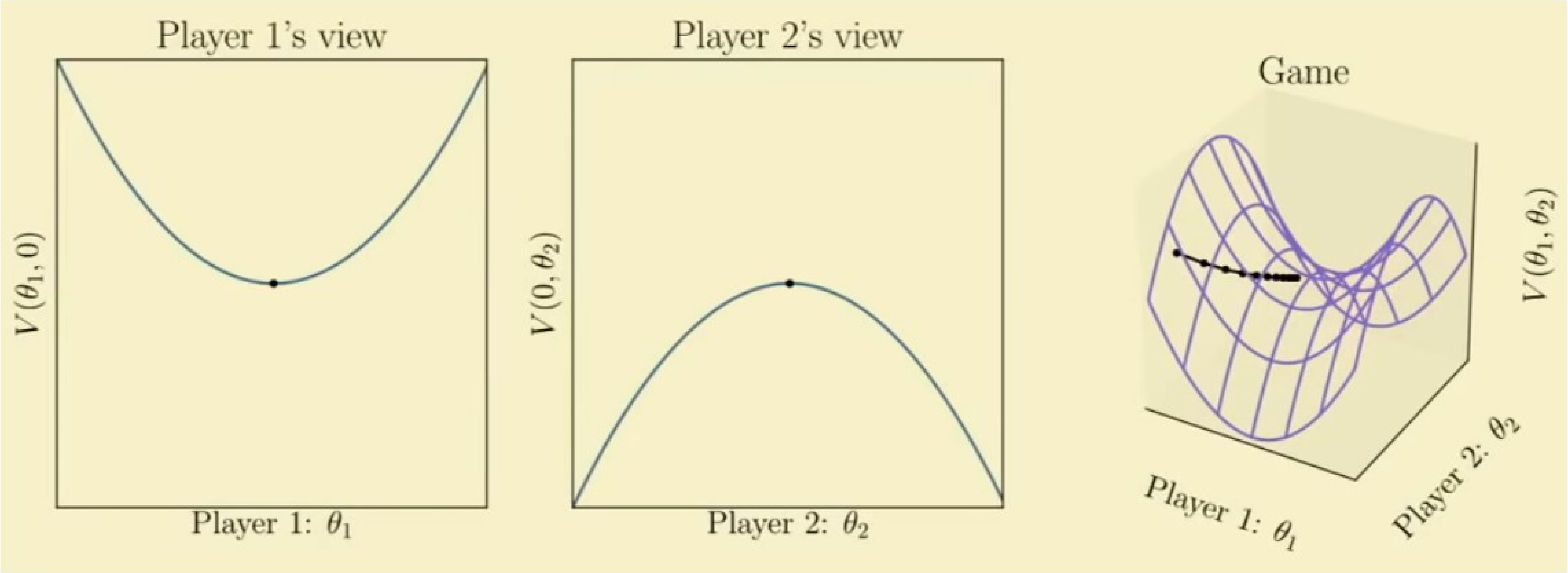
- Compresses observed data to some smaller representation
- Unsupervised setting
- Reparametrization trick for end-to-end training
- Force latent representation to imitate a gaussian distribution (KL divergence)
- The latent variables can be interpreted by pertubation their values
- Can be used to generate new samples

GANs

What is a GAN?

- **G**enerative
  - You can sample novel input samples
  - E.g., you can literally “create” images that never existed
- **A**dversarial
  - Our generative model **G** learns adversarially, by fooling an discriminative oracle model **D**
- **N**etwork
  - Implemented typically as a (deep) neural network
  - Easy to incorporate new modules
  - Easy to learn via backpropagation

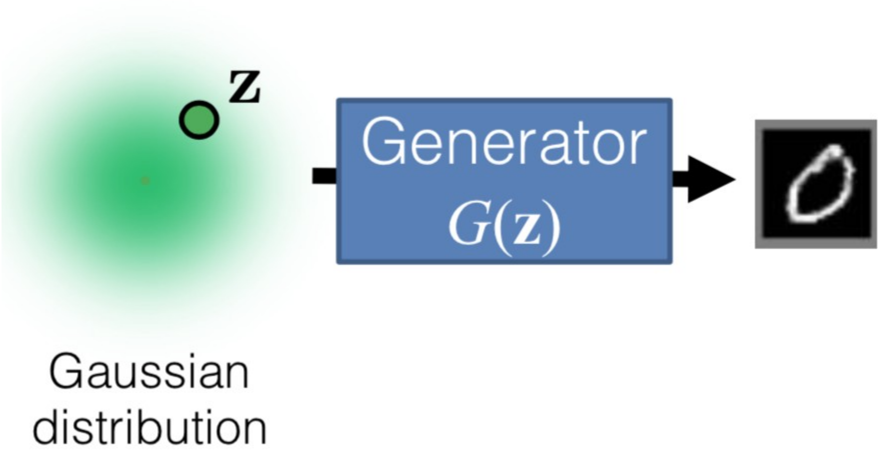
Adversarial Learning



Goodfellow, 2019

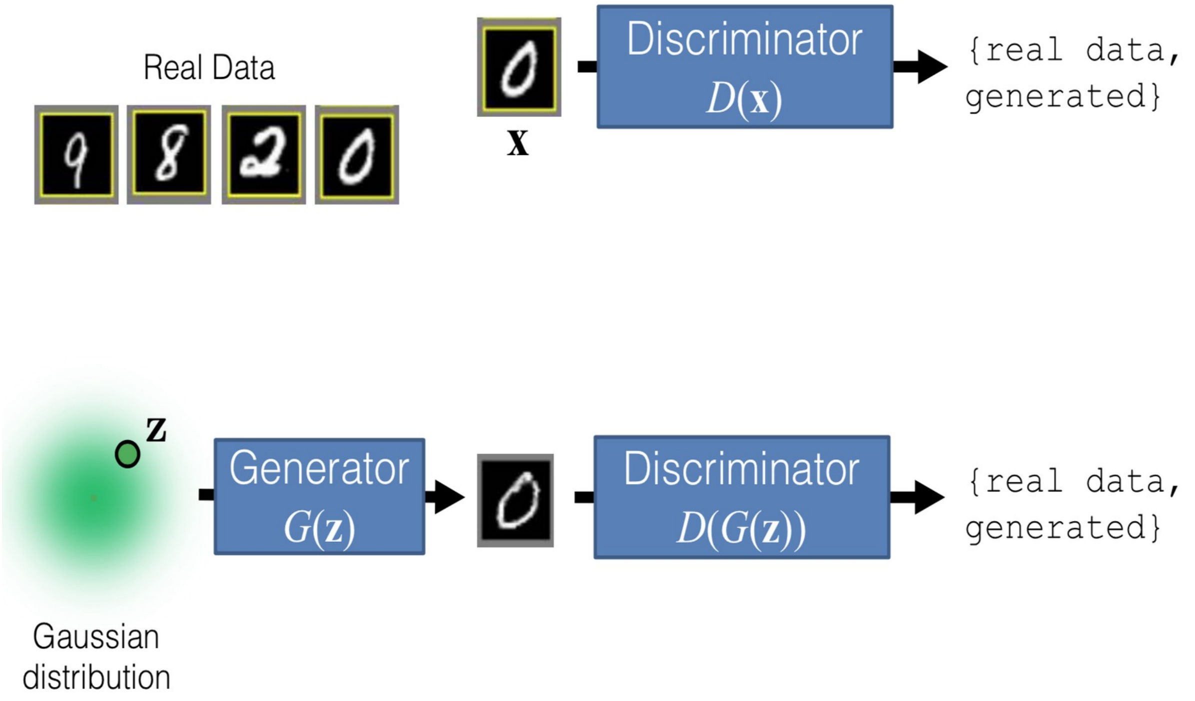
Generative Adversarial Networks

- We would like to train a network G to generate images from some domain from random vectors z:

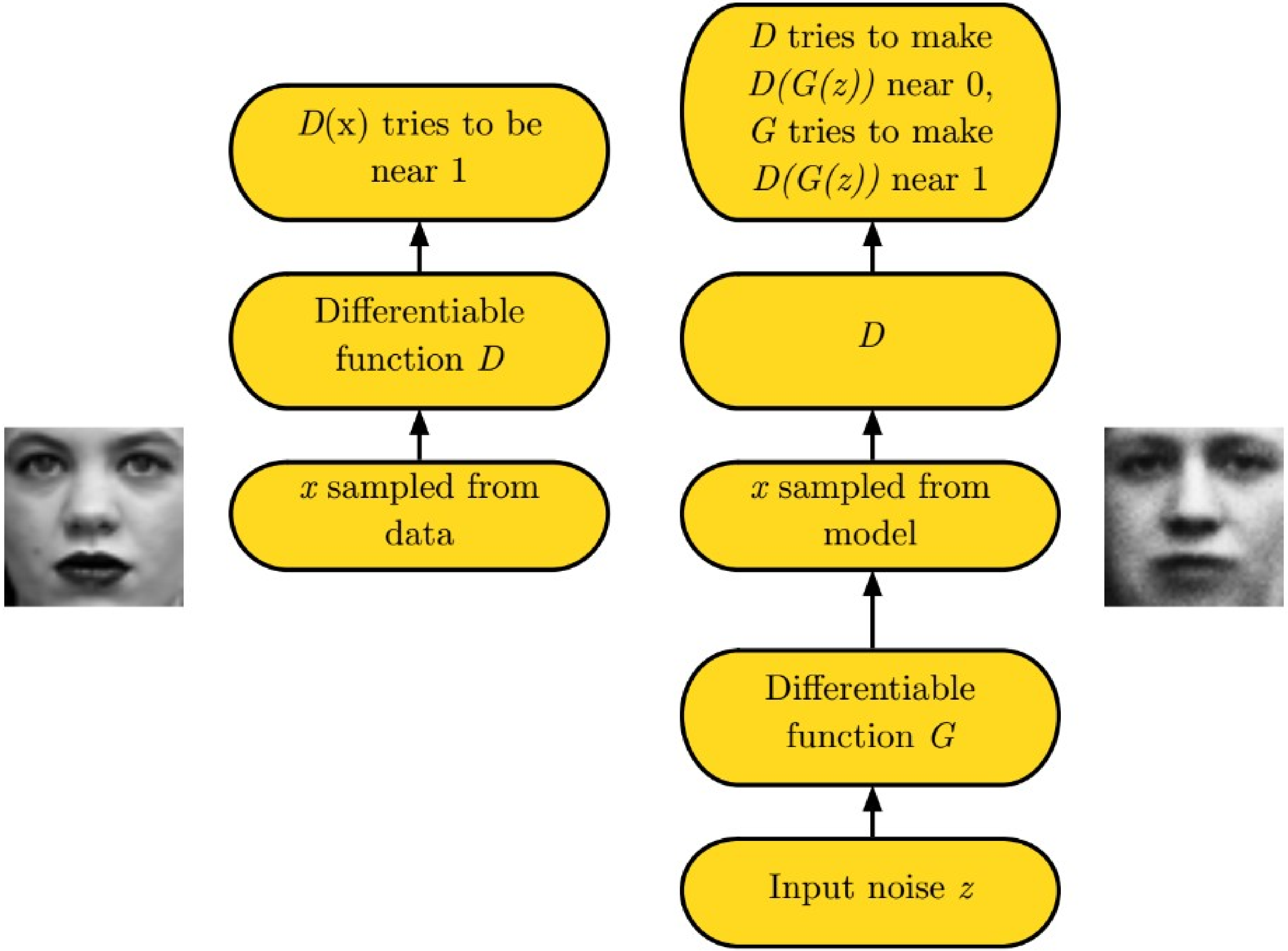


Generative Adversarial Networks

- Idea: Add a second network (Discriminator D) jointly trained with the Generator G to recognize if an input is a real sample from the domain of interest or if it was created by the Generator.
- When the Discriminator cannot distinguish the generated images from the real ones, the Generator generates realistic images

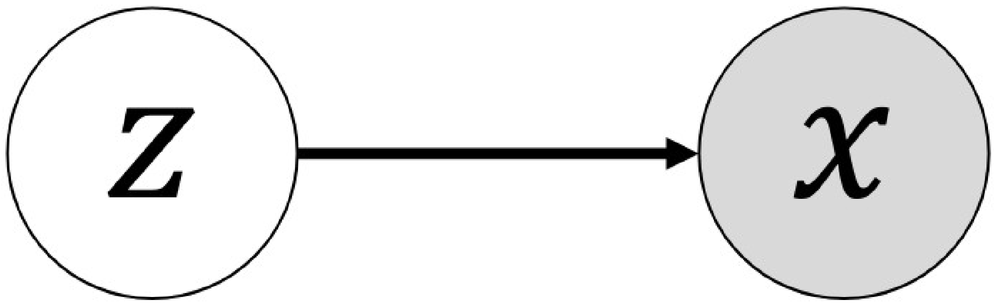


GAN: Pipeline



Generator network $x = G(z;\theta^{(G)})$

- Must be differentiable
- No invertibility requirement
- Trainable for any size of z
- Can make conditionally Gaussian given z, but no strict requirement



Generator & Discriminator: Implementation

- The discriminator is just a standard neural network
- The generator looks like an inverse discriminator

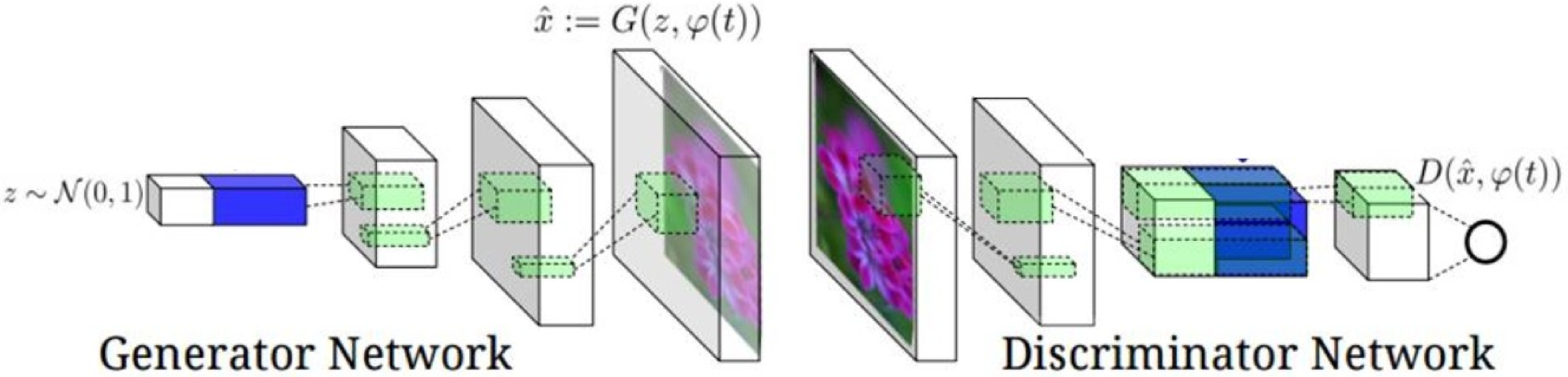


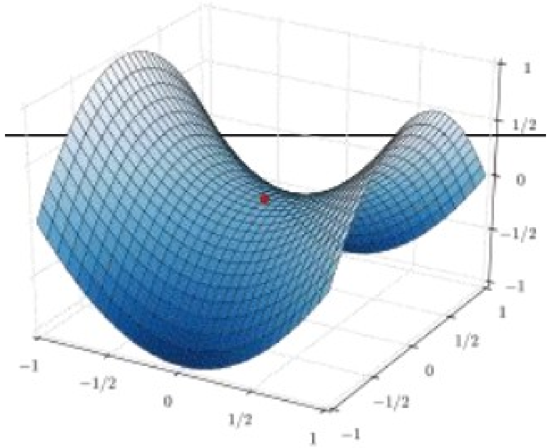
Figure 2. Our text-conditional convolutional GAN architecture. Text encoding $\varphi(t)$ is used by both generator and discriminator. It is projected to a lower-dimensions and depth concatenated with image feature maps for further stages of convolutional processing.

Network Architecture

Training definitions

- Minimax
- Maximin
- Heuristic, non-saturating game
- Max likelihood game

Minimax Game



- $J^{(D)} = -\frac{1}{2}\mathbb{E}_{x\sim p_{data}} \log D(x) \; -\frac{1}{2}\mathbb{E}_{z\sim p_z} \log(1 - D(G(z))$

- $D(x) = 1$ → The discriminator believes that x is a true image
- $D(G(z)) = 1$ → The discriminator believes that G(z) is a true image

- Equilibrium is a saddle point of the discriminator loss
- Final loss resembles Jenssen-Shannon divergence

https://arxiv.org/pdf/1701.00160.pdf

Minimax Game

- For the simple case of zero-sum game

$$J^{(G)} = -J^{(D)}$$

- So, we can summarize game by

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

- Easier theoretical analysis

Minimax Game

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

- Easier theoretical analysis

- In practice not used → when the discriminator starts to recognize fake samples, then generator gradients vanish

Heuristic non-saturating game

- $J^{(D)} = -\frac{1}{2}\mathbb{E}_{x\sim p_{data}} \log D(x) \; -\frac{1}{2}\mathbb{E}_{z\sim p_z} \log(1 - D(G(z))$
- $J^{(G)} = -\frac{1}{2}\mathbb{E}_{z\sim p_z} \log(D(G(z))$

- Equilibrium not any more describable by single loss
- Generator maximizes the log-probability of the discriminator being mistaken
  - Good G(z) → D(G(z)) =1 → $J^{(G)}$ is maximized
- Heuristically motivated; generator can still learn even when discriminator successfully rejects all generator samples

Original Algorithm

for number of training iterations **do**

for k steps **do**

Sample minibatch of m noise samples $\{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)}\}$

Sample minibatch of m real samples $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$

Update the discriminator D by stochastic gradient ascend.

Gradient:

$$\frac{\partial}{\partial D}\left(\frac{1}{m}\sum_{i=1}^{m}\log D(\mathbf{x}^{(i)}) + \frac{1}{m}\sum_{i=1}^{m}\log(1 - D(G(\mathbf{z}^{(i)})))\right).$$

end for

Sample minibatch of m noise samples $\{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)}\}$

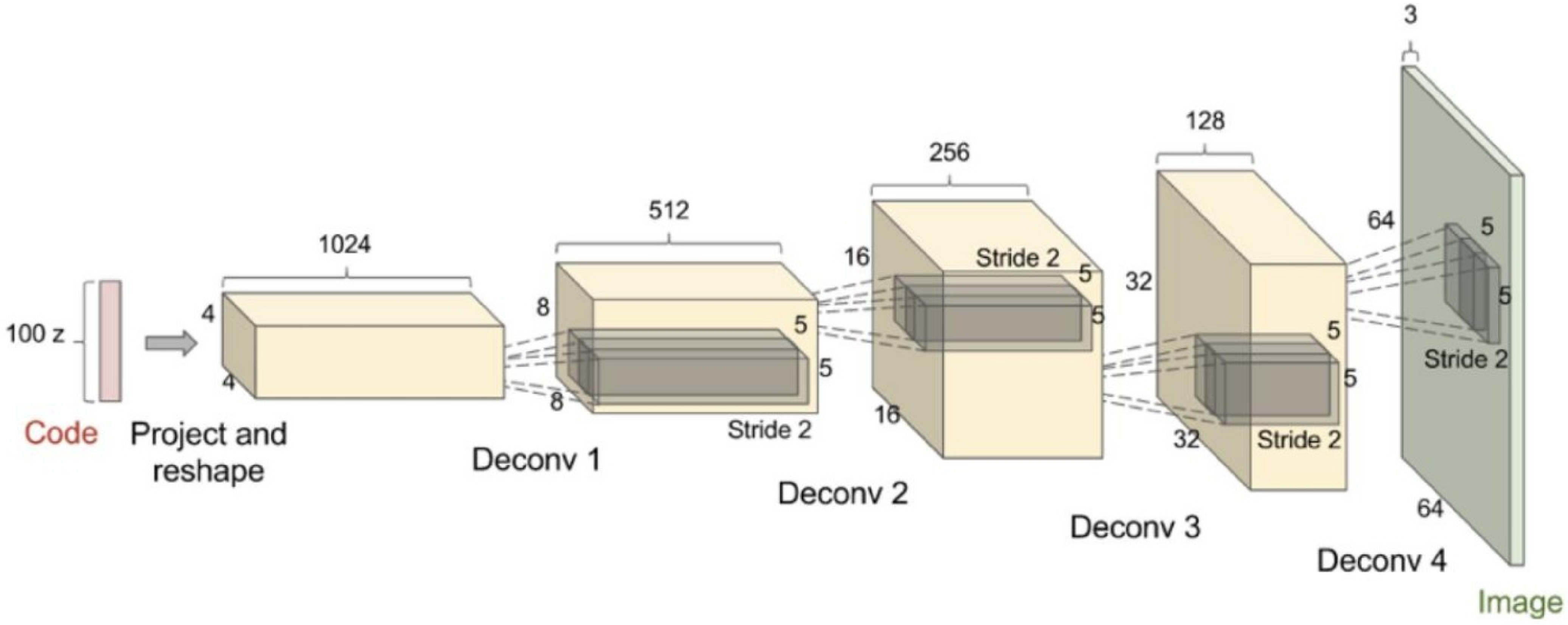
Update the generator G by stochastic gradient ascend.

Gradient:

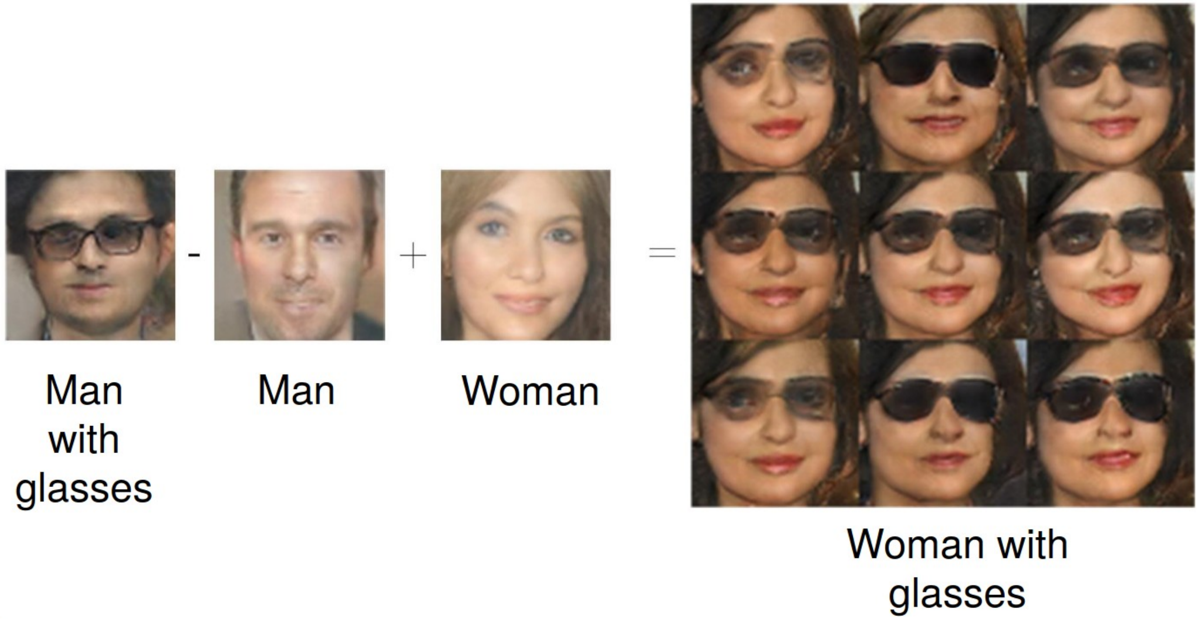
$$\frac{\partial}{\partial G}\left(\frac{1}{m}\sum_{i=1}^{m}\log(D(G(\mathbf{z}^{(i)})))\right).$$

end for

DCGAN Architecture



Examples *[up to 2015]*



Modifying GANs for Max-Likelihood

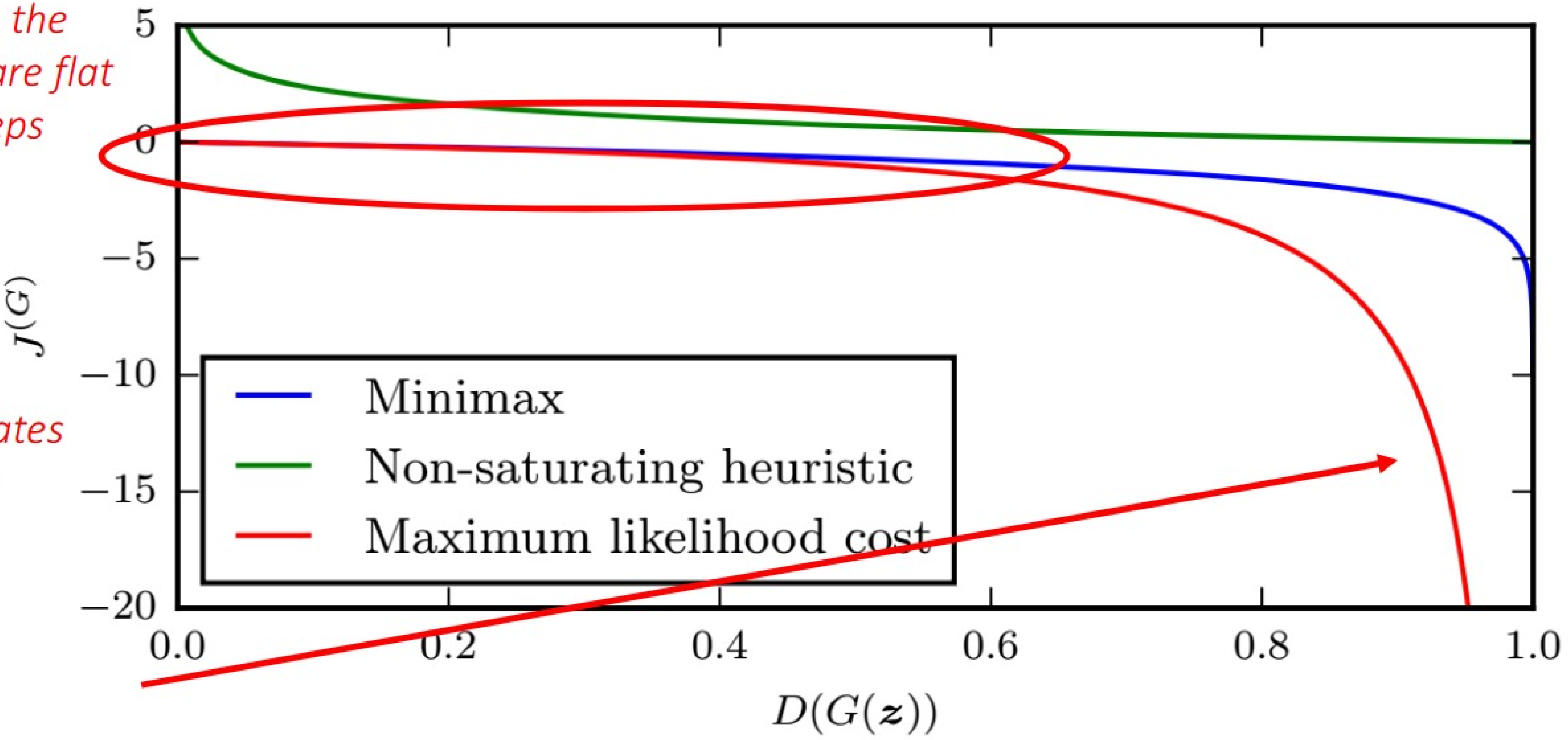
- $J^{(D)} = -\frac{1}{2}\mathbb{E}_{x\sim p_{data}} \log D(x) \ -\frac{1}{2}\mathbb{E}_{z\sim p_z} \log(1 - D(G(z)))$
- $J^{(G)} = -\frac{1}{2}\mathbb{E}_z \log(\sigma^{-1}(D\big(G(z)\big))$

When discriminator is optimal, the generator gradient matches that of maximum likelihood

https://arxiv.org/abs/1412.6515

Comparison of Generator Losses

When sample is likely fake, the minimax and the ML cost are flat
→ no gradients in early steps



The ML cost variant generates gradients mostly from the "good generations"
→ all gradients from few samples
→ high variance
→ Variance reduction?

GAN Problems: Vanishing Gradients

- $J^{(D)} = -\frac{1}{2}\mathbb{E}_{x\sim p_{data}} \log D(x) \; - \frac{1}{2}\mathbb{E}_z \log(1 - D(G(z))$
- $J^{(G)} = -\frac{1}{2}\mathbb{E}_z \log(D(G(z)))$
- If the discriminator is quite bad
  - No accurate feedback for generator
  - No reasonable generator gradients
- But, if the discriminator is perfect, $D(x) = D^*(x)$
  - Gradients go to 0
  - No learning anymore
- Bad when this happens early in the training
  - Easier to train the discriminator than the generator

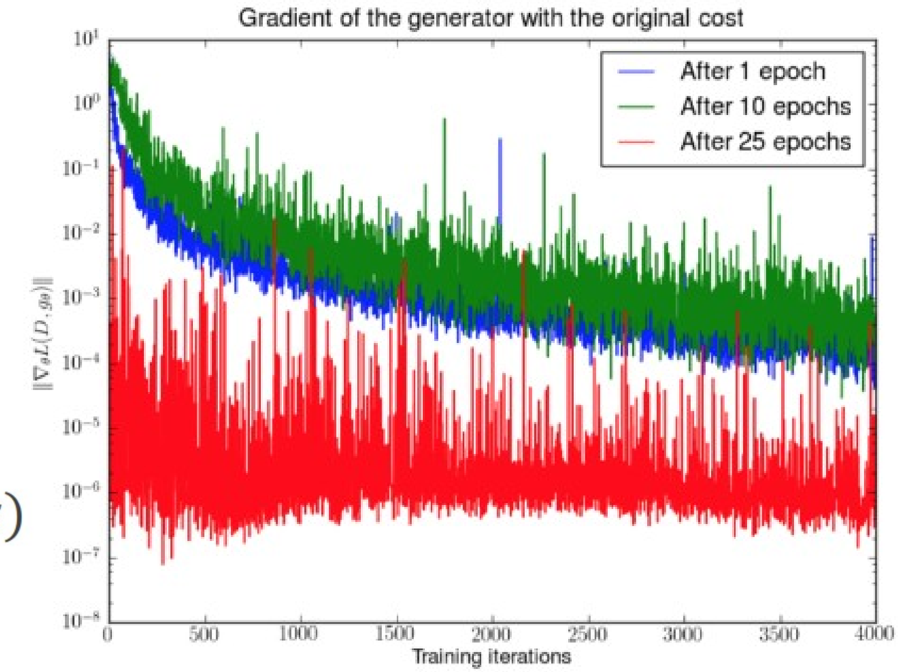
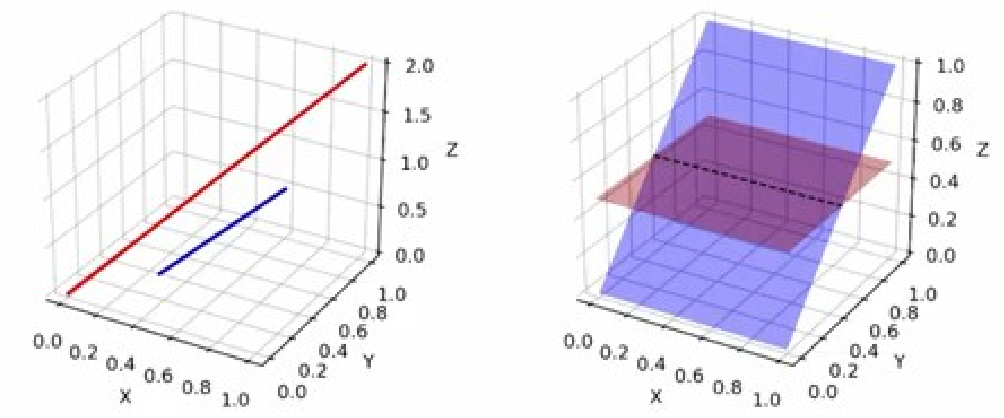


Figure from Arjovsky and Bottou 2016. DCGAN after training 1, 10 and 25 epochs

GAN Problems:Low dimensional supports

- Data lie in low-dim manifolds
- However, the manifold is not known
- During training p_g is not prefect either, especially in the start
- So, the support of p_r and p_g is non-overlapping and disjoint
- Easy to find a discriminating line



GAN Problems: Batch Normalization does not work right way

- Batch-normalization causes strong intra-batch correlation
  - Activations depend on other inputs
  - Generations depend on other inputs
- Generation looks smooth but awkward, strong intra batch correlation

Reference Batch Normalization

- Fix a reference batch $R = \{r_1, r_2, \ldots, r_m\}$
- Given new inputs $X = \{x_1, x_2, \ldots, x_m\}$
- Compute mean and standard deviation of feature of R
- Normalize the features of X using the mean and standard deviation from R
- Every x_1 is always treated the same, regardless of which other examples appear in the minibatch

Visual Batch Normalization

- Reference batch norm can overfit to the reference batch. A partial solution is virtual batch norm
- Fix a reference batch $R = \{r_1, r_2, \ldots, r_m\}$
- Given new inputs $X = \{x_1, x_2, \ldots, x_m\}$
- For each x_i in X:
  - Construct a virtual batch V containing both x_i and all of R
  - Compute mean and standard deviation of features of V
  - Normalize the features of x_i using the mean and standard deviation from V

Balancing generator and discriminator

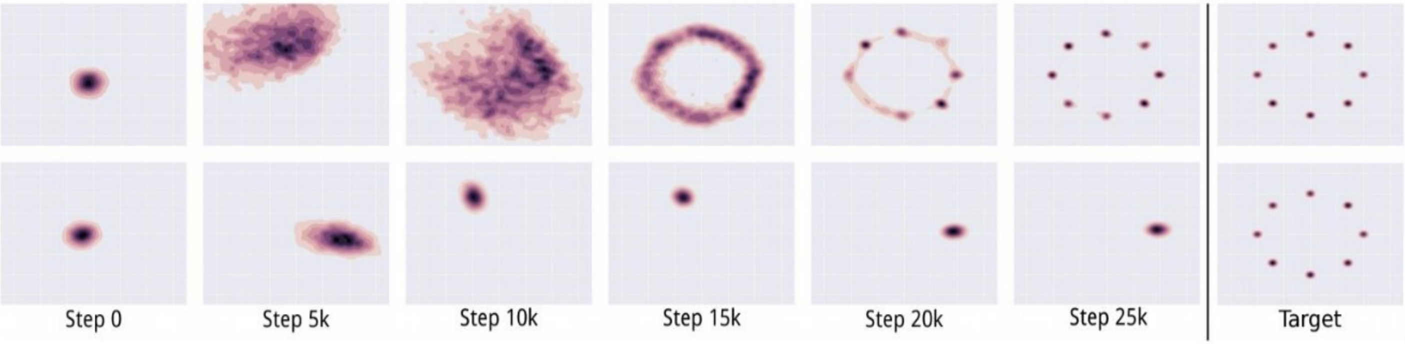
- Usually the discriminator wins
  - Good, as the theoretical justification assumes a perfect discriminator
- Usually the discriminator network is bigger and deeper than the generator
- Sometimes running discriminator more often than generator works better
  - However, no real consensus
- Do not limit the discriminator to avoid making it too smart
  - Making learning “easier” will not necessarily make generation better
  - Better use non-saturating cost
  - Better use label smoothing

Challenge: Convergence

- Optimization is tricky and unstable
  - Finding a saddle point does not imply a global minimum
  - A saddle point is also sensitive to disturbances
- An equilibrium might not even be reached
- Mode-collapse is the most severe form of non-convergence

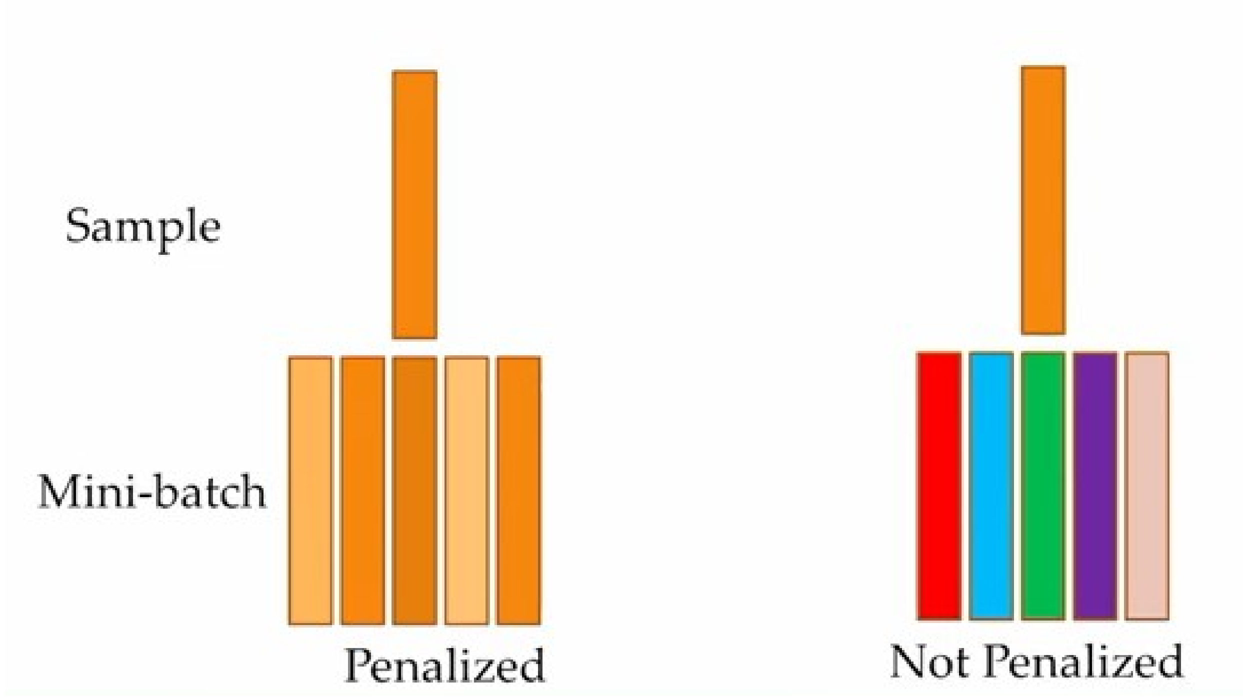
GAN Problems: Mode collapse

- Discriminator converges to the correct distribution
- Generator however places all mass in the most likely point
- All other modes are ignored
  - Underestimating variance
- Low diversity in generating samples



Minibatch features

- Classify each sample by comparing to other examples in the mini-batch
- If samples are too similar, the model is penalized



Challenge: how to evaluate?

- Despite the nice images, who cares?
- It would be nice to quantitatively evaluate the model
- For GANs it is hard to even estimate the likelihood
- In the absence of a precise evaluation metric, do GANs do truly good generations or generations that appeal/ fool to the human eye?
  - Can we trust the generations for critical applications, like medical tasks?
  - *Are humans a good discriminator for the converges generator?*

Training procedure

- Use SGD-like algorithm of choice
  - Adam Optimizer is a good choice
- Use two mini-batches simultaneously
  - The first mini-batch contains real examples from the training set
  - The second mini-batch contains fake generated examples from the generator
- Optional: run k-steps of one player (e.g. discriminator) for every step of the other player (e.g. generator)

Feature matching

- Instead of matching image statistics, match feature statistics

$$J_D = \left\| \mathbb{E}_{\boldsymbol{x} \sim p_{data}} f(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{z} \sim p(\boldsymbol{z})} f\big(G(\boldsymbol{z})\big) \right\|_2^2$$

- f can be any statistic of the data, like the mean or the median

Use labels if possible

- Learning a conditional model p(y|x) is often generates better samples
  - Denton et al., 2015
- Even learning p(x,y) makes samples look more realistic
  - Salimans et al., 2016
- Conditional GANs are a great addition for learning with labels

Summary

- GANs are generative models using supervised learning to approximate and intractable cost function
- GANs can simulate many cost functions, including max likelihood
- Finding Nash equilibria in high-dimensional, continuous, non-convex games is an important open research problem
- GAN research is in its infancy, most works published only in 2016. Not mature enough yet, but very compelling results

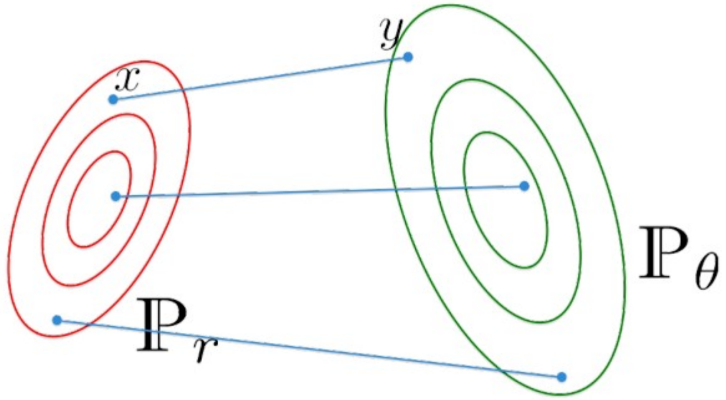
2014 2015 2016 2017 2018

Models

- Wasserstein GAN
- Progressive GANs
- InfoGAN
- Conditional GAN
- StyleGAN
- CycleGAN

Wasserstein GAN [Intuition]

- The distribution of the generated data should be as close as possible to the distribution of the real data [M. Arjovsky et al. 2017]
- The Wasserstein metric is the cost of optimal transport between the two distributions.



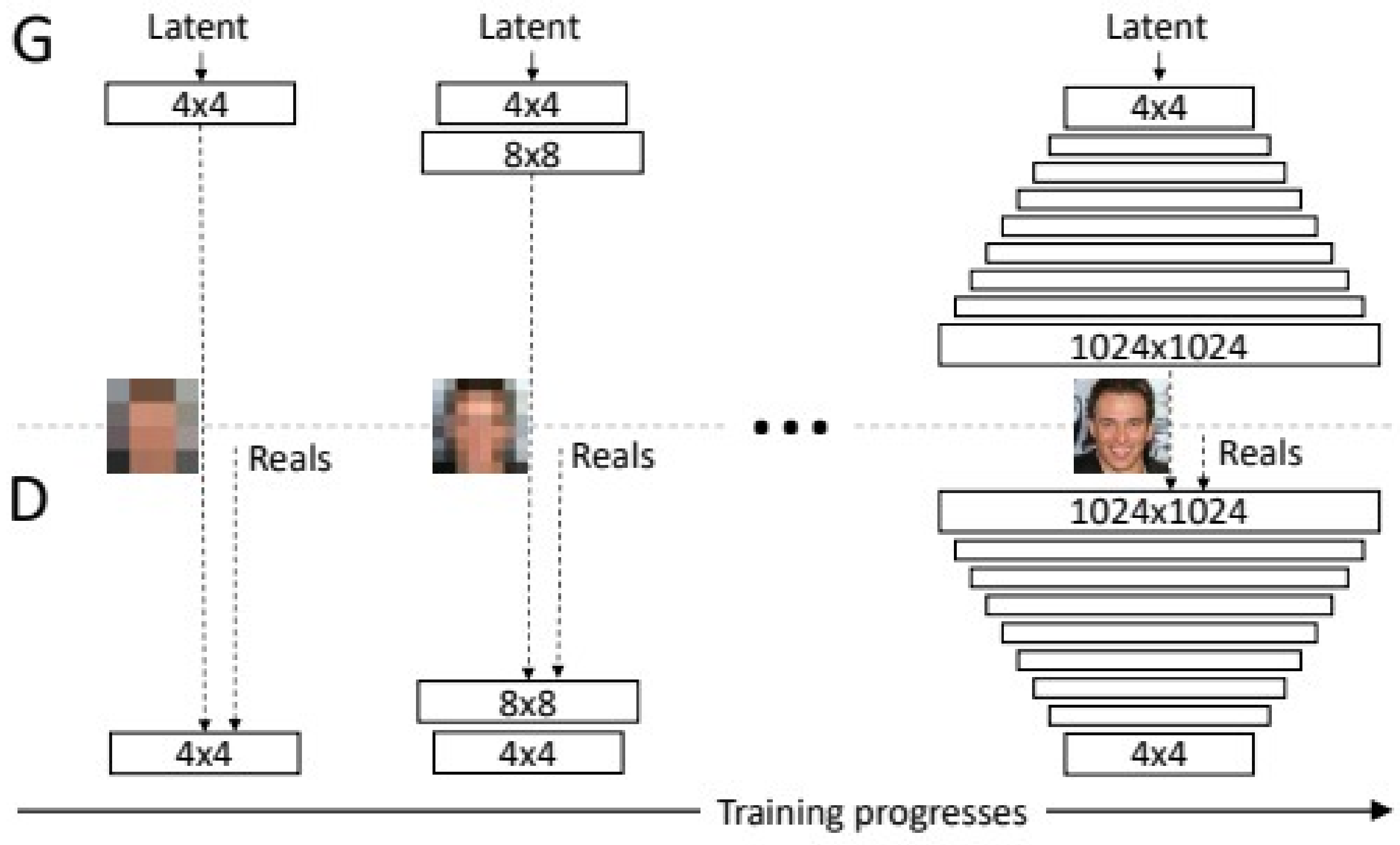
Intuitive (but imperfect) view:

$$W(\mathbb{P}_r, \mathbb{P}_\theta) = \min_{\gamma \in \Gamma} \sum_{(x,y) \in \gamma} [\|x - y\|],$$

where Γ is the set of all possible sets of correspondences between x and y.

Progressive GANs

- T. Karras et al. 2018



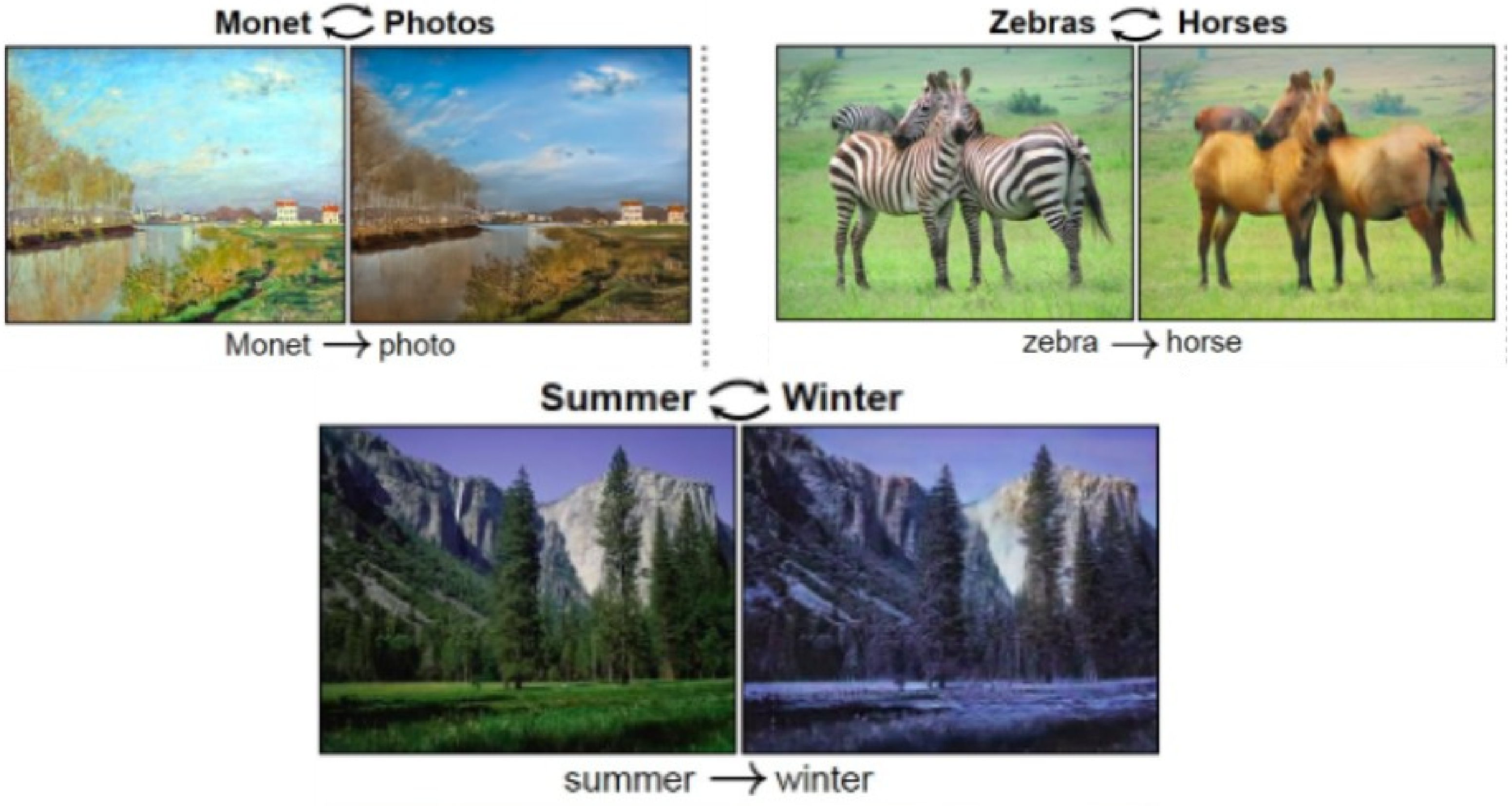
Progressive GANs: Results

Generated Image

Nearest Neighbor in the training set

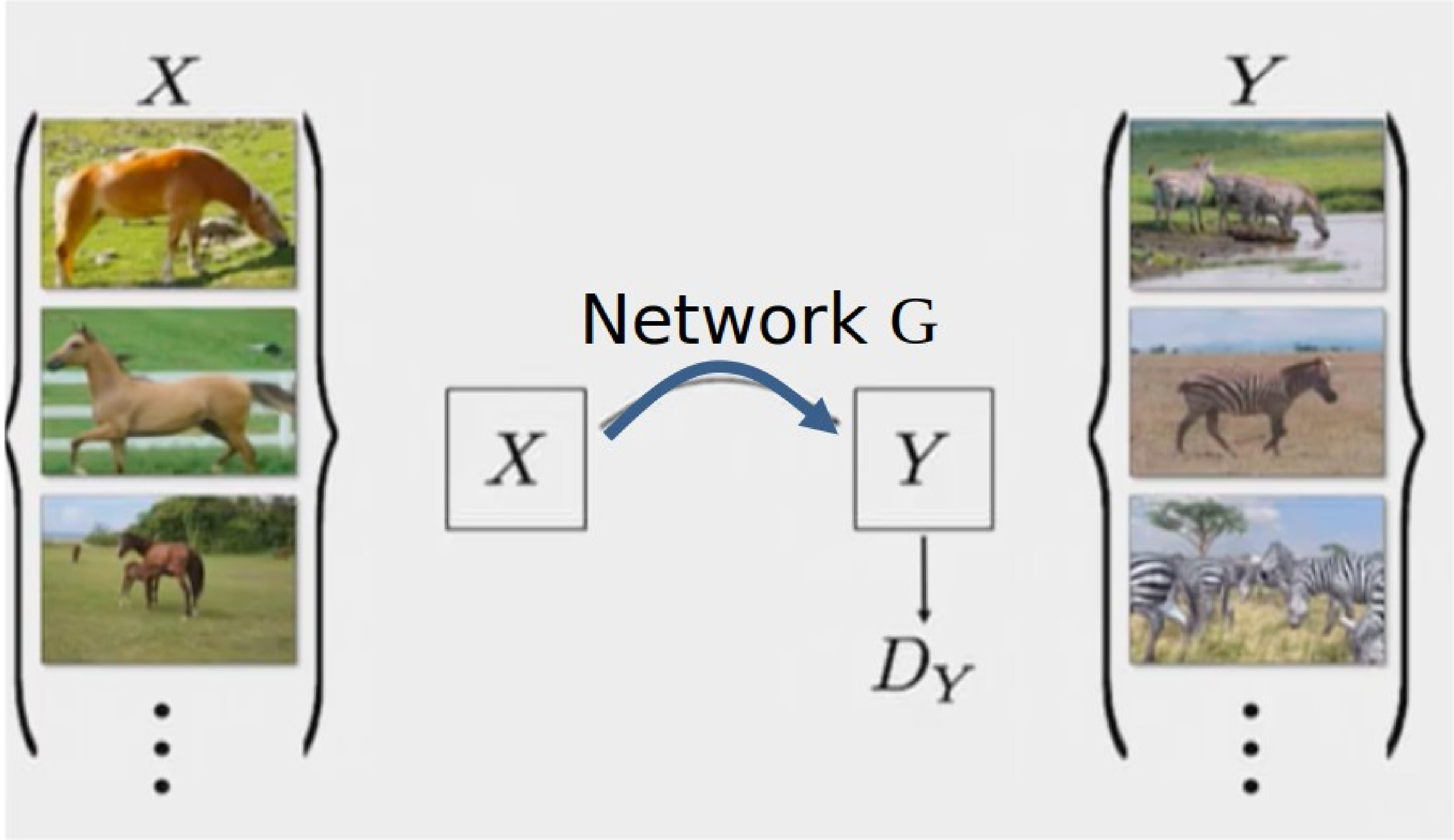
CycleGAN

- How can we make sure we preserve the content of an input image?



CycleGAN

- J.-Y. Zhu et al. 2017



CycleGAN

- J.-Y. Zhu et al. 2017