OEAW AI SUMMER SCHOOL

DEEP LEARNING IV

(Variational) Autoencoders, GANs

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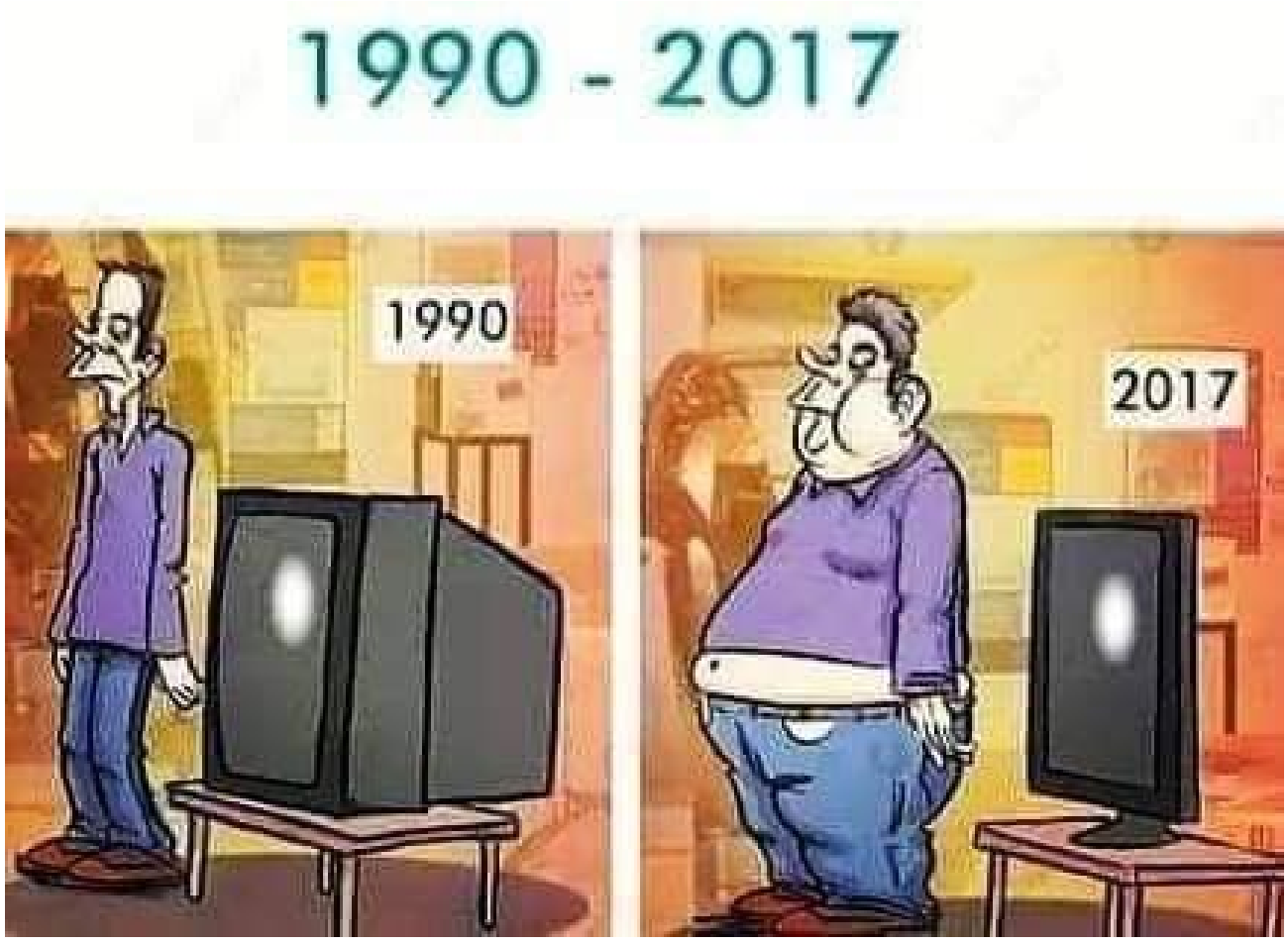
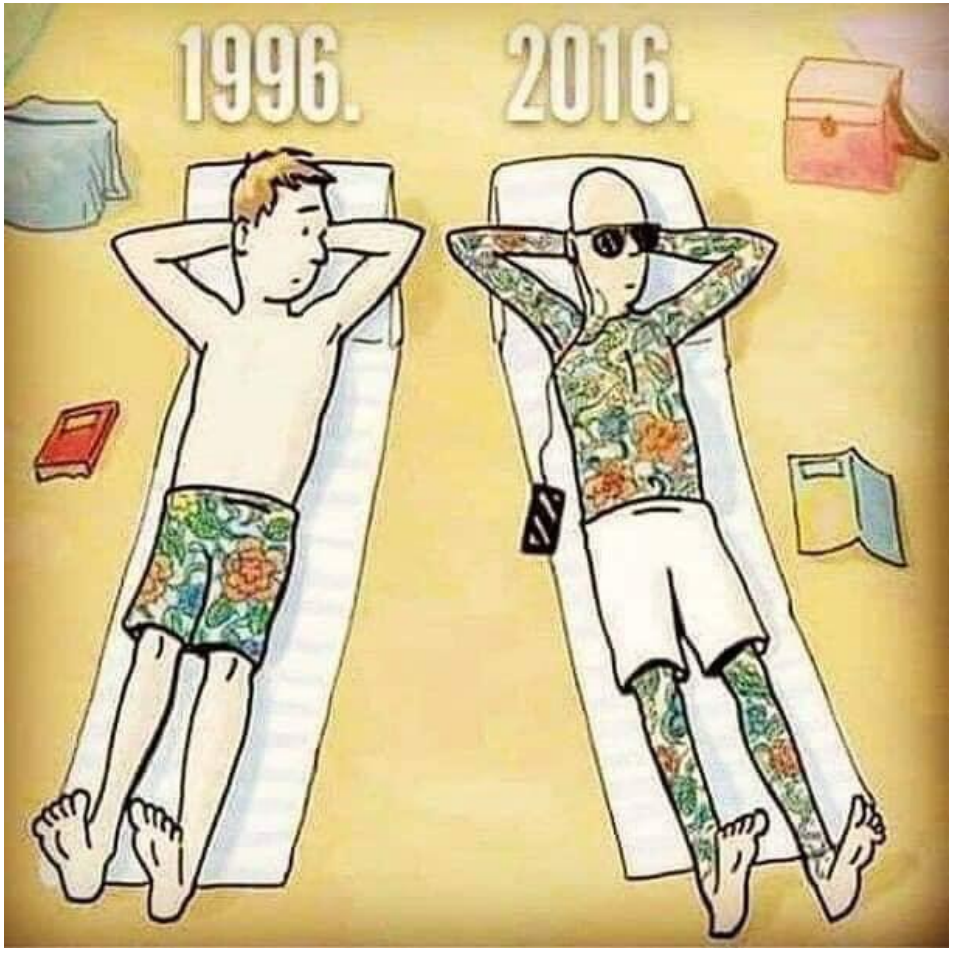
Then and now



Then and now



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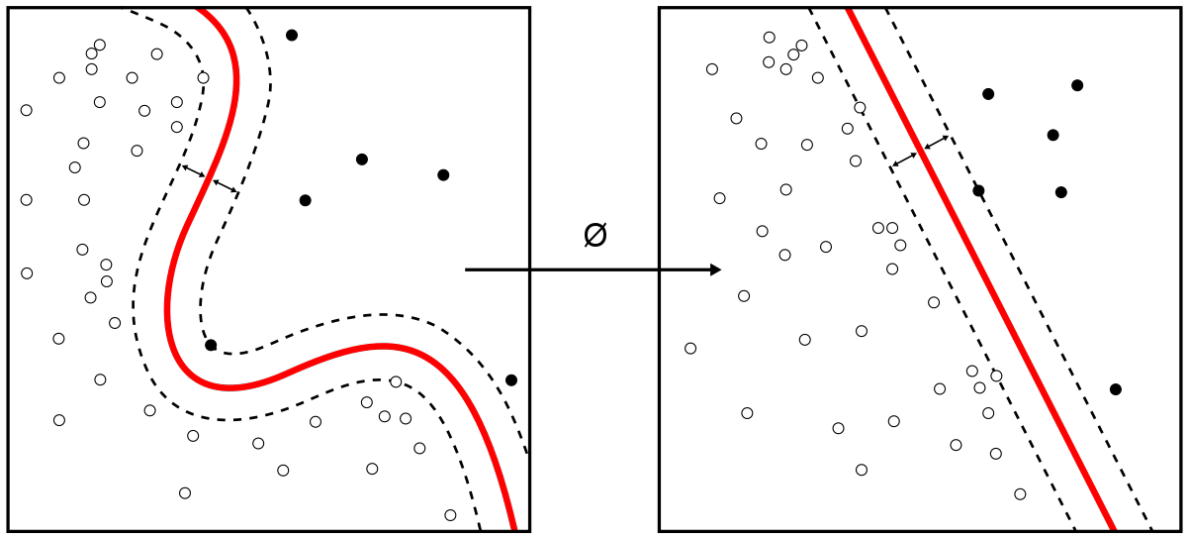


Timeline of Machine Learning

- First serious neural network efforts started in the 1980s.
- 1984 Leo Breiman: **Classification and regression trees**
- 1992-1995: profound mathematical foundation of **Support Vector Machines**:
  - kernel trick
  - soft margin classifier
- 2006-2008: **Restricted Boltzman Machines** started the Deep Learning hype
- 2012: **AlexNet**
- 2013: Speech recognition with **LSTMs**
- 2013 onwards:
  - **Tricks of the Trade**
  - **VAE**
  - **GAN**
  - ...

We are Deep Learning

- (Deep) Machine Learning has the potential to revolutionize your field of science ...
- ... BUT (Deep) Machine Learning is no black box magic which always works:
  - Not every problem is a ML problem:
    - Sometime “simple” statistics is all you need
  - Not every ML problem is a Deep Learning problem:
    - You have to know your data
    - You have to know the statistics
    - You have to know what algorithm to use
    - You have to know how to control the beast (especially in Deep Learning)
- Doesn’t matter what you are doing, you can do really cool things with (Deep) Learning!

Lecture IV: (Variational) Autoencoders, GANs

Autoencoders

Hidden representations

- Each hidden layer of the neural net calculates a new representation of the data.
- Each hidden layer sees the data only via the representation of the layer below.

Hidden representations

- Each hidden layer of the neural net calculates a new representation of the data.
- Each hidden layer sees the data only via the representation of the layer below.
- Imagine a neural net for classification with 1 hidden layer:
  - Neural network gives better performance than logistic regression ...
  - ... but the output layer is actually a logistic regression that uses the representation of the hidden layer.
  - $\Rightarrow$ **Learning a hidden representation normally helps**.

Autoencoders

Goal: Can we use this "representation learning" property of neural nets without needing a label to predict (i.e. in an unsupervised fashion)?

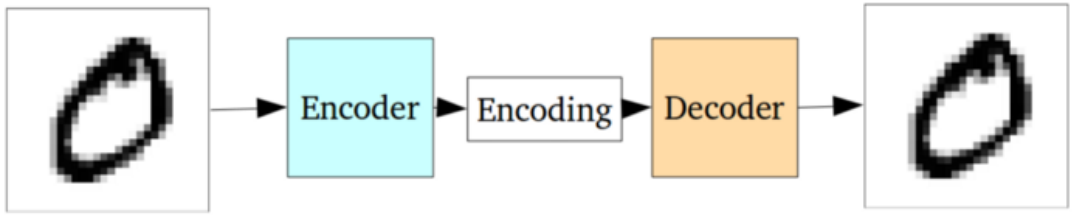
Idea: Let the network predict the input data again.
(The input data is re-used as label.)

Result: The hidden layer will learn a representation of the input that encodes all its major features.
(So it's easy to reconstruct the input again.)

Use: This can be used as a general feature construction method, but e.g. also to compress the input data.

This is called an **Auto-Encoder (AE)** or **Auto-Associator**.

General remarks



Most often, autoncoders have only one hidden layer:

$$\mathbf{h} = f_1(\mathbf{W1} \cdot \mathbf{x}) \qquad \text{”encoding“ step}$$

$$\mathbf{o} = f_2(\mathbf{W2} \cdot \mathbf{h}) \qquad \text{”decoding“ step}$$

- For binary inputs (and target outputs), f_2 is often a sigmoid.
- For unconstrained or approximately Gaussian inputs, f_2 is often the identity function.
- Sometimes tied weights are used, i.e. $\mathbf{W2} = \mathbf{W1}^T$ (reduces the number of parameters and often doesn't hurt performance).

Linear autoencoder

In the simplest case, $f1$ is the identity as well:

$$\mathbf{h} = \mathbf{W1} \cdot \mathbf{x}$$

$$\mathbf{o} = \mathbf{W2} \cdot \mathbf{h}$$

- Essentially $o = \mathbf{W2} \cdot \mathbf{W1} \cdot \mathbf{x} = \hat{\mathbf{W}} \cdot \mathbf{x}$
- Only interesting if we have less hidden units than inputs, otherwise trivial solution $\mathbf{W1} = \mathbf{W2} = \mathbf{I}$.
- Very similar to PCA:
  - Linear AE learns representation that lives in the same linear subspace as the PCA solution.

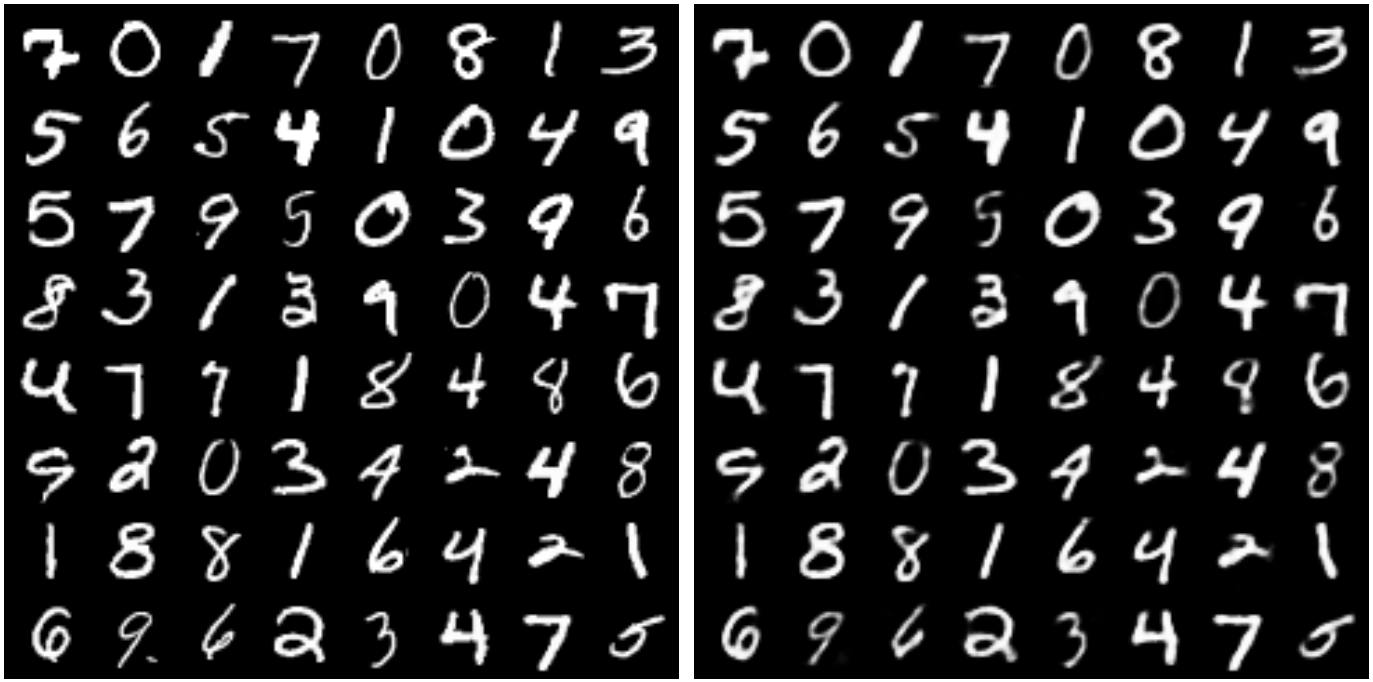
    (Proof: ”Neural networks and principal component analysis“, Baldi & Hornik, 1989)

Pytorch implementation non-linear AE

```
class autoencoder(nn.Module):
    def __init__(self, ae_input_dim):
        super(autoencoder, self).__init__()
        # encoder
        self.encoder_linear1 = nn.Linear(ae_input_dim, 256)
        self.encoder_linear2 = nn.Linear(256, 10)
        # decoder
        self.decoder_linear1 = nn.Linear(10,256)
        self.decoder_linear2 = nn.Linear(256, ae_input_dim)

    def encoder(self, x):
        x = self.encoder_linear1(x)
        x = F.relu(x)
        x = self.encoder_linear2(x)
        x = F.relu(x)
        return x

    def decoder(self, x):
        x = self.decoder_linear1(x)
        x = F.relu(x)
        x = self.decoder_linear2(x)
        x = torch.sigmoid(x)
        return x

    def forward(self, x):
        hidden = self.encoder(x)
        encoded = self.decoder(hidden)
        return hidden, encoded
```

“Traditional” non-linear autoencoder

- Autoencoder with 28×28 dimensional input vector of MNIST examples (left), 10 hidden states, and 28×28 dimensional output vector (right).
- Reconstruction error $\sum_i (\mathbf{o}_i - \mathbf{x}_i)^2$ is almost perfect.

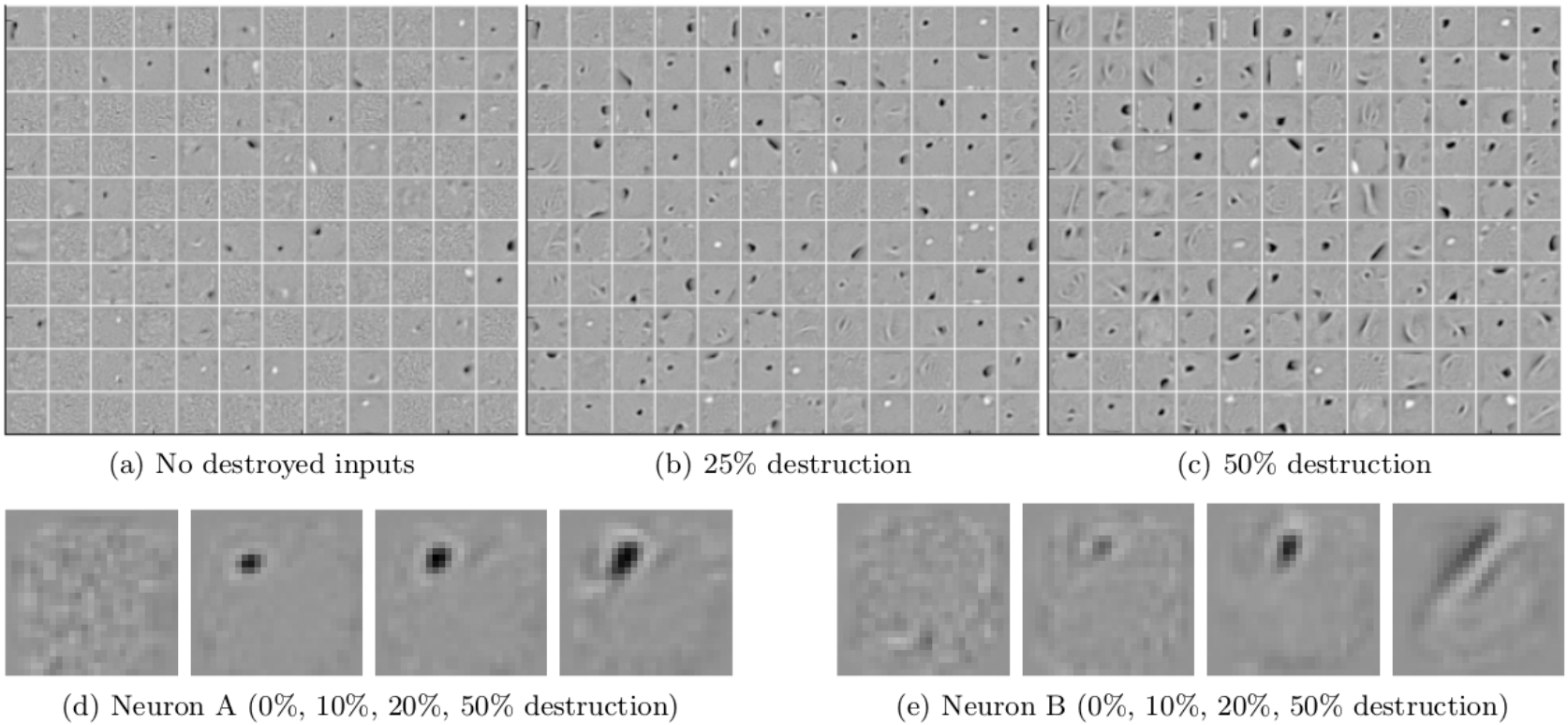


Denoising autoencoders

- Add noise to input, force autoencoder to reconstruct a noise-free version:
  - AE must learn to recognize structures.
  - AE must learn not to focus on noise.
  - Usually ”drop-out“ noise: simply set some inputs to zero (This works best on binary data.)

Denoising autoencoder on MNIST

- Patches correspond to rows of learnt weight matrices.
- With increasing level of corruption, an increasing number of filters resembles sensible feature detectors.



(a) No destroyed inputs (b) 25% destruction (c) 50% destruction

(d) Neuron A (0%, 10%, 20%, 50% destruction)

(e) Neuron B (0%, 10%, 20%, 50% destruction)

Vincent, Larochelle, Bengio, Manzagol. Extracting and Composing Robust Features with Denoising Autoencoders. ICML 2008

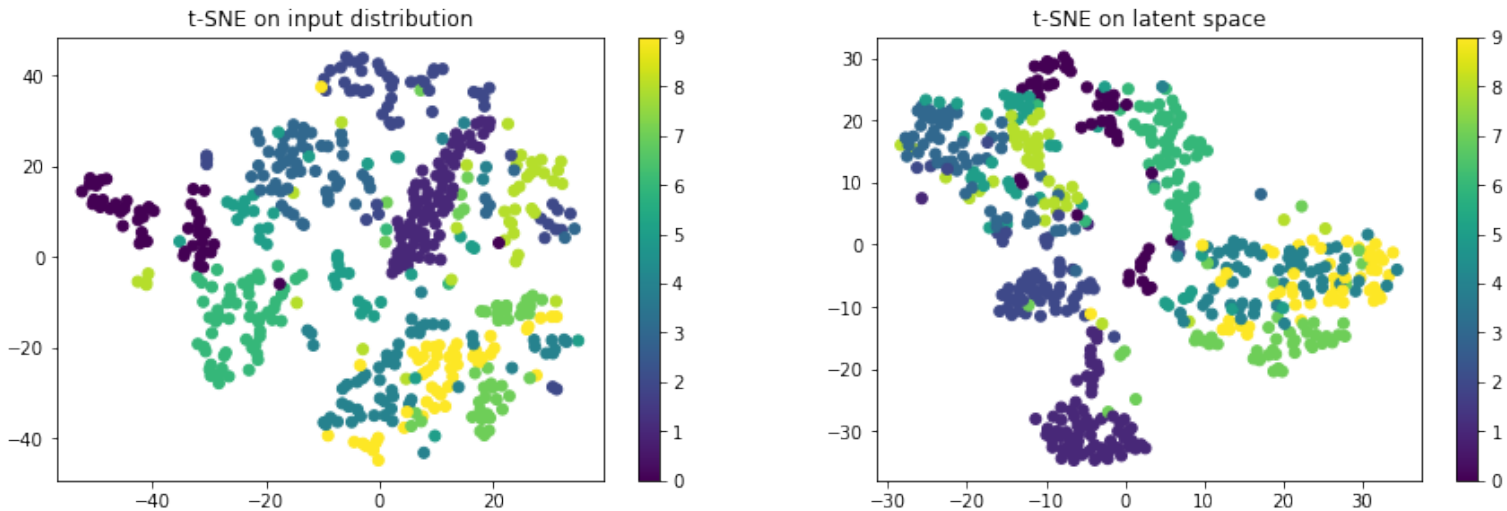
Autoencoders summarized

- Linear AEs are easy to analyze, but doing PCA isn't very exciting.
- Non-linear activation functions learn more interesting patterns.
- Many different AEs exist:
  - "Traditional" autoencoders
  - Denoising autoencoders
  - Sparse autoencoders: forcing hidden units to be inactive most of the time; instead of many large features, we will learn many small ones.
  - ...
- **However**: Autoencoders are limited in their applications: we will discuss why!
- $\Rightarrow$ **Variational autoencoders (VAE)**

Variational autoencoders

Limits of autoencoders

- The latent space of autoencoders is not continuous, or does not allow easy interpolations.
- Continuous latent space is what you need when **building generative models**:
  - Generative models: unsupervised learning
  - You don't want to replicate the input, our classify the input. **You want to generate new samples**.



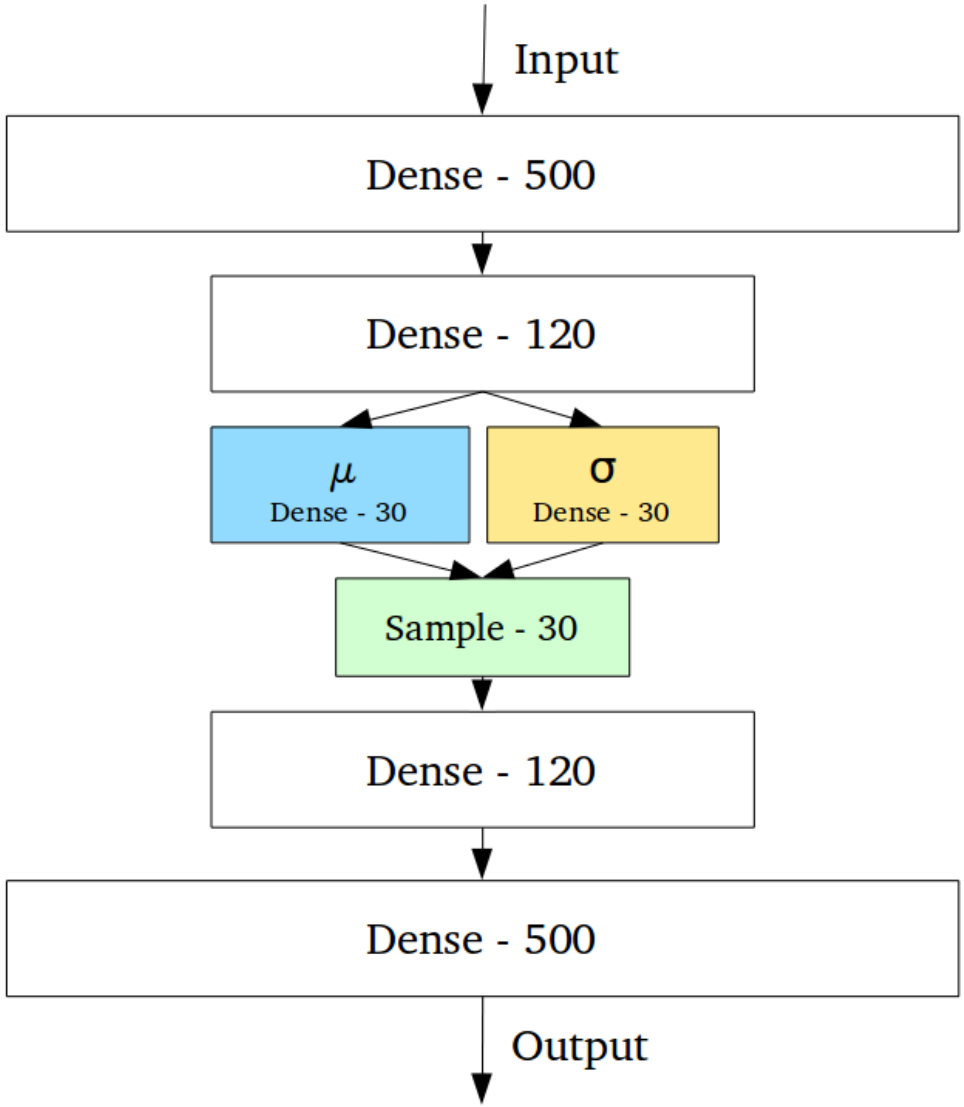
T-SNE visualization of the encodings from the above MNIST examples show distinct clusters.

Variational autoencoders

- By sampling from discontinuous latent space (gaps between clusters), decoder generates unrealistic outputs.
- Latent space of VAEs is by design continuous.
  - Encoder outputs two vectors:
    - vector of means of distribution
    - vector of standard deviations of distribution
  - Force this distribution to be standard normal distribution.
  - Sample from this distribution and pass the obtained sampling onward to the decoder.
- Through stochastic generation, the encoding will vary on every single pass simply due to sampling.
- The decoder is not only able to decode single encodings in the latent space, but ones that slightly vary too.

Kingma, Diederik P and Welling, Max. Auto-Encoding Variational Bayes. In The 2nd International Conference on Learning Representations (ICLR), 2013

Variational autoencoders



Understanding-variational-autoencoders

Pytorch implementation VAE

```python
class VAE(nn.Module):
    def __init__(self, ae_input_dim):
        super(VAE, self).__init__()
        # encoder
        # 10-dimensional hidden space
        self.encoder_linear1 = nn.Linear(ae_input_dim, 400)
        self.encoder_linear2_1 = nn.Linear(400, 10)
        self.encoder_linear2_2 = nn.Linear(400, 10)
        # decoder
        self.decoder_linear1 = nn.Linear(10, 400)
        self.decoder_linear2 = nn.Linear(400, ae_input_dim)


    def encoder(self, x):
        x = self.encoder_linear1(x)
        x = F.relu(x)
        return self.encoder_linear2_1(x), self.encoder_linear2_2(x)

    def sampling(self, mu, log_var):
        if self.training:
            std = torch.exp(0.5*log_var)
            eps = torch.randn_like(std)
            return eps.mul(std).add_(mu)
        else:
            # During inference, we simply spit out the mean of the
            # learned distribution for the current input.
            return mu

    def decoder(self, x):
        x = self.decoder_linear1(x)
        x = F.relu(x)
        x = self.decoder_linear2(x)
        return torch.sigmoid(x)

    def forward(self, x):
        mu, log_var = self.encoder(x)
        x = self.sampling(mu, log_var)
        return self.decoder(x), mu, log_var
```

The loss function

- L = Cross Entropy Error $H_y(g(\mathbf{x}; \mathbf{W}))$
  + Kullback-Leibler divergence D_{KL} between all the components of $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ and the standard normal
  - $H_y(g(\mathbf{x}; \mathbf{W}))$ is calculated for every pixel (output percentage of target value).
  - D_{KL}: measure of how two probability distributions differ from each other

```
def loss_function(x_hat, x, mu, log_var):
    BCE = F.binary_cross_entropy(x_hat, x, reduction='sum')
    KLD = -0.5 * torch.sum(1 + log_var - mu.pow(2) - log_var.exp())
    return KLD + BCE
```

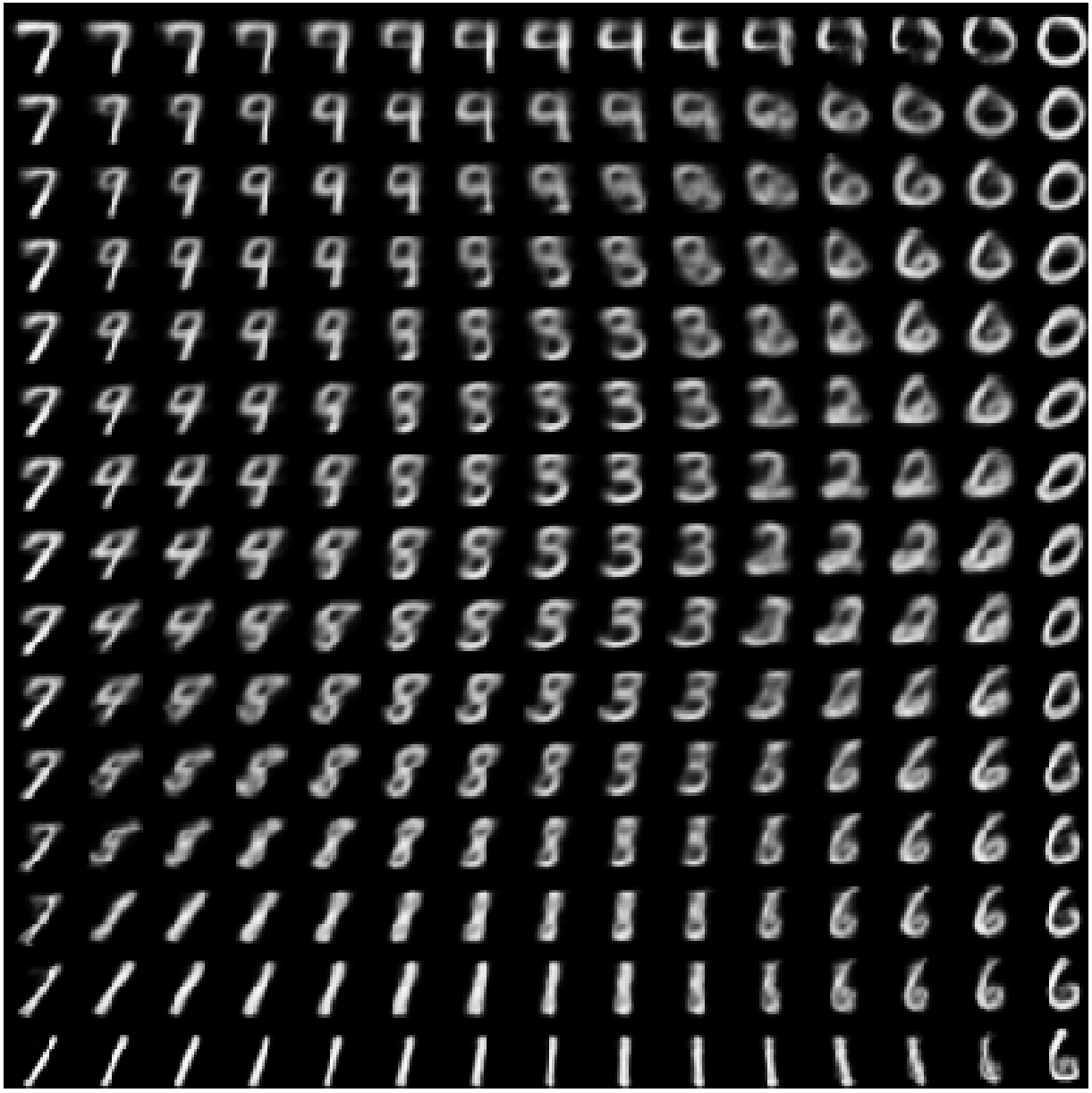
Making the loss differentiable

- $\mathbf{x} = \text{sample}(\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}))$ is not backpropable with respect to $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$
- However, it can be rewritten as:
  - $\mathbf{x} = \boldsymbol{\mu} + \boldsymbol{\sigma} \cdot \text{sample}(\mathcal{N}(\mathbf{0}, \mathbf{1}))$
  - This is backpropable now! :)

Variational autoencoders on MNIST

- Variational autoencoder with a 28×28 dimensional input vector for every MNIST example, 10 hidden states, and a 28×28 dimensional output vector (left)
- 64 random vectors of a 10-dimensional $\mathcal{N}(\mathbf{0}, \mathbf{1})$ are drawn and handed to the decoder (right)

VAE walking around in the latent space



VAE image generation

Larsen and Sønderby. Blog. Generating Faces with Torch, 2015

VAEs vs GANs

- Variational autoencoders ...
  - ... are usually easier to train and easier to get working.
  - ... are relatively easy to implement and robust to hyperparameter choices.
  - ... have an explicit inference network. So we can do reconstruction.
- However, variational autoencoders collapse all the dimensions in the latent, which are not needed:
  - This limits the generative power to a certain degree.
  - $\Rightarrow$ Generative adversarial networks ...

Generative adversarial networks

Cool idea

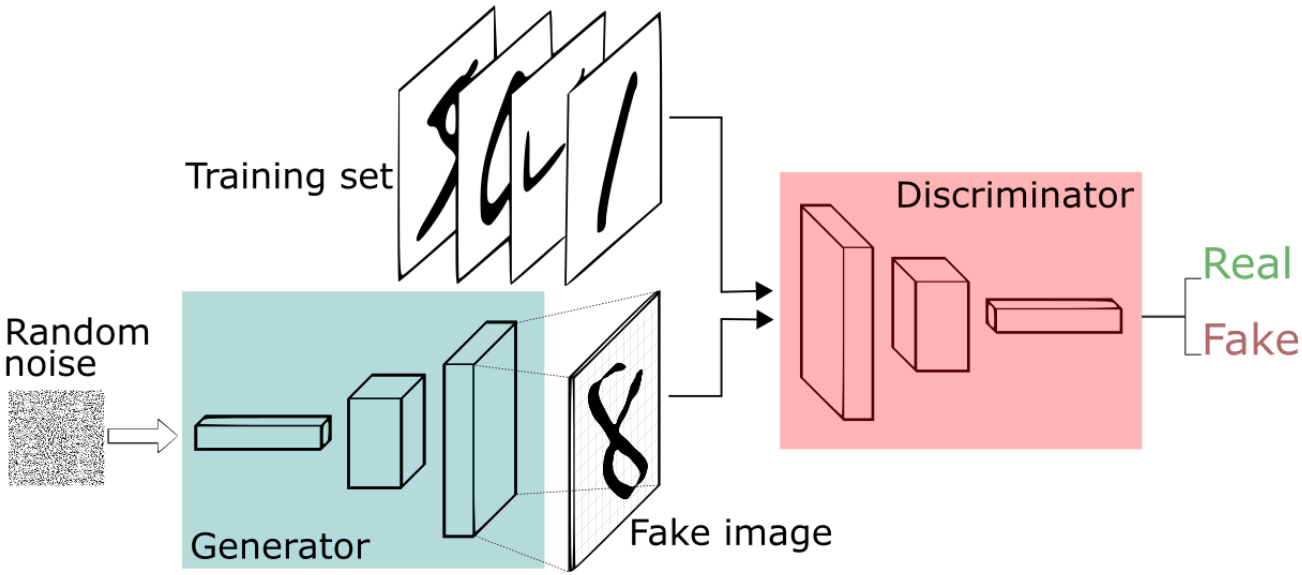
"The coolest idea in machine learning in the last twenty years."
(Yann LeCun)

Kerras et al (Nvidia). Progressive Growing of GANs for Improved Quality, Stability, and Variation. ICLR (2018)

The guy behind GANs

Min-max game

- Two networks play against each other.
- Automatically labeled data: generated, real
- Generator: tries to generate realistic images, tries to fool the discriminator
- Discriminator: tries to tell apart real and generated images, tries to outsmart the generator



Goodfellow et al. Generative adversarial nets. In Advances in Neural Information Processing Systems, 2014

GAN loss discriminator

- Remember cross entropy error:

$$L = -\sum_i y_i \log g(\mathbf{x}_i; \mathbf{W}) + (1 - y_i) \log(1 - g(\mathbf{x}_i; \mathbf{W}))$$

- In the GAN setting:

$$\underbrace{min}_{D} L(D) = -\mathbb{E}_{\mathbf{x} \sim p_{\text{real}}(\mathbf{x})} [\log D(\mathbf{x})] - \mathbb{E}_{\mathbf{z} \sim p_{\text{gen}}(\mathbf{z})} [\log (1 - D(\mathbf{z}))]$$

$$\underbrace{max}_{D} L(D) = \mathbb{E}_{\mathbf{x} \sim p_{\text{real}}(\mathbf{x})} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\text{gen}}(\mathbf{z})} [\log (1 - D(\mathbf{z}))]$$

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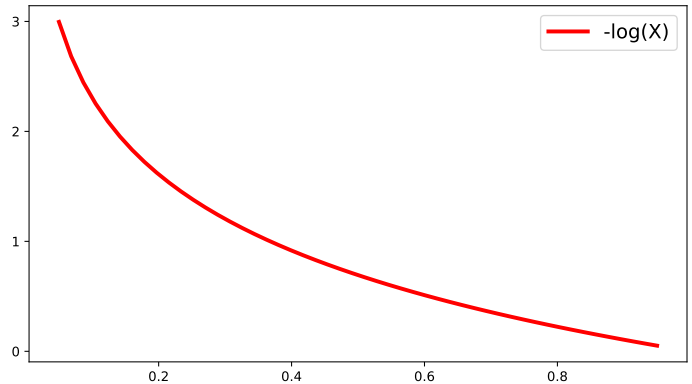

- Probability of D(real)

GAN loss discriminator

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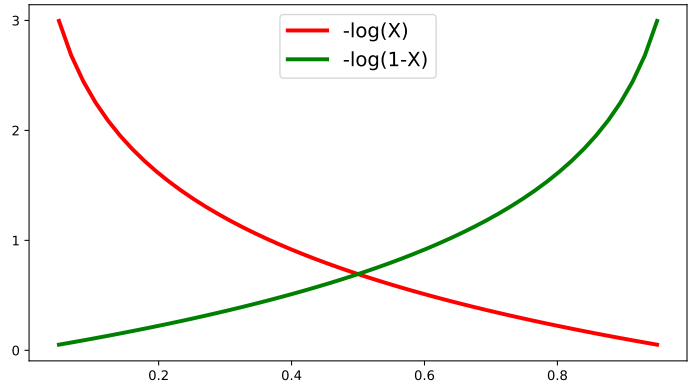


- Probability of D(real)
- Probability of D(fake)

GAN loss generator

- Discriminator loss:

$$\underbrace{max}_{D} L(D) = \mathbb{E}_{\mathbf{x}\sim p_{\text{real}}(\mathbf{x})} \left[\log D(\mathbf{x})\right] + \mathbb{E}_{\mathbf{z}\sim p_{\text{gen}}(\mathbf{z})} \left[\log \left(1 - D(G(\mathbf{z}))\right)\right]$$

- Generator loss:

$$\underbrace{min}_{G} L(D, G) = \mathbb{E}_{\mathbf{z}\sim p_{\text{gen}}(\mathbf{z})} \left[\log \left(1 - D(G(\mathbf{z}))\right)\right]$$

$$\simeq \underbrace{max}_{G} \mathbb{E}_{\mathbf{z}\sim p_{\text{gen}}(\mathbf{z})} \left[\log \left(D(G(\mathbf{z}))\right)\right]$$

- Putting it all together:

$$\underbrace{min}_{G} \underbrace{max}_{D} L(D) = \mathbb{E}_{\mathbf{x}\sim p_{\text{real}}(\mathbf{x})} \left[\log D(\mathbf{x})\right] + \mathbb{E}_{\mathbf{z}\sim p_{\text{gen}}(\mathbf{z})} \left[\log \left(1 - D(\mathbf{z})\right)\right]$$

Pytorch implementation GAN

```
class Generator(nn.Module):
    def __init__(self, g_input_dim, g_output_dim):
        super(Generator, self).__init__()
        self.linear1 = nn.Linear(g_input_dim, 256)
        self.linear2 = nn.Linear(256, 512)
        self.linear3 = nn.Linear(512, 1024)
        self.linear4 = nn.Linear(1024, g_output_dim)

    def forward(self, x):
        x = self.linear1(x)
        x = F.relu(x)
        x = self.linear2(x)
        x = F.relu(x)
        x = self.linear3(x)
        x = F.relu(x)
        x = self.linear4(x)
        return torch.tanh(x)

class Discriminator(nn.Module):
    def __init__(self, d_input_dim):
        super(Discriminator, self).__init__()
        self.linear1 = nn.Linear(d_input_dim, 1024)
        self.linear2 = nn.Linear(1024, 512)
        self.linear3 = nn.Linear(512, 256)
        self.linear4 = nn.Linear(256, 1)

    def forward(self, x):
        x = self.linear1(x)
        x = F.relu(x)
        x = F.dropout(x, 0.3)
        x = self.linear2(x)
        x = F.relu(x)
        x = F.dropout(x, 0.3)
        x = self.linear3(x)
        x = F.relu(x)
        x = F.dropout(x, 0.3)
        x = self.linear4(x)
        return torch.sigmoid(x)
```

Pytorch implementation generator

```
def train_discriminator(x):
    D.zero_grad()

    # discriminator loss on real
    x_real, y_real = x.view(-1, mnist_dim), torch.ones(x.view(-1, mnist_dim).shape[0], 1)
    x_real, y_real = Variable(x_real.to(device)), Variable(y_real.to(device))

    D_output = D(x_real)
    D_real_loss = criterion(D_output, y_real)
    D_real_score = D_output

    # discriminator loss on fake
    z = Variable(torch.randn(args.batch_size, z_latent).to(device))
    x_fake, y_fake = G(z), Variable(torch.zeros(args.batch_size, 1).to(device))

    D_output = D(x_fake)
    D_fake_loss = criterion(D_output, y_fake)
    D_fake_score = D_output

    # gradient backprop
    D_loss = D_real_loss + D_fake_loss
    D_loss.backward()
    D_optimizer.step()

    return  D_loss.data.item()
```

Pytorch implementation discriminator

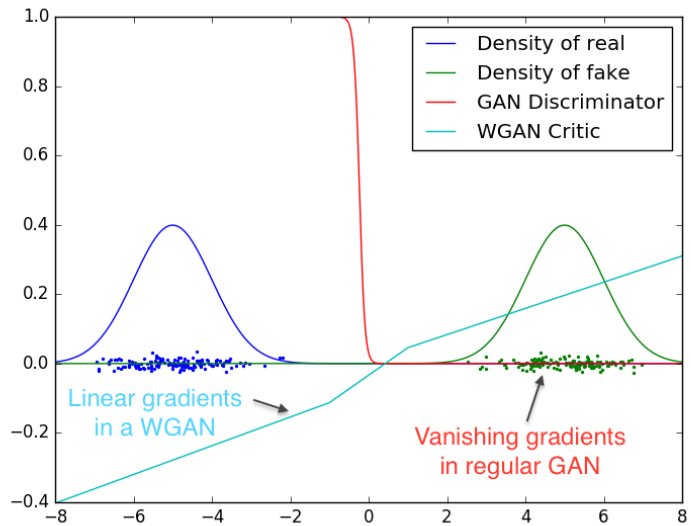
```
def train_generator():
    G.zero_grad()

    z = Variable(torch.randn(args.batch_size, z_latent).to(device))
    y = Variable(torch.ones(args.batch_size, 1).to(device))

    G_output = G(z)
    D_output = D(G_output)
    G_loss = criterion(D_output, y)

    # gradient backprop
    G_loss.backward()
    G_optimizer.step()

    return G_loss.data.item()
```

Loss as divergence

- For solving the optimization problem of the generator the loss can be interpreted as Jensen-Shannon divergence $JSD(p_{real}(\mathbf{x}), p_{gen}(\mathbf{x}))$, which has to be minimized.
- Jensen-Shannon divergence is the symmetrized Kullback-Leibler divergence.
- Both are measures of the similarity between probability distributions.
- This has put up the questions if their are maybe better similarity measurements?

Wasserstein distant

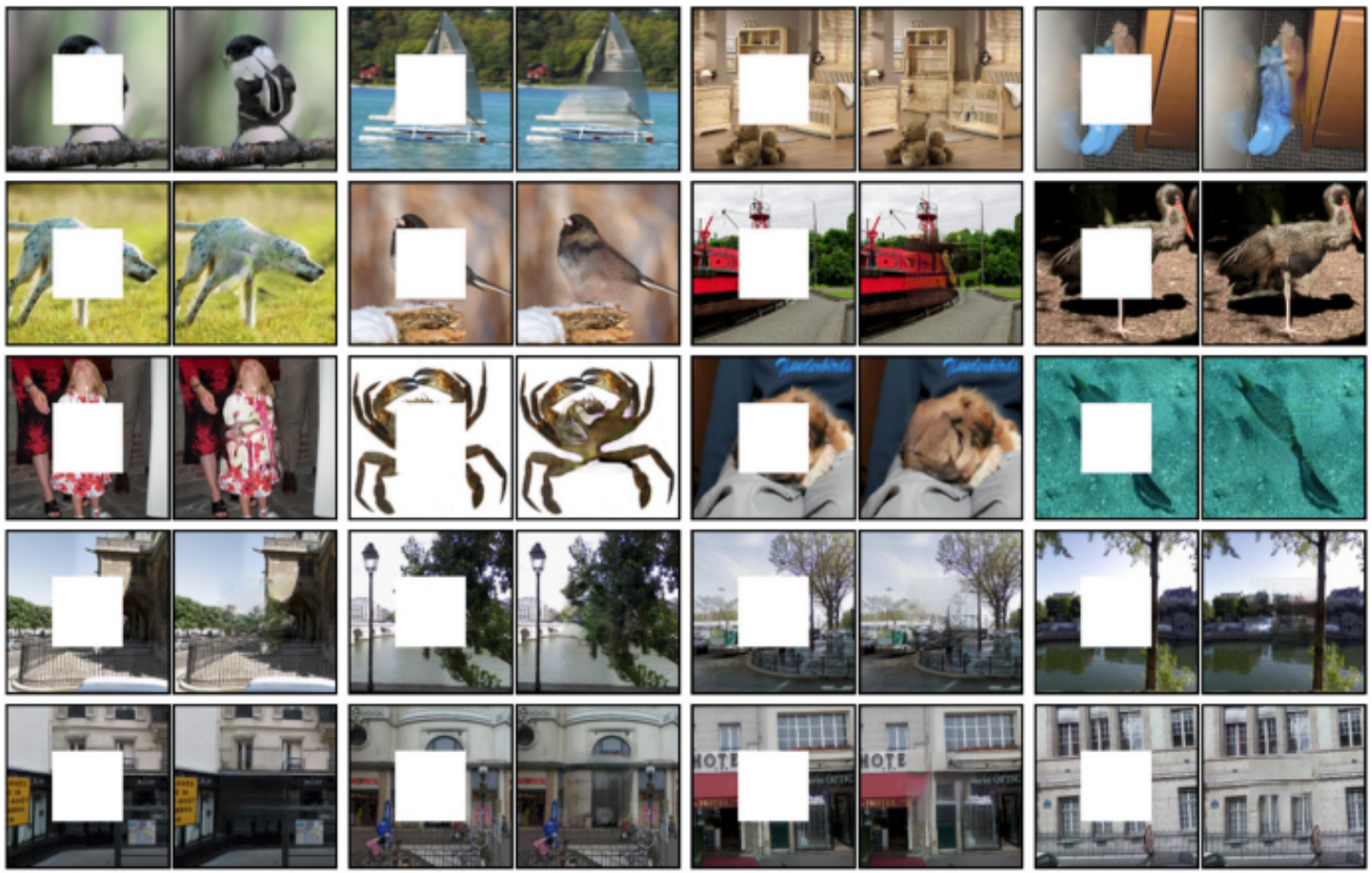
- Out of thousands the Wasserstein GAN worked best.
- The reason is twofold:
  - Wasserstein distance has gradients even if distributions are not overlapping.
  - A penalty term (free when clever implemented) allows to move distributions towards regions of largest change:
    - similar to the spectral norm and the largest eigenvalue



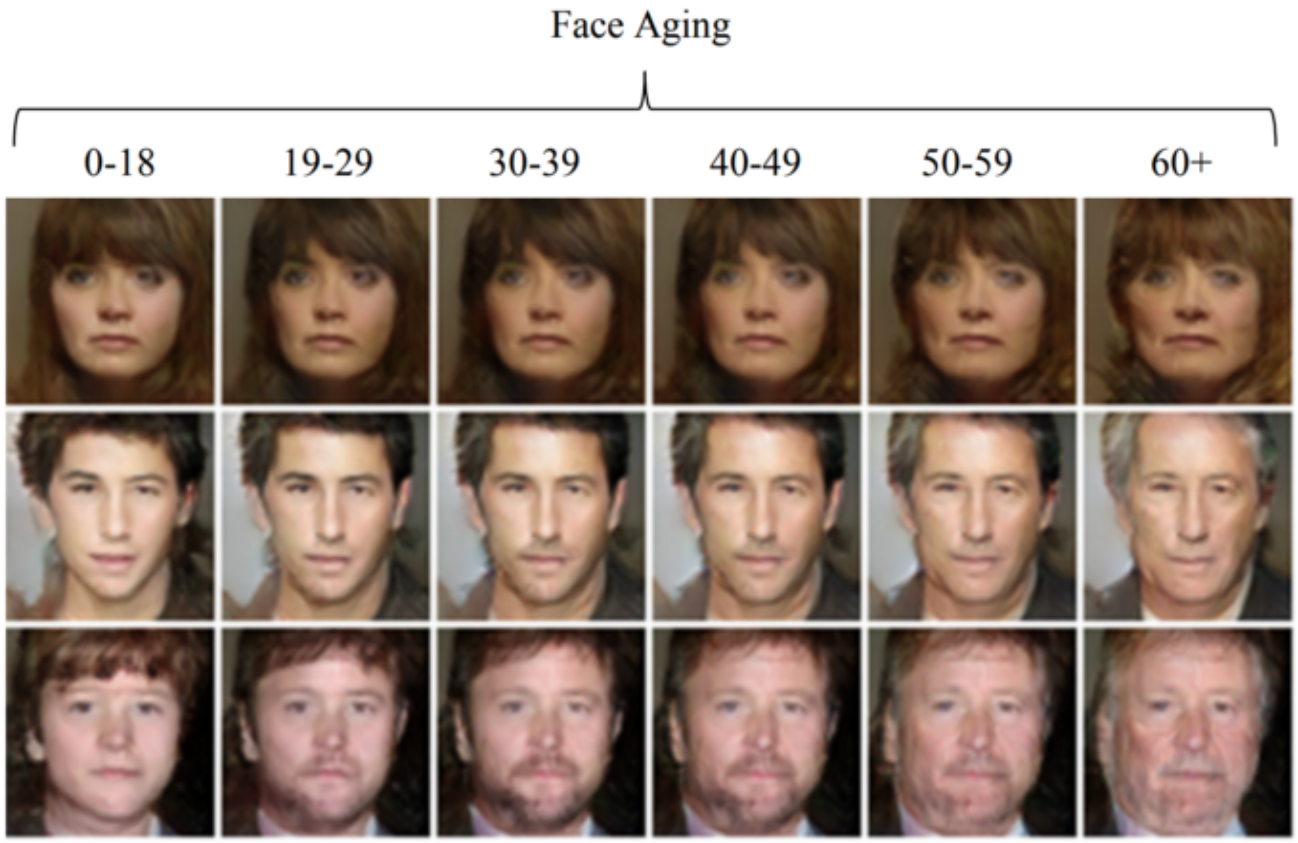
M. Arjovsky, S. Chintala, and L. Bottou. Wasserstein generative adversarial networks. Proceedings of the 34th International Conference on Machine Learning (ICML), 2017.

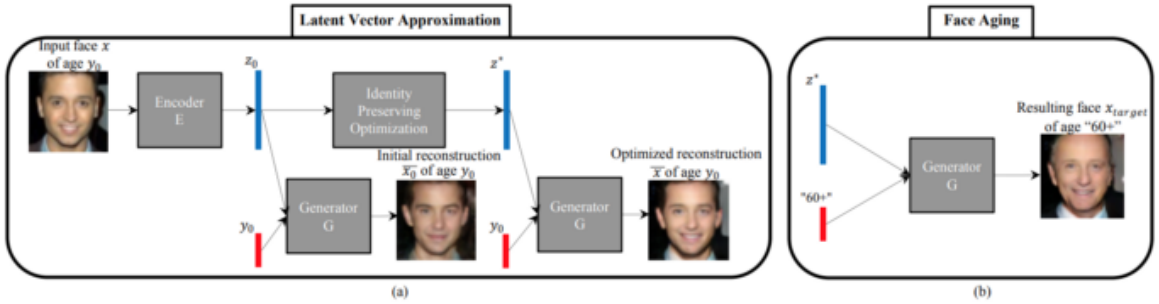
Image inpaiting

- Repairing images has been an important subject decades ago. GANs are ideally suited for filling the missing part with created “content”.

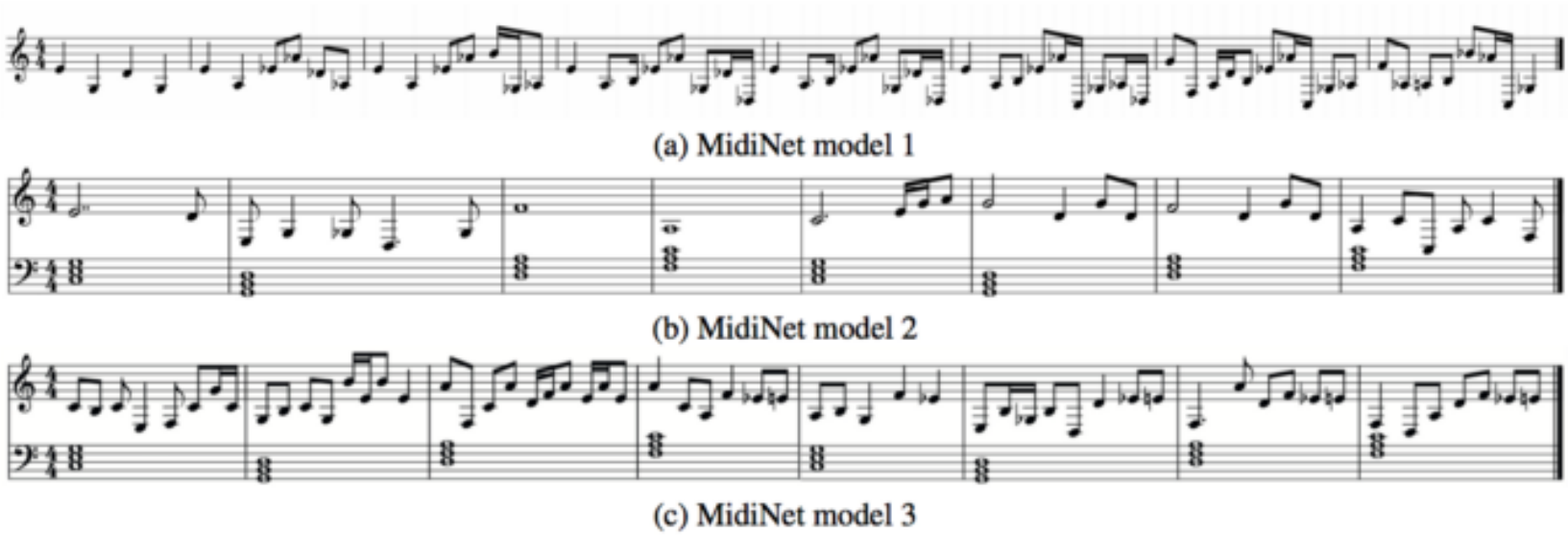


Face aging


Face Aging
0-18
19-29
30-39
40-49
50-59
60+


Latent Vector Approximation
Input face x of age y_0
Encoder E
z_0
Identity Preserving Optimization
z^*
Initial reconstruction $\overline{x_0}$ of age y_0
Optimized reconstruction $\overline{x}$ of age y_0
y_0
Generator G
y_0
Generator G
(a)
Face Aging
z^*
"60+"
Generator G
Resulting face x_{target} of age "60+"
(b)

Music generation

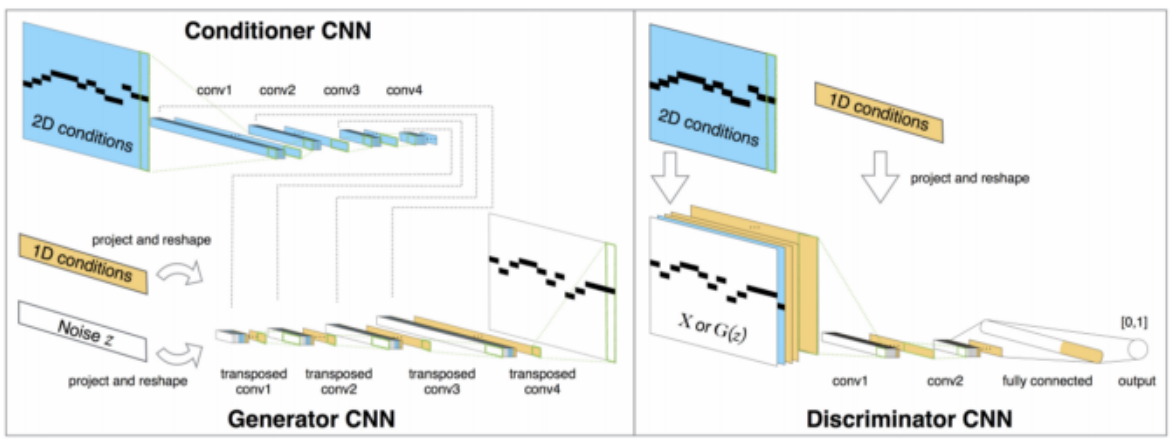


(a) MidiNet model 1

(b) MidiNet model 2

(c) MidiNet model 3

Figure 3. Example result of the melodies (of 8 bars) generated by different implementations of MidiNet.



Emojis from pictures

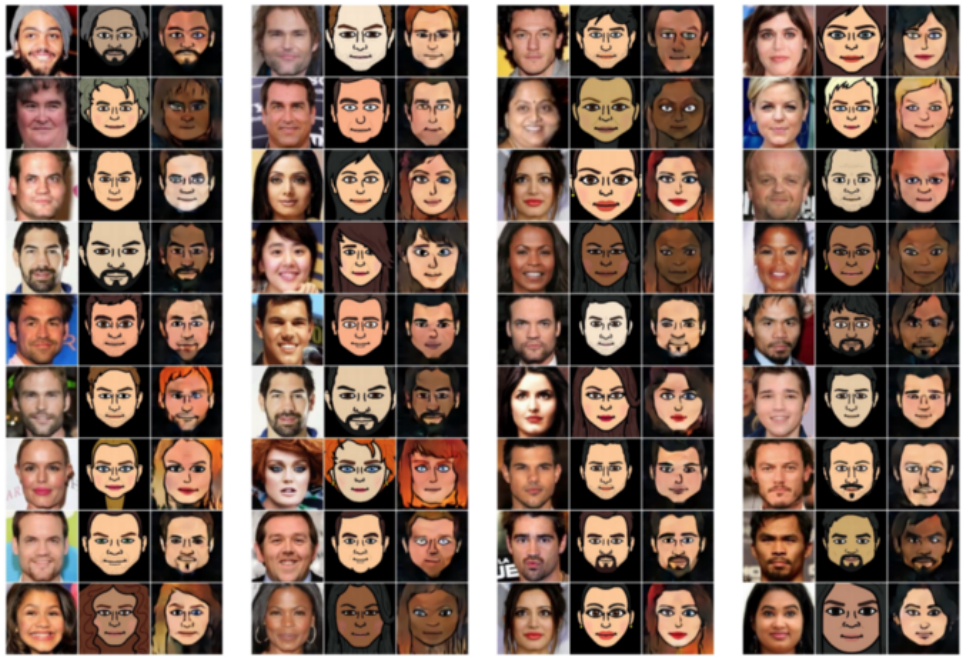


Figure 4: Shown, side by side are sample images from the CelebA dataset, the emoji images created manually using a web interface (for validation only), and the result of the unsupervised DTN. See Tab. 4 for retrieval performance.

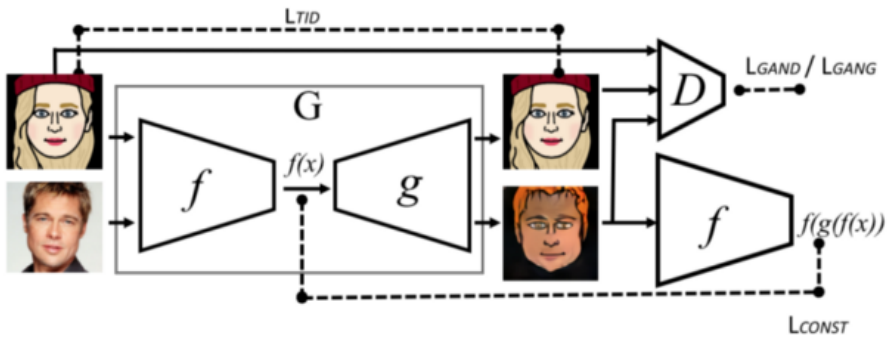


Figure 1: The Domain Transfer Network. Losses are drawn with dashed lines, input/output with solid lines. After training, the forward model G is used for the sample transfer.

Text to image

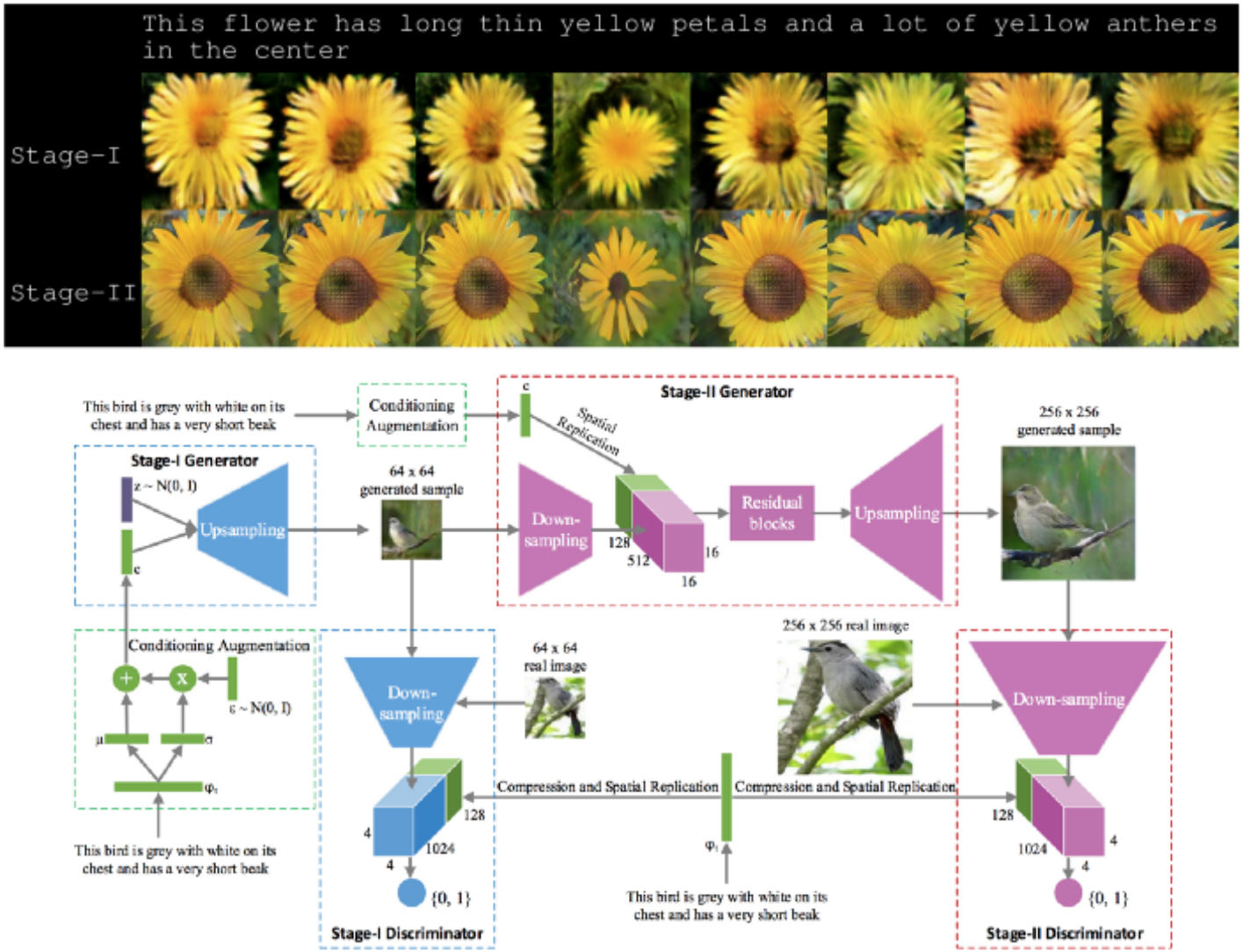
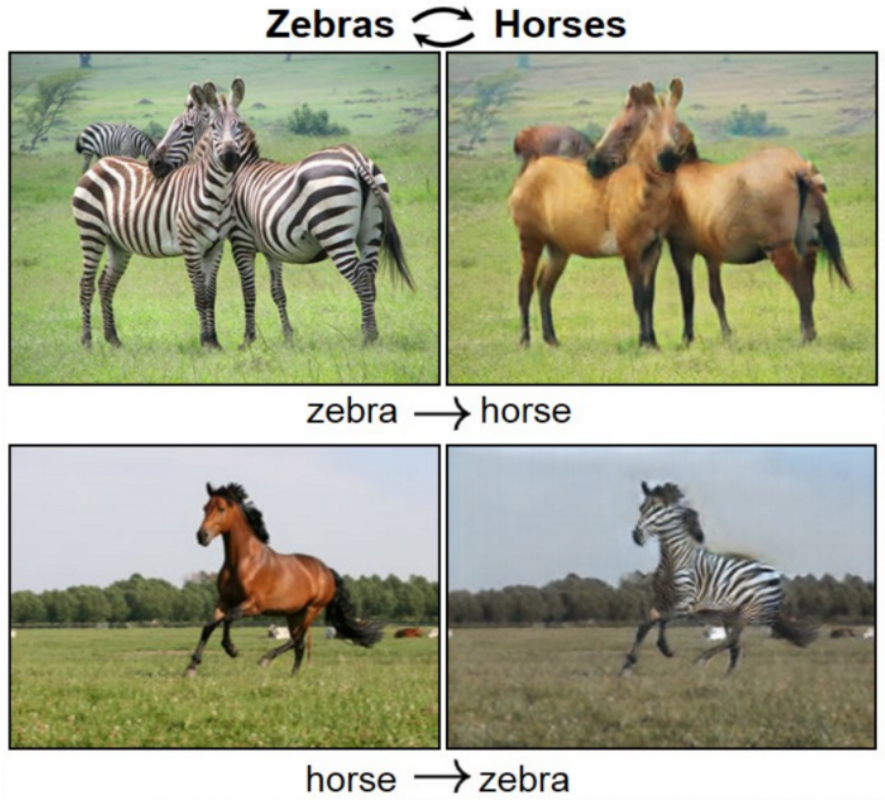


Figure 2. The architecture of the proposed StackGAN. The Stage-I generator draws a low resolution image by sketching rough shape and basic colors of the object from the given text and painting the background from a random noise vector. The Stage-II generator generates a high resolution image with photo-realistic details by conditioning on both the Stage-I result and the text again.

CycleGAN


Photograph
Monet
Van Gogh
Cezanne
Ukiyo-e


Zebras ⇄ Horses
zebra → horse
horse → zebra

DiscoGAN

(b) Handbag images (input) & **Generated** shoe images (output)

High-resolution image synthesis