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Saint Petersburg, Russia

Специализированные технологии машинного обучения / Advanced Machine learning Technologies

Lecture 4 – Generative Models

Outline

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1. Autoencoders (AEs): “encode -> code -> decode”
2. Latent variables and latent space;
3. Variational autoencoders (VAEs);
4. Generative Adversarial Networks (GANs).
5. Conditional Adversarial Networks (CGANs).

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Unsupervised Learning

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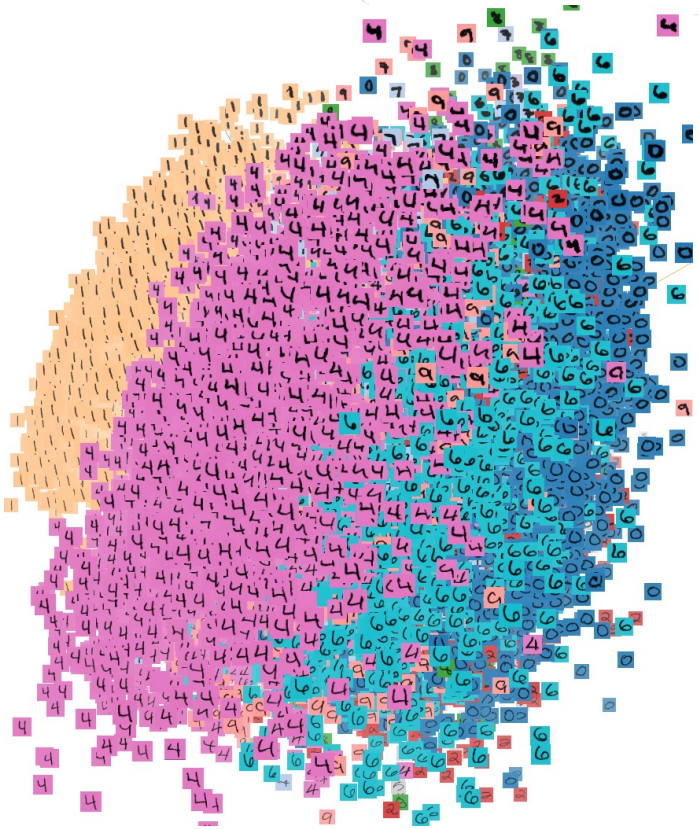
Unsupervised Learning

Data: X (no labels!)

Goal: Learn the structure of the data (density estimation)

- Clustering/grouping,
- Density estimation,
- Dimensionality reduction,

? Autoencoders (AE),
? Variational AE (VAE)
? Generative Adversarial Networks (GAN)



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Why Generative Models?

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- **Supervised learning models are discriminative models**
  - Given an image **X**, predict a label **Y**
  - Estimates **P(Y|X)**
- **Discriminative models have several key limitations**
  - Can't model **P(X)**, i.e. the probability of seeing a certain image
  - Thus, can't sample from **P(X)**, i.e. **can't generate new objects**
- **Unsupervised models**
  - Estimate **P(x)** as density distribution but cannot sample new objects with desired properties
- **Generative models (in general) cope with all of above**
  - Can model **P(X)**
  - Can generate new objects

Autoencoders

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- The autoencoder idea was a part of NN history for decades *(LeCun et al, 1987).*

- Traditionally an autoencoder was used for dimensionality reduction and feature learning.

- Recently, the connection between autoencoders and latent space modeling has brought variational autoencoders (VAEs) to the front of generative modeling.

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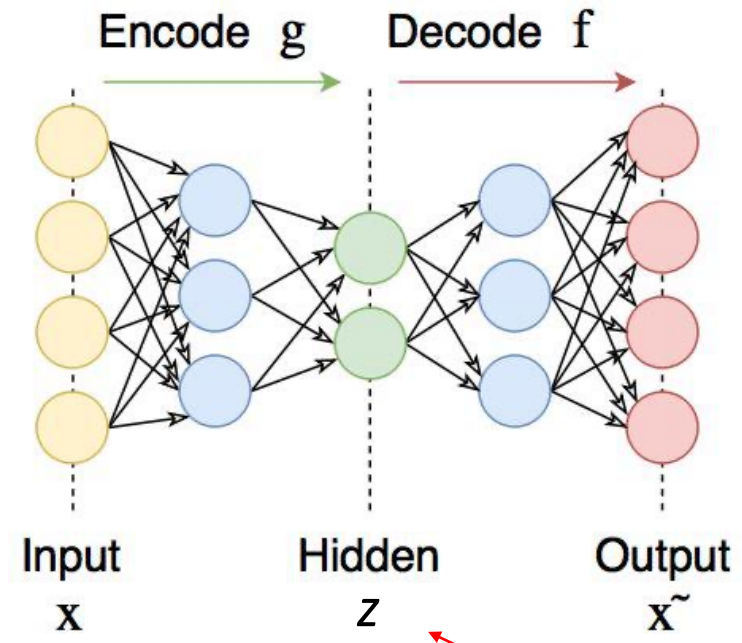
Autoencoders



Autoencoders try to learn **Identity function**, so that:

$$\tilde{x} = f(g(x)) = f(z) \cong x$$

“dense” autoencoder

“latent variables”, “latent space”

Autoencoders

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- Given data x *(no labels)* we would like to learn the functions *g (encoder) and f (decoder)* where:

$$\mathrm{g}(x) = s(wx + b) = z$$

$$\mathrm{f}(z) = s(w'\mathrm{z} + b') = \hat{x}$$

so that $h(x) = f\big(g(x)\big) = \hat{x}$

where h is an **approximation** of the identity function.

z is some **latent representation** or **code** and s is a non-linearity such as the sigmoid

($\hat{x}$ is x's reconstruction)

- Add some regularization not to learn trivial reconstruction

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Undercomplete AE vs overcomplete AE

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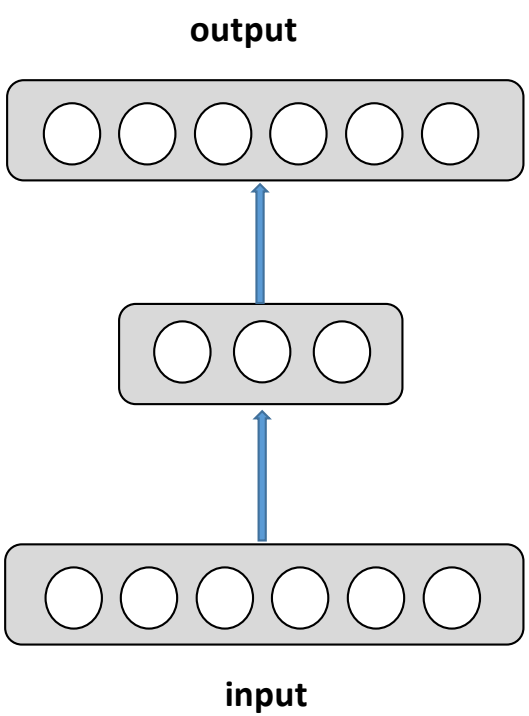
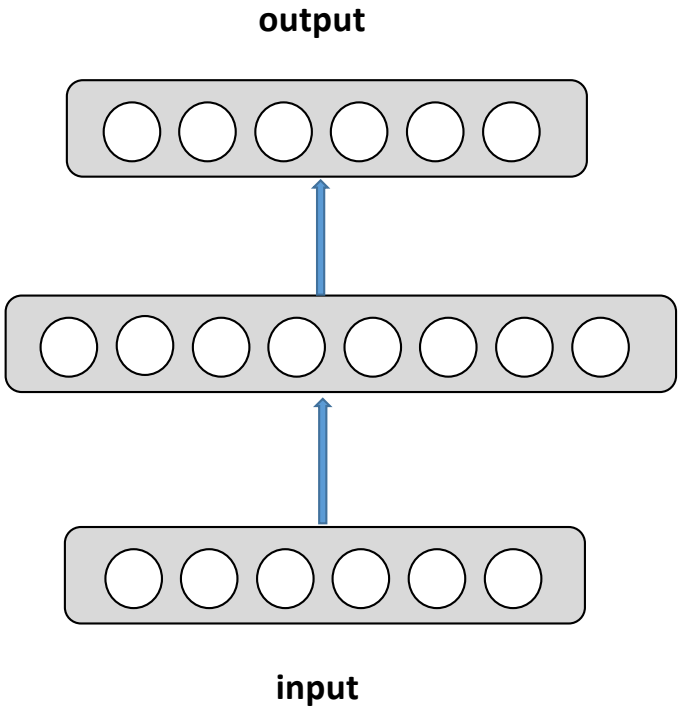
Two basic types of AE structures:





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Undercomplete AE

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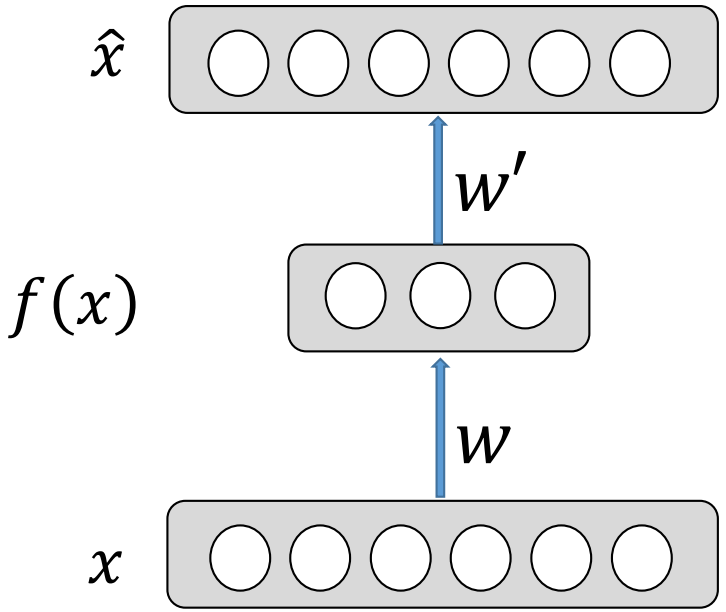
Hidden layer is **undercomplete** if smaller than the input layer

- Compresses the input => dimension reduction
- Good features for representation of meaningful characteristics of the input data.



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Overcomplete AE

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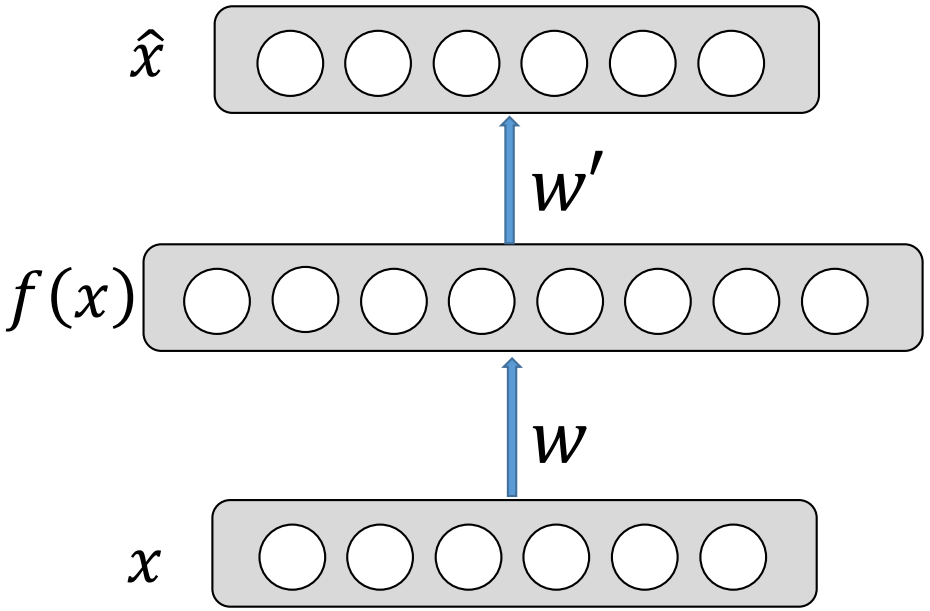
Hidden layer is **overcomplete** if its dimension is greater than the input layer

- No compression in hidden layer.
- Each hidden unit could copy a different input component.
- No guarantee that the hidden units will extract meaningful structure.
- A higher dimension code helps to model a more complex distribution.
- Overfitting?



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Convolutional AE

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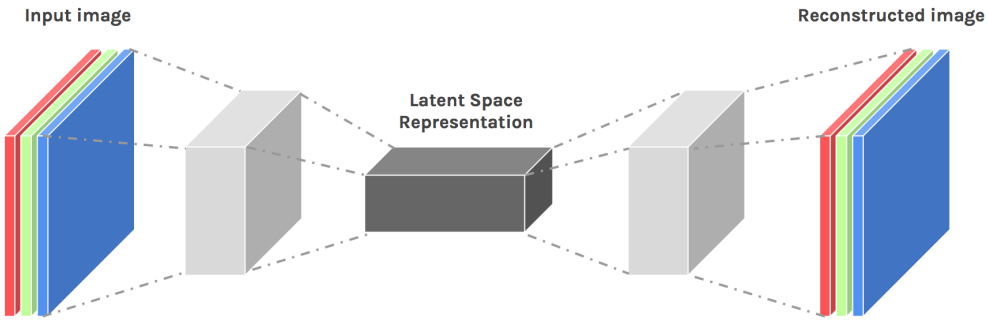

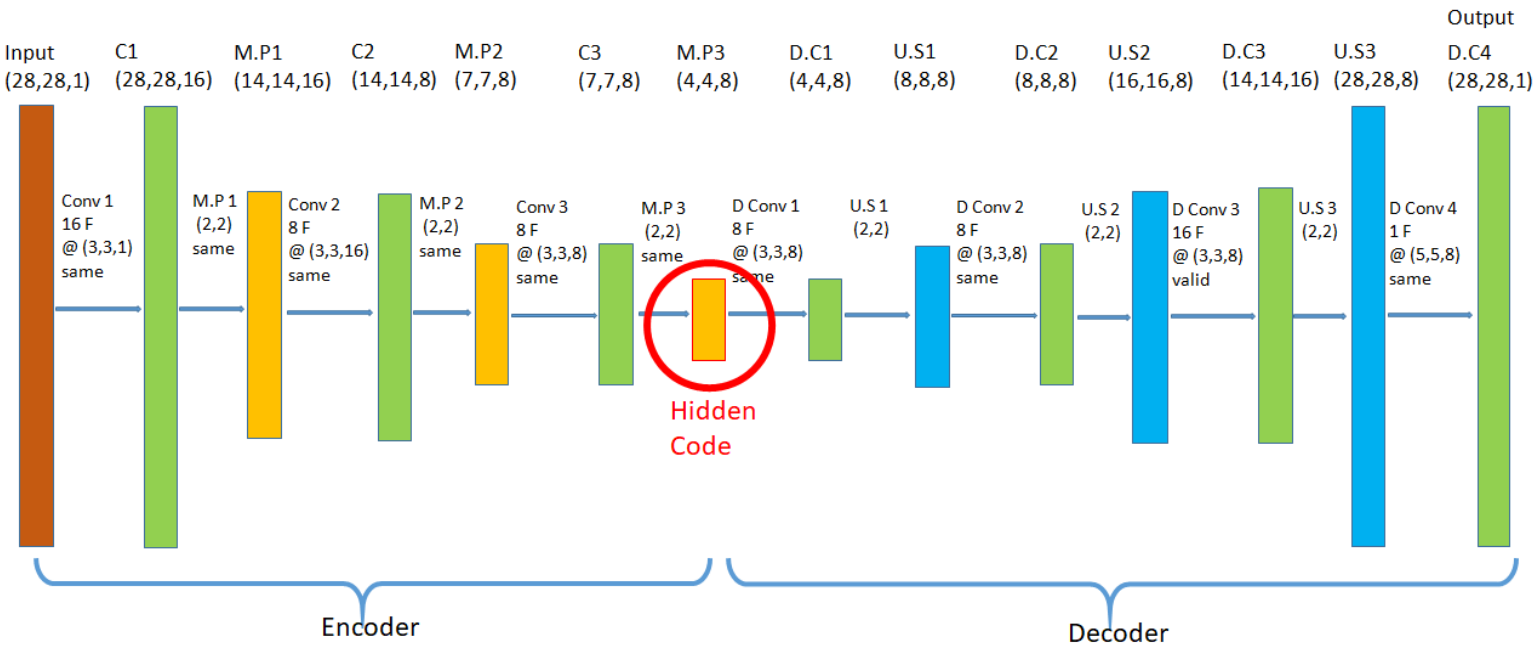

Keras example results

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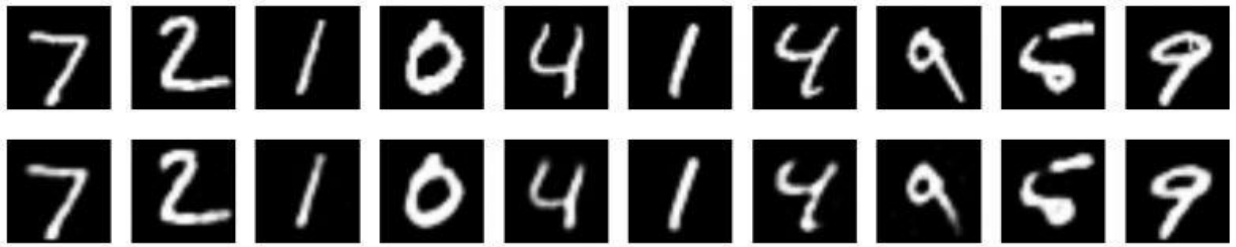
Dense AE:



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Keras example results

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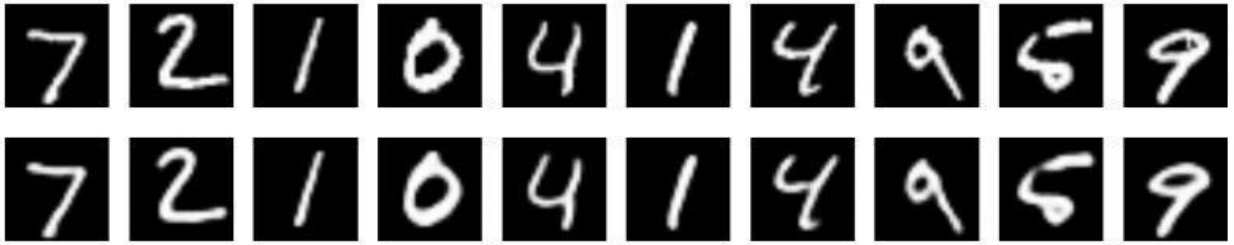
Dense AE:

Conv AE:



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Regularization

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Motivation:

- We would like to learn meaningful features **without** varying the code's dimensions (Overcomplete or Undercomplete).

Solution: apply other constraints to the training process.

→ Add regularization term to the loss function:

$$L(x, f(g(x))) + \Omega(h),$$

For example, $\Omega(h) = \lambda * |h|$

- prevent overfitting;
- more robust and meaningful codes (latent variables);
- prevent learning trivial identity function;

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Denoising Autoencoders

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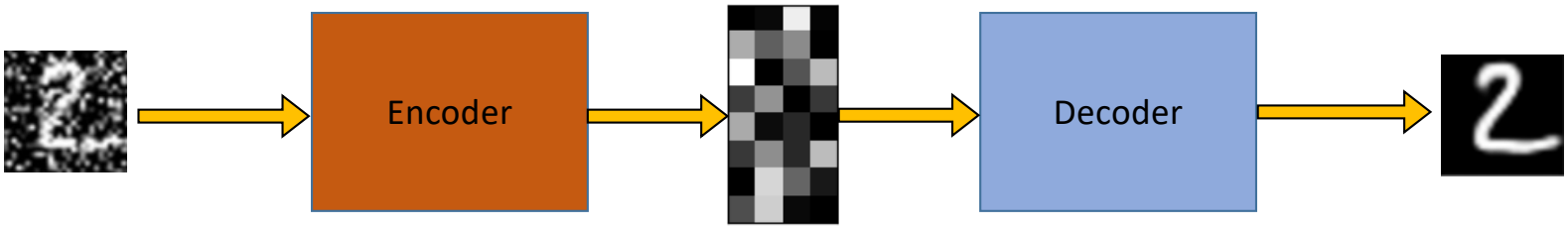
Intuition:

- Add some noise to the input and compare with clean data (train to reconstruct initial image)

$$L(x, f(g(\hat{x}))).$$

A more robust model



Noisy Input

Latent space representation

Denoised Input

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Denoising Autoencoders

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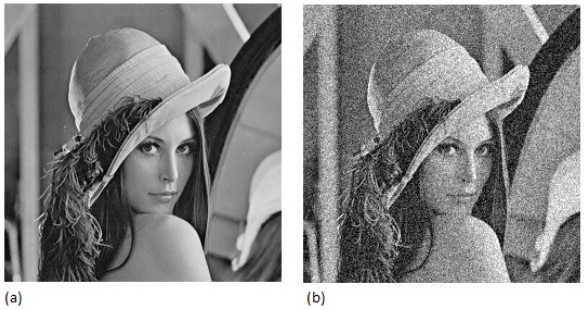
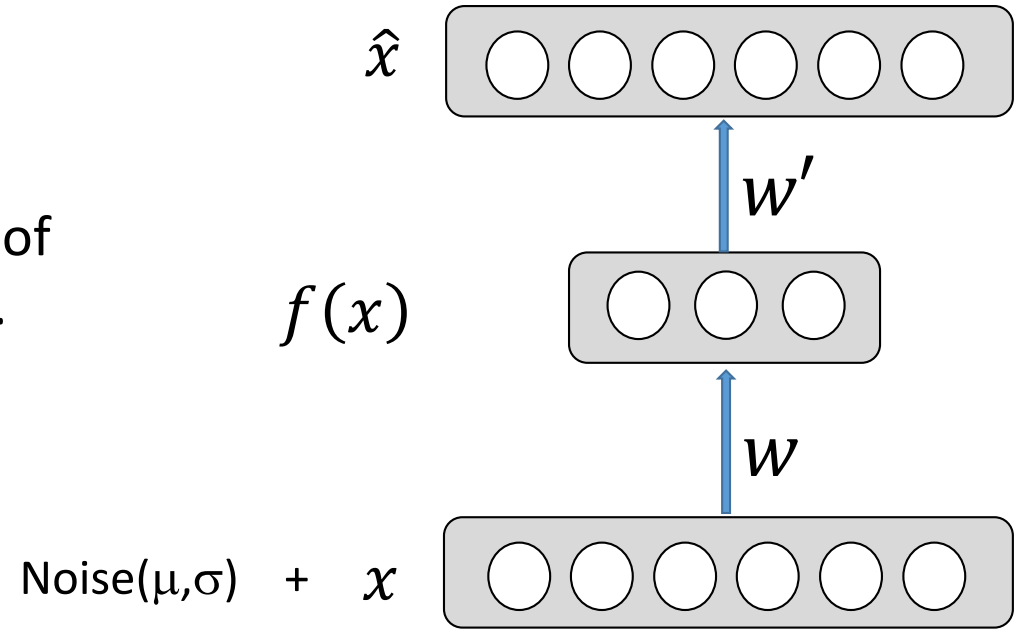
Idea: A robust representation against noise:

- Random assignment of subset of inputs to 0, with probability v.
- Gaussian additive noise.





Denoising Autoencoders

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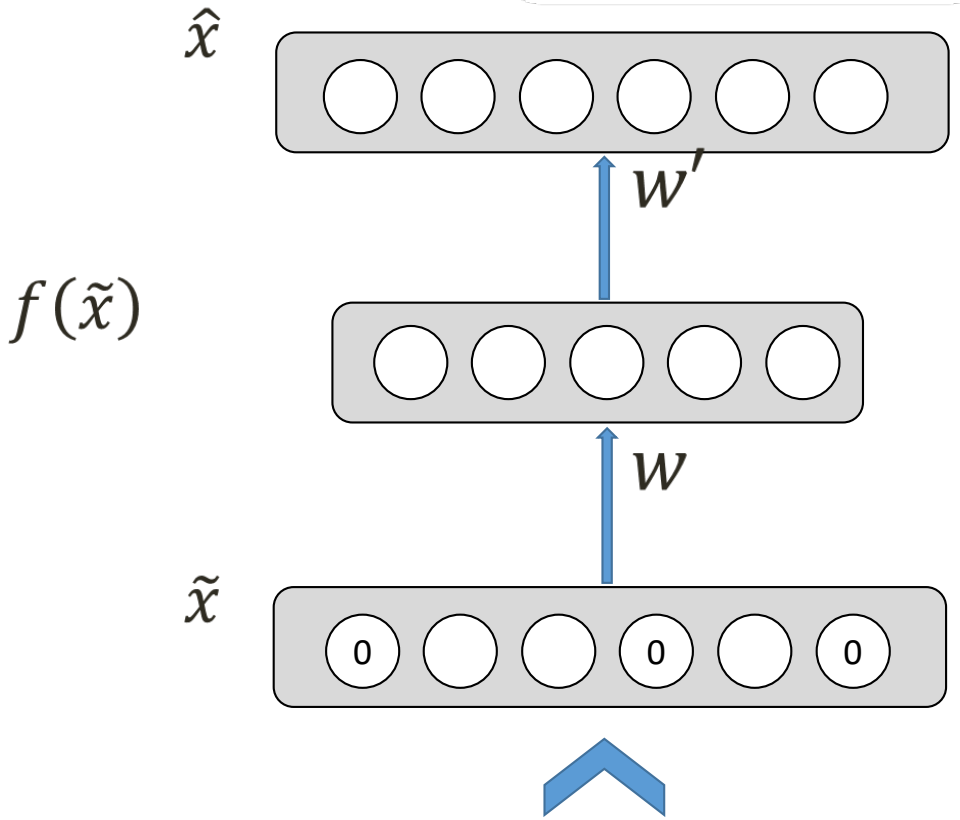
- Reconstruction is computed from noisy image;
- Loss function compares prediction with the noiseless image;
- We are forcing the hidden layer to learn a generalized structure of the data!



Denoising Autoencoders - process

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Taken some input x Apply Noise $\tilde{x}$

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Denoising convolutional AE - example

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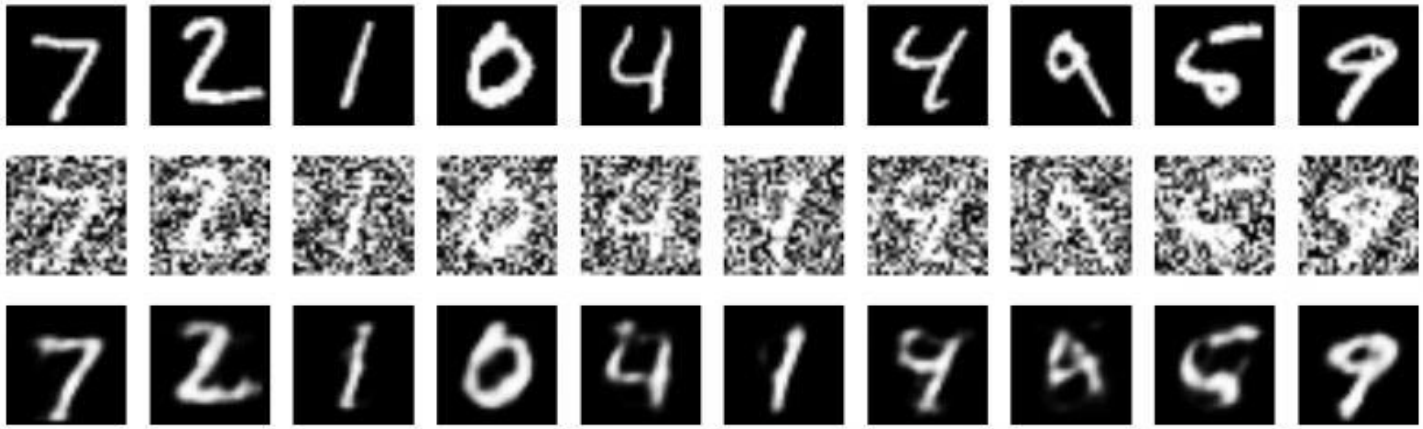
Keras implementation result:



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Latent space: motivation

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Learning the identity function seems trivial, but with added constraints on the network (such as limiting the number of hidden neurons or/and regularization) we can learn information about the structure of the data

→ Trying to capture the **distribution of the data**

Let's take a look at the codes….

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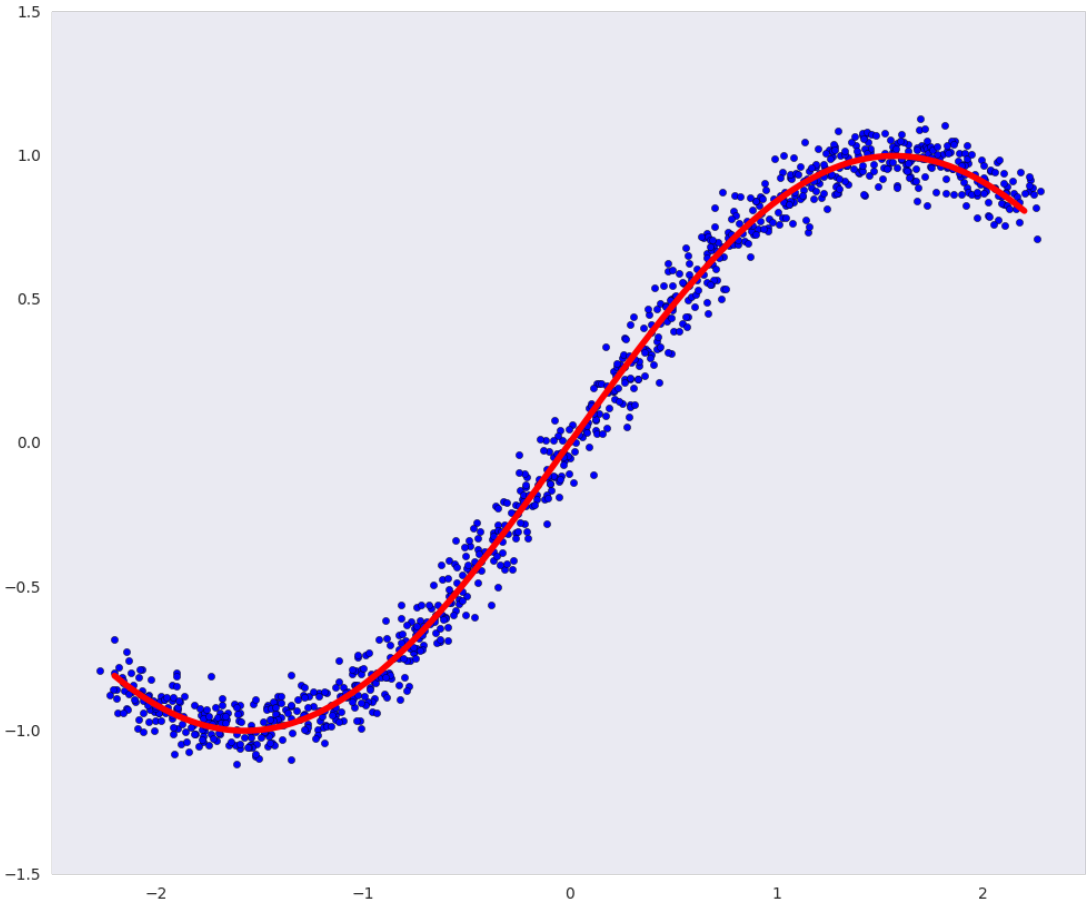
Latent space



- Dots – initial distribution of the samples;
- Red line – desirable manifold

(objects near the line are ~digit images)

https://habr.com/ru/post/331500/

Latent space

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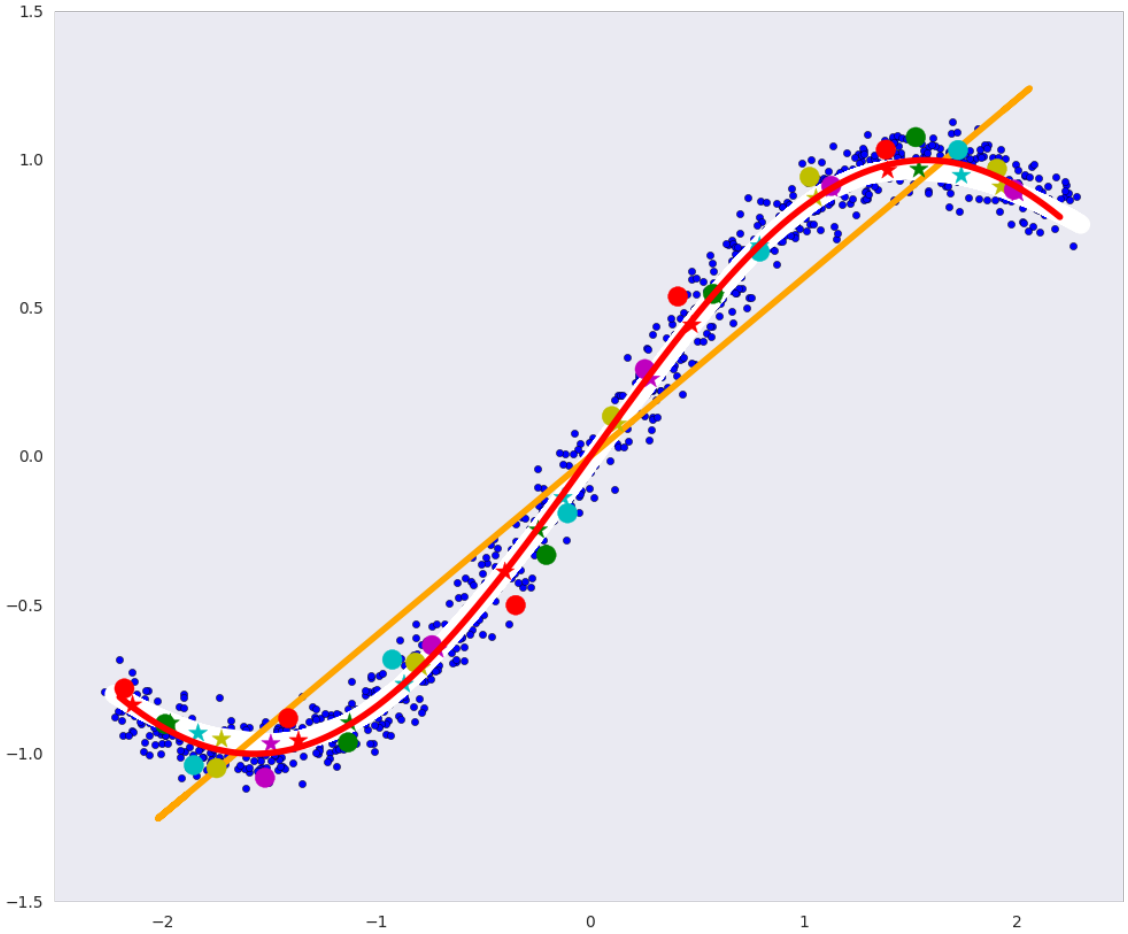

- the white line is the manifold to which the blue data points after the auto-encoder go, that is, the auto-encoder's attempt to construct the manifold that determines the most variations in the data;
- The orange line is the manifold to which the blue data points go after the PCA;
- colored circles - points that turn into asterisks of the corresponding color after encoding;
- colored asterisks - respectively, the images of the circles after the auto-encoder.

White line – is “encoded manifold” or “latent space”

https://habr.com/ru/post/331500/

Latent variables

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➢ We can consider the general population as a process of generating data, which depends on a number of hidden variables (random variables).

➢ The dimension of the data can be much higher than the dimension of the hidden random variables that these data define. Consider the process of generating the next digit: how the digit will look can depend on many factors:

- **desired numbers;**
- **thickness of the stroke;**
- **tilt**
- **neatness;**

➢ Each of these factors has its own prior distribution.

➢ For example, the probability that a figure of **8** will be drawn is the Bernoulli distribution with a probability of 1/10,

➢ The **thickness of the stroke** also has some distribution and may depend on both accuracy and its hidden variables, such as the **thickness of the handle** or the **temperament of a person** (again with his distributions).

➢ The auto-encoder itself in the learning process will (somehow) learn the hidden factors, for example, such as those listed above, some of their complex combinations.

Various types of “2”

However, the joint distribution that auto-encoder learns does not have to be simple, it can be some kind of complex curved area.

Code manifold and real world manifold:

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If we take two objects and look at objects lying on an arbitrary curve between them, then most likely intermediate objects will not belong to the general population, since the variety on which the general population lies can be very curved and small.

moving in a straight line in the space of numbers from one “8” to another

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Code manifold and real world manifold:

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If we take two objects and look at objects lying on an arbitrary curve between them, then most likely intermediate objects will not belong to the general population, since the variety on which the general population lies can be very curved and small.

moving in a straight line in the space of numbers from one “8” to another

But if we move along a curve between codes (and if the code’s manifold is well parametrized), then the decoder will translate this curve from the code space to a curve that does not leave the defining manifold in the space of objects. That is, intermediate objects on the curve will belong to the entire population.

moving in a straight line in the space of codes from one “8-code” to another

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Learning latent space

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- **X** — random sample (single image) from the dataset of 28x28 pixels images,
- **Z** - a random value of hidden factors that determine the number in the picture
- **P(X)** - the probability distribution of the images of the figures in the pictures, i.e. the probability of a particular image of a digit *generally* to be drawn (if the picture is not like a digit, then this probability is extremely small);
- **P(Z)** - the probability distribution of hidden factors, for example, the distribution of the thickness of the stroke;
- **P(Z|X)** - the probability distribution of hidden factors for a given picture (a different combination of hidden variables and noise can lead to the same picture);
- **P(X|Z)** - the probability distribution of pictures for given hidden factors; the same factors can lead to different pictures (the same person in the same conditions does not draw exactly the same numbers);
- **P(Z,X)** - joint distribution and, the most complete understanding of the data needed to generate new objects.

Learning latent space

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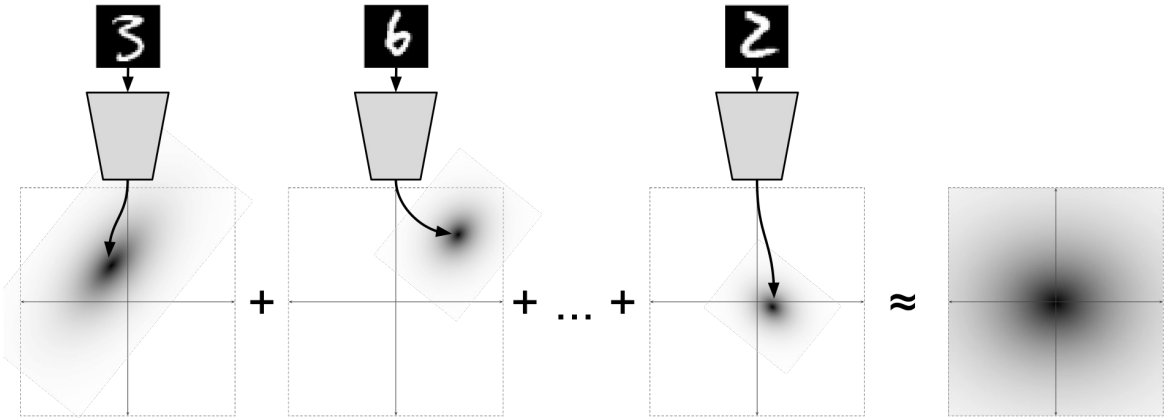
http://ijdykeman.github.io/ml/2016/12/21/cvae.html

It can be shown (introducing specific loss function to encoder) that:

$$P(Z|X) = N(\mu(X), \Sigma(X))$$



Encoder predict the parameters of some Normal distribution!

A variational autoencoder (VAE) is a generative model that learns to map objects into a given hidden space and than to generate the new objects as decoded samples from this hidden space.

Variational Autoencoders

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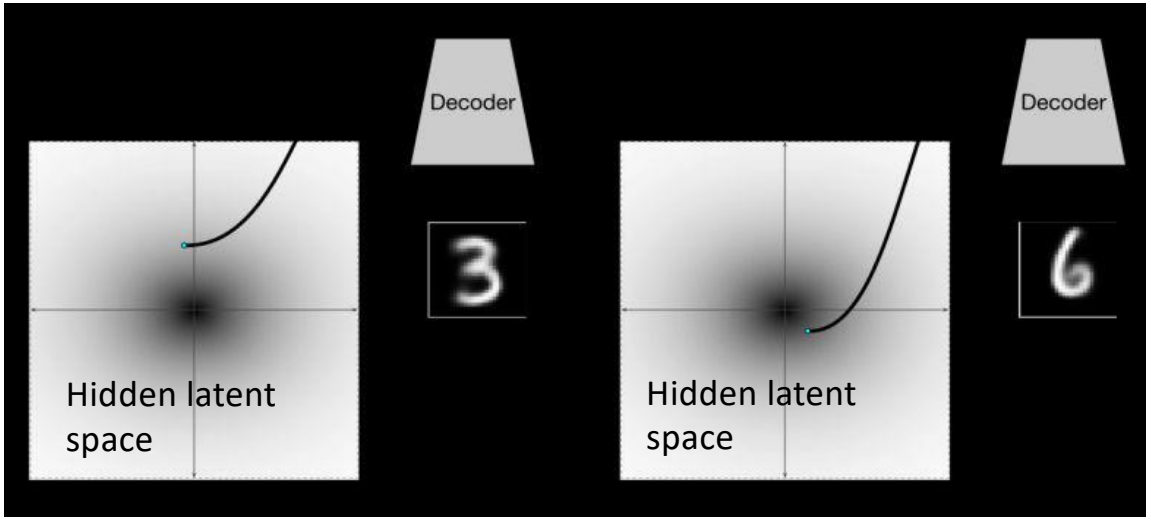
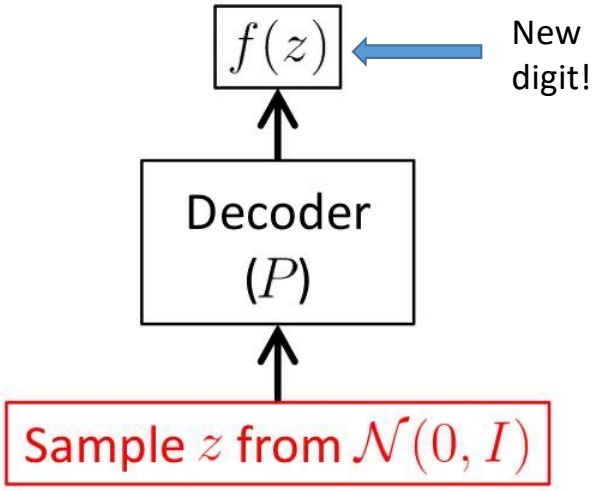
In order to be able to generate new objects, the space of hidden variables (latent variables) must be predictable.
VAE are autoencoders that learn to map objects into a given latent space and, therefore, sample them.

Therefore, variational autoencoders are also referred to the family of generative models.

For example, we can sample from ***P(z) ~ N(0,1)*** distribution to decode new digits:





Conditional VAE: add new information to the input → new objects with desirable features (thickness or style)!

http://ijdykeman.github.io/ml/2016/12/21/cvae.html https://habr.com/ru/post/331664/

VAE architecture

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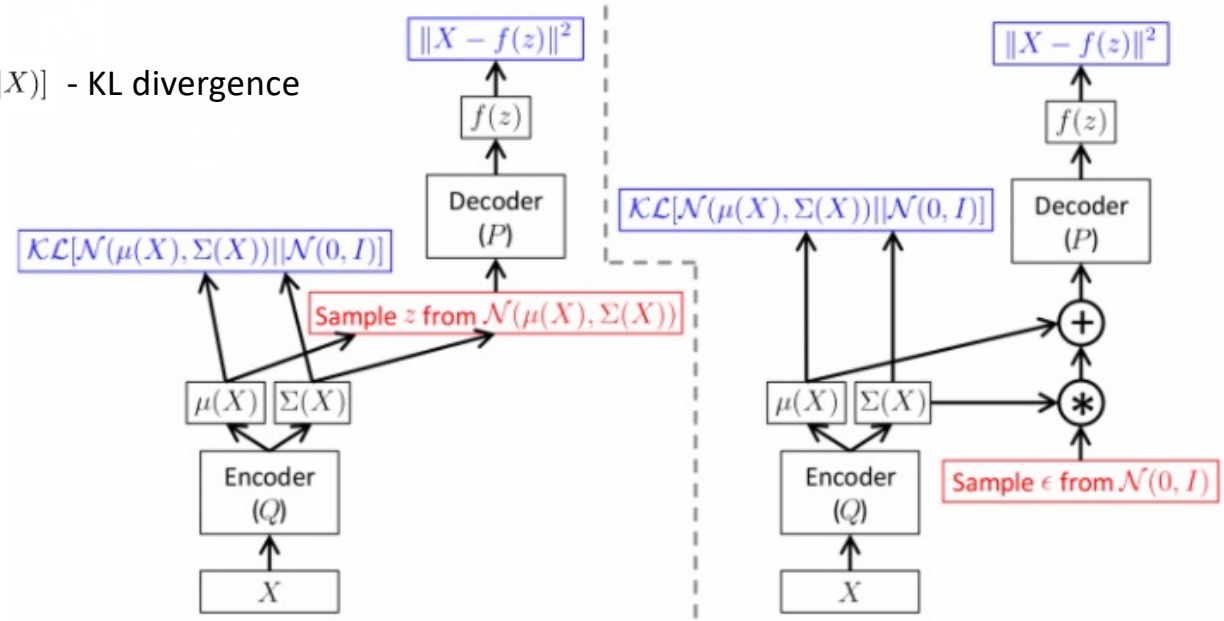
$P(X;\theta) = \int_z P(X|Z;\theta)P(Z)dZ$ - want to maximize

$P(X|Z;\theta) = N(X|f(Z;\theta), \sigma^2 I),$

$KL[Q(Z|X)||P(Z|X)] = \mathbb{E}_{Z\sim Q}[\log Q(Z|X) - \log P(Z|X)]$ - KL divergence

We can fix that encoder should generate hidden parameters from the multivariate Gaussian distribution:

$Q(Z|X;\theta_1) = N(\mu(X;\theta_1), \Sigma(X;\theta_1))$



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It can be shown that:

$\log P(X) - KL[Q(Z|X)||P(Z|X)] = \mathbb{E}_{Z\sim Q}[\log P(X|Z)] - KL[Q(Z|X)||P(Z)]$

VAE example

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GANs

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GANs

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- **Generative**
  - Learn a generative model – to generate smth new
- **Adversarial**
  - Trained in an adversarial setting: generator vs. discriminator
- **Networks**
  - Use Deep Neural Networks

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Magic of GANs…

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Generate 2D/3D shapes ➔ helpful for designers (rendering)

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Ledig, Christian, et al. "Photo-realistic single image super-resolution using a generative adversarial network." *arXiv preprint arXiv:1609.04802* (2016).

Magic of GANs…

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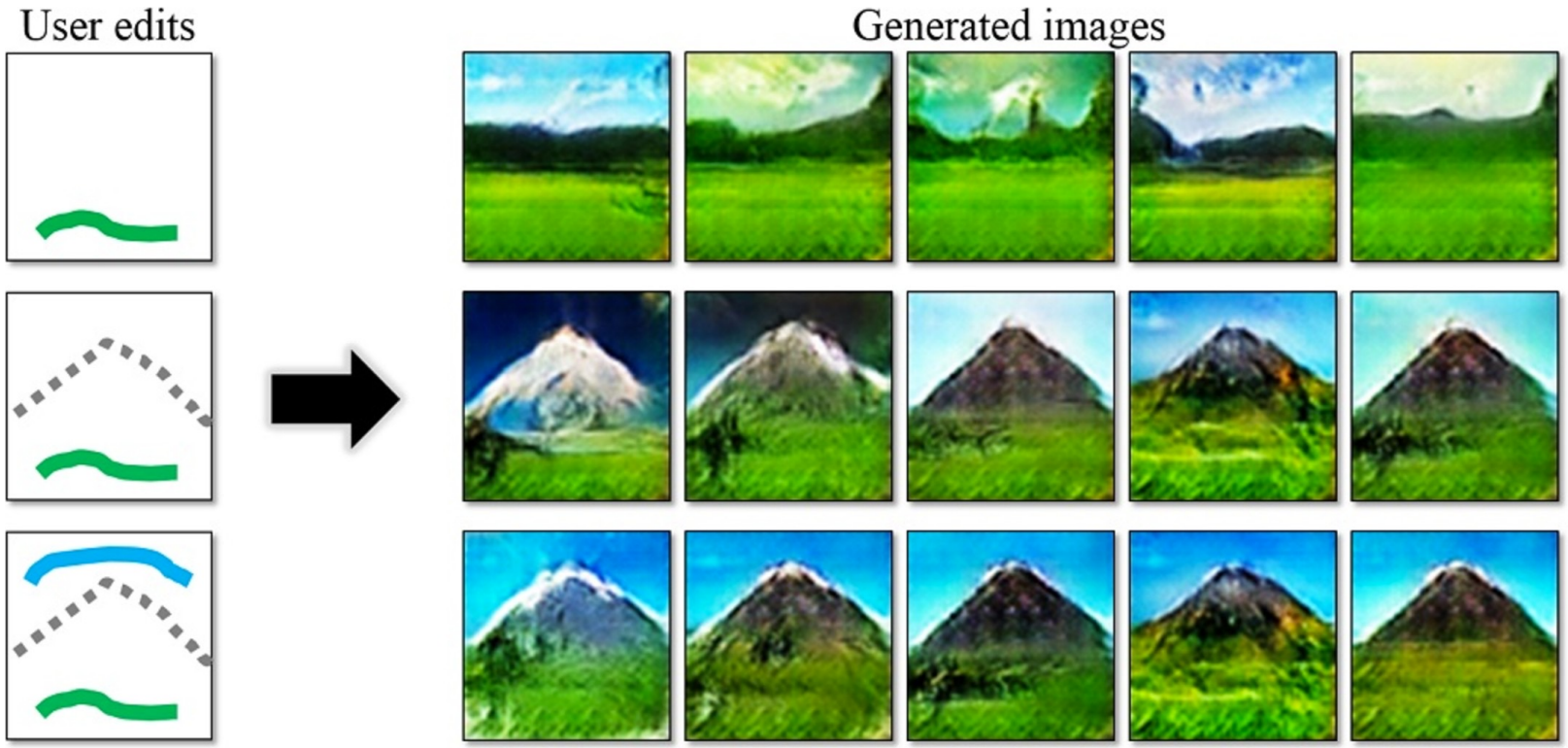
Generate new images and videos ➔ helpful for artists



http://people.eecs.berkeley.edu/~junyanz/projects/gvm/

Applications using GANs

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- Font generation
- Anime character generation
- Interactive Image generation
- Text2Image (text to image)
- 3D Object generation
- Image Editing
- Face Aging
- Human Pose Estimation
- Domain-transfer (e.g. style-transfer, pix2pix, sketch2image)
- Image Inpainting (hole filling)
- Super-resolution
- High-resolution image generation (large-scale image)
- Adversarial Examples (Defense vs Attack)
- Visual Saliency Prediction (attention prediction)
- Robotics
- Video (generation/prediction)
- Synthetic Data Generation
- Real-time face reconstruction
- Photorealistic Image generation (e.g. pix2pix, sketch2image)
- Human Pose Estimation
- …

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Adversarial Training

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- **GANs extend the idea of discriminative modeling:**
  - **Generator:** generate fake samples, tries to fool the Discriminator
  - **Discriminator:** tries to distinguish between real and fake samples
  - Train them against each other (separately)
  - Repeat this and we get better Generator and Discriminator
  - => receive more realistic generated objects!

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Policeman vs. Counterfeiter

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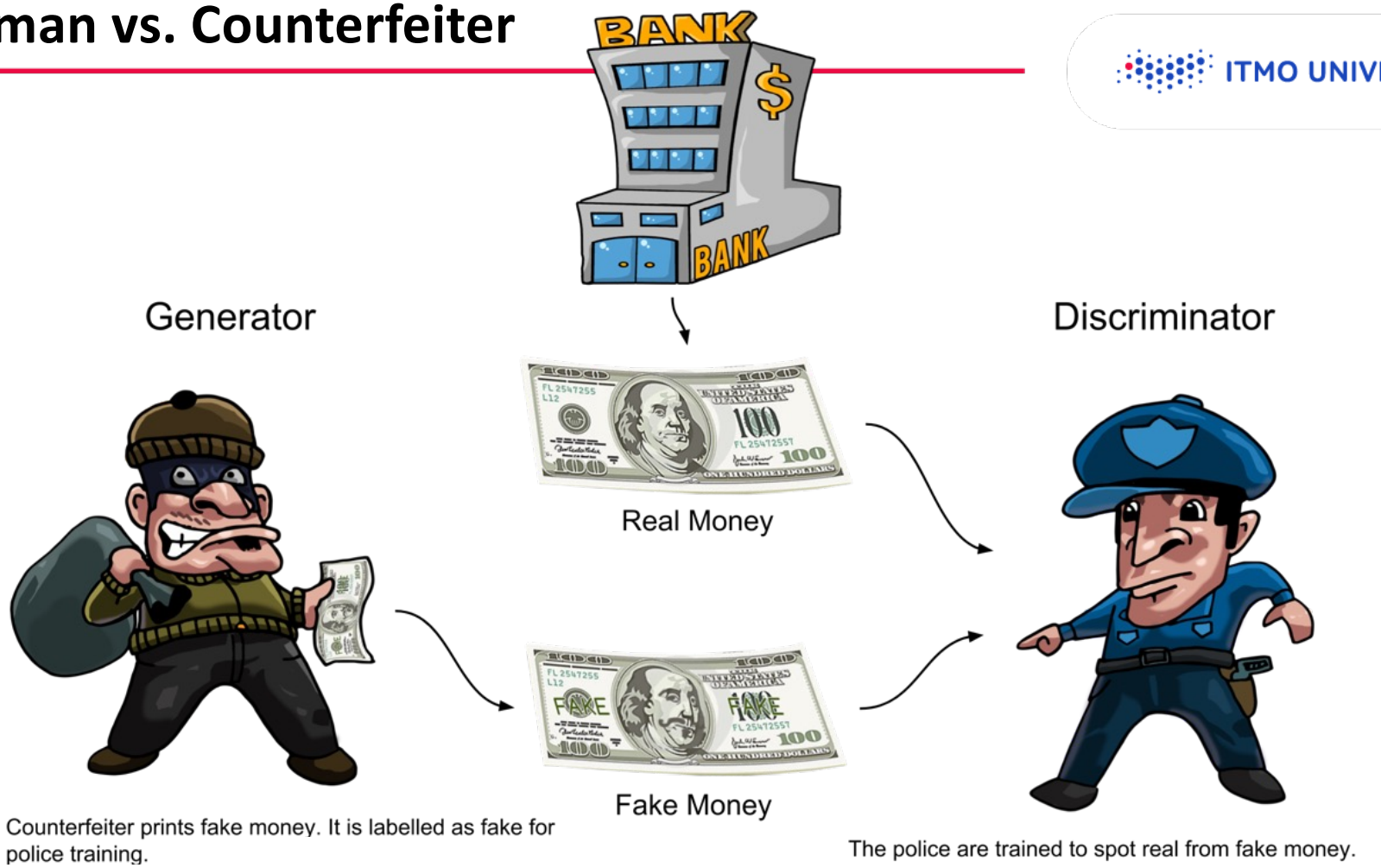

GAN's Architecture

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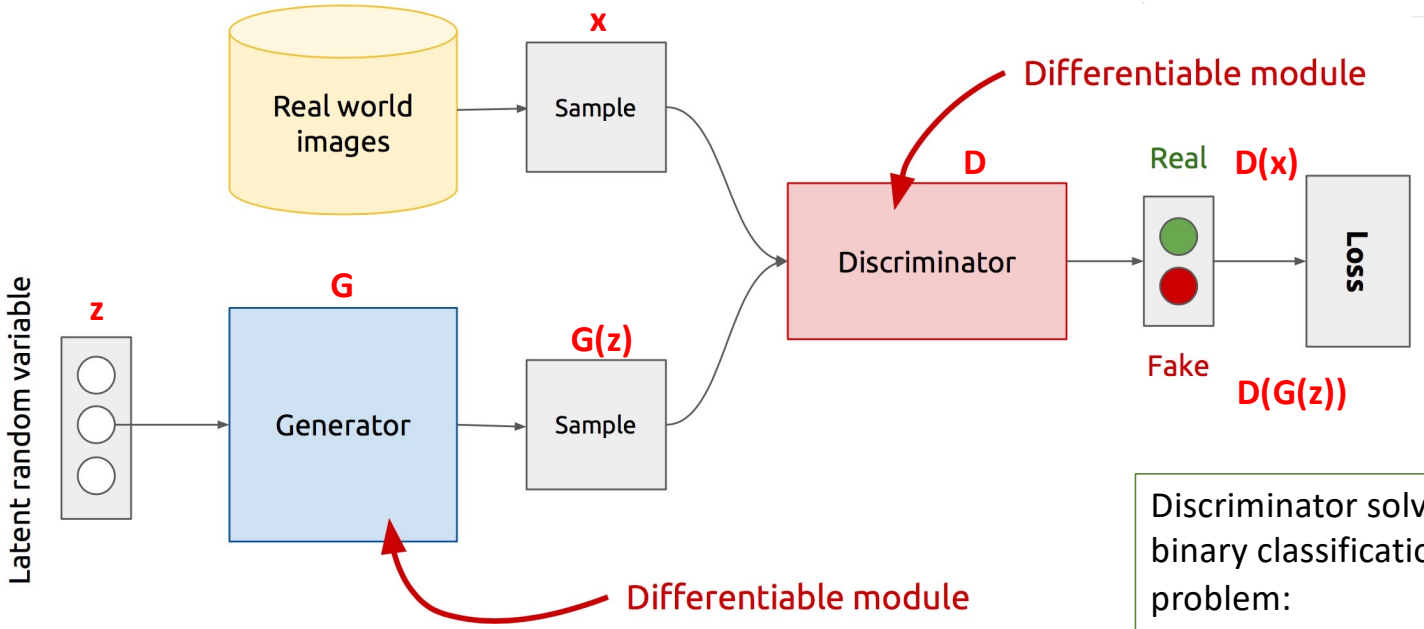

Discriminator solve binary classification problem:
«0» - is for the fake
"1" – is for the real

- **Z** is some random noise (Gaussian/Uniform).
- **Z** can be thought as the latent representation of the image.

https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

Training Discriminator

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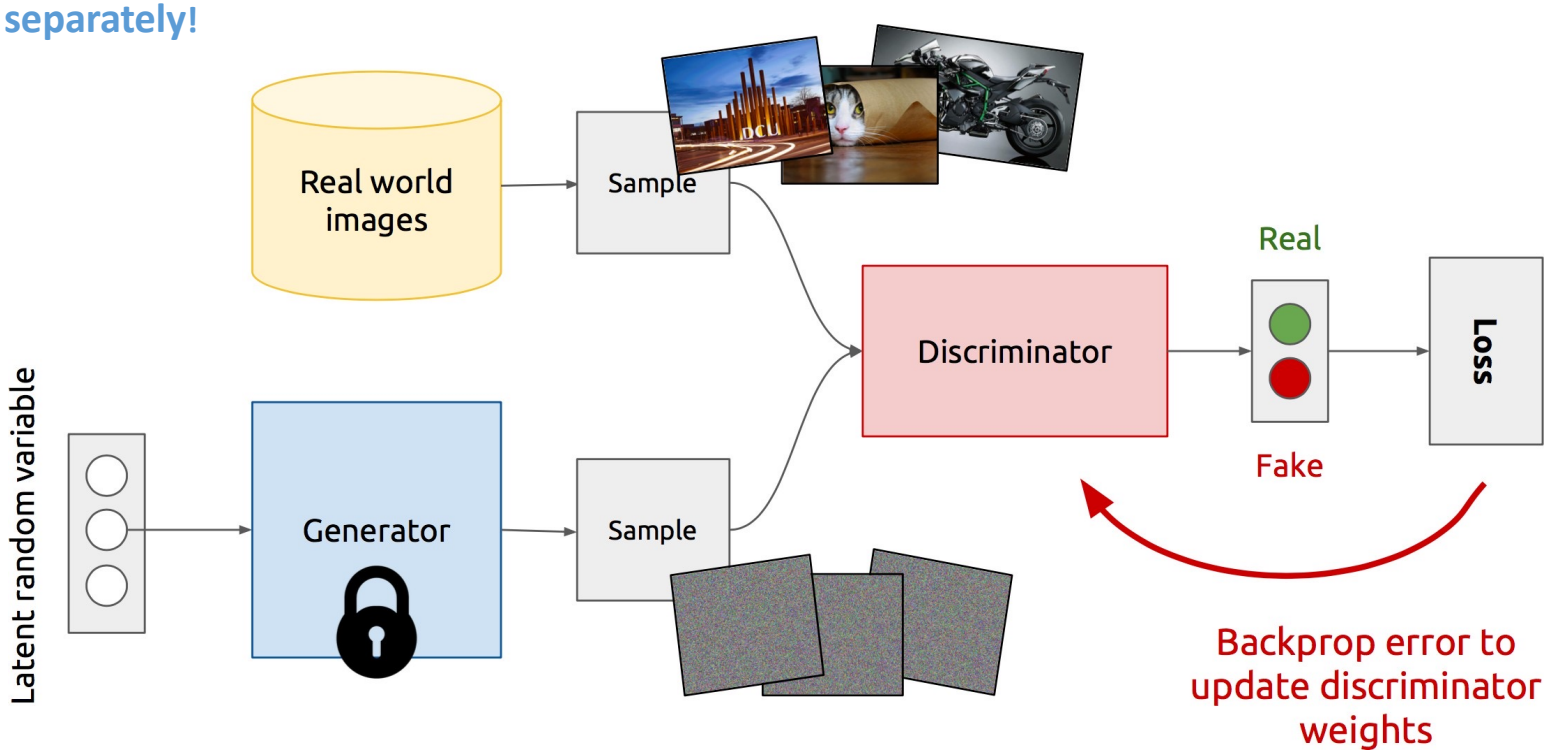
Training separately!



https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

Training Generator

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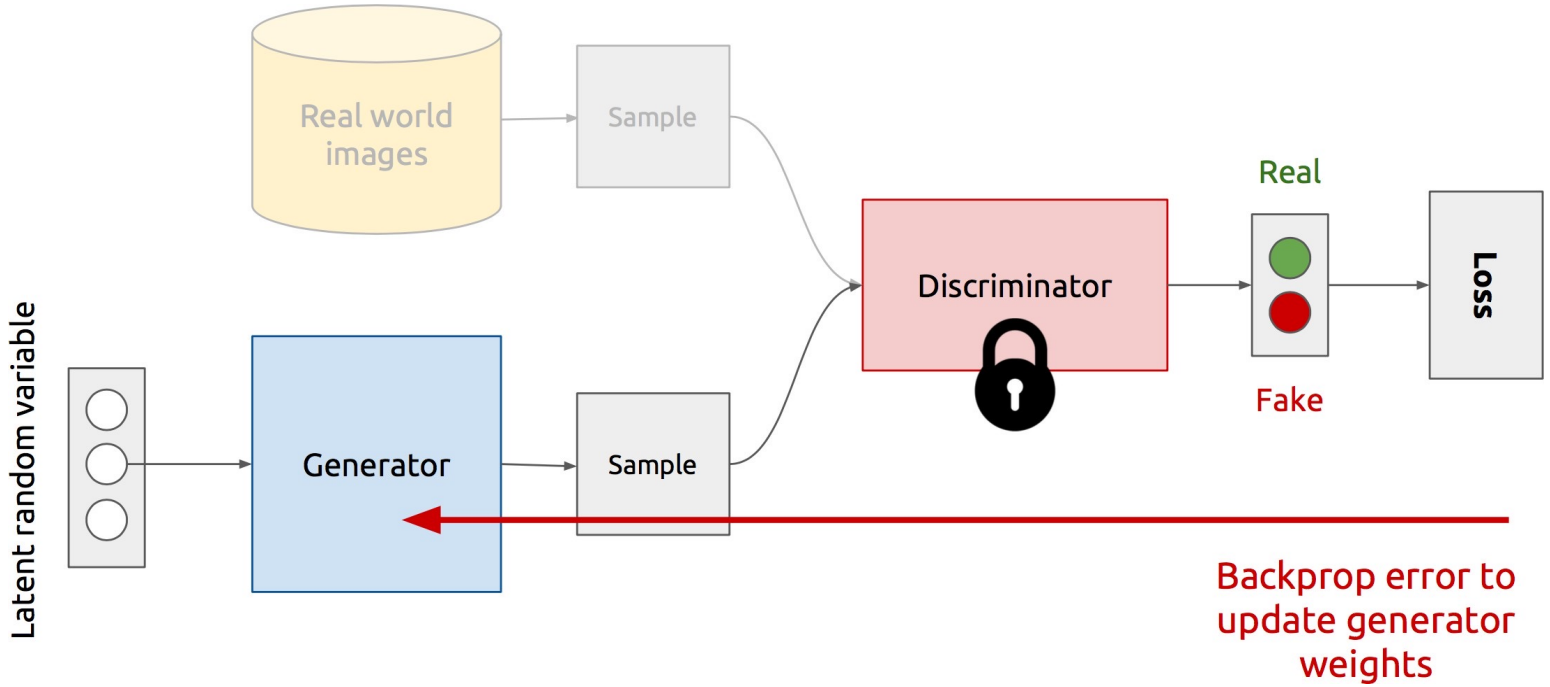
Training separately!



https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

GAN's formulation

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GANs training process is formulated as a **minimax game**, where:

- The **Discriminator** is trying to maximize its reward $\boldsymbol{V}(\boldsymbol{D}, \boldsymbol{G})$
- The **Generator** is trying to minimize Discriminator's reward (== maximize its loss)

$$V(D,G) = \mathbb{E}_{x\sim p(x)}[\log D(x)] + \mathbb{E}_{z\sim q(z)}[\log(1 - D(G(z)))]$$

where:

x $\subset$ X – real samples

G(z) – generated samples

1 – $D(G(z))$ – probability of predicting "real" label

G – generator

D – discriminator

D(x)=1, if discriminator has labeled x as real

D(x)=0, if discriminator has labeled x as fake

GAN's training algorithm

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Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

Discriminator updates

for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

end for

Generator updates

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for

Deep Convolutional GANs (DCGANs)

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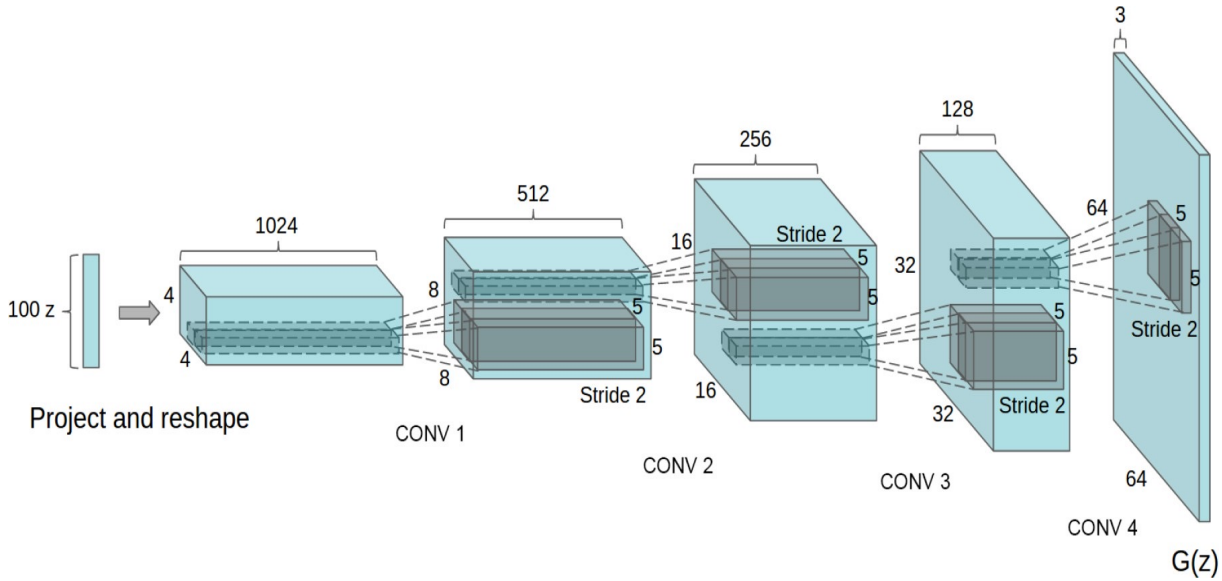
Generator Architecture



Key ideas:

- Replace FC hidden layers with Convolutions
- **Generator:** Fractional-Strided convolutions
- Use Batch Normalization after each layer
- **Inside Generator**
  - Use ReLU for hidden layers
  - Use Tanh for the output layer

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Radford, Alec, Luke Metz, and Soumith Chintala. "Unsupervised representation learning with deep convolutional generative adversarial networks." arXiv:1511.06434 (2015).

Example

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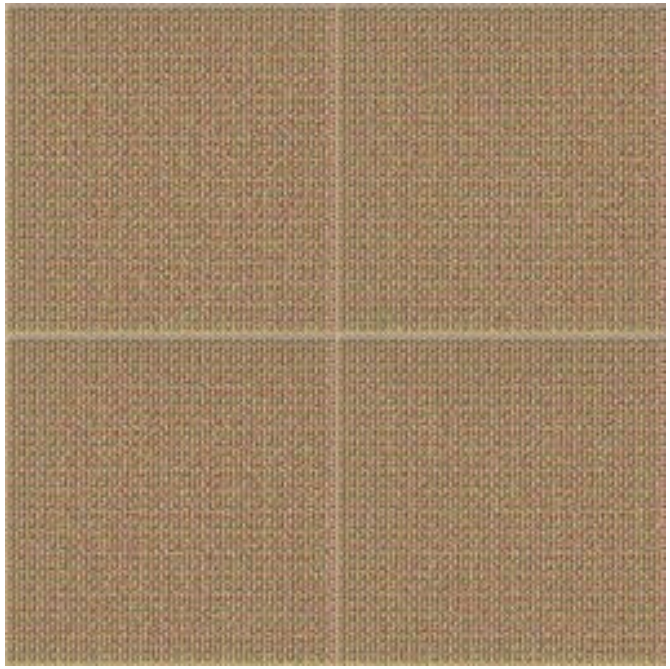

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DCGAN: bedroom images

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Radford, Alec, Luke Metz, and Soumith Chintala. "Unsupervised representation learning with deep convolutional generative adversarial networks." arXiv:1511.06434 (2015).

Learning meaningful latent space

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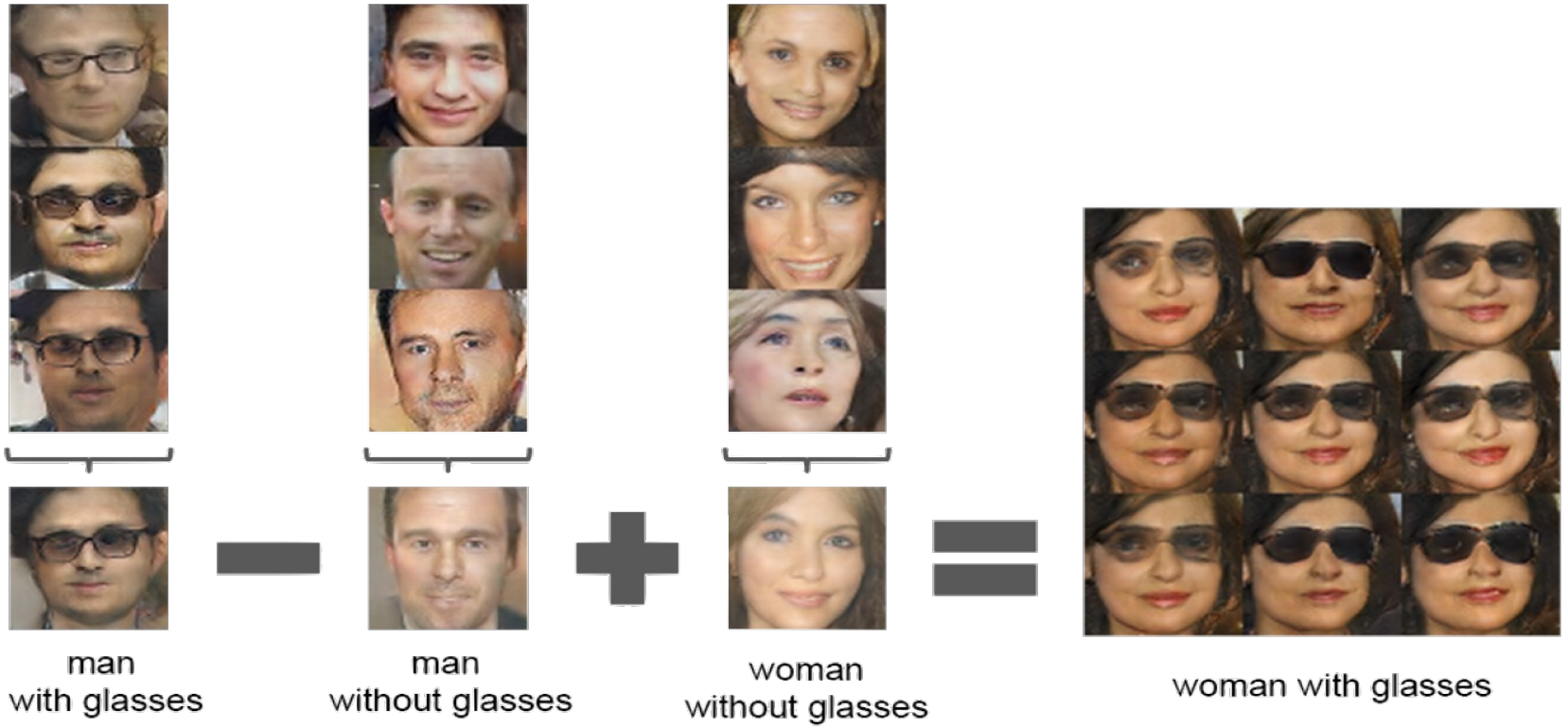
Latent vectors with additional labels capture interesting patterns…



Radford, Alec, Luke Metz, and Soumith Chintala. "Unsupervised representation learning with deep convolutional generative adversarial networks." arXiv:1511.06434 (2015).

GANs and cGANs (I)

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GANs: $\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))].$

G – a generative model;
D – a discriminative model;
x – training real data;
z – data generated by G;

If both the generator and the discriminator are conditioned on some extra information *y*:

$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x}|\boldsymbol{y})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}|\boldsymbol{y})))].$ - conditional GAN (cGAN);

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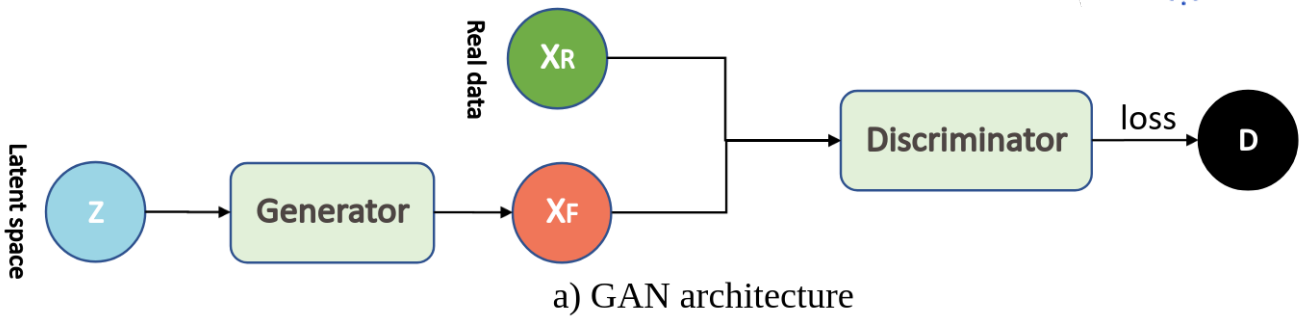
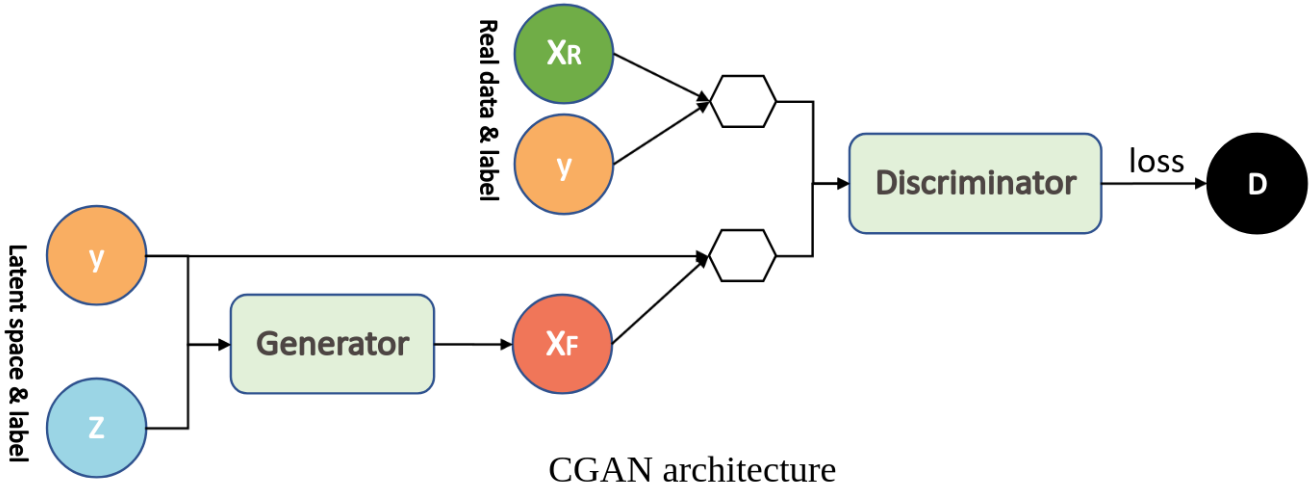
GANs and cGANs (II)

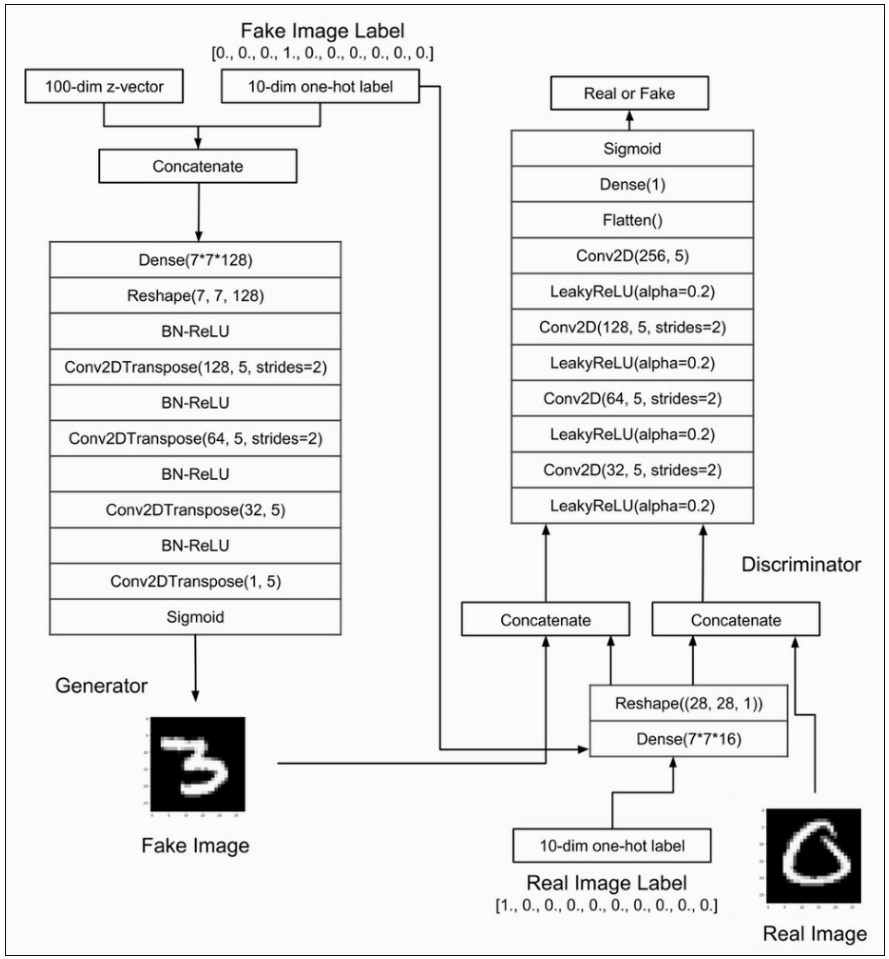


a) GAN architecture



CGAN architecture

GANs and cGANs (III)



https://medium.com/datadriveninvestor/an-introduction-to-conditional-gans-cgans-727d1f5bb011