shorturl.at/hoA38 ← Tutorial web page

# Generative Models: Part I

- Variational Autoencoders
- Generative Adversarial Networks


**Jonas Glombitza,** Martin Erdmann

RWTH Aachen

21.03.2022
Deep Learning Weeks, Uppsala

# Outline

Monday

I. Deep Learning Basics – short hands-on

II. Convolutional Neural Networks – short hands-on

*BREAK*

III. Introduction to Generative Adversarial Networks (GANs)

IV. Tutorial: Implementation of GANs

Wednesday

V. Latest developments & advanced techniques

- Wasserstein GANs

VI. Application in physics research

- Simulation acceleration, domain adaption

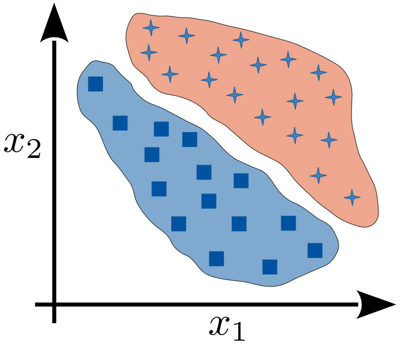
*BREAK*

VII. Tutorial: Implementation of Wasserstein GANs

**Feel free to ask questions during the seminar!**
**Just "raise" your hand...**

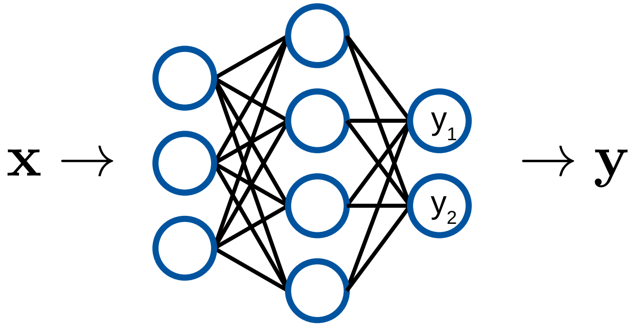
# Supervised and Unsupervised Learning

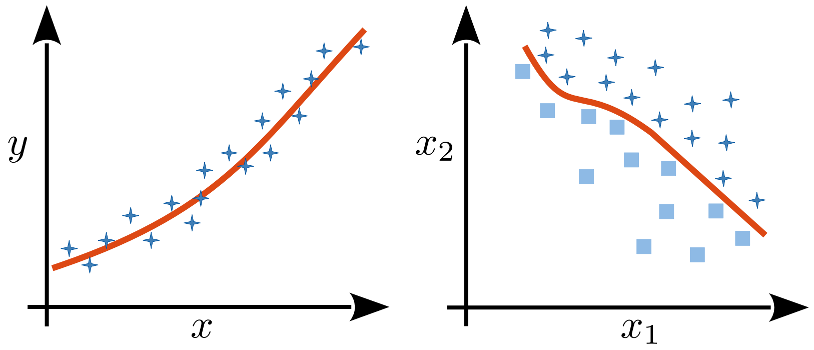
- Generative Models
    - Variational Autoencoders
    - Generative Adversarial Networks



# Supervised Learning

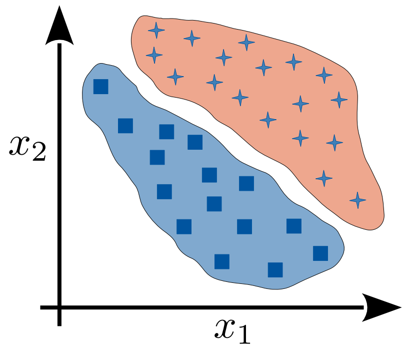
- Situation
  - Large labeled data set (pair of input $\mathbf{x}$ and output $\mathbf{y}$)
- Typical Task:
  - Learn function to map input to specific output
  - Train model to predict the associated label
  - Achieve best generalization performance
  - Infer *conditional* probability density $p(\mathbf{x}|\mathbf{y})$



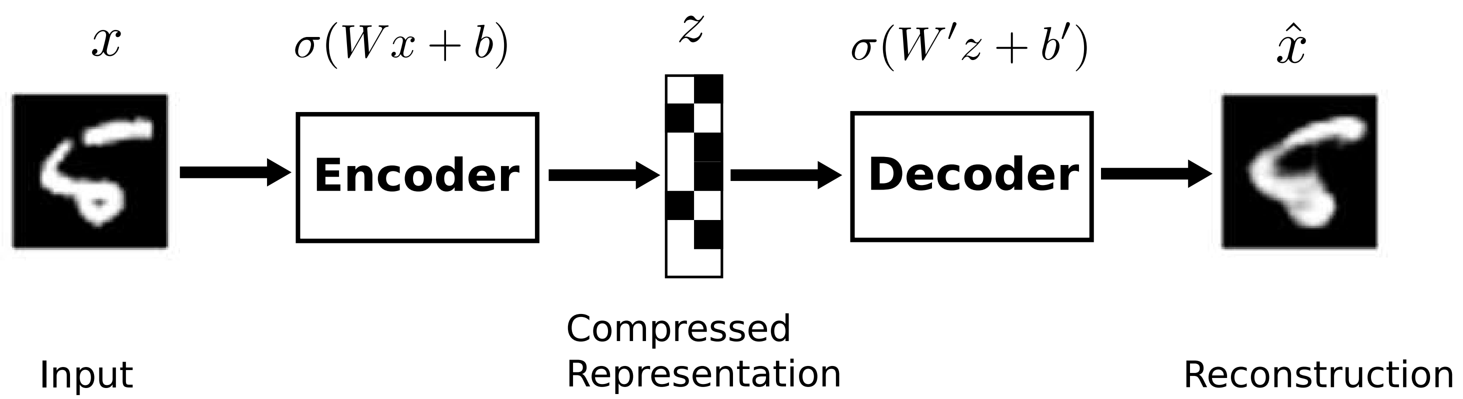



# Unsupervised Learning

- Typical situation: non labeled data set
- Tasks:
  - Learn (low dimensional) data encodings → *autoencoders*
  - Estimate underlying probability density → *generative models*
  - Clustering, anomaly detection – find (non-) similar samples
- Infer *a priori* probability density $p(x)$
- Models typical trained without label information
  - Contrast: semi-supervised learning



# Recap: Autoencoders




- Reconstruction of input data (approximation of identity function)
- Learning interesting representation (constraints to hidden layer)
- Objective function:

$$\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}) = \frac{1}{N} \sum_{i=1}^{N} (\hat{\mathbf{x}}_i - \mathbf{x}_i)^2$$

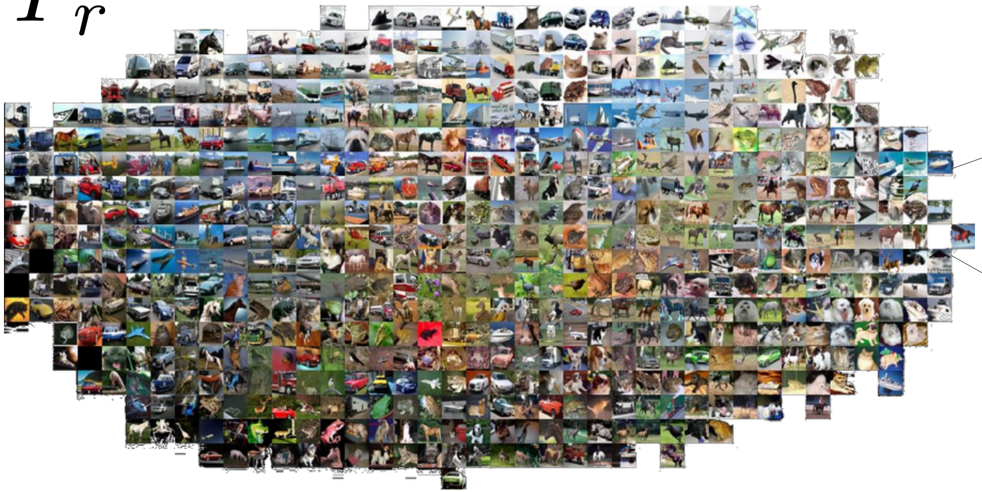
- Deep autoencoders often show underfitting → use shortcuts!

# Generative Models

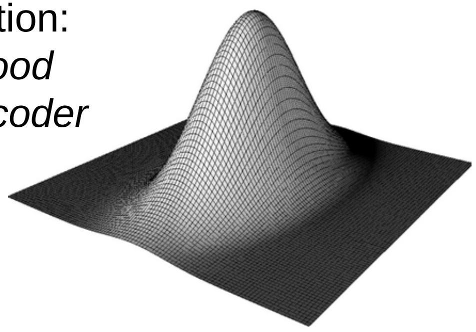
Approximate data distribution $P_r$ with another distribution $P_\theta$

$\theta$ = distribution parameters

$P_r$

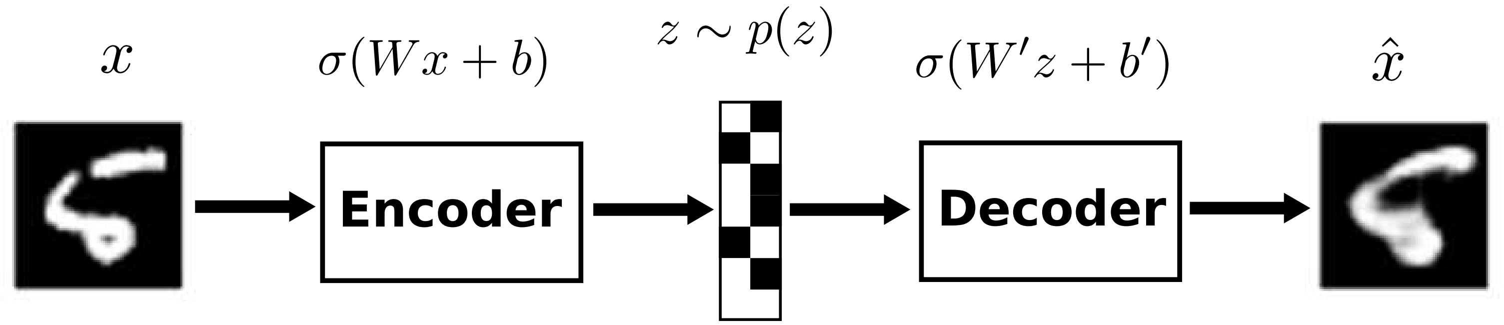


Learn prior distribution:
*Maximizing Likelihood*
*Variational Autoencoder*



Learn to generate samples following $P_\theta$
Without using directly $P_\theta$
*Train a generator only* $\rightarrow$ *GANs*

# Variational Autoencoder

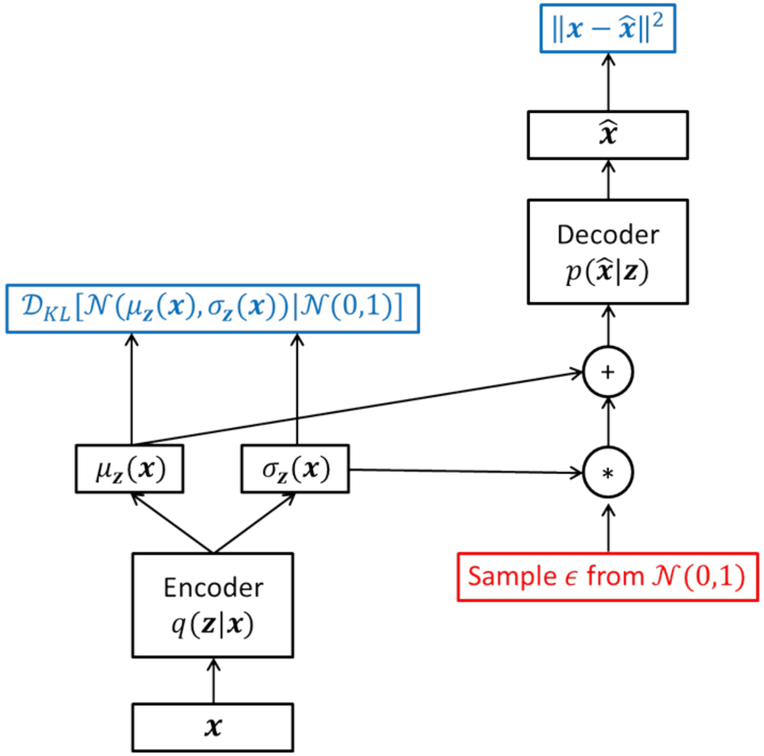



- Learned representation is not an arbitrary function
  - Impose *prior distribution* on the hidden (low dimensional) representation
- Trained decoder part can be used as *generator* (sample from prior distribution)
- Objective function = reconstruction error + divergence of hidden representation from a prior

$$\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}, \mathbf{z}) = \mathcal{L}_{recon.}(\mathbf{x}, \hat{\mathbf{x}}) + \mathcal{D}_{KL}[q(\mathbf{z}|\mathbf{x})|p(\mathbf{z})]$$
$$= \frac{1}{N}\sum_{\mathbf{x}}\left[||\mathbf{x} - \hat{\mathbf{x}}||^2 + \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})}\right]$$

Kullback-Leibler Divergence: $\mathcal{D}_{KL}$
Measure of information loss if $p(\mathbf{z})$ is used instead of $p(\mathbf{z}|\mathbf{x})$

# Variational Autoencoder




**Gaussian prior:** $z \sim \mathcal{N}(0,1)$

- Encoder $q(\mathbf{z}|\mathbf{x})$ learns latent parameters $\mu_{\mathbf{z}}(\mathbf{x}), \sigma_{\mathbf{z}}(\mathbf{x})$ of Gaussian distribution
- Re-parametrization $z = \mu_{\mathbf{z}}(\mathbf{x}) + \sigma_{\mathbf{z}}(\mathbf{x})\epsilon$ with $\epsilon \in \mathcal{N}(0,1)$
- Example: 2D Gaussian
  - Only two independently normal distributed parameters in hidden layer for each input
- $\mathcal{D}_{KL}[\mathcal{N}(\mu_z(\mathbf{x}),\sigma_z(\mathbf{x}))|\mathcal{N}(0,1)]$

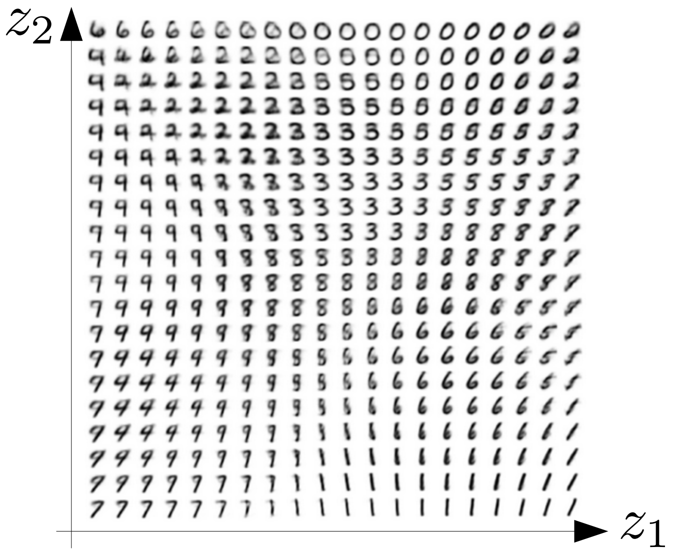
$$= \frac{1}{N}\sum_{\mathbf{x}}\int_{\mathbf{z}} dz\, \mathcal{N}(\mu_{\mathbf{z}},\sigma_{\mathbf{z}}) \log\frac{\mathcal{N}(0,1)}{\mathcal{N}(\mu_{\mathbf{z}}(\mathbf{x}),\sigma_{\mathbf{z}}(\mathbf{x}))}$$

$$= \frac{1}{N}\sum_{\mathbf{x}}\frac{1}{2}(1+\log\sigma^2_{\mathbf{z}}(\mathbf{x}) - \mu^2_{\mathbf{z}}(\mathbf{x}) - \sigma^2_{\mathbf{z}}(\mathbf{x}))$$

# Variational Autoencoder

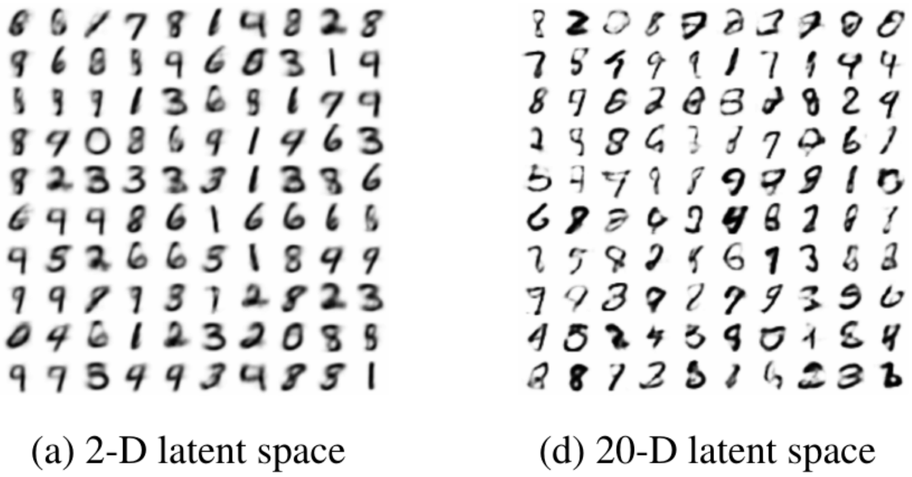
Objective: $\mathcal{L}(\mathbf{x}, \hat{\mathbf{x}}, \mathbf{z}) = MSE(\mathbf{x}, \hat{\mathbf{x}}) + \mathcal{D}_{KL}[q(\mathbf{z}|\mathbf{x})|p(\mathbf{z})]$

- Mean-squared-error: → How accurate input can be reconstructed
- KL-divergence: → How close the latent variables match (unit Gaussian)
- Allows walk in latent space

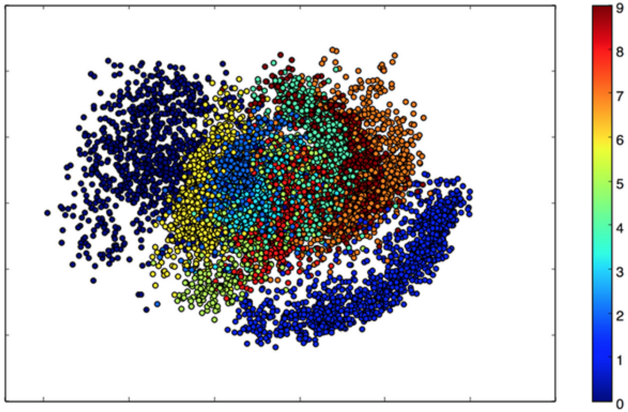



VAE trained on MNIST using 2D Gaussian prior

Improved quality for increased size of latent space



# Variational Autoencoder



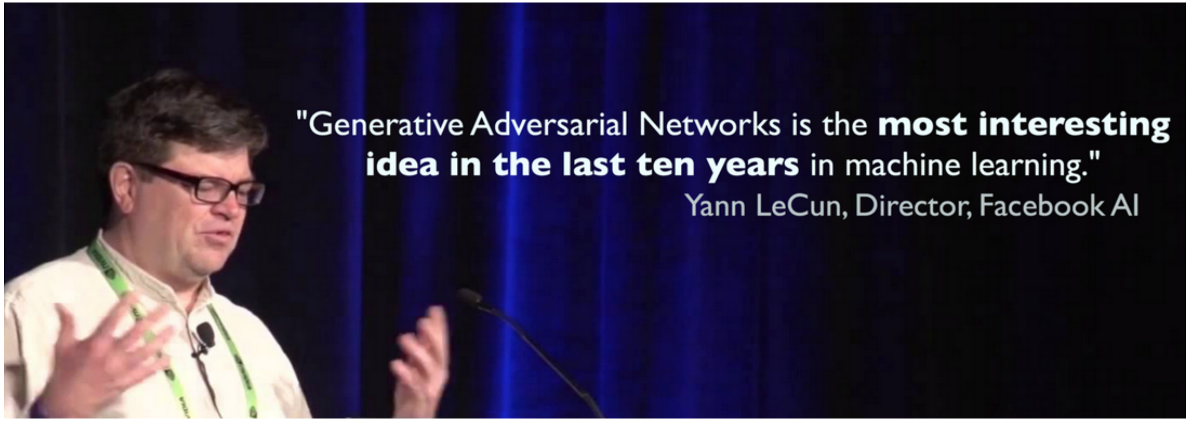
Latent space of VAE trained on MNIST

- Samples of Variational Autoencoders often look noisy
  - Gaussian prior not always best choice / can use arbitrary prior distribution
  - Gaussian distributions can not capture all modes of the data
  - Mean-squared-error loss very inflexible

➢ Try adversarial approach → Only train a generator

# Introduction to GANs

- Adversarial training
- Design of GANs
- Conditioning



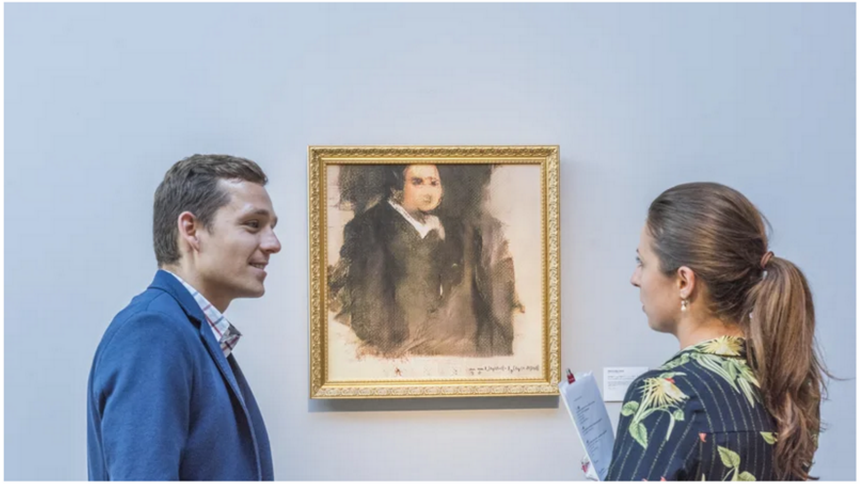
# Generative Adversarial Networks - GANs

Künstliche Intelligenz

## Auktionshaus versteigert erstmals KI-Gemälde

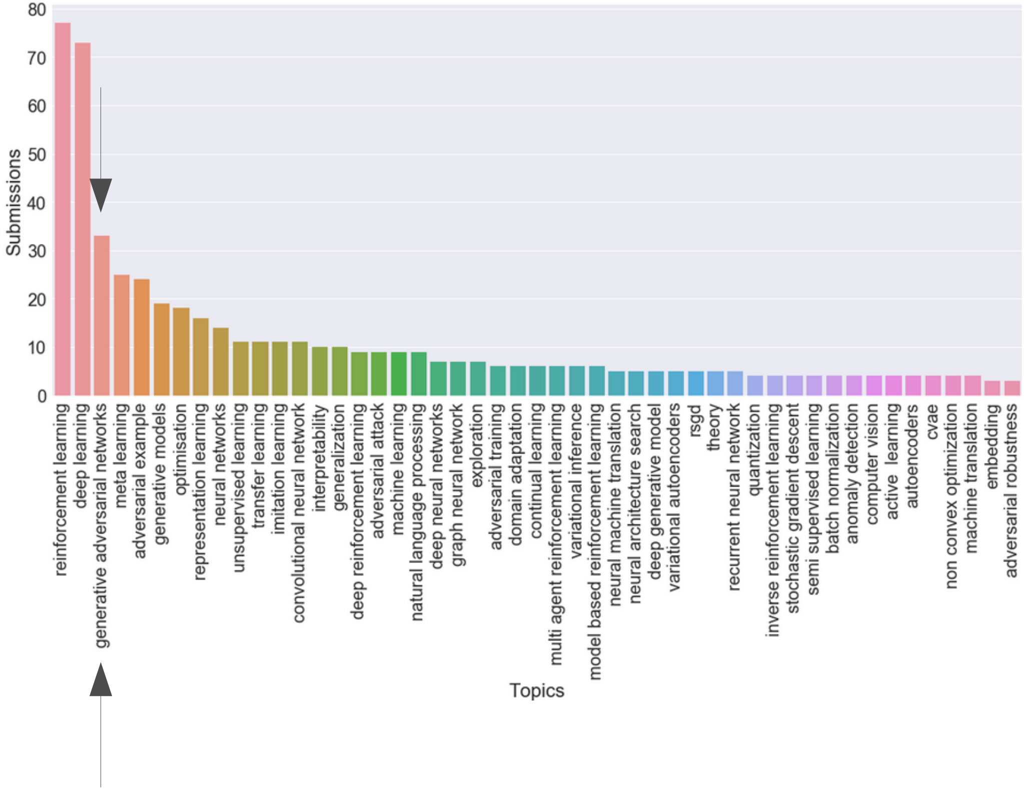
Kein Maler sondern ein Computer-Algorithmus hat das Porträt "Edmond de Belamy" erschaffen. Beim Auktionshaus Christie's zahlte ein Interessent dafür knapp 400.000 Euro.

26. Oktober 2018, 9:00 Uhr / Quelle: ZEIT ONLINE, AFP, fo / 75 Kommentare



*Der verschwommene Druck "Edmond de Belamy" zeigt einen Mann in dunkler Kutte mit weißem Kragen, der an einen französischen Geistlichen erinnert.* © Christie's/dpa

https://ailab.criteo.com/iclr-2019-stats-trends-and-best-papers/



# How to train a Generator

I. Objective: learn to generate new samples following $P_\theta$

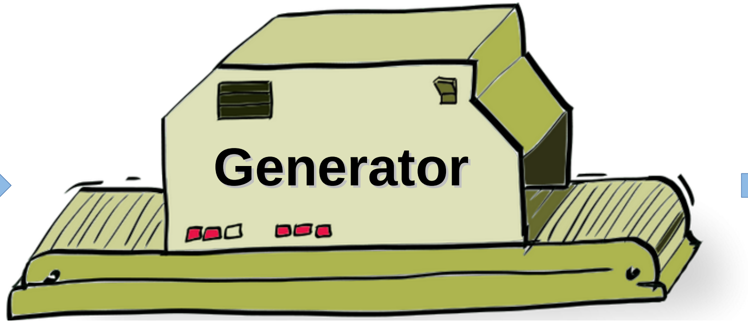
II. Learn a function that transform a distribution $p(\mathbf{z})$ into $P_\theta$ using a generator $G_\theta$

$\mathbf{z} \in Z$ → latent space

III. Generator $G_\theta$ is implemented as neural network with weights $\theta$

**Noise input**

$\mathbf{z} \sim p(\mathbf{z})$




**Samples following $P_\theta$**

# Generative Adversarial Networks

I. Hard to formulate a supervised training loss

II. Use **unsupervised training** to train the generator

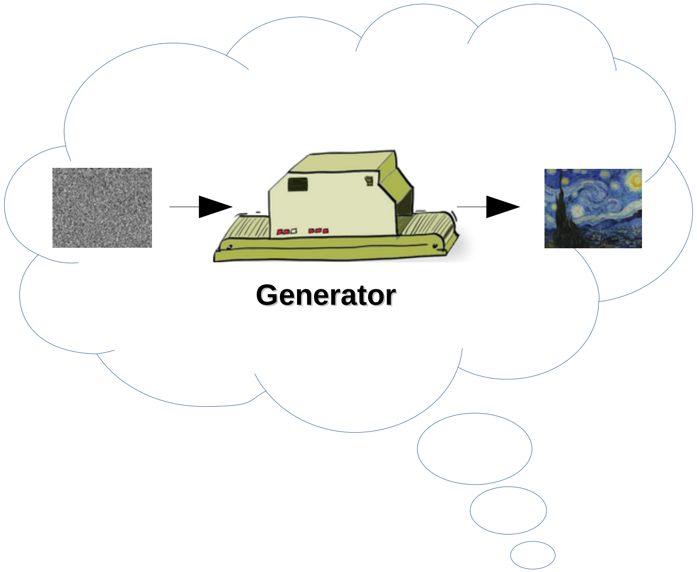
- Objective: $P_\theta \approx P_r$
- Measure: given by **second neural network**

→ Generated samples of generator should be similar to real samples after training

- without reproducing training data

→ **Adversarial approach:**

Train 2 networks adversarial (against each other)




Art forger

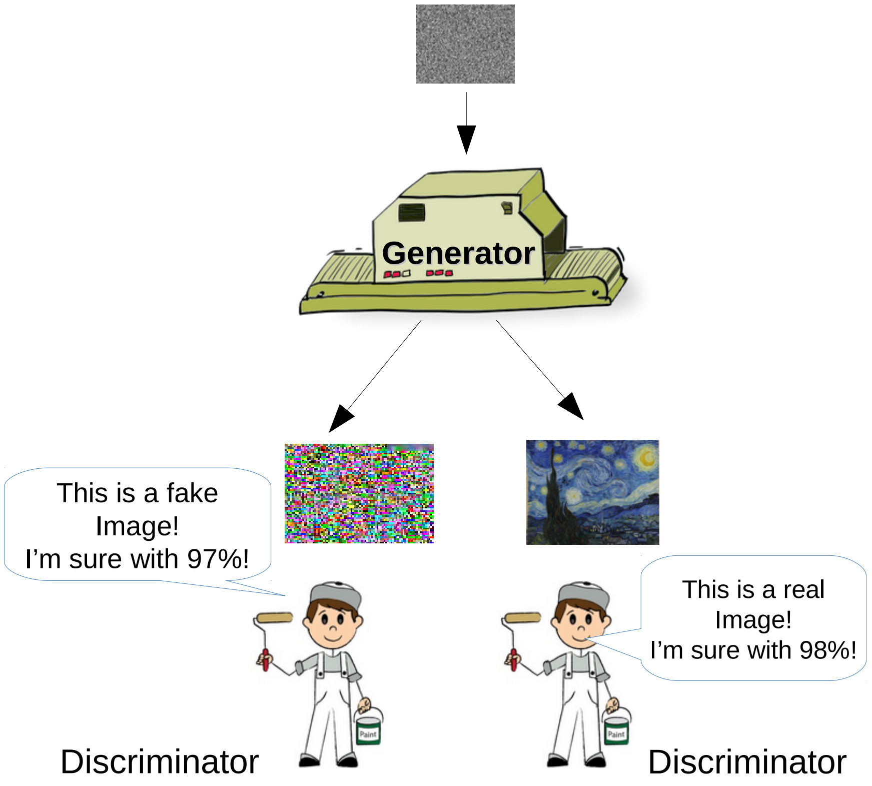
Wants to create some fake images

# Generative Adversarial Networks

I. Generator
- Try to generate realistic samples

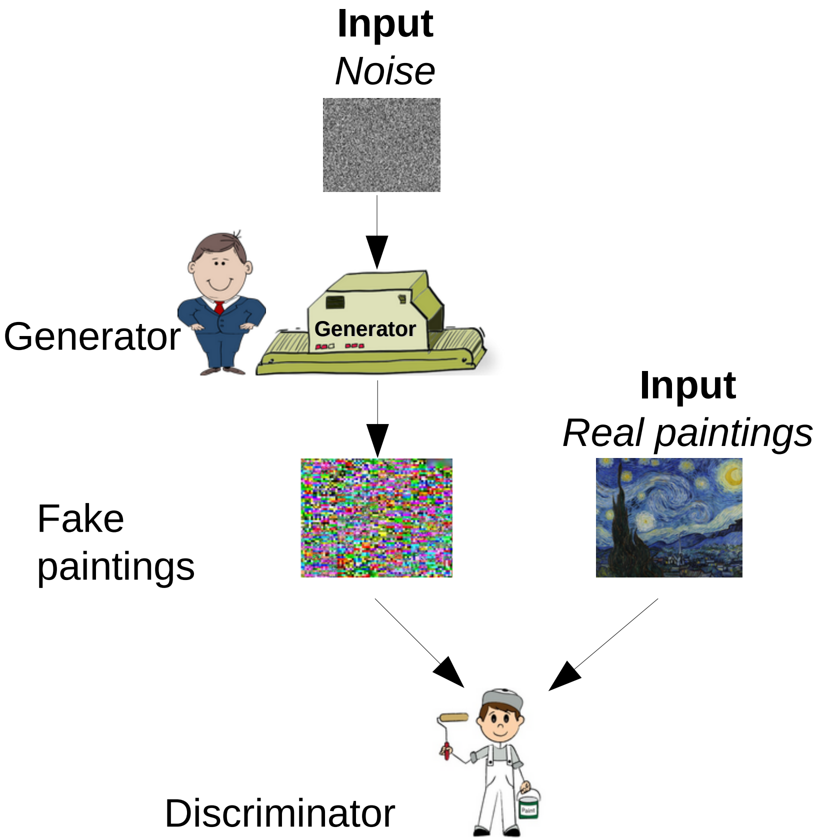
II. Discriminator
- Try to discriminate between fakes and realistic images
- Evaluate if $P_\theta \approx P_r$

III. Discriminator returns probability if generated sample is real

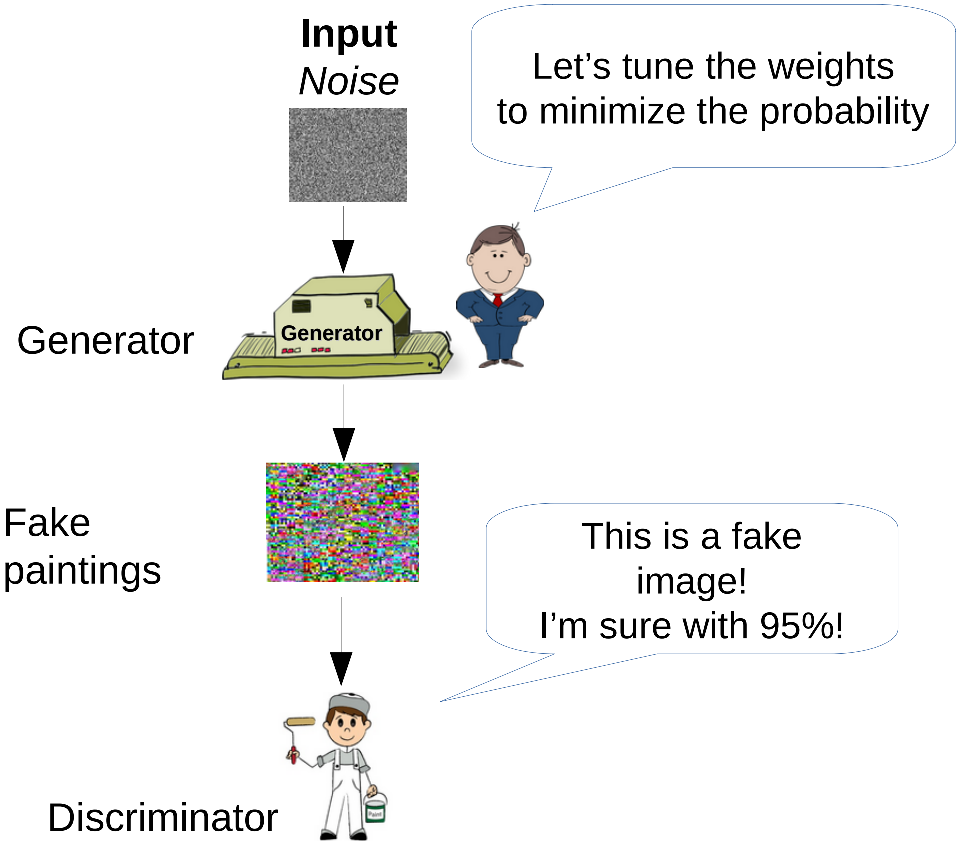



*"GANs is the most interesting idea in the last ten years in machine learning."* *- Y. LeCun*

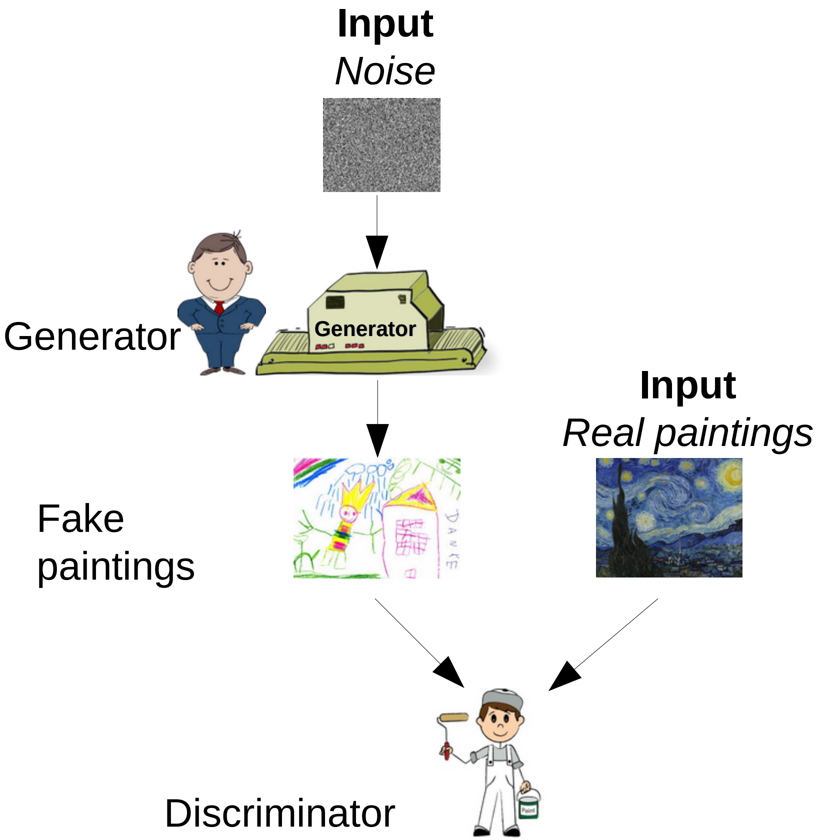
# Train Discriminator



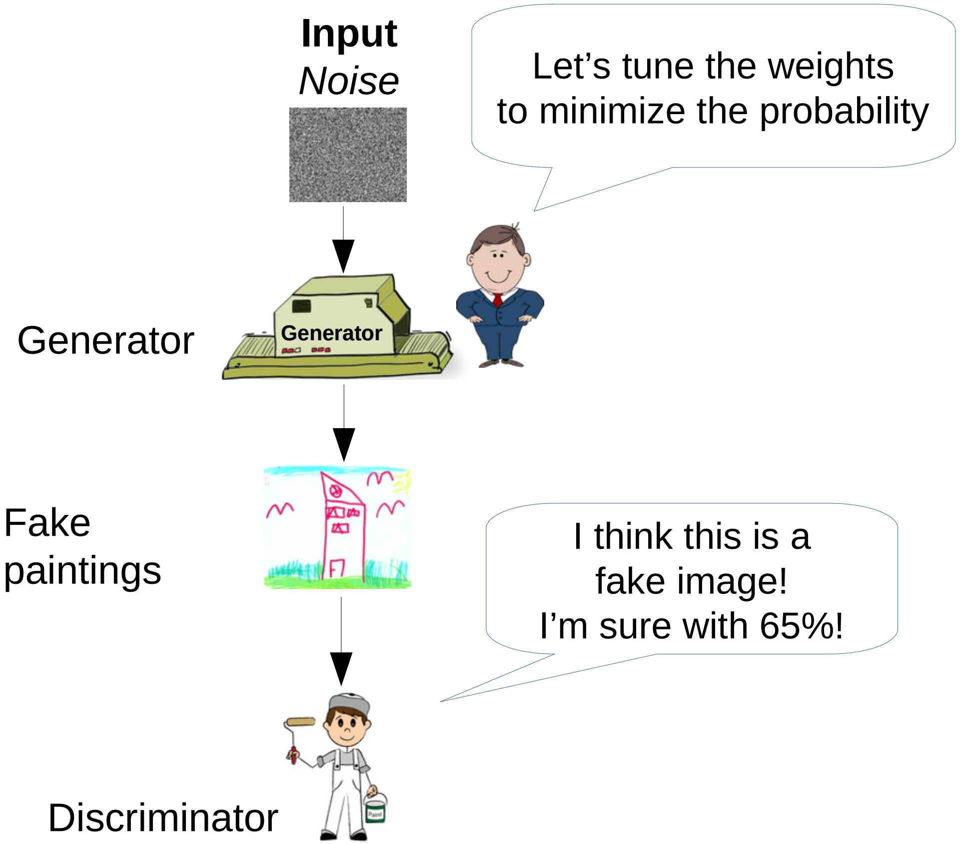

# Train Generator



## Train Discriminator




## Train Generator



# Train the Discriminator

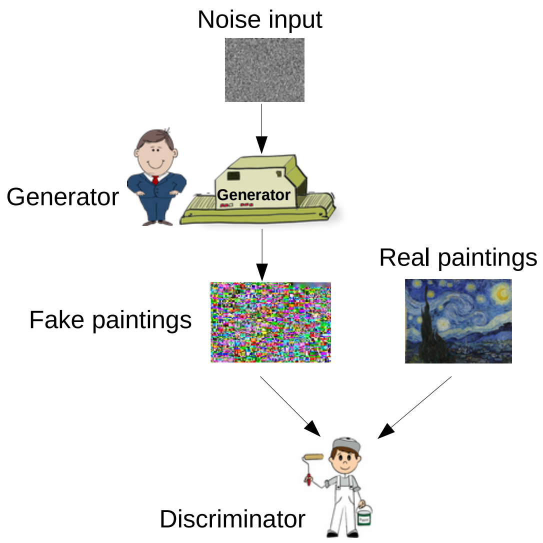
I. Implemented as neural network $D$ having weights $w$

Expectation value

$$Loss = \mathbb{E}_{\mathbf{x}\sim p_{data}(\mathbf{x})}[log(D_w(\mathbf{x}))] + \mathbb{E}_{\mathbf{z}\sim p_z(\mathbf{z})}[log(1 - D_w(G(\mathbf{z})))]$$

Real samples

Generated fake samples




II. **Maximize** loss → minimize binary cross entropy

- Tuning discriminator weights

III. Typical classification task for neural network

- Learns to separate two classes

# Train the Generator

I. Optimal discriminator is freezed

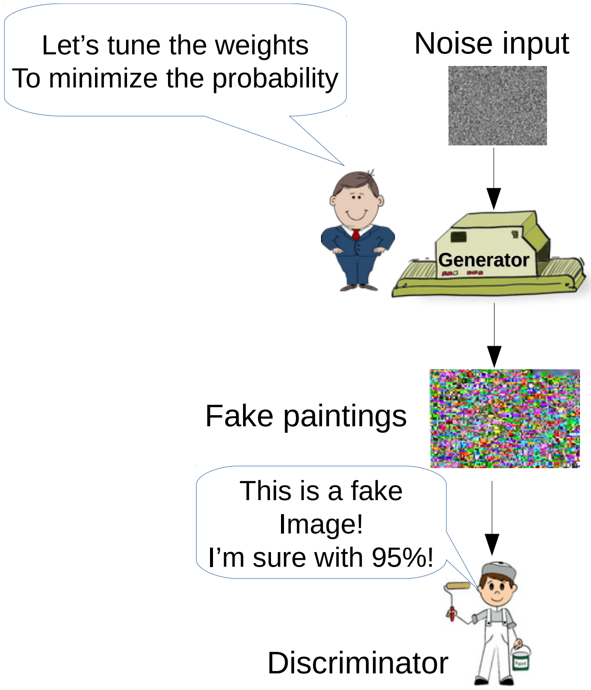
$$Loss = \mathbb{E}_{\mathbf{z}\sim p_z(\mathbf{z})}[log(1 - D(G_\theta(\mathbf{z})))]$$

II. **Minimize** loss: $\rightarrow$ maximize binary cross entropy

- Tuning the generator weights $\theta$
- Discriminator should fail to discriminate

III. Best case: coin flipping

$$D(G(\mathbf{z})) = \frac{1}{2} \qquad D(\mathbf{x}) = \frac{1}{2}$$

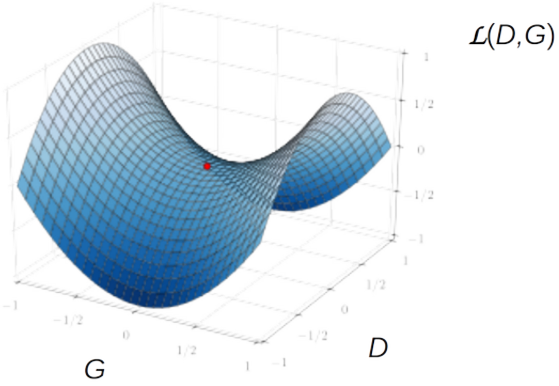


# GAN Training

$$\min_G \max_D L(D, G) = \mathbb{E}_{\mathbf{x}\sim p_{data}(\mathbf{x})}[log(D(\mathbf{x}))] + \mathbb{E}_{\mathbf{z}\sim p_z(\mathbf{z})}[log(1 - D(G(\mathbf{z})))]$$

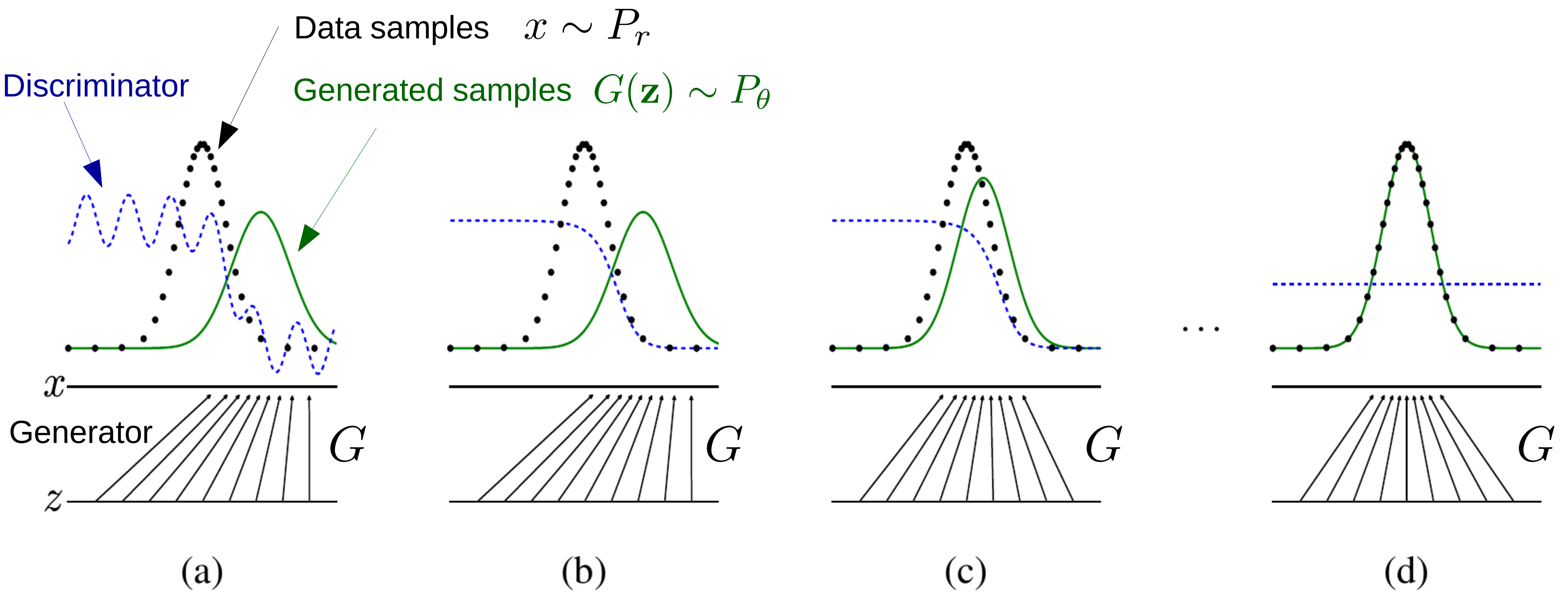
Training 2 networks at the same time is challenging
Losses of discriminator and generator are highly dependent

I. Train generator and discriminator alternating
   - Min/Max game
   - Sum of both players is zero




II. Finding Nash equilibrium is hard
   - Discriminator and generator need to have same quality
   - Minimize Jensen-Shannon divergence (assume optimal discriminator)

# Optimal Evolution of GAN Training




Goodfellow et al. - arXiv:1406.2661

Gradient of discriminator guides generator
→ G generates samples which are more likely identified as data

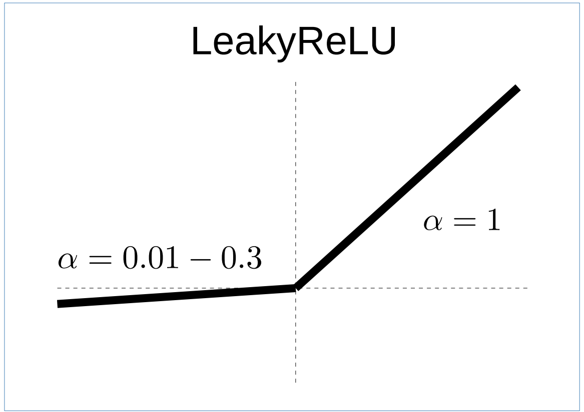
**Epochs**

# Network Design

- Discriminator / classical DCNN for classification
  - Use sigmoid (1 output node) / softmax (2 output nodes) after last layer

- DCGANs (Deep Convolutional GANs) show improved stability

- Use Deep Convolutional generator and discriminator:
  I. Use batch normalization
  II. Remove fully connected hidden layers
  III. Use ReLU in the generator
  IV. Use LeakyReLU in the discriminator
  V. Use transposed convolutions



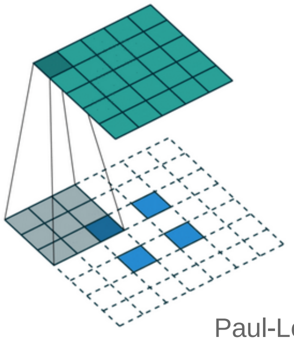
# Deep Convolutional GAN (DC-GAN)

I. Topology of the generator:
   - Decrease feature space
   - Increase spatial extent

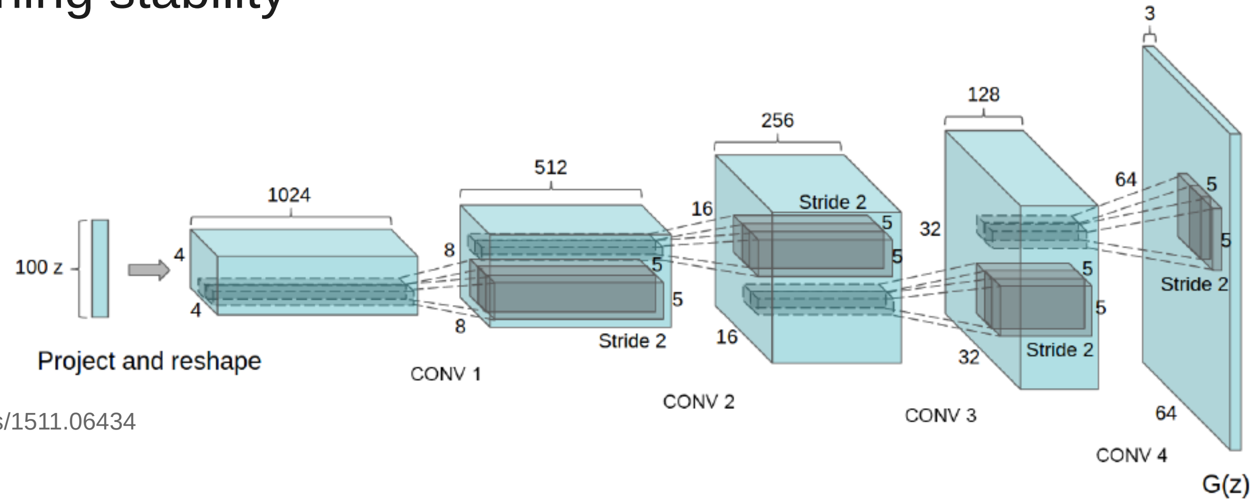
II. Supports a simple structured latent space

III. Use transposed convolutions + striding

➔ Shows improved training stability



Paul-Louis Pröve,
Towards Data Science




A. Radford, L. Metz, S. Chintala - https://arxiv.org/abs/1511.06434

# Implementation: Adversarial Training

Generate fake samples $\tilde{x}$ similar to real samples $x$

I. Train discriminator
  - Sample noise $z$, feed it into the generator to generate fake samples $G(z) = \tilde{x}$
  - Train discriminator to classify fake $\tilde{x}$ and real samples $x$

II. Train generator using the discriminator feedback
  - Freeze parameters of discriminator
  - Generate fake samples $G(z) = \tilde{x}$ and pass it to the discriminator
  - Adapt weights of $G$ by fooling the discriminator $D$

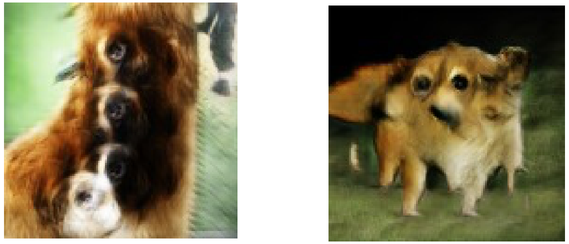
III. Unfreeze parameters of the discriminator

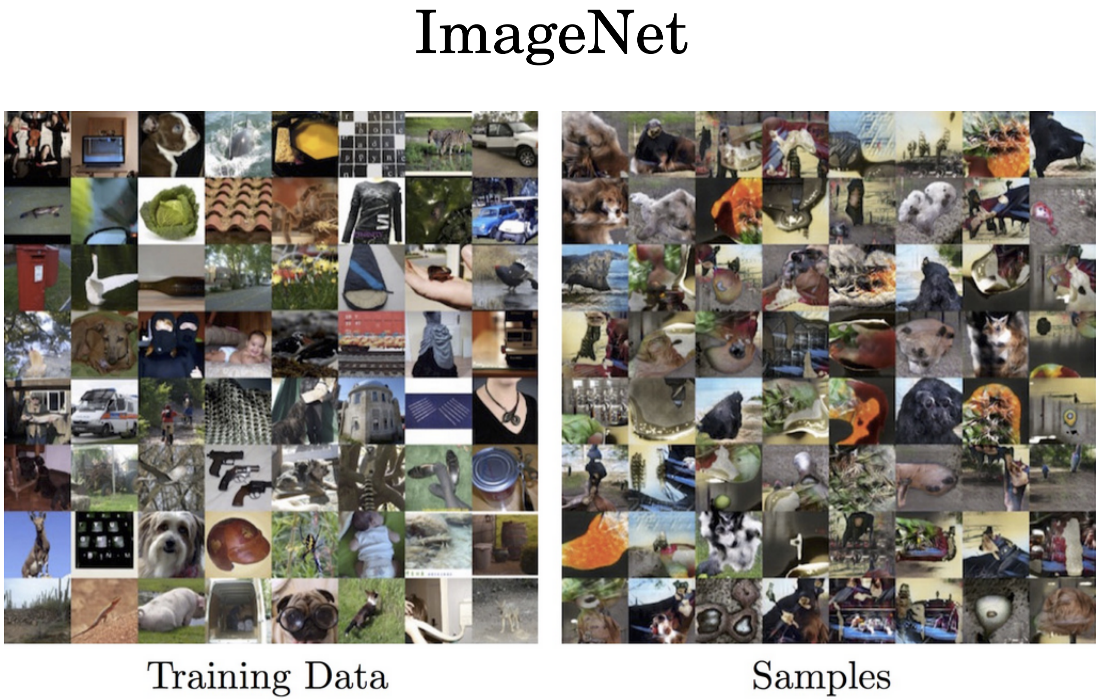
```
# freeze / unfreeze layers in a model
for layer in model.layers:
    layer.trainable = True    # False
# update parameters for a single batch
loss = model.train_on_batch(x, y)
```

# Generative Adversarial Networks

- Wrong global structure

- Wrong body parts





# Manifold Hypothesis

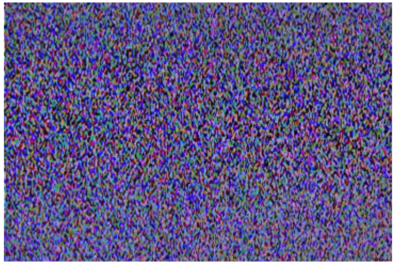
**Idea:** Manifolds of meaningful pictures are highly concentrated with very little volume and embedded in a very high dimensional space

I. Generation of images is a very challenging task

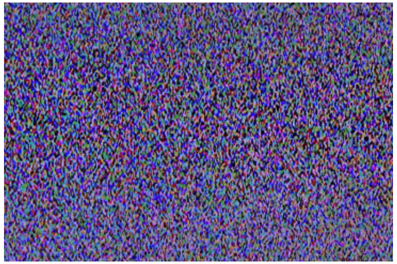
II. Correlations / probability dimension are high dimensional

**Example:** Try to generate images randomly:

Goal



Sample 1

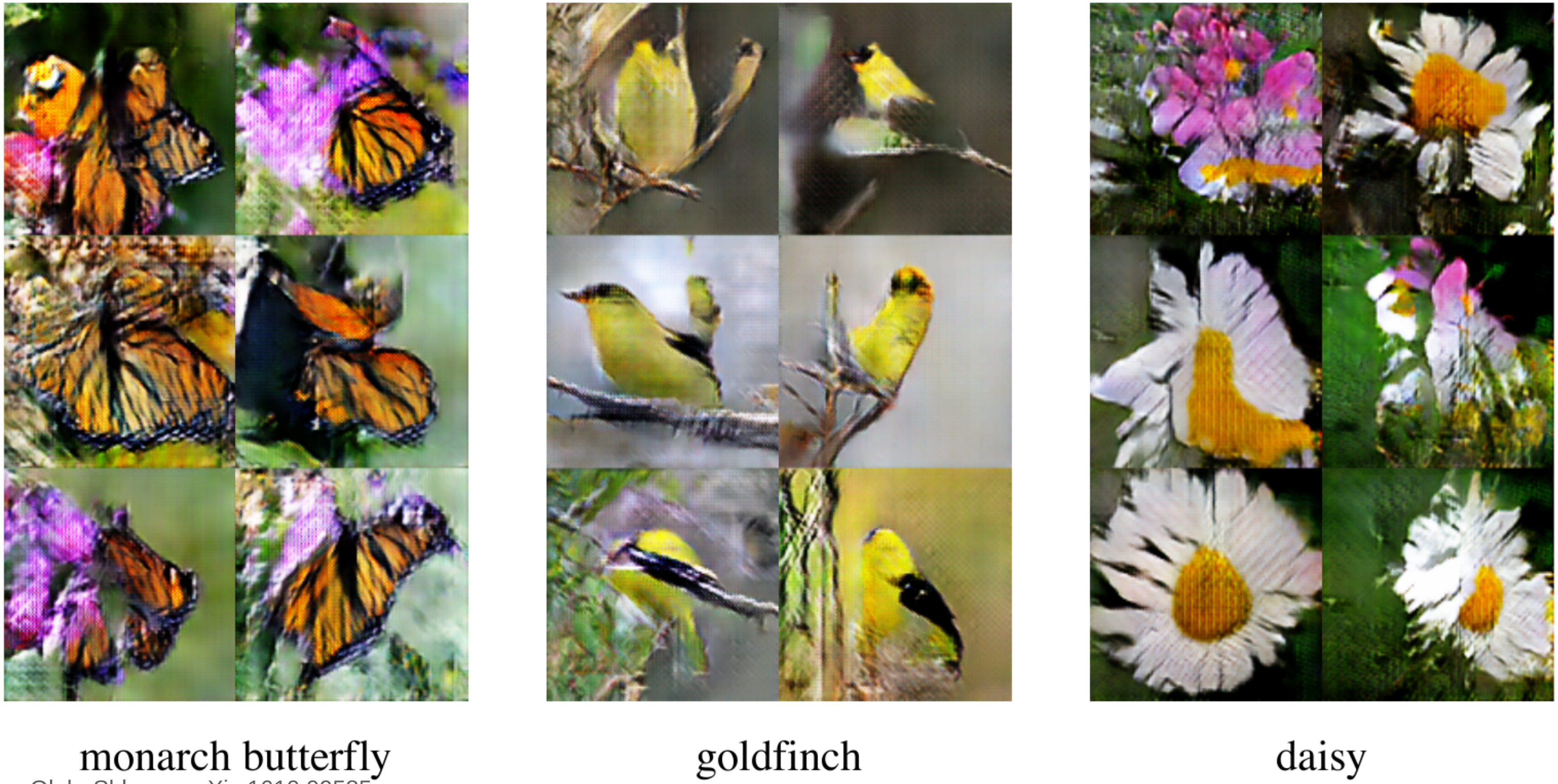


Sample 100,000

You will even never reach this "neighborhood sample"

*"To deal with a 14-dimensional space, visualize a 3-D space and say 'fourteen' to yourself very loudly. Everyone does it." - G. Hinton*

# Evolution of GANs - 2016




Odena, Olah, Shlens - arXiv:1610.09585

# Evolution of GANs

goldfish

bunting

Zhang, Goodfellow, Metaxas, Odena - arXiv:1805.08318

# GANs not perfect...



Brock, Donahue, Simonyan - https://arxiv.org/abs/1809.11096

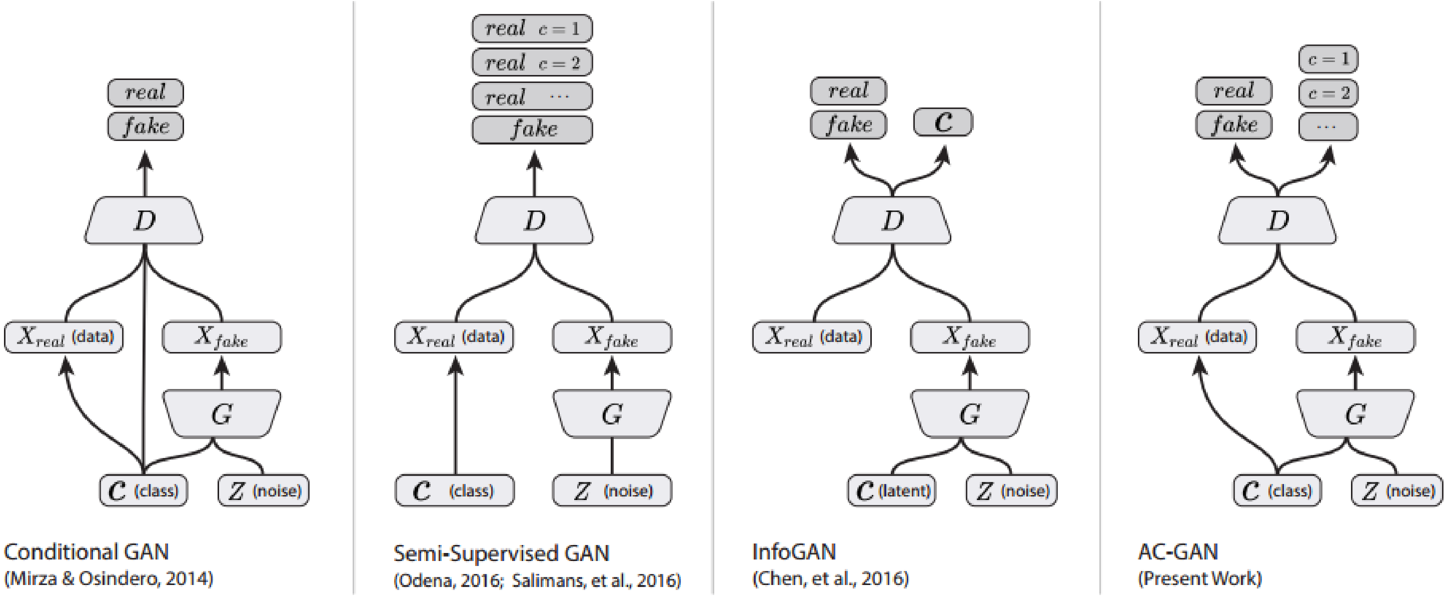



Karras, Alla, Laine, Lehtinen - arXiv:1710.10196

→ Much better images in the next lecture...

# Conditioning of GANs – Semi Supervised

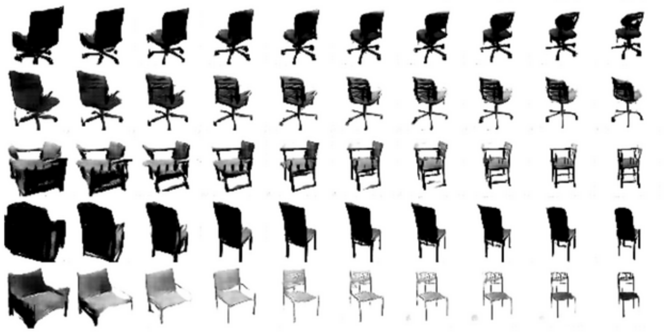
- Constrain generator to learn conditional probability distribution
  - Reduce complexity of latent space, allow for interpretations
- ➢ Feed generator and discriminator additional information (e.g. class labels: dog)
  - Force generated samples show specific characteristics (label dependencies)



# Conditioning of GANs

## InfoGAN

(a) Rotation



(b) Width

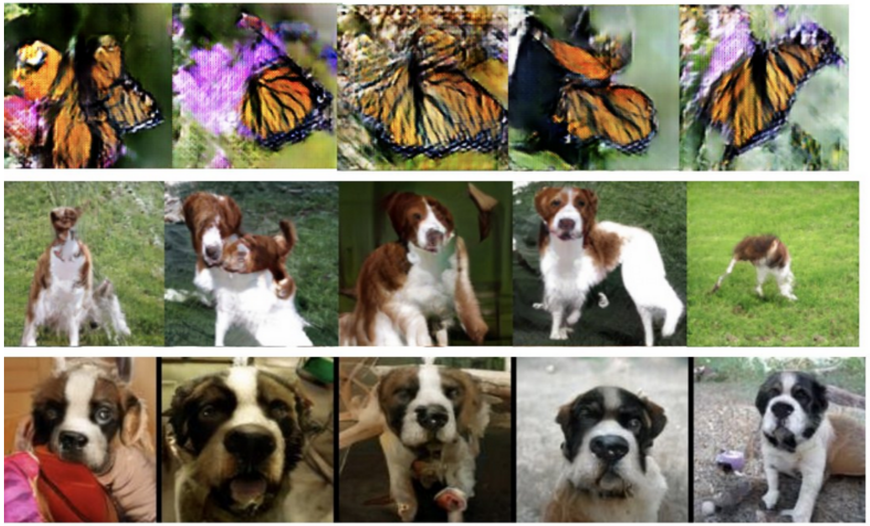
Chen et al. 2016

## Conditional image synthesis

A. Odena et al. 2016

T. Miyato et al. 2017

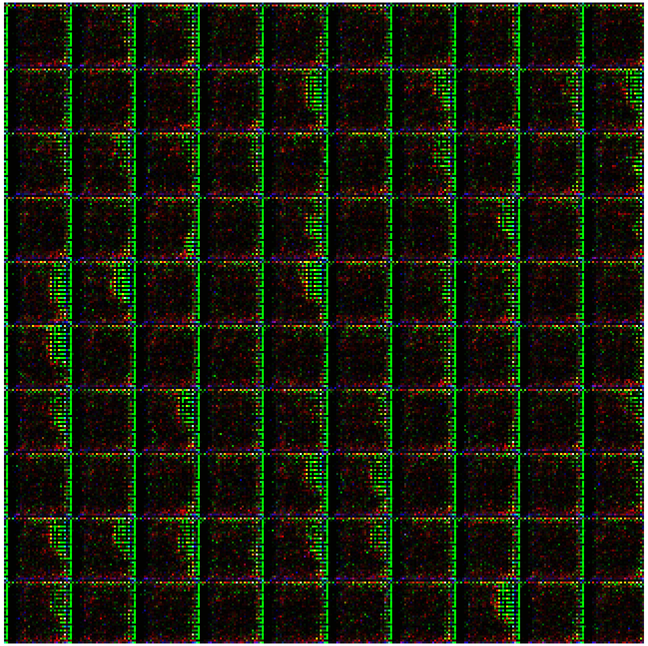
H. Zhang et al. 2018



- Field of generative model is growing very fast

# VAE vs GAN

VAE



GAN

https://blog.openai.com/generative-models/

# Next Lecture: Advanced Techniques

https://www.whichfaceisreal.com/

- Which picture is generated, which picture is part of CELEB A data set?

# Summary

- **Generative Models**
  - Generation of new samples using approximation of underlying data distribution

- **Variational Autoencoder**
  - Hidden representation follows low dimensional arbitrary prior distribution
  - Trained decoder part can be used as generator to produce new samples

- **Generative Adversarial Networks**
  - Hand-coded loss is replaced by discriminator (tries to discriminate between fake samples and real samples)
  - Adversarial training: generator and discriminator trained against each other
  - Generator tries to fool discriminator
  - Use conditioning to create prior on latent space

# References & Further Reading


- M. Erdmann, J. Glombitza, G. Kasieczka, U. Klemradt, Deep Learning for Physics Research, World Scientific, 2021, www.deeplearningphysics.org/
- I. Goodfellow, Y. Bengio, A. Courville, Deep Learning, Chapter 7 / 8 / 9, MIT Press, 2016, www.deeplearningbook.org
- Kingma, Welling: Variational Autoencoder - https://arxiv.org/abs/1312.6114
- Makzhani et al.: Adversarial Autoencoders - https://arxiv.org/abs/1511.05644
- Goodfellow et al.: Generative Adversarial Networks - https://arxiv.org/abs/1406.2661
- Odena et al.: AC-GAN - https://arxiv.org/abs/1610.09585
- Radford et al.: DCGAN - https://arxiv.org/abs/1511.06434
- Zhang et al.: SAGAN - https://arxiv.org/pdf/1805.08318.pdf

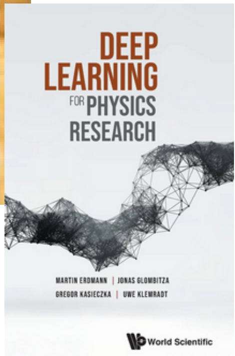
# Tryout
# Deep Learning
# Yourself!

**Find many physics examples at:**

http://www.deeplearningphysics.org/

For example:

- CNNs, RNNs, GCNs
- GANs and WGANs
- Anomaly detection, Denosing AEs
- Visualization & introspection and more

# Tutorial

Open jupyter notebooks in google colab:

You can find the repository at:
https://github.com/jglombitza/tutorial_generative_models
Open PART I: Vanilla_GAN.ipynb

Open in Colab

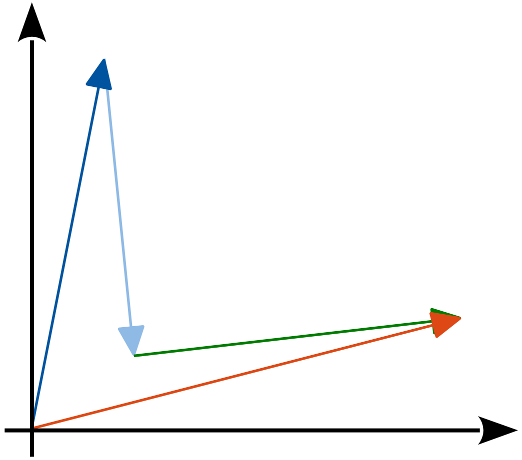
# Arithmetic in Latent Space

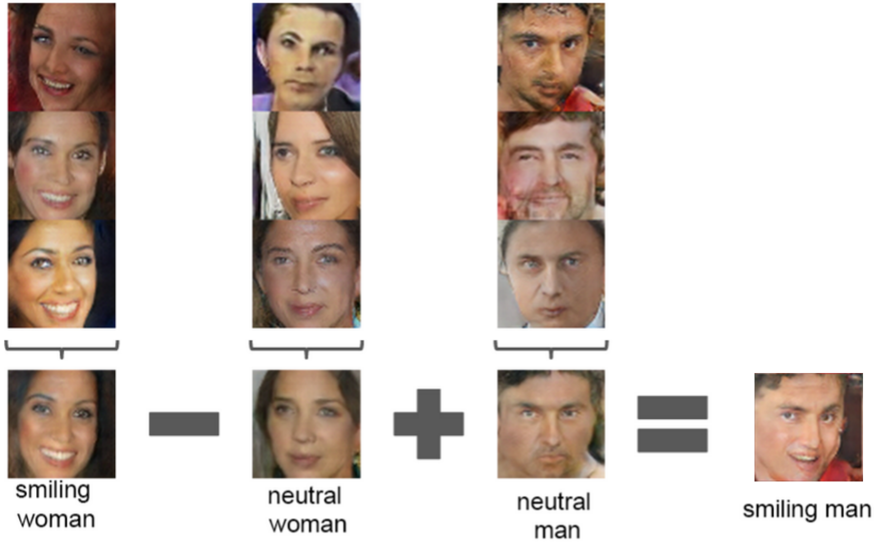
**Idea:** Discover structure of the latent space

- Can we do arithmetic with latent vectors of generated samples which represent different characteristics?

$$\mathbf{z}_{king} - \mathbf{z}_{man} + \mathbf{z}_{women} = \mathbf{z}_{queen}?$$

- Average over several samples to get representation vector






A. Radford, L. Metz, S. Chintala - https://arxiv.org/abs/1511.06434