

Variational Auto Encoders

Introduction to Deep Learning al Auto Encoders
on to Deep Learning
Fall 2024

Attendance: @1582

A new problem

- From a large collection of images of faces, can a network learn to generate new portraits
	- Generate samples from the distribution of "face" images
		- How do we even characterize this distribution?

A new problem

- From a large collection of landscapes, can a network learn to *generate* new landscape pictures
	- Generate samples from the distribution of "landscape" images
		- How do we even characterize this distribution?

- **Hypothesis:** The data are distributed about a curved or otherwise non-linear manifold in high dimensional space
	- The principal components of all instances of the target class of data lie on this manifold
- To generate data for this class, we must select a point on this manifold

• Problems:

- Characterizing the manifold
- Having a good strategy for selecting points from it

Recall : The AE

- The autoencoder captures the underlying manifold of the data
	- "Non linear" PCA
	- Deeper networks can capture more complicated manifolds
		- "Deep" autoencoders states of the state of the stat

- The decoder represents a source-specific generative dictionary
- Exciting it will produce data similar to those from the source!

• Train AE with the pictures…

The face dictionary

• The decoder can now be used to generate instances from the "faces" manifold

The problem with AEs

- Improper choice of input to the decoder can result in incorrect generation
- How do we know what inputs are reasonable for the decoder?
- Solution : only choose input $(z's)$ that are typical of the class
	-
	-

Poll 1 (@1573, @1574)

- The decoder in an AE can only generate data on a lowdimensional surface/manifold of the space
	- True
	- False
- What is true of the dimensionality of this manifold
	- It cannot be predicted and can be anything
	- It is no greater than the dimensionality of the latent representation that is input to the decoder
	- It will be the same as the input to the encoder

Poll 1

• The decoder in an AE can only generate data on a lowdimensional surface/manifold of the space

– True

– False

- What is true of the dimensionality of this manifold
	- It cannot be predicted and can be anything
	- It is no greater than the dimensionality of the latent representation that is input to the decoder
	- It will be the same as the input to the encoder

Impose distribution on z

When training the autoencoder, explicitly impose the constraint that the hidden representation z must follow a specific distribution - E.g $P(z)$ is standard Gaussian $(N(0,I))$

Generation

- To generate novel values, sample z from the prescribed distribution $(N(0,I))$
- If the network is properly trained, and z is properly sampled, the output should be a reasonable generation
	- E.g. of a face

How to train the model

• Problem: How does one train an AE to ensure that the hidden representation z has a specific distribution, e.g. $N(0, I)$

How to train the model

- Problem: How does one train an AE to ensure that the hidden representation z has a specific distribution, e.g. $P(z) = N(0, I)$
- Encoder and decoder may have arbitrarily complex structure and their own parameters $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$

A property of isotropic Gaussians

- $P(Z) = N(0, I)$
- The distribution is perfectly symmetric in every direction
	- The different variables (subvectors Z_1 and Z_2 of Z) are independent!

$$
- P(Z_1, Z_2) = P(Z_1)P(Z_2)
$$

– Each individually will also be isotropic: $P(Z_1) = N(0, I)$

Log likelihood on an isotropic Gaussian

•
$$
P(Z) = \frac{1}{\sqrt{(2\pi)^d}} \exp(-0.5|Z|^2)
$$

- $\log P(Z) = -0.5d \log 2\pi 0.5|Z|^2$
- $-\log P(Z) = 0.5d \log 2\pi + 0.5|Z|^2$

Training with statistical constraints

- Minimize the error between X and \hat{X}
- Minimize the KL divergence between the distribution of z and the standard Gaussian $N(0, I)$
	- $-$ Minimize the negative log likelihood of z as computed from a standard Gaussian

Training with statistical constraints

$$
\min \sum_{z} -\log N(z; 0, I) = \min 0.5 \sum_{x} |z|^2
$$

= $\min \sum_{x} |E(X; \theta)|^2$
Minimize the negative log likelihood of z as computed
from a standard Gaussian

Training with statistical constraints

$$
\min_{\theta,\phi}\sum_{X}|X-\hat{X}|^2+\lambda|E(X,\theta)\big|^2
$$

Poll 2 (@1575, @1576)

- A regular AE trained to also minimize the length of the hidden (latent) representation implicitly imposes an isotropic Gaussian distribution on the latent representation
	- True
	- False
- The output of an AE trained in this manner is no longer constrained to lie on a low dimensional manifold
	- True
	- False

Poll 2

• A regular AE trained to also minimize the length of the hidden (latent) representation implicitly imposes an isotropic Gaussian distribution on the latent representation

– True

- False
- The output of an AE trained in this manner is no longer constrained to lie on a low dimensional manifold
	- True
	- False

This model does not capture the entire distribution

$$
\min_{\theta,\phi}\sum_{X}|X-\hat{X}|^2+\lambda|E(X,\theta)\big|^2
$$

• This simple formulation does not adequately capture the variation in the data

The problem

- The generative portion of the model is just the decoder
	- Inputting Gaussian data into it still only produces what the decoder is capable of producing!

The problem

- space
	- Of the same dimension as the input
	- -

The problem

- The actual dimensionality of the data manifold may be (and generally will be) greater than the dimensionality of z
- Even if we capture the dimensionality of the principal manifold perfectly,
	- dimensional
- Our simple model captures none of the variation off the manifold!

Accounting for the noise

 $x = D(z) + e$

- Assume that the actual data is obtained by adding noise to the output of the decoder Source that the actual data is obtained by adding noise to the output of the

ecoder

- The noise accounts for the variation off the manifold

he model itself must be trained to minimize this noise

- Ensuring that it has e $\sim P(e)$

ime that the actual data is obtained by adding noise to

oder

The noise accounts for the variation off the manifold

model itself must be trained to minimize this noise

Ensuring that it has captured the princi **Example 12**
 Example 12
 Example 3
 Example 3
	- The noise accounts for the variation off the manifold
- The model itself must be trained to minimize this noise
	- - This is the smallest amount of noise to be added, such that the distribution at the output of the decoder fully explains the distribution the training data
- = Couer
 \blacksquare The noise accounts for the variation off the manifold
 \blacksquare The noise accounts that thas captured the principal manifold most effectively
 \blacksquare This is the *smollest* amount of noise to be added, suc
	-

Accounting for the noise

 $x = D(z) + e$

- Assume that the actual data is obtained by adding noise to the output of the decoder **Example 12**

• The enoise accounts for the variation off the manifold
 odel itself must be trained to minimize this noise
 odel itself must be trained to minimize this noise

• This is the *smallest* amount of noise
	- The noise accounts for the variation off the manifold
- The model itself must be trained to minimize this noise
	- Ensuring that it has captured the principal manifold most effectively
		- This is the smallest amount of noise to be added, such that the distribution at the output of the decoder fully explains the distribution the training data
- Typical Assumption: The noise is uncorrelated Gaussian $N(0, C)$ (i.e. it has maximum entropy) and is independent of z – The noise accounts for the variation off the manifold

– The noise accounts for the variation off the manifold

– Ensuring that it has captured the principal manifold most effectively

• This is the *smollest* amount
	-
- This has a consequence: x is no longer a deterministic outcome of z
	-

The actual model

- -
- A K-dimensional vector z is drawn from a standard K-dimensional Gaussian and passed through the decoder
	- This results in data lying on a K -dimensional non-linear surface in the data space
- Then a full-rank, low-amplitude noise is added to it, to generate the final data
	- $-$ The actual data distribution is a fuzzy region around the surface. $\frac{29}{29}$

If the z that went into the decoder to produce any training data

$$
\underset{\phi}{\text{argmin}} E[\|D(z;\phi) - x\|^2]
$$

• The encoder estimates the to permit us to estimate **From the barpat of the model to march the framing data** Since, by assumption, e is the smallest amount of noise needed for the output of the model to match the training data

If the z that went into the decoder to produce any training data Example 1 went into the decoder to produce any training data
s known along with x, the decoder (ϕ) can be estima
argmin $E[||D(z; \phi) - x||^2]$
by assumption, e is the smallest amount of noise needed
equiput of the model to m Example 1: went into the decoder to produce are
s known along with x, the decoder (α
argmin $E[||D(z; \phi) - x||^2]$
by assumption, e is the smallest amount
equiput of the model to match the train
Unfortunately, we don't have

$$
\underset{\phi}{\text{argmin}} E[\|D(z;\phi) - x\|^2]
$$

• The encoder estimates the to permit us to estimate **From the barpat of the model to march the framing data** Since, by assumption, e is the smallest amount of noise needed for the output of the model to match the training data

Unfortunately, we don't have the z for each x .

If the z that went into the decoder to produce any training data instance x is known along with x, the decoder (ϕ) can be estimated

$$
\underset{\phi}{\text{argmin}}\, E[\|D(z;\phi)-x\|^2]
$$

The encoder estimates the z to permit us to estimate ϕ

• If the z that went into the decoder to produce any data instance x is known

 ϕ 21

- The encoder estimates the z to permit us to estimate ϕ
- Problem: Several \hat{x} values exist that could be modified by noise to produce a given x
	- The z that could produce a given x is not unique

- -
	-
- Instead of finding the unique z for any x, we will find the distribution $P(z|x)$

- -
	-
- Instead of finding the unique z for any x, we will find the distribution $P(z|x)$
- The variational autoencoder
	- So named because the learning procedure utilizes a variational bound on the likelihood of the data

The variational autoencoder

$$
\begin{array}{ccc}\nX & \longrightarrow & \text{Encoder} \\
E(X; \theta) & & P(Z|X) \\
\end{array}\n\longrightarrow\n\begin{array}{ccc}\nZ \sim P(Z|X) & & \text{Decoder} \\
D(z; \phi) & & \text{N}\n\end{array}\n\longrightarrow\n\begin{array}{ccc}\n\text{Decoder} & & \text{Decoder} \\
D(z; \phi) & & \text{N}\n\end{array}\n\longrightarrow\n\begin{array}{ccc}\n\text{Decoder} & & \text{N} \\
\hline\nX & & \text{N} \\
\end{array}
$$
\n\nThe decoder tries to convert the expected output for zs drawn from this distribution to *x* — More practically, it tries to convert a typical sample *z* from *P*(*z*|*x*) to *x*.\n

- The encoder computes the distribution $P(z|x)$ for any x
- The *decoder* tries to convert the *expected* output for zs drawn from this distribution to x
	- More practically, it tries to convert a typical sample z from $P(z|x)$ to x
$$
\begin{array}{c|c|c|c|c} \hline X & \text{Encoder} & \longrightarrow P(z|X) & \text{Z} \sim P(z|X) & \longrightarrow & \text{Decoder} & \longrightarrow & \widehat{X} \\ \hline E(X;\theta) & \text{I} & \text{Z} \sim P(z|X) & \longrightarrow & D(z;\phi) & \longrightarrow & \widehat{X} \end{array}
$$

- The encoder computes the distribution $P(z|x)$ for any x
- The *decoder* tries to convert a typical sample z from $P(z|x)$ to x
- Training the encoder:
	- Estimate θ to make the zs that can be encoded \hat{x} values that are closer to x more probable

- The encoder computes the distribution $P(z|x)$ for any x
- The *decoder* tries to convert a typical sample z from $P(z|x)$ to x
- Training the encoder:
	- Estimate θ to make the zs that can be encoded \hat{x} values that are closer to x more probable
- Training the decoder:
	- Estimate ϕ to make the noise e between $\hat{x} = D(z)$ and x more probable
		- I.e. make it as small as possible

- The encoder computes the distribution $P(z|x)$ for any x
- The *decoder* tries to convert a typical sample z from $P(z|x)$ to x
- Training the encoder:
	- Estimate θ to make the zs that can be encoded \hat{x} values that are closer to x more probable
- Training the decoder:
	- Estimate ϕ to make the noise e between $\hat{x} = D(z)$ and x more probable
		- I.e. make it as small as possible
- **Constraint on z: ?**

What it means…

• The combined posterior distribution $P(z|X)$ over all possible values of X is a standard normal distribution

$$
\int_{-\infty}^{\infty} P(X)P(\mathbf{z}|\mathbf{X})d\mathbf{X} = N(0,I)
$$

• I.e. we must train the model such that the combined posterior over According to the model:
 $\int_{-\infty}^{\infty} P(X)P(z|X)dX = N(0, I)$

I.e. we must train the model such that the combined

all Xs is a standard normal

Learning the Encoder

- The encoder actually computes an *estimate* $Q(z|X)$ of the actual posterior $P(z|X)$ (in whichever way we do it) for each X
- We must minimize the divergence between the estimate $Q(z|X)$ and the *true* posterior $P(z|X)$ (over all X)

 $= E_X KL(Q(Z|X), P(Z|X))$

This is intractable in general because $P(Z|X)$ is unknown $\qquad \qquad _{43}$

Bayes and the Decoder to the rescue

$$
\varphi^* = \underset{\varphi}{\operatorname{argmin}} \, KL(Q(z|X)P(z|X)) \qquad \qquad \text{NLL of Decode} \\ = \underset{\varphi}{\operatorname{argmin}} \, KL(Q(z|X), P(z)) - E_{z \sim Q} \log P(X|z) \qquad \qquad
$$

• The modification gives us the simpler optimization

 $= E_X KL(Q(\mathbf{z}|\mathbf{X}), N(0, I))$

• We must minimize the expected divergence between the distribution $Q(z|X)$ modelled by the encoder and the standard normal $N(0,I)$ to get a good approximation of $P(z|X)$

The variational Encoder

Reverting to the $P(z|X)$ notation for uniformity

$$
\begin{array}{c|c}\nX & \text{Encoder} \\
E(X; \theta) & \n\end{array}\n\longrightarrow P(z|X)
$$

- We must train the encoder to minimize the *expected KL divergence* between $P(z|X)$ and the standard normal $N(0, I)$ verting to the $P(z|X)$ notation for uniformity
 $\frac{X}{E(X;\theta)} \longrightarrow P(z|X)$

• We must train the encoder to minimize the expected KL divergence

between $P(z|X)$ and the standard normal $N(0, I)$

• Empirically (since we perform Em
-

$$
E_XKL(P(\mathbf{z}|\mathbf{X}), N(0, I)) \approx \frac{1}{N} \sum_{\mathbf{X}} KL(P(\mathbf{z}|\mathbf{X}), N(0, I))
$$

• We must train the encoder to minimize the expected KL divergence
between $P(z|X)$ and the standard normal $N(0, I)$
• Empirically (since we perform Empirical Risk Minimization)
 $E_X KL(P(z|X), N(0, I)) \approx \frac{1}{N} \sum_{X} KL(P(z|X), N(0, I))$
• between the posterior $P(z|X)$ and the standard normal over the training data

The variational Encoder

Reverting to the $P(z|X)$ notation for uniformity

$$
X \longrightarrow E^{r}(\mathbf{Z}|\mathbf{X})
$$

- We must train the encoder to minimize the expected KL divergence between $P(z|X)$ and the standard normal $N(0, I)$
- Empirically (since we perform Empirical Risk Minimization)

$$
E_XKL(P(\mathbf{z}|\mathbf{X}), N(0, I)) \approx \frac{1}{N} \sum_{\mathbf{X}} KL(P(\mathbf{z}|\mathbf{X}), N(0, I))
$$

We must train the encoder to minimize the average KL divergence between the posterior $P(z|X)$ and the standard normal over the training data

For this, the encoder must model the distribution, $P(z|X)$

 $-$ It is now computing an entire distribution rather than a single value of $z = \frac{47}{4}$

The problem for the encoder lies in
the decoder... the decoder…

- (since we don't know the exact e that was added to \widehat{X})
	-
- determine the corresponding set of z values
	- I.e. cannot characterize the set of z values that resulted in the set of \hat{X} values that could have produced \boldsymbol{X}

The problem for the encoder lies in the decoder…

- The decoder that converts z to \widehat{X} is highly nonlinear
	- $-$ Difficult to characterize the distribution of the z values that could produce a given X
- Though $P(\widehat{X}|X)$ is Gaussian (since *e* is Gaussian), going back through the decoder, $P(z|X)$ is generally not characterizable!
	- We need to make some simplifying assumptions

Z is an isotropic Gaussian

• $P(Z) = N(0, I)$

- Independence $\rightarrow P(Z_1|Z_2) = P(Z_1)$
- $P(Z_1|Z_2) = N(0,I)$
- The conditional distribution of Z_1 given Z_2 is also an isotropic Gaussian regardless of the value of Z_2

- This property will hold regardless of the line/hyperplane along which you consider the conditional
	-

- This property will hold regardless of the line/hyperplane along which you consider the conditional
	-
- More generally, for "nearly linear" functions, the conditional distribution is still well approximated by a Gaussian (but the mean and variance may not be standard)
	-
	- probability regions of (Z)
		- $E(|f(Z)-linear(Z)|^2) < \epsilon$

- More generally, for "nearly linear" functions $-P(Z|f(Z) = c) \approx N(\mu, \Sigma)$
- But μ and Σ will depend on c (and $f()$)

Poll 3 (@1577, @1578)

- The Z is a random vector with an isotropic Gaussian distribution,
the conditional distribution of the projection of Z on any affine
plane is also isotropic **Poll 3 (@1577, @1578)**
The Z is a random vector with an isotropic Gaussian distribution,
the conditional distribution of the projection of Z on any affine
— True plane is also isotropic
	- True
	- False
- If Z is a random vector with an isotropic Gaussian distribution, the conditional distribution of Z on any curved surface is also approximately Gaussian for surfaces of low curvature
	- True
	- False

Poll 3

• The Z is a random vector with an isotropic Gaussian distribution, the conditional distribution of the projection of Z on any affine plane is also isotropic

– True

- False
- If Z is a random vector with an isotropic Gaussian distribution, the conditional distribution of Z on any curved surface is also approximately Gaussian for surfaces of low curvature
	- True
	- False

Encoder Decoder

- The encoder computes the distribution $P(z|X)$ for any X
- The *decoder* tries to convert a randomly sampled z from $P(z|X)$ to X
- Training the encoder:
	- Estimate θ to make the zs that can be encoded \widehat{X} values that are closer to X more probable
- Training the decoder:
	- Estimate ϕ to make the noise between $\widehat{X} = D(z)$ and X more probable
- Constraint on z: Make the average $P(z|X)$ as close to the standard Gaussian as possible

The encoder computes the distribution $P(z|X)$ for any X

- The *decoder* tries to convert a randomly sampled z from $P(z|X)$ to X
- Training the encoder:
	- $-$ Estimate θ to make the zs that can be encoded $\widehat{\bm{X}}$ values that are closer to \bm{X} more probable
- Training the decoder:
	- Estimate ϕ to make the noise between $\widehat{X} = D(z)$ and X more probable
- Constraint on z: Make the average $P(z|X)$ as close to the standard Gaussian as possible

 $\mu(x;\varphi)$ and $\Sigma(x;\varphi)$ are parametric functions of x, with parameters that we jointly represent as φ

We approximate $P(z|X)$ as

 $P(z|X) \approx Q(z|X) = Gaussian N(z; \mu(X), \Sigma(X))$

- where $\mu(X; \varphi)$ and $\Sigma(X; \varphi)$ are estimated such that $Q(z|X)$ approximates $P(z|x)$ as closely as possible
- For convenience, we will assume $\Sigma(X; \varphi)$ is a diagonal matrix, represented entirely by its diagonal elements
- We will use $Q(z|X)$ as our proxy for $P(z|X)$

- The encoder computes the distribution $P(z|X)$ for any X
- The *decoder* tries to convert a randomly sampled z from $P(z|X)$ to X
- Training the encoder:

- Training the decoder:
	- Estimate ϕ to make the noise between $\hat{X} = D(z)$ and X more probable
- Constraint on z: Make the average $P(z|X)$ as close to the standard Gaussian as possible

$$
-\frac{d}{2}\log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

$$
\theta^* = \underset{\theta}{\operatorname{argmax}} \sum_{(X,z)} -\frac{d}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

$$
\theta^* = \underset{\theta}{\text{argmax}} \sum_{(X,z)} -\frac{d}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

• We can learn the parameters using backpropagation, which minimizes the following loss

$$
\theta^* = \underset{\theta}{\operatorname{argmax}} \sum_{(X,z)} -\frac{d}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

rn the parameters using backpropagation, which minimizes the following loss

$$
L(\theta, \phi, \sigma^2) = \sum_{(X,z)} d \log(\sigma^2) + \frac{1}{\sigma^2} ||X - D(z; \phi)||^2
$$

$$
\theta^* = \underset{\theta}{\text{argmax}} \sum_{(X,z)} -\frac{d}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

• We can learn the parameters using backpropagation, which minimizes the following loss

$$
\theta^* = \underset{\theta}{\operatorname{argmax}} \sum_{(X,z)} -\frac{d}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} ||X - D(z; \phi)||^2
$$

ne parameters using backpropagation, which minimizes the following loss

$$
L(\theta, \phi, \sigma^2) = \sum_{(X,z)} d \log(\sigma^2) + \frac{1}{\sigma^2} ||X - D(z; \phi)||^2
$$

this with respect to θ

$$
\theta^* = \underset{\theta}{\operatorname{argmin}} L(\theta, \phi, \sigma^2)
$$

Must minimize this with respect to θ

$$
\theta^* = \operatorname*{argmin}_{\theta} L(\theta, \phi, \sigma^2)
$$

Sampling Z

- For each training input X , z is obtained as a sample from $N(z; \mu(X; \theta), \Sigma(X; \theta))$
- We use a standard "reparametrization" step to sample z
	- Draw K-dimensional vector ε from $N(0,I)$
	- Compute $z = \mu(X; \theta) + \Sigma(X; \theta)^{0.5} \varepsilon$

Remember this one $\nabla_{\theta} z = \nabla_{\theta} \mu(X; \theta) + diag(\varepsilon) \nabla_{\theta} \Sigma(X; \theta)^{0.5}$ 0.5 This will be specific to X and to the specific sample of z for that X (via ε)

 $X = D(z; \phi) + e$

$$
L(\theta, \phi, \sigma^2) = d \log \sigma^2 + \sum_{(x,z)} \frac{1}{\sigma^2} ||X - D(z; \phi)||^2
$$

$$
- z = \mu(X; \theta) + \Sigma(X; \theta)^{0.5} \varepsilon
$$

 $- \varepsilon$ is sampled from $N(0, I)$

$$
\theta^* = \underset{\theta}{\text{argmin}} \ L(\theta, \phi, \sigma^2)
$$

- The derivative of $L(\theta, \phi, \sigma^2)$ with respect to θ can be computed using the chain rule $\nabla_{\theta}L(\theta,\phi,\sigma^{2})=\sum_{(X,Z)}\nabla_{z}L(\theta,\phi,\phi)$ $Z^L(\theta,\phi,o^-)$ V $_\theta Z$ $\sqrt{2} \sqrt{2}$ (X,Z) $V_ZL(\sigma, \varphi, o^-)$ $V_{\theta}Z$
	- For use in backpropagation 69

X	Encoder	$P(z X)$	$z \sim P(z X)$	Decoder
• The encoder computes the distribution $P(z x)$ for any x				
• The decoder tries to convert a randomly sampled z from $P(z x)$ to x				
• Training the encoder:				
• Estimate θ to make the zs that can be encoded to x more probable				
• Training the decoder:				

- The encoder computes the distribution $P(z|x)$ for any x
- The *decoder* tries to convert a randomly sampled z from $P(z|x)$ to x
- Training the encoder:
	-
- Training the decoder:
	- Estimate ϕ to make the noise between $\hat{x} = D(z)$ and x more probable
- The *encoder* computes the *alstribution* $P(Z|X)$ for any x

 The *decoder* tries to convert a randomly sampled z from $P(z|x)$ to x

 Training the encoder:

 Estimate θ to make the zs that can be encoded to Gaussian as possible

 $X = D(z; \phi) + e$ $Z \sim N(0, I)$
 $D(z; \phi)$ $\longrightarrow X$

 $P(X|z) = N(X; D(z; \phi), \sigma^2 I)$

$$
L(\theta, \phi, \sigma^2) = d \log \sigma^2 + \sum_{(X, z)} \frac{1}{\sigma^2} ||X - D(z; \phi)||^2
$$

$$
\phi^*, \sigma^{2^*} = \operatorname*{argmin}_{\phi, \sigma^2} L(\theta, \phi, \sigma^2)
$$

• The derivative of this w.r.t ϕ and σ^2 is trivially computed for backprop

- The encoder computes the distribution $P(z|X)$ for any X
- The *decoder* tries to convert a randomly sampled z from $P(z|X)$ to X
- Training the encoder:
	-
- Training the decoder:
	- Estimate $\boldsymbol{\phi}$ to make the noise between $\widehat{X} = D(z)$ and X more probable

Constraint on z: Make the average $P(z|X)$ as close to the standard Gaussian as possible
The constraint on P(z) **•** The KL between $Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))$ and the standard Gaussian $N(z; 0, I)$ works out to
 $KL(Q(z, x; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(x; \theta)^T \mu(x; \theta) - d - \log|\Sigma(x; \theta)|)$ **The constraint on** $P(z)$

between $Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))$ and the standard Gaussian $N(z; KL(Q(z, x; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(x; \theta)^T \mu(x; \theta) - d - \log|\Sigma|)$

is is a function of encoder parameters θ

The constrained on P(z)
the KL between
$$
Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))
$$
 and the standard Gaussian $N(z; 0, I)$ works out to

$$
KL(Q(z, x; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(x; \theta)^T \mu(x; \theta) - d - \log|\Sigma(x; \theta)|)
$$
This is a function of encoder parameters θ

– This is a function of encoder parameters θ

The constraint on P(z) **•** The KL between $Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))$ and the standard Gaussian $N(z; 0, I)$ works out to
 $KL(Q(z|X; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(X; \theta)^T \mu(X; \theta) - d - \log|\Sigma(X; \theta)|)$ **The constraint on** $P(z)$
between $Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))$ and the standard Gaussian $N(z;$
 $KL(Q(z|X; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(X; \theta)^T \mu(X; \theta) - d - \log|\Sigma|)$
is is a function of encoder parameters θ
parall loss thus become

The constraint on P(z)
\n
$$
P(z)
$$
\n
$$
P(z)
$$
\n
$$
P(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))
$$
\nand the standard Gaussian $N(z; 0, I)$ works out to
$$
KL(Q(z|X; \theta), N(z; 0, I)) = \frac{1}{2} (tr(\Sigma(x; \theta)) + \mu(X; \theta)^T \mu(X; \theta) - d - \log|\Sigma(X; \theta)|)
$$
\nis is a function of encoder parameters θ
\n
$$
P(z)
$$
\n
$$
P(z
$$

- This is a function of encoder parameters θ
- The overall loss thus becomes:

 $L_{VAE}(\theta, \varphi, \sigma^2)$ $2₁$

The KL between
$$
Q(z|X) = N(z; \mu(X; \theta), \Sigma(X; \theta))
$$
 and the standard Gaussian $N(z; 0, I)$ works out to
\n
$$
KL(Q(z|X; \theta), N(z; 0, I)) = \frac{1}{2} \left(tr(\Sigma(x; \theta)) + \mu(X; \theta)^T \mu(X; \theta) - d - \log|\Sigma(X; \theta)| \right)
$$
\n- This is a function of encoder parameters θ
\nThe overall loss thus becomes:
\n
$$
L_{VAE}(\theta, \phi, \sigma^2)
$$
\n
$$
= \sum_{X} \left(tr(\Sigma(X; \theta)) + \mu(X; \theta)^T \mu(X; \theta) - d - \log|\Sigma(X; \theta)| \right) + \frac{1}{\sigma^2} \sum_{(x, z) \in [X, z]} ||(X - D(z; \phi))||^2 + d \log \sigma^2
$$
\nThis must be minimized to train the VAE
\n- The derivatives of all terms w.r.t. are easily computed using backprop

- This must be minimized to train the VAE
	-

The complete training pipeline

- Initialize θ and φ
- Iterate:
	- Sample $z_{\chi,\varepsilon}$ from $N(z;\mu(x;\varphi),\Sigma(x;\varphi))$ for each training instance

— Reestimate *θ*, *φ*, *σ*² from

$$
L_{VAE}(\theta, \phi, \sigma^2)
$$

$$
= \sum_{x \in X} \bigl(tr(\Sigma(x; \theta)) + \mu(x; \theta)^T \mu(x; \theta) - d
$$

$$
-\log|\Sigma(x;\theta)| + \frac{1}{\sigma^2} \sum_{(x,z)\in[X,Z]} ||(x - D(z;\phi))||^2
$$

+ $d \log \sigma^2$

But where are the neural nets?

- $D(z; \theta)$ is a neural network
- $\mu(x;\theta)$ and $\Sigma(x;\theta)$ are generally modelled $e^{\alpha N(0,\sigma^2)}$ by a common network with two outputs
	- The combined parameters of the network are θ

The VAE for generation

• Once trained the encoder can be discarded

- The rest of the network gives us a generative model for x
- Generating data using this part of the model should (ideally) give us data similar to the training data

Recap: The VAE

- An autoencoder with statistical constraints on the hidden representation
	- The encoder is a statistical model that The encoder is a statistical model that
computes the parameters of a Gaussian $D(z; \phi)$
	- The decoder converts samples from the Gaussian back to the input
- The *decoder* is a generative model that, when excited by standard Gaussian inputs, generates samples similar to the training data

The Variational AutoEncoder

The decoder is the actual generative model.

The encoder is primarily needed for training.

It can also be used to generate the (approximate) distribution of latent space representations conditioned on specific inputs (much like a regular autoencoder).

z is a *latent-space* representation of the data.

 $\mu(x)$ can also be used as an expected latent representation of x .

Poll 4 (@1579, @1580)

- A variational autoencoder is a generative extension of autoencoders that **Poll 4 (@1579, 0**
A variational autoencoder is a generative externodels probability distributions
- True – False
	-
	-
- Select the true statements
	- The standard VAE assumes a latent representation that has an isotropic Gaussian PDF
	- The VAE model requires addition of Gaussian noise to the output of a regularized AE in order to permit the output to fill space beyond a lowerdimensional manifold
	- The decoder of the VAE can be used to generate samples from the distribution of the data it is trained on, if the input to the decoder is drawn from a standard Gaussian

Poll 4

- A variational autoencoder is a generative extension of autoencoders that **Poll 4**
A variational autoencoder is a generative externodels probability distributions
- True
- False
	-
	-
- Select the true statements
	- The standard VAE assumes a latent representation that has an isotropic Gaussian PDF
	- The VAE model requires addition of Gaussian noise to the output of a regularized AE in order to permit the output to fill space beyond a lowerdimensional manifold
	- The decoder of the VAE can be used to generate samples from the distribution of the data it is trained on, if the input to the decoder is drawn from a standard Gaussian

VAE examples

• Top: VAE trained on MNIST and used to generate new data

• Below: VAE trained on faces, and used to generate new data

From C. Doei

From J. Rocco

VAE and latent spaces

- The latent space z often captures underlying structure in the data x in a smooth manner
	- $-$ Varying z continuously in different directions can result in plausible variations in the drawn output
- Reproductions of an input x can be manipulated by wiggling z around its expected value $\mu(x)$

VAE conclusions

- Simple statistical extension of the autoencoder
- Excellent generative models for the distribution of data $P(x)$
	- Various extensions such as Conditional VAEs, which model conditional distributions, such as $P(x|y)$
		- Straight-forward extension where the conditioning variable y is an additional input to the encoder and decoder
- Read the literature on the topic, it is vast

VAE limitations

- The decoder is not generally invertible
-
- The decoder is not generally invertible

 Cannot get a closed form for $P(z|X)$

 This requires an Encoder that *approximates* $P(z|X)$

 Solution: "**Normalizing flow models**" Invertible

decoders that give you close decoders that give you closed forms for $P(z|X)$

VAE limitations

Next Class!

- The decoder must transform a standard Gaussian all the way to the target distribution in one step
	- This is often too large a gap
	-
- - - Whose seed model is a VAE
			-

» …

