Autoencoders and Generative Models

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MVA - DELIRES

Introduction

- Neural networks are often used for :
  - Classification/detection (MLPs, CNNs)
  - Modelling time-series, sequences (RNNs)
- All of these networks rely on the extraction of features to analyse data
- Idea : the network's internal representation of the data can be useful !
- **Autoencoders** and more generally **generative models** use this idea

Introduction

- What do you think of these faces ?

Introduction

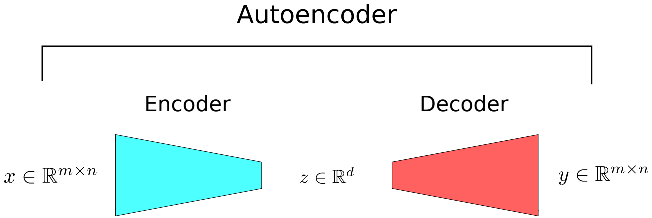
- What do you think of these faces ?

- These are all **generated by a generative model !!**
- In the next two lessons, we are going to see how this is possible

Autoencoders

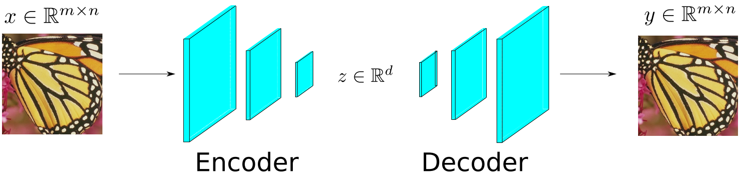
Autoencoders

- Autoencoders consist of two networks : an **encoder** and a **decoder**
  - Encoder : map data x to a smaller **latent space**
  - Decoder : map point z back from latent space to original data space
- Main idea : the latent space is a space where it is **easier to manipulate/understand data**
- More powerful and compact representation of data



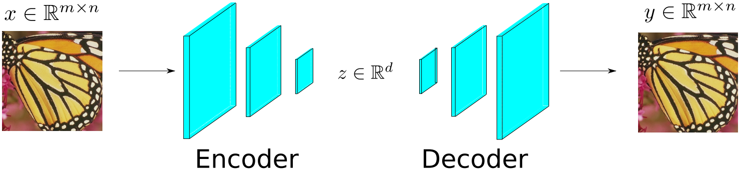
Autoencoders

- The autoencoder is trained to minimise some norm between the input x and the output y of the decoder
- In almost all cases, we have $d << mn$
- This forces the autoencoder to learn a compact and powerful latent space



Autoencoders

- Uses of autoencoders :
  - Data compression, dimensionality reduction
  - Classification (easier in latent space)
  - **Data generation/synthesis**



Autoencoders - some notation

- An AE is a neural network consisting of two sub-networks
  - The encoder Φ_e,

$$\begin{aligned}\Phi_e \colon \mathbb{R}^{mn} &\to \mathbb{R}^d \\ x &\mapsto \Phi_e(x) = z\end{aligned}$$

  - The decoder Φ_d,

$$\begin{aligned}\Phi_d \colon \mathbb{R}^{d} &\to \mathbb{R}^{mn} \\ z &\mapsto \Phi_d(z) = y\end{aligned}$$

- As in other neural networks, the main components of AEs are **mlp's/convolutions**, **biases** and **non-linearities**

Autoencoders

- The autoencoder is trained to reproduce the input x as an output y, in the sense of some norm, having gone through the bottleneck of the network
- The norm most often used is the sum of squared differences (ℓ_2-norm)

Autoencoding training minimisation problem

$$\begin{aligned}\mathcal{L}(x) &= \|y - x\|_2^2 \\ &= \sum_i^m \sum_j^n \Big((\Phi_d \circ \Phi_e(x))_{i,j} - x_{i,j} \Big)^2\end{aligned}$$

- Put simply : **output should look like input !**

Autoencoders - upsampling

- Most often, the autoencoder uses convolutions
- A key question is how to create the bottleneck : **downsampling**
- We know how to downsample :
  - Strided convolutions
  - Max pooling
- How about **upsampling** ?

Autoencoders - upsampling

- Upsampling can be carried out in several ways :
  - Simple interpolation (linear, bilinear, bicubic)
  - Transposed convolution
- **Transposed convolution** is probably the most common upsampling
  - Simultaneously upsamples and “convolves”
- Let’s take a look at how this works

Autoencoders - transposed convolution

- Recall that we can write the convolution as a matrix/vector multiplication (see lecture on CNNs)
- For example, take the convolution with the Laplacian operator

$$w = \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix} \rightarrow A_w = \begin{pmatrix} -4 & 1 & \overset{0}{\cdots} & -1 & \overset{0}{\cdots} & & \\ 1 & -4 & 1 & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} & \\ 0 & 1 & -4 & 1 & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} & 1 & -4 \end{pmatrix}$$

- To carry out convolution + stride with subsampling s, we just remove certain rows from the matrix A_w (the elements not retained during subsampling)

Autoencoders - transposed convolution

$$A_{w,s} = \begin{pmatrix} -4 & 1 & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} & & \\ 1 & -4 & 1 & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} & \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \overset{0}{\cdots} & 1 & \overset{0}{\cdots} & 1 & -4 \end{pmatrix}$$

- A_w now becomes a $\frac{mn}{s} \times mn$ matrix $A_{w,s}$
- Transposed convolution just consists of $A^T_{w,s}$

Autoencoders - transposed convolution

- Let's take a concrete example :
  - We wish to upsample a 1D signal x of size 2 to size 4
  - Convolutional filter $w = [1, 2, 1]^T$
- First, we look at the convolution matrix at the higher resolution signal size 4

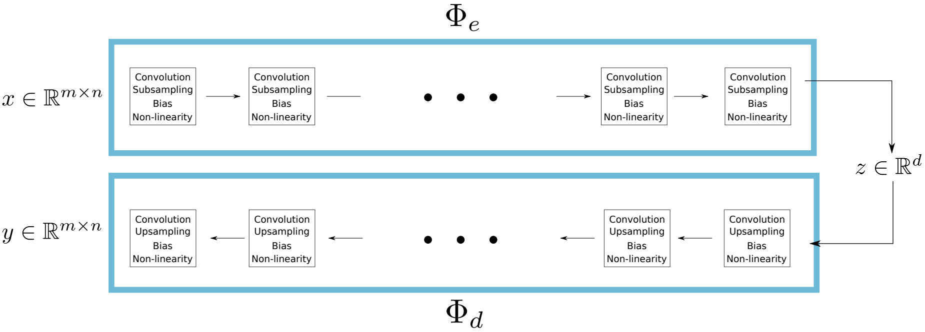
$$A_w = \begin{pmatrix} \mathbf{2} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ 1 & 2 & 1 & 0 \\ \mathbf{0} & \mathbf{1} & \mathbf{2} & \mathbf{1} \\ 0 & 0 & 1 & 2 \end{pmatrix}$$

- Therefore, we have :

$$A_{w,s} = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 \end{pmatrix} \quad A^T_{w,s} = \begin{pmatrix} 20 \\ 11 \\ 02 \\ 00 \end{pmatrix}$$

Autoencoders

A generic autoencoder architecture



- $d << m * n$

Autoencoder variants

- Autoencoders come in many flavours, differ mainly by their loss functions
- Naive autoencoder loss $\mathcal{L}$ can lead to certain problems
  - Overfitting to data, poor robustness
  - Latent space difficult to interpret, not necessarily meaingful w.r.t data space
- As is often the case in deep learning, this can be addressed using **regularisation**
- In practice, this means adding extra terms to $\mathcal{L}$

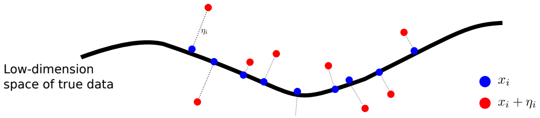
Denoising autoencoder

- First example : the denoising autoencoder
- We would like to make the encoder/decoder robust to **small perturbations** in the input data
- One solution : the **denoising autoencoder**

Denoising autoencoder

- Idea : add noise η to the input

$$\mathcal{L}(x) = \|\Phi_d \circ \Phi_e(x + \ \eta) - x\|_2^2$$



Sparse autoencoder

- Ideally, we want the code to be as **sparse** as possible
- Why ? We want the smallest vector which accurately describes the data
  - Combinations of elements more difficult to interpret
  - Useful for classification

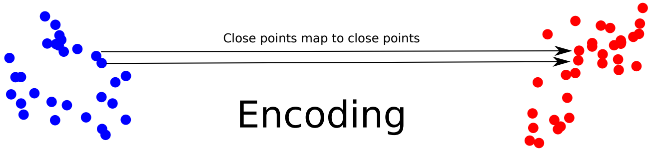
Sparse autoencoder

$$\mathcal{L}(x) = \|\Phi_d \circ \Phi_e(x) - x\|_2^2 + \lambda \|z\|_1$$

- The $\|z\|_1$ norm encourages sparsity in z

Contractive autoencoder

- Another approach to regularisation : contractive autoencoder
- Close points in data space map to close points in latent space (thus, contractive)



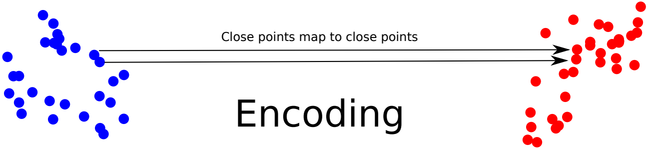
- How can we impose this ?
- $\frac{\partial z_j}{\partial x_i}$ should be small, for all couples (i, j)

Contractive autoencoder

- Add the Frobenius (ℓ_2) norm of the Jacobian of z w.r.t. x, $J_x z$, to the cost function

$$\begin{aligned}\mathcal{L}(x) &= \|\Phi_d \circ \Phi_e(x) - x\|_2^2 + \lambda \|J_x E(x)\|_F^2 \\ &= \|\Phi_d \circ \Phi_e(x) - x\|_2^2 + \lambda \|J_x z\|_F^2\end{aligned}$$

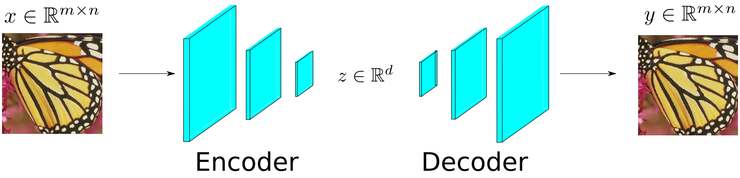
- Reminder, Jacobian : $J_x(z) = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_{mn}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_d}{\partial x_1} & \cdots & \frac{\partial z_d}{\partial x_{mn}} \end{pmatrix}$



Autoencoders - summary

Important points to remember

- Autoencoder consists of two networks : encoder and decoder
- These compress to and from a **smaller dimension latent space**
- This latent space represents data more **powerfully and compactly**



- Example of autoencoder use : interpolation of complex data

Interpolation of complex data[†]

[†] ***Generative Visual Manipulation on the Natural Image Manifold***, *J-Y. Zhu, P. Krähenbühl, E. Schechtman, A. Efros, CVPR 2016*

Generative models

Generative models

- In many applications, it is desirable to **synthesise** data
  - Video post-production
  - Data augmentation

- Several types of generative models exist :
  - Restricted Bolzmann machines, Deep Belief models
  - **Variational autoencoders**
  - **Generative Adversarial Networks**;
  - Texture synthesis and style transfer models;

- The common idea in these models is the internal representation/latent space of the network

Generative models

- Modern generative models produce highly realistic, (relatively) high-definition images

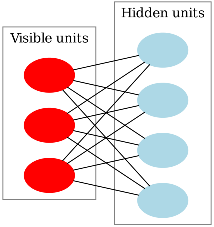

Synthesis examples from “Real NVP”†

- Before, we take a small detour to present Restricted Bolzmann Machines

† ***Density estimation using Real NVP***, *L. Dinh, J. Sohl-Dickstein, S. Bengio, arXiv:1605.08803 2016*

Restricted Bolzmann machines

- A **Restricted Bolzmann machine** is a collection of binary random variables
- The variables' probability distribution is learned during training
- The variables form a bipartite graph



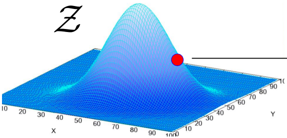
- Restricted Bolzmann machines are used less nowadays in favour of **variational autoencoders** and **Generative Adversarial Networks**, which we will see now

Variational autoencoder

- Suppose we want to produce **random examples of data**, how would we go about this ?

Variational autoencoder

- Suppose we want to produce **random examples of data**, how would we go about this ?
- We can model the latent space in a **probabilistic manner**
- Synthesis will then consist of :
  1. Sampling in the latent space
  2. Decoding to produce the random image



Generator

Probabilistic model in latent space

Synthesis of random image

Variational autoencoder - variational Bayesian approach

- The Variational Autoencoder (VAE) encourages the latent code z to follow a certain distribution, via the loss function
- This is in turn achieved by using a **Variational Bayesian** approach

Variational autoencoder - variational Bayesian approach

- The Variational Autoencoder (VAE) encourages the latent code z to follow a certain distribution, via the loss function
- This is in turn achieved by using a **Variational Bayesian** approach
- The Variational Bayesian approach is a methodology to approximate the **posterior distribution** of unobserved variables in graphical models
- We will need some tools from statistics : conditional probability, Bayes theorem, marginal distributions, distribution divergences ...
- Keep in mind that the main goal here is to **choose a loss function which will encourage the latent space to follow a probability distribution**

Variational autoencoder - variational Bayesian approach

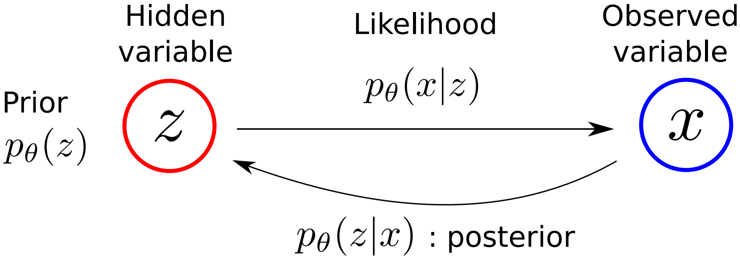
- Let's take an example. Suppose we have a student A, who comes to lessons or not. The event of A's presence in the lesson is x. This is the **observed variable**
- We also know that sometimes it rains, and that A's presence in the class depends on whether it rains or not. Let us denote the event of it raining with z. This is the **latent variable**
- Suppose that we do not directly know whether it is raining (we cannot look out of the window), but can only observe whether the student A is in the lesson

Variational autoencoder - variational Bayesian approach

- The probability of A being in the lesson, $\mathbb{P}(x)$, is the **marginal probability**
- The probability of it raining $\mathbb{P}(z)$ is the **prior probability**
- The probability of A being in the lesson given z, $\mathbb{P}(x|z)$ is the **likelihood**
- The probability of it raining, given x, $\mathbb{P}(z|x)$ is the **posterior probability**

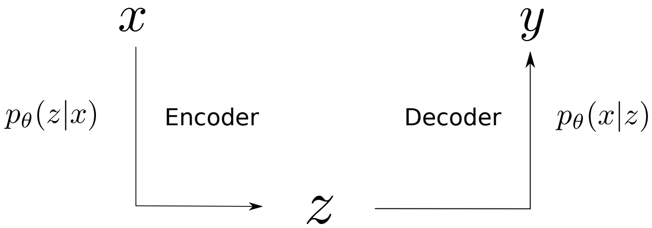
Variational autoencoder - variational Bayesian approach

- At this point, we assume that all the probabilities discussed have a **probability density function**
- We suppose that the distributions come from families of distrbutions parameterised by the parameters θ ($p_\theta(x)$, $p_\theta(x|z)$ etc)



Variational autoencoder - variational Bayesian approach

- There are some clear analogies with the autoencoder
- Encoder : posterior $p_\theta(z|x)$
- Decoder : likelihood $p_\theta(x|z)$



- We want to **impose the prior $p_\theta(z)$** !!

Variational autoencoder - variational Bayesian approach

- Often, we know (or we can at least estimate) the likelihood $p_\theta(x|z)$
- However, often the posterior distribution $p_\theta(z|x)$ is difficult to calculate, or intractable. Why is this the case ?

Variational autoencoder - variational Bayesian approach

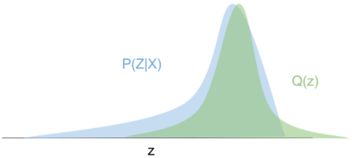
- Often, we know (or we can at least estimate) the likelihood $p_\theta(x|z)$
- However, often the posterior distribution $p_\theta(z|x)$ is difficult to calculate, or intractable. Why is this the case ?

$$\begin{aligned} p_\theta(z|x) &= \frac{p_\theta(x|z)\ \ p_\theta(z)}{p_\theta(x)} && \text{Bayes's rule} \\ &= \frac{p_\theta(x|z)\ \ p_\theta(z)}{\int p_\theta(x,z)dz} && \text{Marginal distribution} \end{aligned}$$

- $\int p_\theta(x,z)dz$ can be a very high-dimensional integral
- Calculating the posterior probability is known as the **inference problem**

Variational autoencoder - variational Bayesian approach

- So, how do we approach the problem of inference ?
- The variational Bayesian approach consists in using an **approximate distribution** $q_\phi(z|x) \approx p_\theta(z|x)$, which is easier to manipulate



- What does it mean for two probability distributions to be **similar** ?
  - Often, this is defined using the **Kullback-Leibler divergence**

Variational autoencoder

Kullback-Leibler divergence

Let p and q be two probability distributions defined over the same domain. The Kullback-Leibler divergence is defined as

$$KL(p \,||\, q) = \int p(x) \log \frac{p(x)}{q(x)} dx \tag{1}$$

Variational autoencoder

Kullback-Leibler divergence

Let p and q be two probability distributions defined over the same domain. The Kullback-Leibler divergence is defined as

$$KL(p \,||\, q) = \int p(x) \log \frac{p(x)}{q(x)} dx \tag{1}$$

The Kullback-Leibler divergence has some interesting properties :

- Non-negative : $KL(p \,||\, q) \geq 0$
- $KL(p \,||\, q) = 0 \iff p = q$ almost everywhere
- Non-symmetric : $KL(p \,||\, q) \neq KL(q \,||\, p)$

The second point is quite important. Why ? Because we know that **by minimising the KL divergence we are necessarily forcing p and q closer together**.

Variational autoencoder

- Let's come back to variational Bayesian methods now. We wish to approximate $p_\theta(z|x)$ with $q_\phi(z|x)$. To do this, we will find a $q_\phi *$:

$$q_\phi^* = \arg\min_{q_\phi} KL\left(q_\phi(z|x) \; || \; p_\theta(z|x)\right) \; ^\dagger \tag{2}$$

- Unfortunately, this does not help us much. Why ? **Because we don't know $p_\theta(z|x)$** !

- We will have to minimise $KL\left(q_\phi(z|x) \; || \; p_\theta(z|x)\right)$ some other way

† *You might notice that the q_ϕ before the p_θ. We do not go into the technical reasons here ...*

Variational autoencoders - The evidence lower bound

Evidence of Lower BOund (ELBO, lower bound of $\log p_\theta(x)$)

$$\text{ELBO}(q_\phi) = \mathbb{E}_{q_\phi}\left[\log(p_\theta(x,z))\right] - \mathbb{E}_{q_\phi}\left[\log q_\phi(z|x)\right]$$

- This is known as the "Evidence of Lower BOund" because :

$$\log p_\theta(x) = \text{ELBO}(q_\phi) + KL(q_\phi(z|x) \;\; || \; p_\theta(z|x)))$$

- KL divergence is positive : the ELBO is a lower bound for $\log p_\theta(x)$ (the "evidence")
- **By maximising the ELBO, we minimise the KL divergence between $q_\phi(z|x)$ and $p_\theta(z|x)$**

Variational autoencoders - Variational Autoencoder loss function

- We can rewrite the ELBO in the following manner*

$$\mathrm{ELBO}(q_\phi) = \mathbb{E}_{q_\phi}\left[\log(p_\theta(x|z))\right] - KL(q_\phi(z|x)\;||\;p_\theta(z))$$

- **We know all of these terms!** : we can use it as a VAE loss function!

Variational Autoencoder loss function

$$\mathcal{L}(x;\theta,\phi) = \overbrace{\mathbb{E}_{q_\phi}\left[\log(p_\theta(x|\;z))\right]}^{\text{Reconstruction error}} - \underbrace{KL(q_\phi(z|x)\;||\;p_\theta(z))}_{\text{Enforce the prior distribution}}$$

- **Important note !** : we want to **maximise** this loss function !

* *This is shown at the end of the slides*

Variational Autoencoder summary

1. We modelled the autoencoding process using a probabilistic (Bayesian) framework, with an observed and a hidden variable
2. We wanted to calculate the posterior distribution $p_\theta(z|x)$, but this is complicated
3. We used an approximation $q_\phi(z|x)$ to $p_\theta(z|x)$
4. We used the ELBO as a loss function to minimise $KL(q_\phi(z|x)||p_\theta(z))$
    - Ensures a good reconstruction
    - Encourages the latent space to follow our chosen distribution (the prior $p_\theta(z)$)

Variational Autoencoder

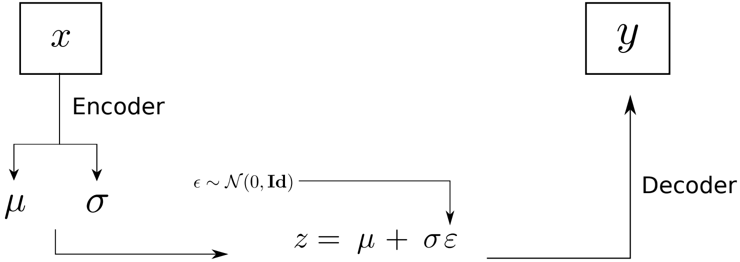
- There remains one more important detail : how to backpropagate through samples of z ? **Random variable, not differentiable**
- Solution : **"reparametrisation trick"**, make the random element an network input
- In the Gaussian case, where q_ϕ is a multivariate Gaussian vector, with mean μ and diagonal covariance matrix $\sigma\mathsf{Id}$, this gives

$$z = \mu + \sigma\epsilon, \quad \epsilon \sim \mathcal{N}(0, \mathsf{Id})$$

- μ and σ are produced by the encoder
- Thus, backpropagation can be carried out w.r.t to the parameters ϕ and θ

Variational autoencoder **in practice**

- The variational autoencoder is actually quite simple to implement
- Take the case of Gaussian $q_\phi(z|x)$

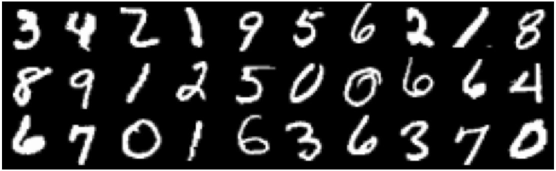


- Encoder and decoder can be MLPs, CNNs ...
- What is the loss in practice ?

Variational autoencoder **in practice**

- Let us take the following case, well-adapted to the **mnist dataset** :
  - Prior : $p_\theta(z) \sim \mathcal{N}(0, \text{Id})$
  - Variational approximation : $q_\phi(z|x) \sim \mathcal{N}(\mu, \sigma\text{Id})$, where $(\mu, \sigma) = \Phi_e(x)$
  - Likelihood : $p_\theta(x|z) \sim Ber(y)$, where $y = \Phi_d(z)$

$$\mathcal{L} = \overbrace{\sum_{i=1}^{mn} x_i \log y_i + (1 - x_i) \log(1 - y_i)}^{\text{Reconstruction error}} - \underbrace{\frac{1}{2} \sum_{j=1}^{d} \left(\mu_j^2 + \sigma_j^2 - 1 - \log\left(\sigma_j^2\right)\right)}_{\text{KL divergence}}$$



Variational autoencoder results

- Some results of variational autoencoders on mnist data : random samples

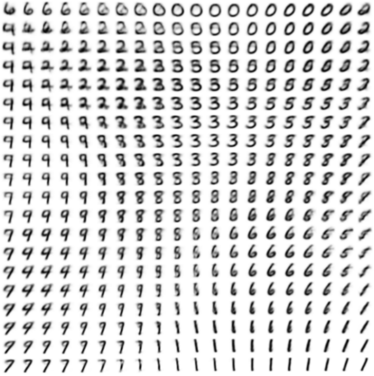
(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Auto-Encoding Variational Bayes, *D. P. Kingma, M. Welling, arXiv preprint arXiv:1312.6114, 2013*

Variational autoencoder results

- Some results of VAEs on mnist, face data : uniform samples

(a) Learned Frey Face manifold



(b) Learned MNIST manifold

Auto-Encoding Variational Bayes, *D. P. Kingma, M. Welling, arXiv preprint arXiv:1312.6114, 2013*

Variational autoencoder results

- Some results of VAEs on more complex digits data

Variational autoencoder results

- Very recent results of VAEs on more complex digits data

NVAE: A Deep Hierarchical Variational Autoencoder, *A. Vahdat, J. Kautz, arXiv preprint arXiv:2007.03898, 2020*

Variational Autoencoders : summary

- Rigourous framework to autoencode data onto a probabilisitcally modelled latent space
- Advantages
  - Theoretically-motivated, loss function meaningful
  - Learn to and from mapping (encoder and decoder)
- Drawbacks
  - Have to re-write loss function for each different model, not always easy
  - In practice, do not produce as complex examples as **Generative Adversarial Networks**, which we will see next week

Generative Adversarial Networks

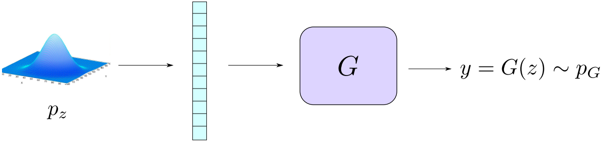
Generative Adversarial networks

- We saw that variational autoencoders were not straightforward to adapt to new situations
- **Generative adversarial networks** (GANs)* are another generative model that generate random examples of high-dimensional data

* ***Generative Adversarial Nets***, *Goodfellow et al, NIPS 2014*

Generative Adversarial networks

- The GAN contains only the **decoder** part of an autoencoder
  - The code z is **explicitly sampled** from a chosen distribution p_z (contrary to the VAE)
- The decoder is referred to here as the "Generator"



- We suppose that the data in the databse follows a distribution p_{data}
- We want to make the distribution of $y = G(z)$, p_G, similar to p_{data}*

* *Why can we not do this via the KL divergence as before ? Too high dimensionality (previously, we worked in the latent space)*

Generative Adversarial networks

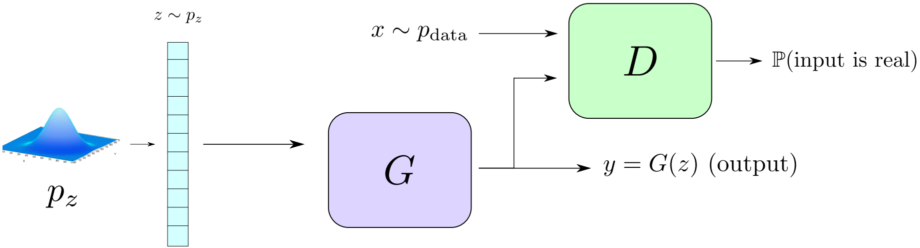
- However, with no reconstruction error, how do we make x look like the data ?
- Answer : Train another network : a **Discriminator** D (or "Adversarial Network")

Generative Adversarial networks

- However, with no reconstruction error, how do we make x look like the data ?
- Answer : Train another network : a **Discriminator** D (or "Adversarial Network")
- $D : \mathbb{R}^{mn} \rightarrow [0, 1]$ is trained to **identify "good" (or "true")** examples of the data
- $G : \mathbb{R}^{z} \rightarrow \mathbb{R}^{mn}$ is trained to **produce realistic data examples**
- The two networks are trained at the same time, and **each try to fool the other !**

Generative Adversarial networks

- The full GAN architecture looks like this



Generative Adversarial networks

- The discriminator is a really interesting idea, why ?
- Reliable and powerful image/data models are difficult to establish
- It is difficult to say whether an image is "good" or not
  - The discriminator acts as a **learned image norm** !
  - It can be used for other purposes also ...
- How is this is achieved ? Via a well-designed loss function

Generative Adversarial networks

GAN loss

- Train generator G and the discriminator D in a minimax optimisation problem

$$\min_G \max_D \overbrace{\mathbb{E}_{x\sim p_{data}}\left[\log D(x)\right]}^{D \text{ is trying to recognize true data}} + \underbrace{\mathbb{E}_{z\sim p_z}\left[\log\left(1 - D(G(z))\right)\right]}_{\substack{G \text{ is trying to fool } D, \\ \text{but } D \text{ is trying not to be fooled}}}$$

Generative Adversarial networks

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  - Second term is low, $\implies 1 - D(G(z))$ is close to 0 $\implies D$ is recognising $G(z)$ as a true data example : G **has fooled** D

Generative Adversarial networks

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- Minimisation w.r.t G
  - Second term is low, $\implies 1 - D(G(z))$ is close to 0 $\implies D$ is recognising $G(z)$ as a true data example : G **has fooled** D
- Maximisation w.r.t D
  - First term is high $\implies D(x)$ is close to 1 : D **is learning to recognize true data**
  - Second term is high $\implies 1 - D(G(z))$ is close to 1 : D **is not getting fooled by** G

Generative Adversarial networks

- At the beginning of the training, the examples from G are not very good : D can spot them easily
- At the end of training, the discriminator should not be able to tell the true data from the generated data : $p_G = p_{data}$
- Optimisation alternates between minimisation and maximisation steps

Generative Adversarial networks

- At the beginning of the training, the examples from G are not very good : D can spot them easily
- At the end of training, the discriminator should not be able to tell the true data from the generated data : $p_G = p_{data}$
- Optimisation alternates between minimisation and maximisation steps
- Are we sure that this loss is well-designed for this purpose ?
- In fact, we can prove that this is the case

- First, we establish the following lemma :

Optimal GAN discriminator D^*

For a fixed G, the optimal D is $D^*(x) = \frac{p_{data}(x)}{p_{data}(x)+p_G(x)}$

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\begin{aligned}
\mathcal{L}(G, D) &= \mathbb{E}_{x \sim p_{data}} [\log D(x)] + \mathbb{E}_{z \sim p_z} [\log(1 - D(G(z)))] \\
&= \int_{\mathcal{X}} p_{data}(x) \log(D(x)) dx + \int_{\mathcal{Z}} p_z(z) \log(1 - D(G(z))) dz \\
&= \int_{\mathcal{X}} p_{data}(x) \log(D(x)) + p_G(x) \log(1 - D(x)) dx.
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- For every x, the maximum of the previous equation w.r.t $D(x)$ is

$$D^*(x) = \frac{p_{data}(x)}{p_{data}(x)+p_G(x)}$$

Generative Adversarial networks

- Given this lemma, we can now state the main optimality theorem

Global optimum of the GAN loss function

The global optimum of the GAN loss function is achieved if and only if $p_G = p_{data}$. At this point $\mathcal{L}(G, D) = -\log 4$.

Generative Adversarial networks

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- First, our previous lemma allows us to rewrite the loss function

$$\max_D \mathcal{L}(G, D) = \mathbb{E}_{x \sim p_{data}} [\log D^*(x)] + \mathbb{E}_{z \sim p_z} [\log(1 - D^*(G(z)))] \quad (3)$$

$$= \mathbb{E}_{x \sim p_{data}} [\log D^*(x)] + \mathbb{E}_{x \sim p_G} [\log(1 - D^*(x))]$$

$$= \mathbb{E}_{x \sim p_{data}} \left[\log \frac{p_{data}(x)}{p_{data}(x) + p_G(x)}\right] + \mathbb{E}_{x \sim p_G} \left[\log \left(\frac{p_G(x)}{p_{data}(x) + p_G(x)}\right)\right]. \quad (4)$$

Generative Adversarial networks

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$$\begin{aligned} &= \mathbb{E}_{x \sim p_{data}} [\log D^*(x)] + \mathbb{E}_{x \sim p_G} [\log(1 - D^*(x))] \\ &= \mathbb{E}_{x \sim p_{data}} \left[\log \frac{p_{data}(x)}{p_{data}(x) + p_G(x)}\right] + \mathbb{E}_{x \sim p_G} \left[\log \left(\frac{p_G(x)}{p_{data}(x) + p_G(x)}\right)\right]. \end{aligned} \tag{4}$$

- Therefore, if $p_G = p_{data}$, then $\mathcal{L}(G, D) = \log \frac{1}{2} + \log \frac{1}{2} = -\log(4)$

Generative Adversarial networks

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- First, we remark that :

$$-\log(4) = \mathbb{E}_{x\ \sim p_{data}}\left[-\log(2)\right] + \mathbb{E}_{x\ \sim p_G}\left[-\log(2)\right]. \quad (5)$$

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- Therefore, by subtracting Equation 5 from Equation 4, we have

$$\begin{aligned}\mathcal{L}(G, D^*) &= -\log(4) + \int p_{data}(x) \log \frac{p_{data}(x)}{\frac{1}{2}\left(p_{data}(x) + p_G(x)\right)} dx \; + \\ &\quad \int p_G(x) \log \frac{p_G(x)}{\frac{1}{2}\left(p_{data}(x) + p_G(x)\right)} dx \\ &= -\log(4) + KL\left(p_{data} \,||\, \frac{p_{data} + p_G}{2}\right) + KL\left(p_G \,||\, \frac{p_{data} + p_G}{2}\right).\end{aligned}$$

Generative Adversarial networks

- This can also be rewritten as

$$\mathcal{L}(G, D^*) = -\log(4) + 2\,\mathbf{JSD}\left(\mathbf{p_{data}} \,||\, \mathbf{p_G}\right).$$

- The **JSD** is the **Jensen-Shannon divergence**
- This is another distance between distributions. For p and q, we have :

$$JSD(p,q) = \frac{1}{2} KL\left(p \,||\, \frac{1}{2}(p+q)\right) + \frac{1}{2} KL\left(q \,||\, \frac{1}{2}(p+q)\right)$$

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- The JSD is **non-negative and equal to zero if and only if** $p_{data} = p_G$
- Therefore $-\log(4)$ is the optimal value, and only reached when $p_{data} = p_G$

Generative Adversarial networks

- To summarise, we know that **by minimising the GAN loss, we are sure to encourage p_G to approximate p_{data}**
- In spite of this theoretical result (and others), training GANs is very difficult and is a current hot topic of research

Generative Adversarial networks

- Here are some results of the original GAN paper*

- In the space of four years, these results have been vastly improved on
- There are many, many GAN variants. We present a few now

* ***Generative Adversarial Nets***, *Goodfellow et al, NIPS 2014*

Conditional Generative Adversarial networks

- The Conditional GAN allows a label $\mathbf{c}$ to be added to the loss function
- It is then possible to generate examples of a given class

$$\min_G \max_D \left[\log D(x|\mathbf{c})\right] + \left[\log\left(1 - D(G(z|\mathbf{c}))\right)\right]$$

* ***Conditional Generative Adversarial Nets**, Mirza, M. and Osindero, S., arXiv preprint arXiv:1411.1784, 2014*

- Examples of results of Conditional GAN

* ***Conditional Generative Adversarial Nets***, *Mirza, M. and Osindero, S., arXiv preprint arXiv:1411.1784, 2014*

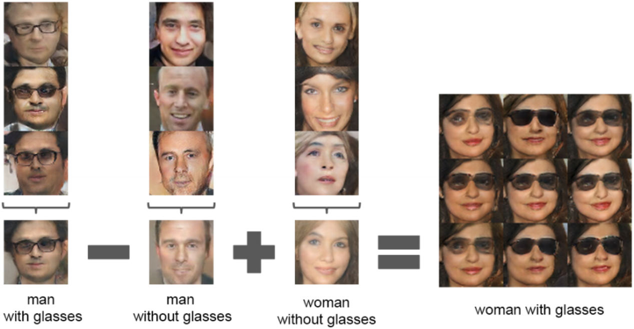
Generative Adversarial networks

- Deep Convolutional Generative Adversarial Networks (DCGAN)
- More complex data, sharper generation

* ***Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks***, *Radford, A. and Chintala, S., arXiv:1511.06434, 2015*

Generative Adversarial networks

- Deep Convolutional Generative Adversarial Networks (DCGAN)
- Linear algebra in the latent space



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Generative Adversarial networks

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Generative Adversarial networks

- A big problem of the GAN is known as **mode collapse**. This occurs when the training leads a GAN to produce the same result all the time
- The "Wasserstein GAN"† modifies the loss function by using a different distance between probabilities : the Wasserstein distance

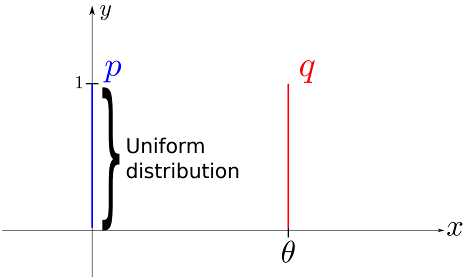
$$W(p,q) = \inf_{\gamma \in \prod(p,q)} \mathbb{E}_{(x,y)\sim\gamma} \left[\|x-y\| \right] \tag{6}$$

- $\prod(p,q)$ is the set of all the joint distributions of (x,y) whose marginals are p and q
- The reason that the Wasserstein distance is useful is that **some sequences of distributions converge under the Wasserstein distance, but not other distances** (the KL divergence, for example)

† ***Wasserstein GAN***, *Ajovsky, M., Chintala, S. and, Bottou, L. arXiv preprint arXiv:1701.07875, 2017*

Generative Adversarial networks

- Consider the following situation (the distribution supports do not intersect) :
  - A distribution $p = (0, \mathcal{U})$ ($\mathcal{U}$ is the uniform distribution)
  - A distribution $q = (\theta, \mathcal{U})$ (θ is a real number)



- In this case $KL(p||q) = +\infty$
- However, $W(p, q) = |\theta|$

Generative Adversarial networks

- The Wasserstein GAN uses the **dual formulation** of the Wasserstein distance

$$W(p,q) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{x\sim p}\left[f(x)\right] - \mathbb{E}_{x\sim q}\left[f(x)\right] \tag{7}$$

- f is a function
- $\|f\|_L \leq 1$ means that f must be 1-Lipschitz

Generative Adversarial networks

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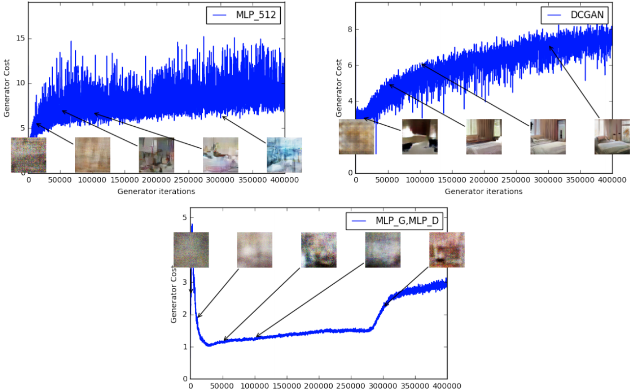
- f is a function
- $\|f\|_L \leq 1$ means that f must be 1-Lipschitz
- Thus, the final modified W-GAN distance is

$$\max_{\theta} \mathbb{E}_{x\sim p_{data}}\left[f_\theta(x)\right] - \mathbb{E}_{z\sim p_z}\left[f_\theta(g_\theta(x))\right] \tag{8}$$

- θ are the parameters of the generator g_θ, and the disriminator f_θ
- f_θ is forced to be a Lipschitz function by clipping the discriminator weights

Generative Adversarial networks

- Wasserstein GAN supposedly improves convergence of GAN training
- Fewer "tricks" (batch-norm etc) needed for good results



Generative Adversarial networks

- Around 2017, "intermediate"-resolution results were achieved by different research teams†

† ***Progressive growing of gans for improved quality, stability, and variation***, *Karras, T., Aila, T., Laine, S., and Lehtine, J., arXiv preprint arXiv:1710.10196, 2017*

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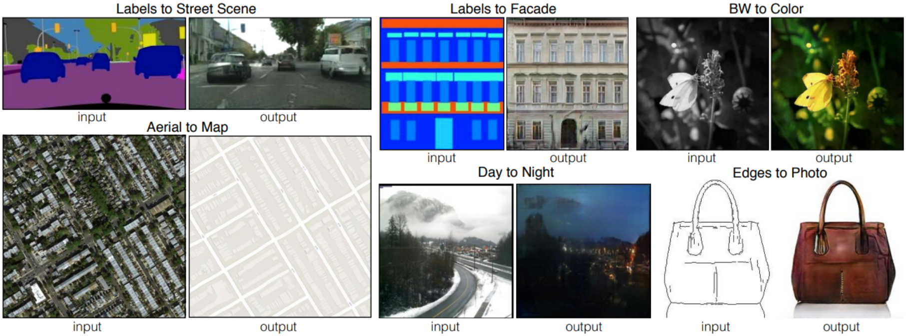
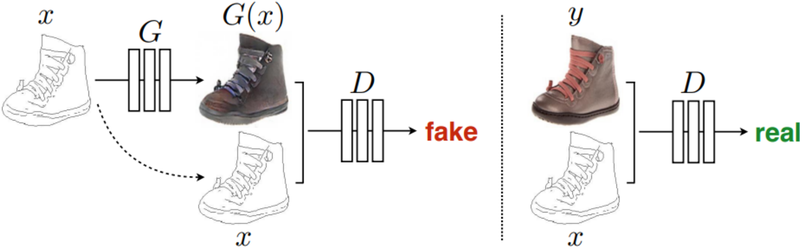
Generative Adversarial networks

- GANs have also been modified to carried out **domain translation**
- One of the most well-known networks is **Pix-To-Pix**†



† ***Image-to-Image Translation with Conditional Adversarial Nets***, *P Isola, J.-Y. Zhu, T. Zhou, A. A. Efros, CVPR, 2017*

- Instead of going from a random code to an image, the GAN learns to map one representation to another



- Can be used for tasks such as data augmentation, image inpainting

† ***Image-to-Image Translation with Conditional Adversarial Nets***, *P Isola, J.-Y. Zhu, T. Zhou, A. A. Efros, CVPR, 2017*

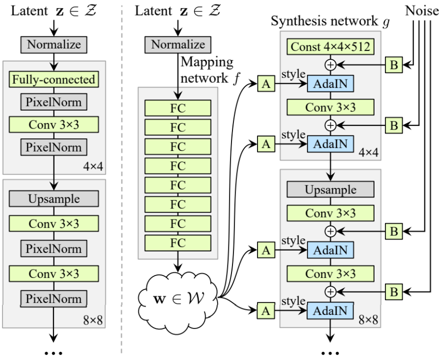
Generative Adversarial networks

- The most recent examples of GANs (in the past ~ 2 years) show realistic results on images of up to $\sim 1000 \times 1000$ pixel resolution
- One of the most impressive is StyleGAN† (there is also another, more recent version, StyleGAN2)
- The main idea of StyleGAN is to transform the **probabilistic** latent space into another, **less entangled** and more **linear**
  - "Entanglement" means mixing up several visual attributes in the latent space
  - If this happens, it is difficult to control attributes separately

† ***A Style-Based Generator Architecture for Generative Adversarial Networks***, *Karras, T., Laine, S., and Aila, T. CVPR, 2019*

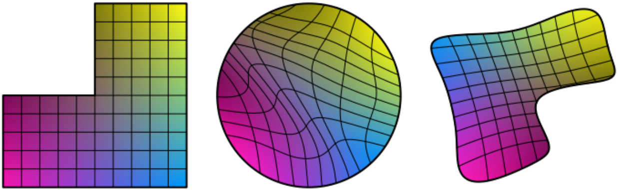
Generative Adversarial networks

- StyleGAN achieves these goals by **inserting the latent code at several resolutions**
- This replaces the purely sequential architecture of classic GANs



(a) Traditional (b) Style-based generator

- The resulting code w is supposedly **more linear**



(a) Distribution of features in training set (b) Mapping from $\mathcal{Z}$ to features (c) Mapping from $\mathcal{W}$ to features

- However, there is as yet no theory to back this up

Generative Adversarial networks

- Some high-resolution examples (from StyleGAN2)

Generative Adversarial networks

- Some high-resolution examples (from StyleGAN2)

- Currently, some of the main goals for researchers working on GANs are the following :
  1. Achieving high-resolution results, **removing visual artefacts**
  2. How to **navigate** correctly in the latent space ? What is the **geometry** of the latent space
  3. How to achieve **disentangled respresentations** in the latent space

Summary on GANs

- GANs are a powerful and generic way of producing **random examples of complex images**
- However, they are **notoriously difficult to train**, this is a current area of research
- A significant disadvantage with respect to variational autoencoders is that **GANs do not train an encoder** : it is a one-way transformation
    - Often, for restoration or other inverse problems, it is useful to have an "inverse" transformation

Summary

Conclusion

We have seen two types of generative models

1. Variational autoencoders
   - An Autoencoder whose latent space is encouraged to follow a certain distribution
   - Variational Bayesian formulation
2. Generative Adversarial Networks
   - A generator trained to create realistic data
   - A discriminator trained to identify true and false data examples

Summary of advantages and weaknesses of Generative Models

Model/method	Advantages	Disadvantages
VAE	• Rigourous formulation • Encoder and decoder trained	• Loss must be rewritten for different probability distributions (not easy) • In practice, more limited applications than GANs
GAN	• Highly flexible • Applied to complex data, impressive results	• Difficult to train • No reverse transformation (encoder)
Texture/style model	• Versatile, simple algorithm • Produces best texture/style results	• Only applicable to limited cases

A few references

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Variational autoencoders - Variational Autoencoder loss function

- We show that the ELBO can be rewritten in the following manner:

$$\text{ELBO}(q_\phi) = \mathbb{E}_{q_\phi}\left[\log(p_\theta(x|z))\right] - KL(q_\phi(z|x) \mid\mid p_\theta(z))$$

- Start out with the initial formulation:

$$\begin{aligned}
\text{ELBO}(q_\phi) &= \mathbb{E}_{q_\phi}\left[\log(p_\theta(x,z))\right] - \mathbb{E}_{q_\phi}\left[\log q_\phi(z|x)\right] \\
&= \int_{q_\phi} \left[\log\left(p_\theta(x|z).p_\theta(z)\right) - \log q_\phi(z|x)\right]\ q_\phi(z|x)dz \qquad \text{Conditional prob.} \\
&= \int_{q_\phi} \log(p_\theta(x|z)).q_\phi(z|x)dz - \int_{q_\phi} \left(\log q_\phi(z|x) - \log p_\theta(z)\right) q_\phi(z|x)dz \\
&= \mathbb{E}_{q_\phi}\left[\log p_\theta(x|z)\right] - KL\left(q_\phi(z|x)||p_\theta(z)\right)
\end{aligned}$$