Deep Learning

Lecture 5: Generative Adversarial, Variational and Implicit Models

Amir Atapour-Abarghouei

amir.atapour-abarghouei@durham.ac.uk

Durham University

Lecture Overview

Generative models

- Unsupervised training
- PixelRNN and PixelCNN

Generative adversarial networks

- Definition
- Common Issues
- Lipschits Continuity
- Spectral Normalisation
- Conditional GANs
- Other Advanced Variants

Variational autoencoders

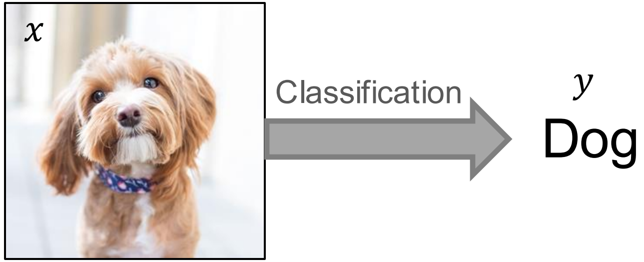
- Autoencoders
- VAEs
- Reparameterisation trick
- ELBO

Implicit networks

- Definition
- SIRENs
- NeRFs

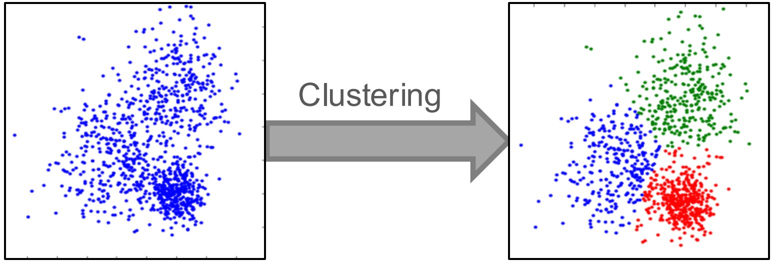
Supervised vs Unsupervised Training

- Supervised Learning:



  - Data x – Labels y
  - Learn mapping function $x \rightarrow y$
  - *e.g.* classification, regression, segmentation, object detection, machine translation, sentiment analysis (and everything else we have talked about so far).

- Unsupervised Learning:



  - Data x – **No** Labels
  - Learn underlying structures and patterns in the data.
  - *e.g.* clustering, dimensionality reduction, feature learning, density estimation.
  - **Generative models** are **unsupervised** as the data used has **no labels**.

Generative Models

Definition:

Given a set of data, capture the probability distribution representing this data and generate new data samples from this distribution.

Training Data ~ $P_{\text{data}}(x)$

https://github.com/NVlabs/ffhq-dataset

Generated Sample ~ $P_{\text{model}}(x)$

https://arxiv.org/pdf/1912.04958.pdf

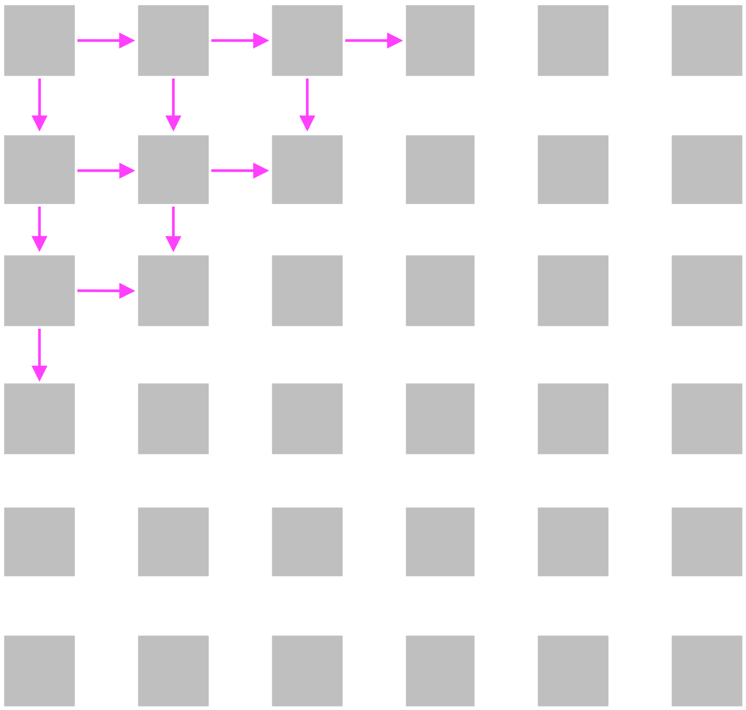
The objective is to learn $P_{\text{model}}(x)$ so it as close as possible to $P_{\text{data}}(x)$.

PixelRNN [van den Oord et al., 2016]

- Explicit tractable density function.
- We generate pixels one by one starting from a corner.
- Dependency on previous pixels is modelled via an RNN.
- During inference, for generation, we initialise the value of the first pixel and the image is generated.

Good results

but RNNs are sequential and thus **inefficient**!



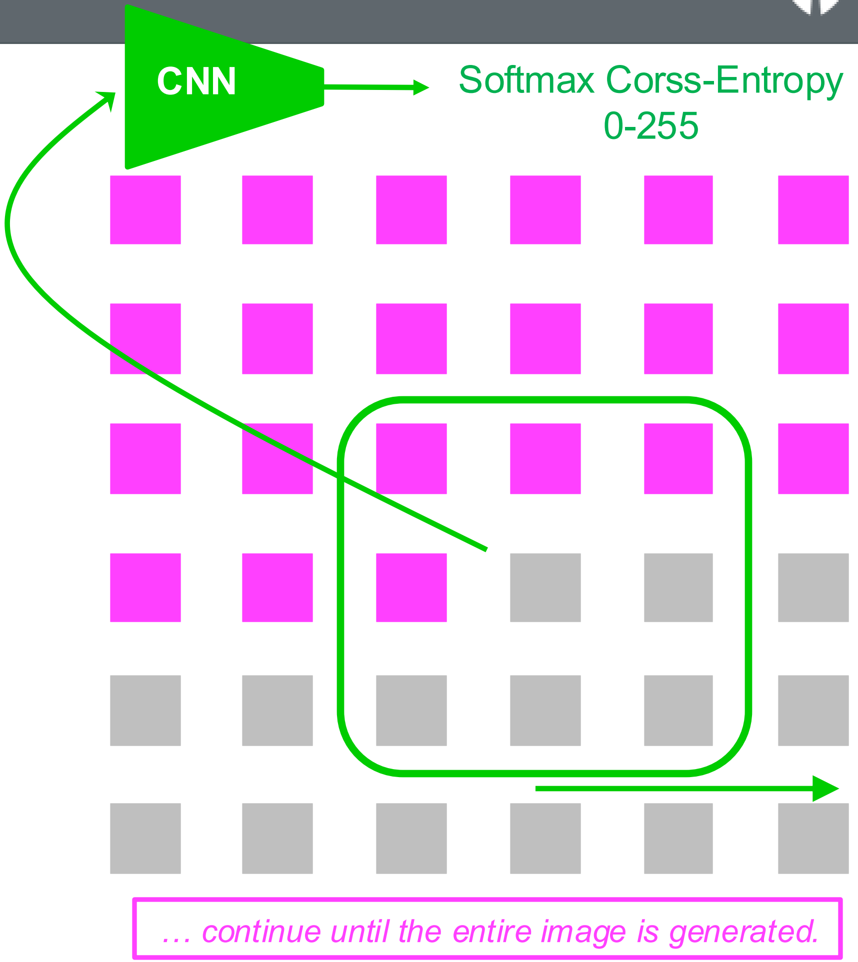
… continue until the entire image is generated.

PixelCNN [van den Oord et al., 2016]

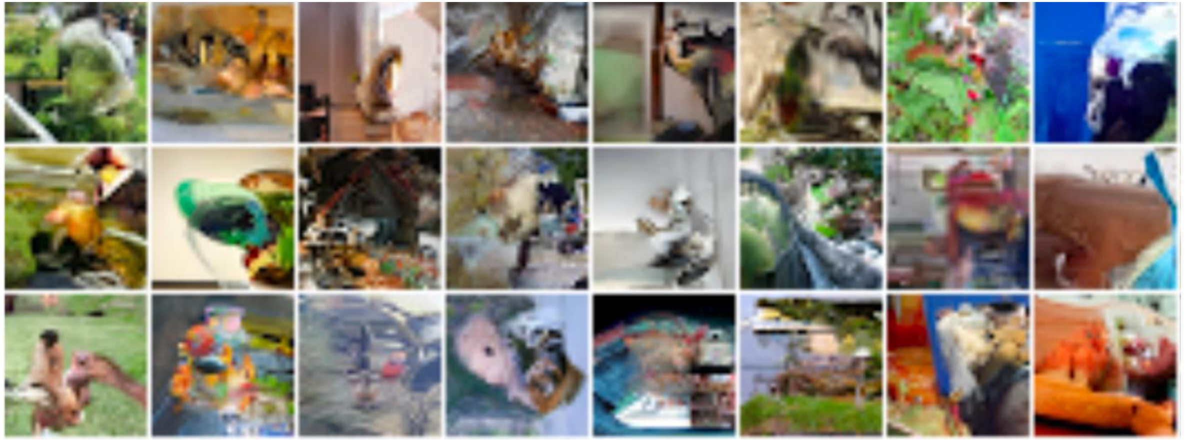
- Explicit tractable density function.
- We generate pixels one by one starting from a corner.
- Dependency on **pixel**s is modelled via a CNN over context patch.

CNN is parallelisable and thus **efficient**!

During inference, generation is sequential and still very slow…!



PixelRNN / PixelCNN [van den Oord et al., 2016]



PixelRNN

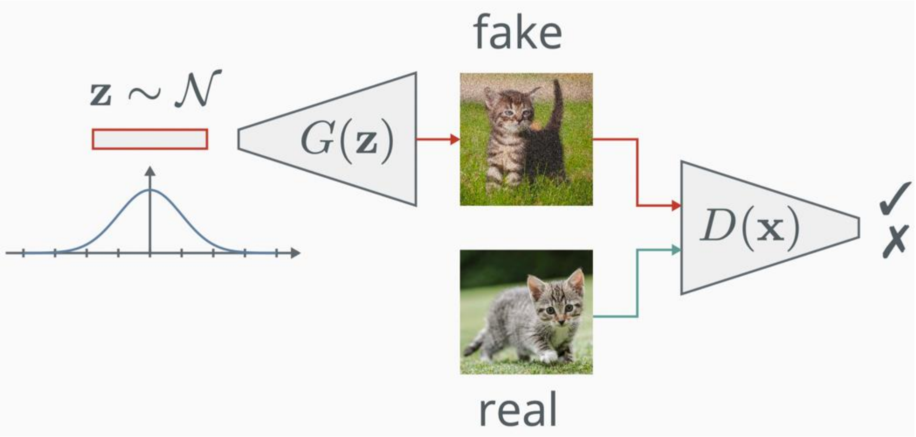
PixelCNN

Generative Adversarial Networks

Definition:

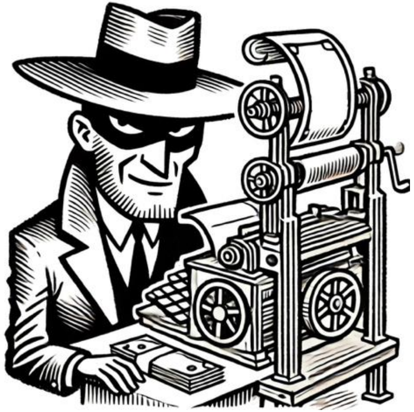
A generative adversarial network (GAN) is a non-coorporative zero-sum game where two networks compete against each other [Goodfellow et al., 2014].

One network $G(z)$ generates new samples, whereas D estimates the probability the sample was from the training data rather than G:



$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{\text{data}}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))\right]$$

Generative Adversarial Networks



1. I see!!

Fake!

2. Hmm!!

Fake!

3. Aha!!

Fake?

4. Success!

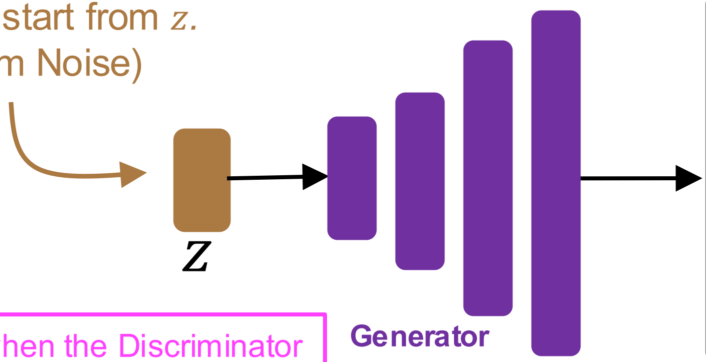
Real?

Generator

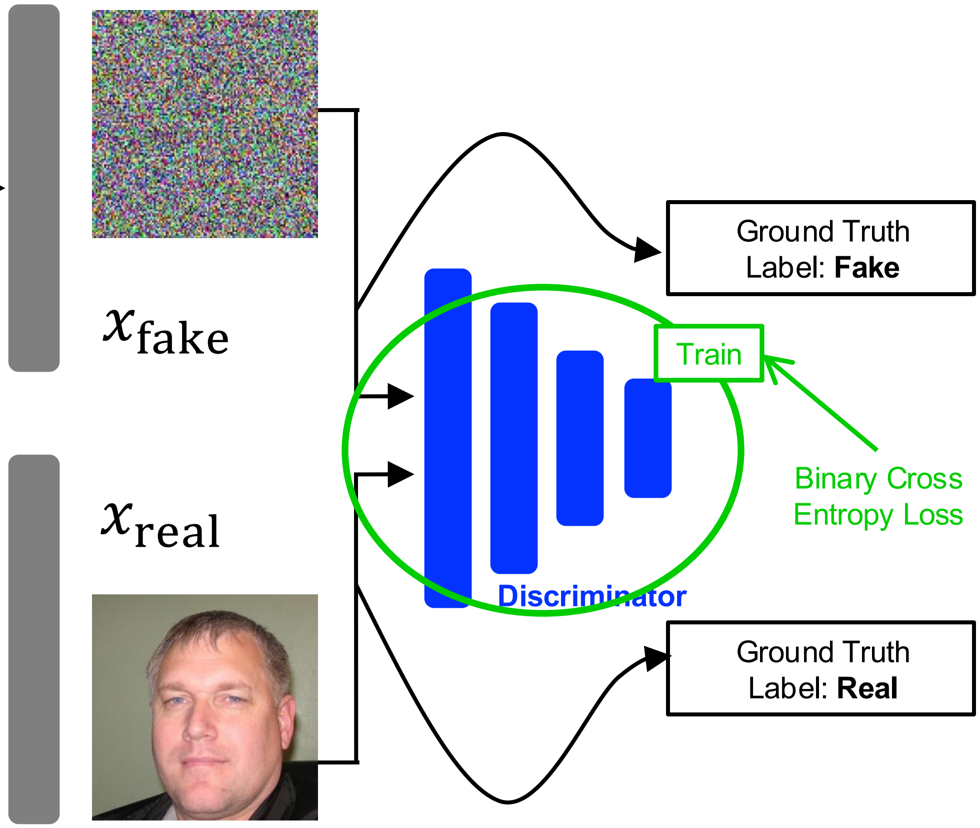
Discriminator

Generative Adversarial Networks Training

We always start from z.
(Random Noise)



Note that when the Discriminator is being trained, the weights of the Generator are not updated.

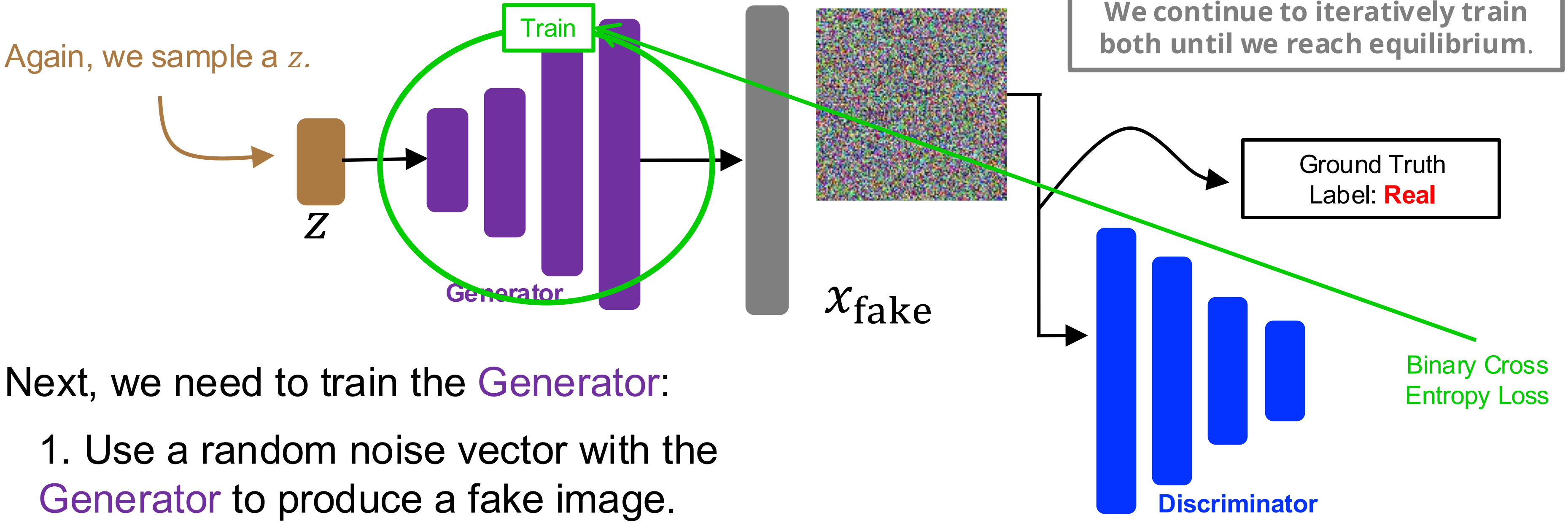


First, we need to train the Discriminator:

1. Use a random noise vector with the Generator to produce a fake image.
2. Use the fake image and a real image to only train the Discriminator.

Generative Adversarial Networks Training

We continue to iteratively train both until we reach equilibrium.



Next, we need to train the Generator:

1. Use a random noise vector with the Generator to produce a fake image.

2. Pass the fake image through the Discriminator, but with a Real label.

3. We then use the gradients from the Discriminator to train the Generator.

Note that we are trying to ***fool*** the Discriminator, which is why the Real label is used for the fake image.

Generative Adversarial Networks Objective

- The objective function:
  - Generator and Discriminator are trained jointly in minimax game:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x\sim p_{\text{data}}} \log \boxed{D_{\theta_d}(x)} + \mathbb{E}_{z\sim p(z)} \log(1 - \boxed{D_{\theta_d}(G_{\theta_g}(z))})\right]$$

Discriminator output for real data x

Discriminator output for fake generated data $G(z)$

- Discriminator (θ_d) wants to **maximise** the objective so $D(x)$ is close to 1 (real) and $D(G(z))$ is close to 0 (fake).
- Generator (θ_g) wants to **minimise** the objective so $D(G(z))$ is close to 1 (the discriminator will think the fake output is real).

Let’s Look at Some Code!

Simple GAN Example

Code on GitHub : https://github.com/atapour/dl-pytorch/blob/main/Simple_GAN_Example/Simple_GAN_Example.ipynb

Code on Colab: https://colab.research.google.com/github/atapour/dl-pytorch/blob/main/Simple_GAN_Example/Simple_GAN_Example.ipynb

Issues:

- **Non-Convergence:** Model is unstable so parameters oscillate and never converge.
- **Diminishing Gradients:** The Discriminator reaches its optimal state too soon and its small gradients cannot train the Generator.
- **Hyperparameter Sensitivity:** The model is too sensitive to any changes in hyperparameters (*e.g.*, learning rate).
- **Mode Collapse:** The Generator collapses and produces a limited variety of samples.

Generative Adversarial Networks

Improvements

Definition: Lipschitz function

A function f is Lipschitz continuous if it is bounded by how fast it can change. Specifically if there exists a positive real constant k where:

$$|f(x) - f(y)| \leq k|x - y|,$$

for all y sufficiently near x. For example, any function with a bounded first derivative is a Lipschitz function.

The slope of any secant line to f is between $-k$ and k

Lower Lipschitz constant makes the function smooth and easy to optimise.

If the inputs x and y are close/similar, we want model outputs, $f(x)$ and $f(y)$ to also be similar.

Generative Adversarial Networks

- Wasserstein GAN [Arjovsky et al., 2017]
  - Limiting the gradients of the discriminator will make it a smoother function.
  - Done by clipping the gradients.

- Improved Wasserstein GAN [Gulrajani et al., 2017]
  - Add a penalty term to penalise the gradients of the discriminator directly.
  - Requires second order differentiation, which PyTorch supports, but it is slow.

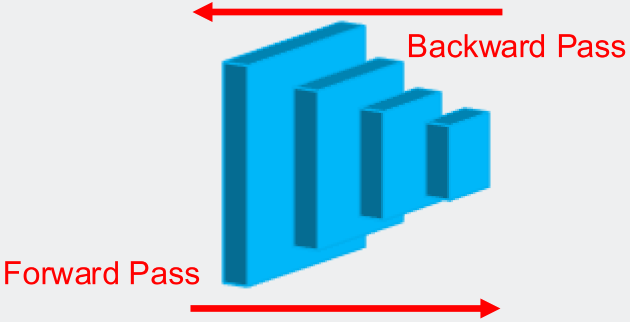
Generative Adversarial Networks

- There is another solution using Normalisation!

First, what is normalisation? – BatchNorm [Ioffe and Szegedy, 2015]

- All layers are updated in the backward pass.
- Every layer assumes other layers are fixed.

The weights of a layer can be updated based on the expectation that the prior layer produces values with a given distribution. However, this distribution is likely to change once that layer is updated.



Batch Normalisation: Layer outputs are rescaled, so they have a mean of *zero* and a standard deviation of *one:*

$$\hat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

- Weight Norm
- Layer Norm
- Instance Norm
- Group Norm
- Switchable Norm

Etc.

Problem: Internal Covariate Shift
(change in the distribution of input during training)

- Spectral Normalisation [Miyato et al., 2018]

Definition: spectral normalisation

The matrix (spectral) norm defines how much a matrix can stretch a vector x:

$$\| A \| = \max_{x \neq 0} \frac{\| Ax \|}{x}$$

Spectral norm normalises the weights for each layer using the spectral norm σ(W) such that the Lipschitz constant for every layer and the whole network is 1.

$$\widehat{W}_{\mathrm{SN}} = W / \sigma(W)$$

$$\sigma\left(\widehat{W}_{\mathrm{SN}}(W)\right) = 1$$

$$\| f \|_{\mathrm{Lip}} = 1$$

Pseudocode: 1-Lipschitz discriminator

```
class Discriminator(nn.Module):
  def __init__(self, f=64):
    super().__init__()
    self.discriminate = nn.Sequential(
      spectral_norm(Conv2d(1, f, 3, 1, 1)),
      nn.LeakyReLU(0.1, inplace=True),
      nn.MaxPool2d(kernel_size=(2,2)),
      spectral_norm(Conv2d(f, f*2, 3, 1, 1)),
      nn.LeakyReLU(0.1, inplace=True),
      nn.MaxPool2d(kernel_size=(2,2)),
      spectral_norm(Conv2d(f*2, f*4, 3, 1, 1)),
      nn.LeakyReLU(0.1, inplace=True),
      nn.MaxPool2d(kernel_size=(2,2)),
      spectral_norm(Conv2d(f*4, f*8, 3, 1, 1)),
      nn.LeakyReLU(0.1, inplace=True),
      nn.MaxPool2d(kernel_size=(2,2)),
      spectral_norm(Conv2d(f*8, 1, 3, 1, 1)),
      nn.Sigmoid()
    )
```

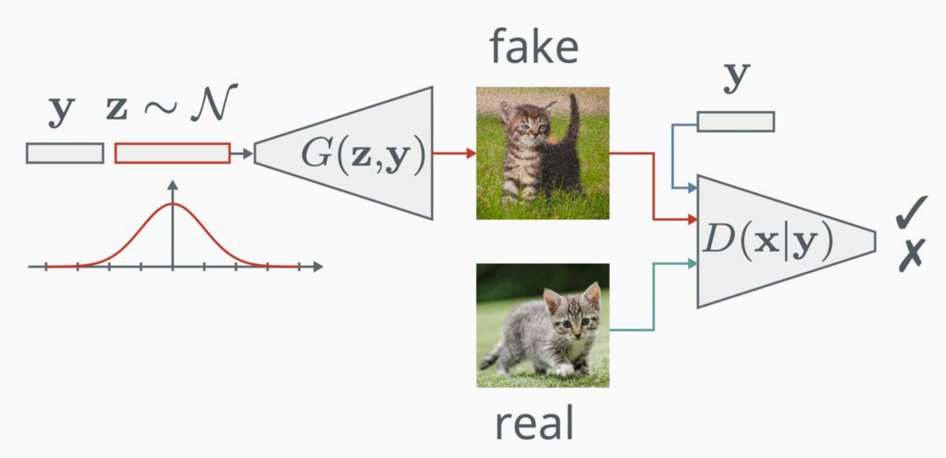
Generative Adversarial Networks

- **DCGAN:** The entire architecture is fully convolutional.
- **Alternative Objective:** Wasserstein GAN - LSGAN.
- **Two Timescale Update:** The Generator is updated more slowly than the Discriminator (SAGAN).
- **Stacking GANs:** Multiple GANs are placed consecutively, and each GAN solves an easier version of the problem (FashionGAN).
- **Progressive Growing GAN:** Higher quality and larger outputs by incrementally increasing the size of the model during training.

Mean squared loss

Definition: Conditional GANs

GANs can be conditioned, for instance with labels y, if available, [Mirza et al., 2014] by feeding the label information into both the generator and the discriminator:



$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x\sim p_{\text{data}}} \log D_{\theta_d}(x|y) + \mathbb{E}_{z\sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z, y|y)))\right]$$

Let's Look at Some Code!

Conditional GAN Example

Code on GitHub : https://github.com/atapour/dl-pytorch/blob/main/Conditional_GAN_Example/Conditional_GAN_Example.ipynb

Code on Colab: https://colab.research.google.com/github/atapour/dl-pytorch/blob/main/Conditional_GAN_Example/Conditional_GAN_Example.ipynb

Generative Adversarial Networks

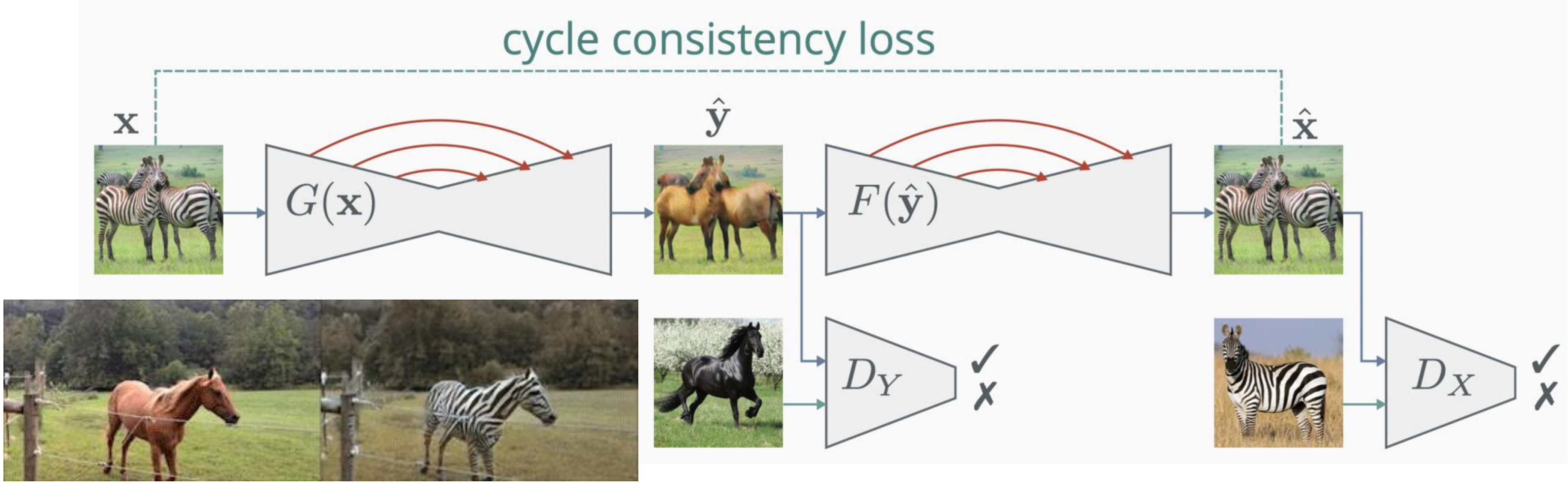
- Auxiliary Classifier GAN (ACGAN)
- InfoGAN
- Least Square GAN (LSGAN)
- Adversarial Autoencoder
- Boundary Equilibrium GAN (BEGAN)
- Energy-Based GAN
- StyleGAN
- etc. etc. etc. ...

Popular Applications

Unpaired Translation (**CycleGAN**)

Definition: CycleGAN [Zhu et al., 2017]

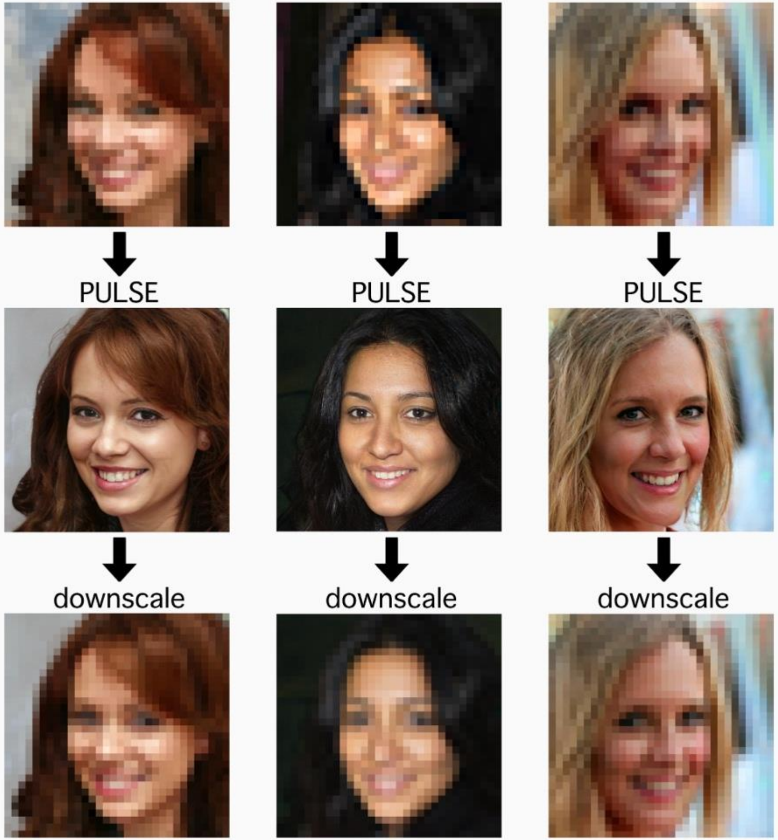
An adversarial architecture for unpaired image translation. It has twin generators with skip connections and two discriminators, which translate between the domains, alongside a cycle consistency loss (L1 distance) to ensure the mapping recovers the original image.



Popular Applications
Super-resolution

Definition: Super-resolution

The objective is to map a single low-resolution input to a distribution of high-resolution outputs. PULSE [Menon et al., 2020] projects points in the search of the latent space of StyleGAN (a large conditional GAN) onto a hypersphere, which ensures probable outputs in the high-dimensional latent space.



Popular Applications Anomaly Detection

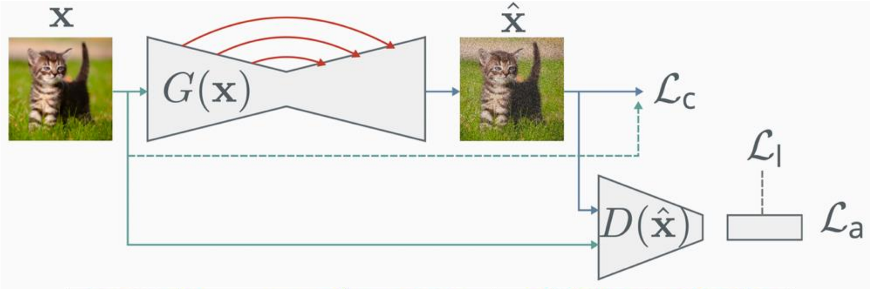
Definition: Anomaly Detection

The objective is to find "anomalies" in the data. Unsupervised anomaly detectors [1,2] learn a normal distribution over (healthy) observations. Then, when they observe something not observed in training (unhealthy/dangerous), they fail to reconstruct - detecting it as an anomaly. Region-based anomaly detectors [3] learn a distribution over inpainted (erased) regions.

[1] Akçay, **Atapour-Abarghouei**, and Breckon. "GANomaly: Semi-Supervised Anomaly Detection via Adversarial Training", ACCV, 2018.

[2] Akçay, **Atapour-Abarghouei**, and Breckon. "Skip-ganomaly: Skip connected and adversarially trained encoder-decoder anomaly detection", IJCNN,. 2019.

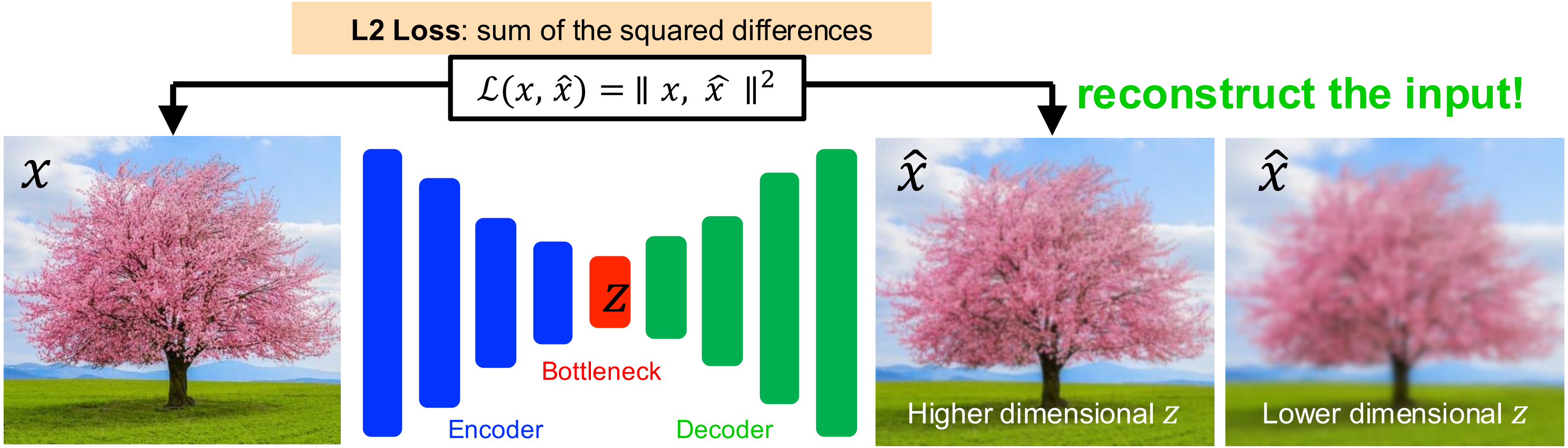
[3] Nguyen, Feldman, Bethapudi, Jennings, and Willcocks. "Unsupervised Region-based Anomaly Detection in Brain MRI with Adversarial Image Inpainting", arXiv:2010.01942.



Autoencoders

- **Not** generative models.
- Designed to obtain latent variables.
- Latent variables inferred by an autoencoder are a lower dimensional feature representation from unlabeled data.

variables that are not directly observed but are rather inferred (through a model)



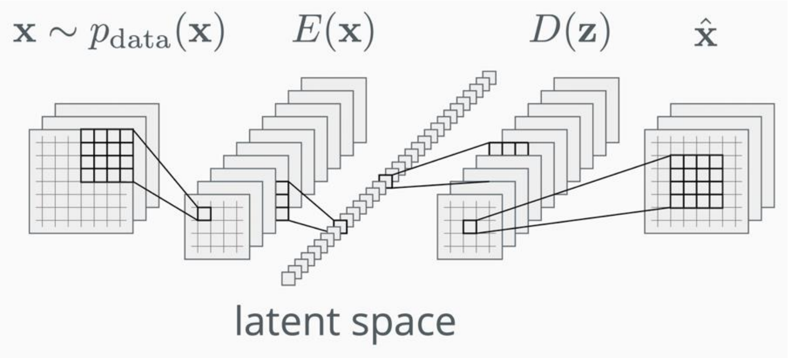
Autoencoders

Definition: Autoencoder

An autoencoder is a feedforward neural network that reconstructs its inputs, thus learning an identity:

$$\mathcal{L}_{AE} = E_{x \sim p_{\text{data}}} [\mathcal{L}(x, D(E(x)))]$$

where $\mathcal{L}$ is a loss function. The encoder function $E : R_n \rightarrow R_m$ compresses the dimensionality of the data $n \ll m$ to a latent encoding $z = E(x)$, which is then recovered by the decoder $D : R_m \rightarrow R_n$, where $\hat{x} = D(z)$.



Autoencoders

Properties: Autoencoder

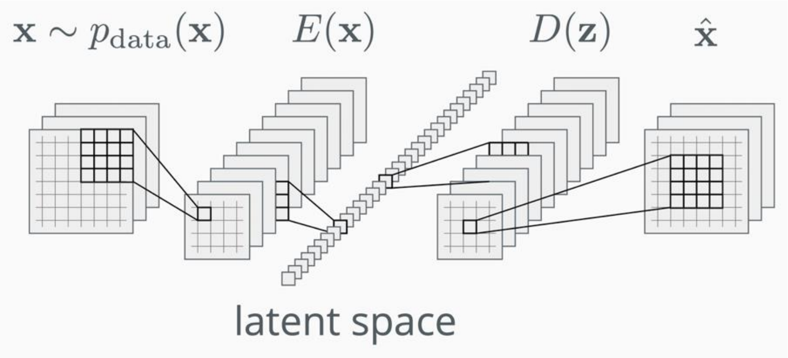
- Very good at representation learning.
- Are being used for data compression.

- Denoising Autoencoders

Reconstruct image from a noisy input.

- Inpainting Autoencoders

Reconstruct image from a input with missing regions.



Let's Look at Some Code!

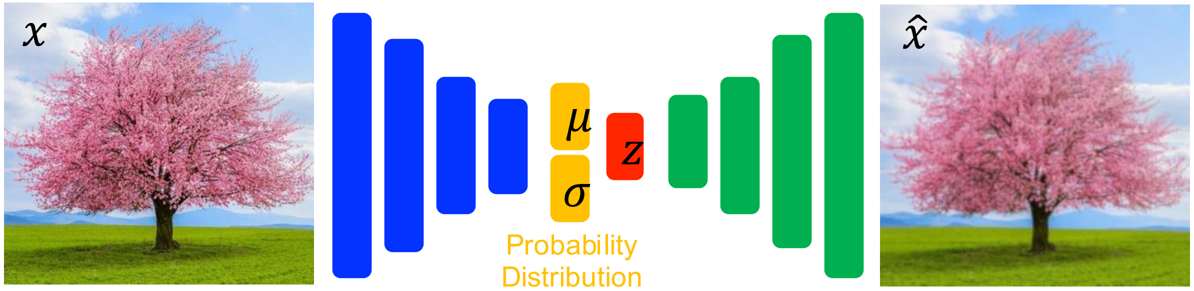
Example of a Simple Autoencoder

Code on GitHub: https://github.com/atapour/dl-pytorch/blob/main/AutoEncoder_Example/AutoEncoder_Example.ipynb

Code on Colab: https://colab.research.google.com/github/atapour/dl-pytorch/blob/main/AutoEncoder_Example/AutoEncoder_Example.ipynb

Variational Autoencoders (VAE) [Kingma and Welling, 2013]

- Explicit approximate variational density function.
- ***Generative Models*** with a probabilistic spin on autoencoders.
- Instead of a fixed latent vector (as in an autoencoder), **VAEs learn a probability distribution** in the latent space that facilitates sampling new data for generation.



Variational Autoencoders (VAE) [Kingma and Welling, 2013]

- The encoder learns:
  - vector μ (**means**)
  - vector σ (**standard deviations**)

describe

Probability Distribution

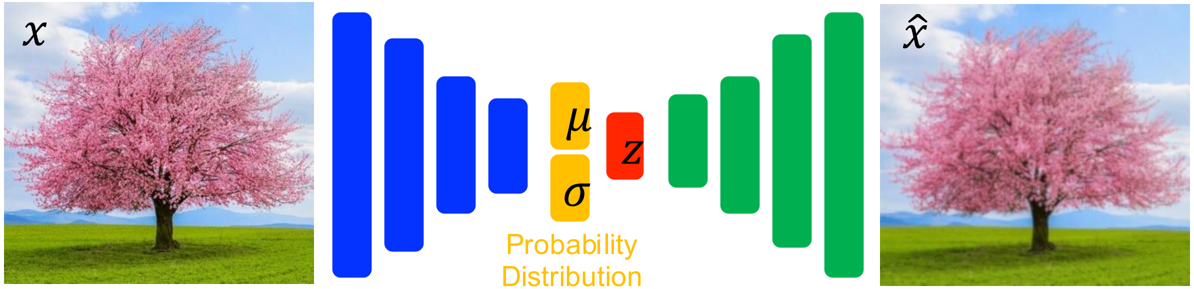
the latent variables in z are sampled

- The loss function will include a reconstruction loss, just like the vanilla autoencoder, but there is more … .

The Encoder computes $p_\phi(z|x)$.

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

The Decoder computes $q_\theta(x|z)$.



Variational Autoencoders (VAE) [Kingma and Welling, 2013]

- The loss function consists of two terms:
  - Reconstruction Loss (L_2 loss)
  - KL Divergence

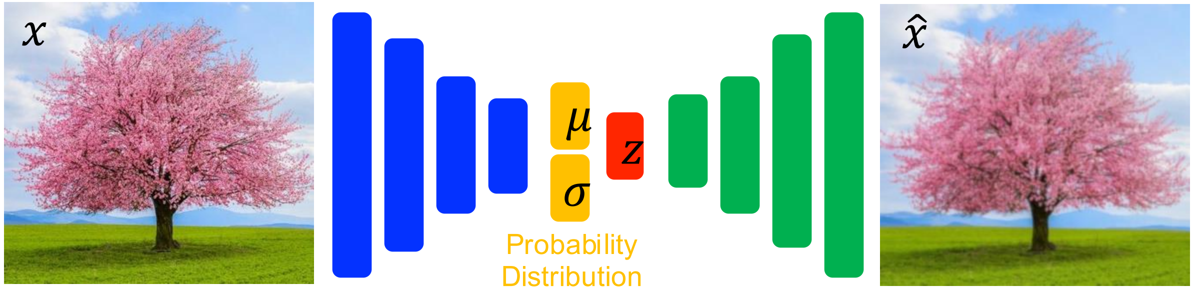
$$\mathcal{L}(\phi,\theta;x,z) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - D_{\mathrm{KL}}(q_\phi(z|x) \parallel p(z))$$

Expectation: we are dealing with random variables

Kullback–Leibler divergence: measure of how one probability distribution is different from another

Reminder: summation or integration of all possible values from a random variable

The Encoder $q_\phi(z|x)$.



The Decoder $p_\theta(x|z)$.

Variational Autoencoders (VAE) [Kingma and Welling, 2013]

We want the probability distribution to be smooth and not to overfit or memorise any of the latent variables within vector z.

$$\mathcal{L}(\phi, \theta; x, z) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}(q_\phi(z|x) \parallel p(z))}$$

- By reducing the distance between the probability distribution and a well-behaved prior distribution (such as a *Normal Gaussian*), we:
  - encourage the latent variables to be evenly distributed around the centre of the latent space
  - and deter the model from clustering points in specific regions and cheat by memorising the data.

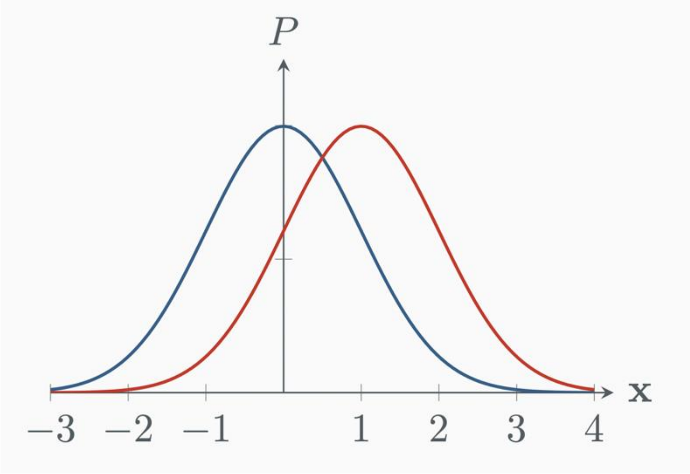
Variational Autoencoders (VAE) [Kingma and Welling, 2013]

Definition: Kullback–Leibler divergence

The Kullback-Leibler divergence (also called relative entropy) measures the difference between distributions and is asymmetric and non-negative:

$$D_{\mathrm{KL}}(p \parallel q) = \int p(x) \log\left(\frac{p(x)}{q(x)}\right) \mathrm{d}x$$

Where $D_{\mathrm{KL}}(p \parallel p) = 0$. Practically, the KL divergence is sensitive at the tails of the distribution.



Desmos Visualisation: https://www.desmos.com/calculator/2sboqbhler

Variational Autoencoders (VAE) [Kingma and Welling, 2013]

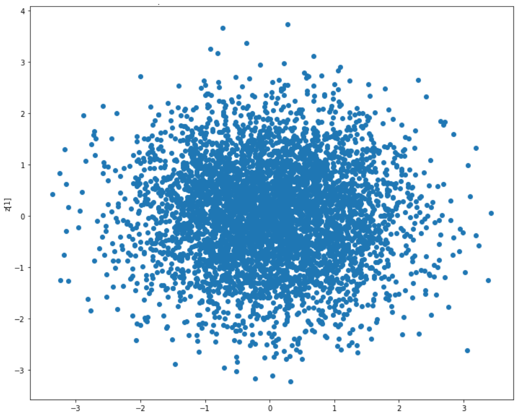
Let's visually inspect how regularisation with the KL term helps.

- We can analyse the effect of the *KL* term by weighting the loss and experimenting with different values:

```
loss = reconstruction_loss + c * kl_loss
```

- We will consider an autoencoder with a latent space of 2 dimensions trained on the MNIST dataset.

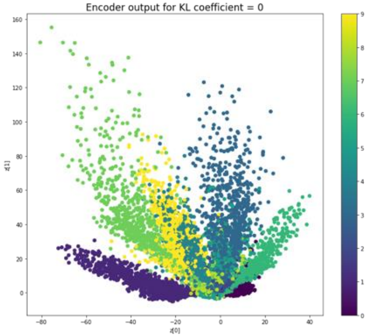
For reference, let's look at points sampled from the *standard Gaussian* in two dimensions.



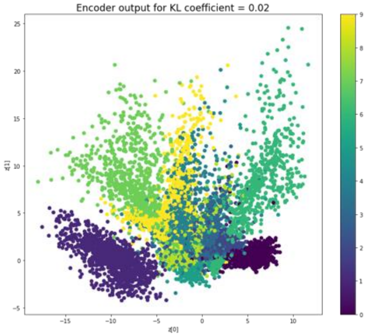
Variational Autoencoders (VAE) [Kingma and Welling, 2013]

We can see how the points begin to cluster with *no* or *a small* `kl_loss`.

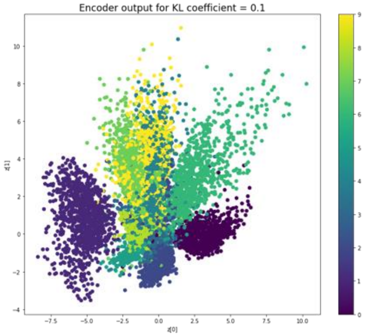
C = 0.0



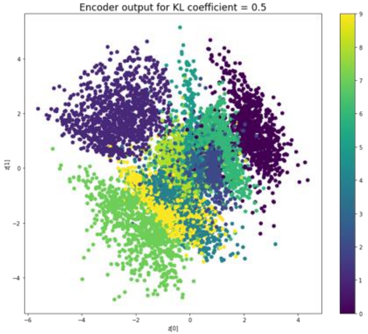
C = 0.02



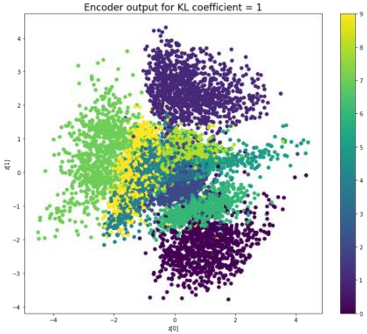
C = 0.1



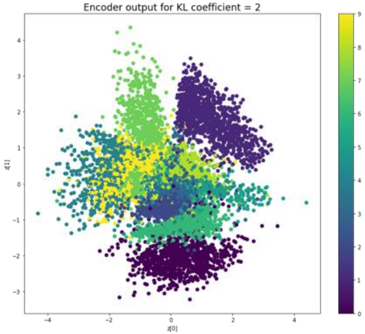
C = 0.5



C = 1.0



C = 2.0



https://www.vincent-lunot.com/post/on-the-use-of-the-kullback-leibler-divergence-in-variational-autoencoders/

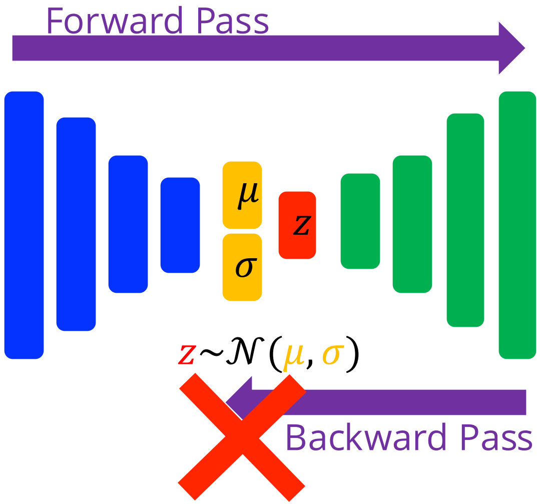
Variational Autoencoders (VAE) [Kingma and Welling, 2013]

Issue to overcome: backpropagation through a sampling layer

Solution: **Reparameterisation Trick**

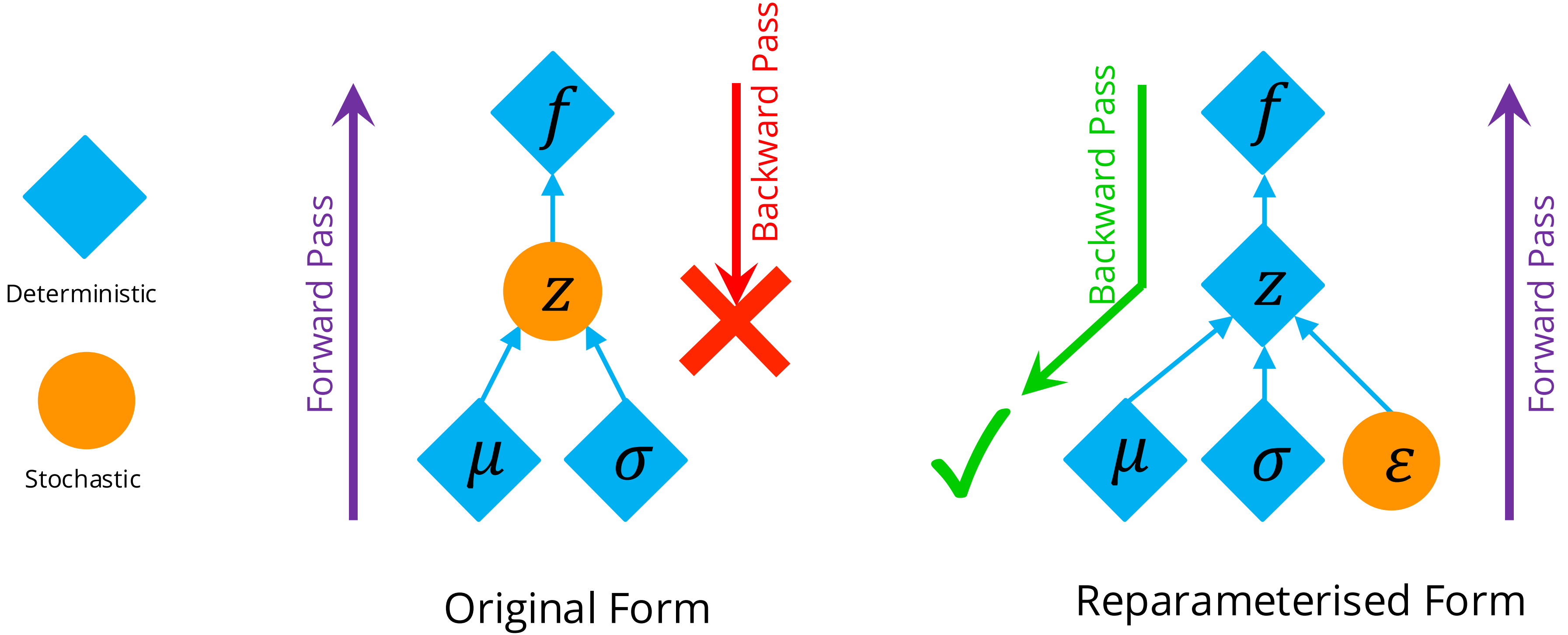
$$z = \mu + \sigma \odot \varepsilon \qquad \text{where } \varepsilon \sim \mathcal{N}(0,1)$$

z will be a sum of a fixed vector μ and a fixed vector σ scaled by random constants ε sampled from the prior distribution (standard Gaussian).



Variational Autoencoders (VAE) [Kingma and Welling, 2013]

- **Reparameterisation Trick**



Variational Autoencoders (VAE) [Kingma and Welling, 2013]

Definition: Evidence Lower Bound (ELBO)

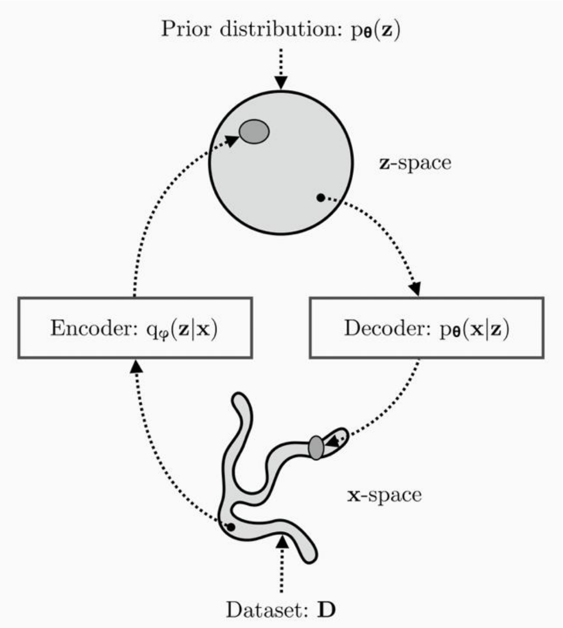
VAEs have three components:

1. The decoder $p_\theta(x|z)$
2. The approximate posterior (encoder) $q_\phi(z|x)$
3. The prior distribution $p_\theta(x)$

They are trained with the reparameterisation trick to maximise the evidence lower bound (ELBO):

$$\log p_\theta(x) \geq \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \mathrm{D}_{\mathrm{KL}}(q_\phi(z|x) \parallel p(z))$$

There are more advanced and state-of-the-art method, such stacking VAEs hierarchically [Child et al., 2021].

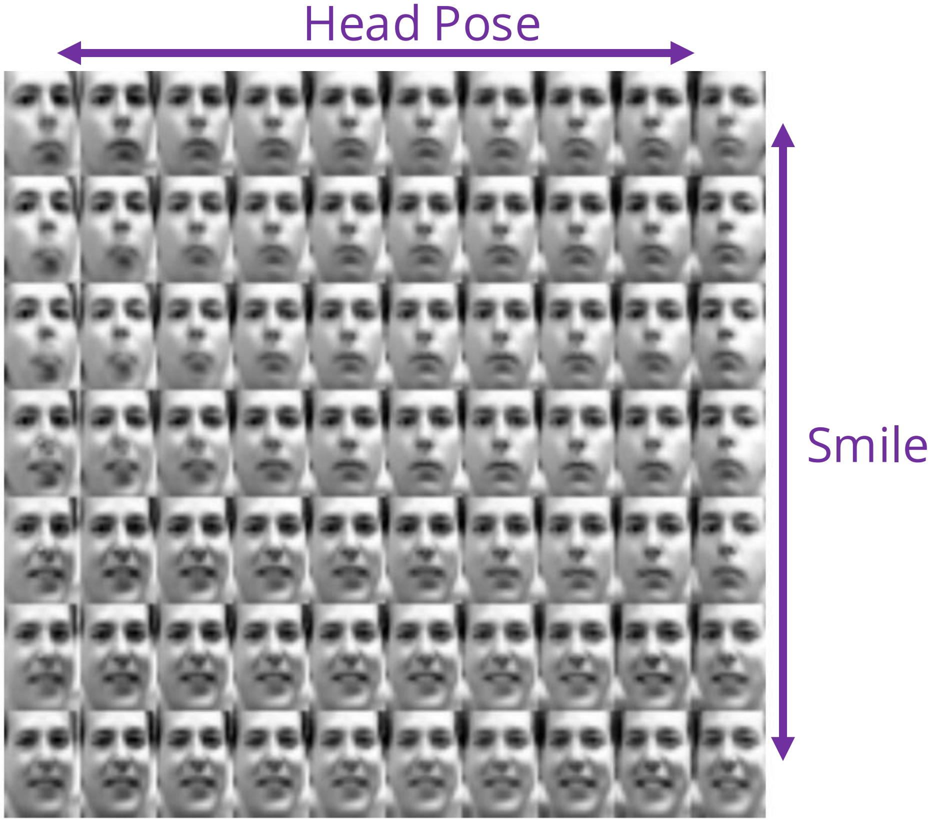


Variational Autoencoders (VAE) [Kingma and Welling, 2013]

- **Results**

The latent variables are forced to be independent of each other.

Different dimensions of z encode interpretable factors of variation.



Let's Look at Some Code!

Example of a Variational Autoencoder

Code on GitHub: https://github.com/atapour/dl-pytorch/blob/main/VAE_Example/VAE_Example.ipynb

Code on Colab: https://colab.research.google.com/github/atapour/dl-pytorch/blob/main/VAE_Example/VAE_Example.ipynb

Implicit Models Definition

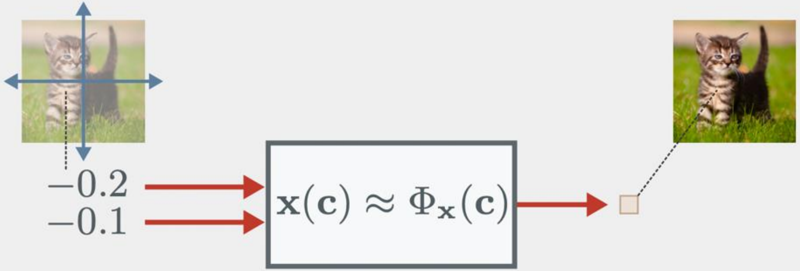
Definition: implicit representations

Consider data $\Phi: \mathbb{R}^m \to \mathbb{R}^n$, like a single image, as a function of coordinates $\mathbf{c} \in \mathbb{R}^m$. The aim is to learn a neural approximation of Φ that satisfies an implicit equation:

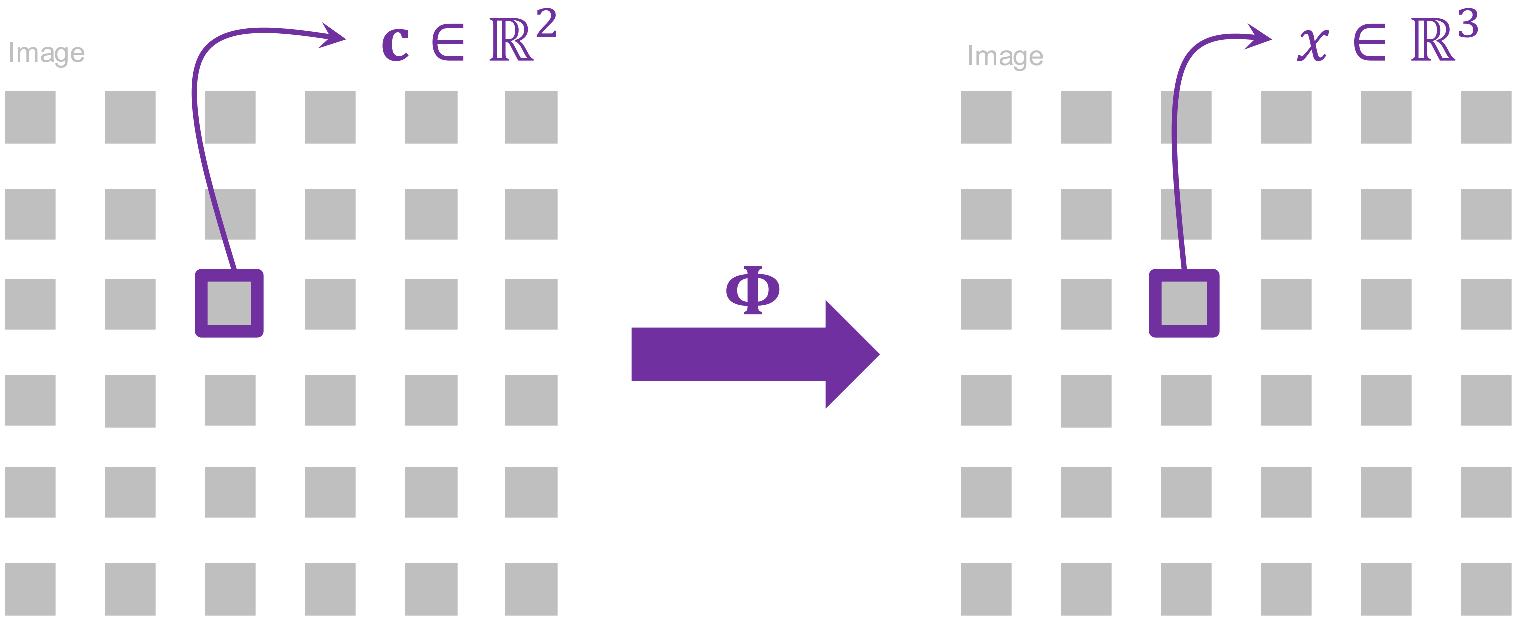
$$R\left(\mathbf{c}, \Phi, \nabla_\Phi, \nabla^2_\Phi, \ldots\right) = 0, \Phi: \mathbf{c} \to \Phi(\mathbf{c})$$

This has applications in 3D modelling, image, video, audio representation.

Example: Implicit Network



Implicit Models



coordinates – (x, y) **pixel value – $\{\mathbf{R}, \mathbf{G}, \mathbf{B}\}$**

$\mathbf{c} \rightarrow$ Neural Network Φ $\rightarrow x$

We can have a neural network approximate the image function.

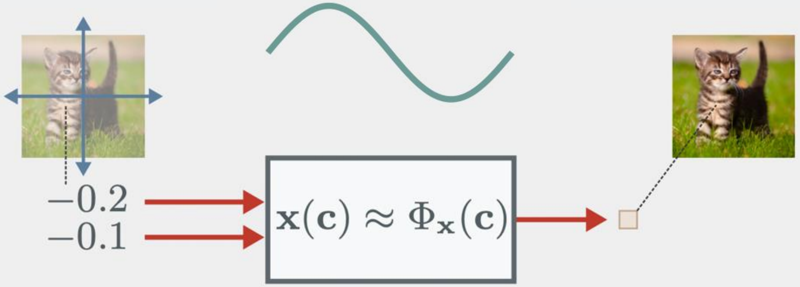
Implicit Representation Networks SIREN

Definition: SIREN

SInusoidal REpresentation Networks (SIREN) are a simple implicit representation network, but use **sin** (with clever initialisation) as their choice of non-linearity [Sitzmann et al., 2020].

sin is periodic, so it allows to capture patterns over all of the coordinate space (translation invariant, like convolutions).

Example: SIREN



https://www.vincentsitzmann.com/siren

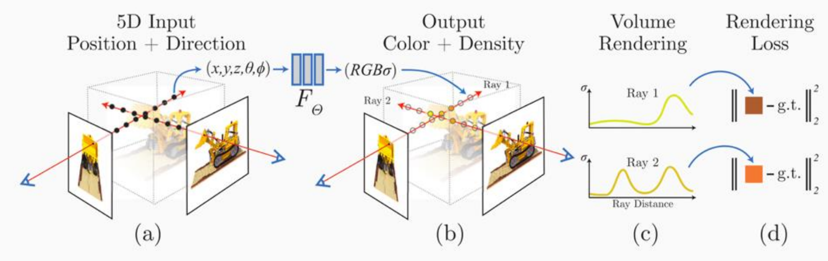
Implicit Representation Networks NeRF

Definition: NeRF

Neural Radiance Fields (NeRF) are similar to SIRENs, but instead of representing an image, they represent a single 3D scene [Mildenhall et al., 2020].

They map from pixel positions (x, y, z) and a viewing direction (θ, ϕ) to a colour and density value σ integrated via a ray on F_θ.

Example: NeRF



https://www.matthewtancik.com/nerf

There are other implicit models:

https://cwkx.github.io/data/GON/

What we learned today!

Generative models

- Unsupervised training
- PixelRNN and PixelCNN

Generative adversarial networks

- Definition
- Common Issues
- Lipschits Continuity
- Spectral Normalisation
- Conditional GANs
- Other Advanced Variants

Variational autoencoders

- Autoencoders
- VAEs
- Reparameterisation trick
- ELBO

Implicit networks

- Definition
- SIRENs
- NeRFs