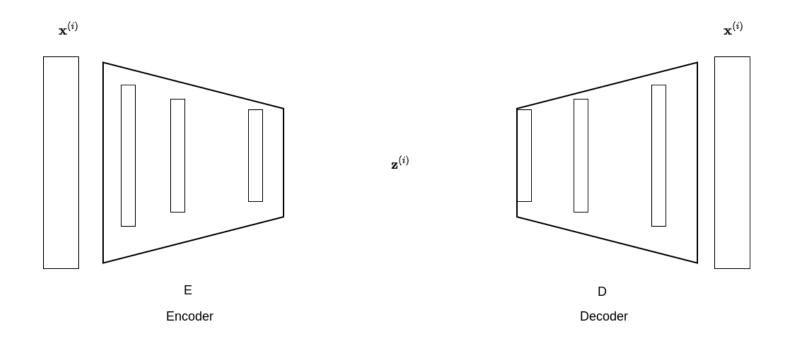
AutoEncoder (AE): High Level

TL;DR

- The Deep Learning analog of Principal Components (PCA)
 - Most of the lessons of AE apply equally to PCA
- Unsupervised: no labels (really semi-supervised)
- Create "synthetic features" from the original set of features
- May be able to use reduced set of synthetic features (dimensionality reduction)
- Generative (vs Discriminative)



An Autoencoder network has two parts

- An Encoder, which takes input x and "encodes" it into z
- A Decoder, which takes the encoding z and tries to reproduce x

Each part has its own weights, which can be discovered through training, with examples

•
$$\langle \mathbf{X}, \mathbf{y} \rangle = \langle \mathbf{X}, \mathbf{X} \rangle$$

That is: we are asking the output to be identical to the input.

z is an alternative latent representation of x.

- Encoded by the Encoder
- Inverted by the Decoder

But when the dimension of z is less than the dimension of x.

- z is a bottle-neck
- the inversion by the Decoder will be imperfect

z becomes a reduced-dimensionality approximation of x.

This is reminiscent of the dimensionality reduction of Principal Components Analysis (PCA).

The main difference from PCA

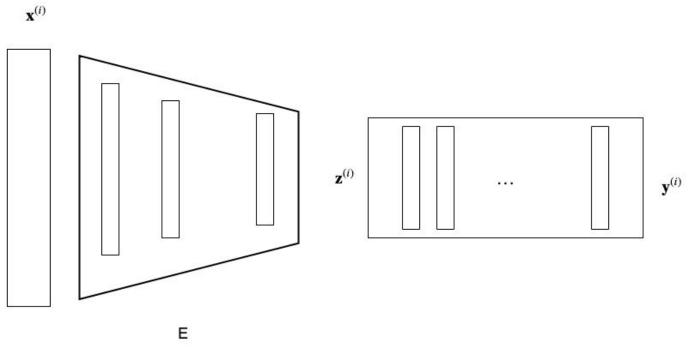
- PCA uses a linear transformation
- NN can use non-linear transformations too
 - PCA as a special case of AE

Autoencoders: Uses

Dimension reduction

After training

- we can discard the Decoder
- use the Encoder output (synthetic features) as reduced dimension inputs to a new task
 - Encoder weights are frozen: non-learnable when training new task
 - \circ It may be easier to solve the new task given ${f z}$ rather than ${f x}$
 - have already discovered "structure" of x
 - Transfer Learning



Encoder with non-learnable weights

New head

In PCA, we eliminated original features that were "less important"

- i.e., explained variation among only a small fraction of the training set
 - recall how we re-denominated explained variance in terms of "number of features"

There is no direct similar concept of feature importance in AE

• other than minimizing a Loss function, which *may* wind up focusing on "important" features

Layer-wise pre-training with Autoencoders

Autoencoders played a vital role in the development of Deep Learning:

- They made it possible to train otherwise untrainable NN's.
- Other innovations supplanted the need for AE's to assist training
 - better initialization
 - better activations functions
 - normalization

Although they are no longer needed for that purpose, it is interesting to see how (and why) they were used.

For a NN with $oldsymbol{L}$ layers that solves a Supervised Learning Problem

- Training attempts to learn the weights of all layers simultaneously
- Layer wise pre-training was an attempt
 - to initialize the weights of each layer
 - in succession
 - so that the task of simultaneously solving for optimal weights had a better chance of succeeding

The idea was to learn an initialization of $\mathbf{W}_{(l)}$, the weights of layer l

ullet After having learned initializations for the weights $\mathbf{W}_{(l')}$ for all layers l' < l.

by creating an Autoencoder from a prefix of the model.

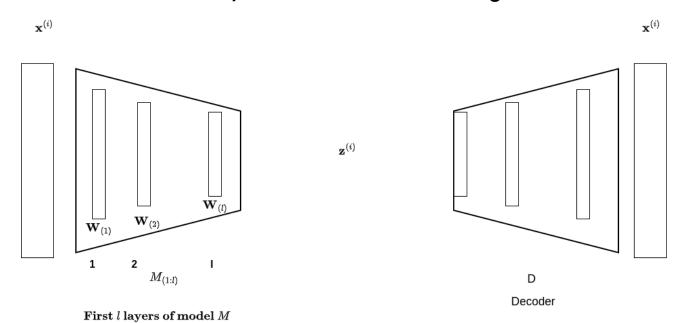
Suppose $oldsymbol{M}$ is a model (sequence of $oldsymbol{L}$ layers plus a head).

Let $M_{\!(1:l)}$ denote the submodel of M consisting of only the first l layers

In order to learn an initialization of $\mathbf{W}_{(l)}$, the weights of layer l

- ullet Create an Autoencoder model $M_{
 m AE}$
- ullet by appending another model (sequence of layers) $oldsymbol{D}$ called the *Decoder* to $M_{(1:l)}$
 - lacksquare the shape of the outputs of D is set to the shape of inputs ${f x}$ of model M

Layerwise Initialization of Weights of model M



We train $M_{\! m AE}$ with an Autoencoder objective

- mapping input $\mathbf{x} \in \mathbf{X}$ to \mathbf{x}
- ullet training set for $M_{\!\!
 m AE}$ is $\langle {f X},{f X}
 angle$

Note that the labels $y^{(i)}$ were not used!

The idea is

- initialization by random weights may not lead to convergence
- The hope is that *any* non-random initialization increases the chance of convergence
- The way to get non-random weights is to train layers of the model with *some* Supervised Learning objective
- Here we use the Autoencoder objective
 - Non-trivial is there is a bottleneck layer of reduced dimension
 - lacktriangle No relationship between f x and f y is entailed
 - \circ Only relationships among members of ${f X}$

Autoencoders and Transfer Learning

Today, autoencoders are useful for another purpose: Transfer Learning.

If we can train an AE network to create features that are useful for reconstruction

it is possible that these features are useful for solving more complicated tasks.

This was in essence what

- Our dimension reduction example (replace the head) was doing
- Layerwise Pre-training was attempting.

So it is not uncommon to approach a complicated problem
 by first constructing an autoencoder to come up with an alternate (and smaller) representation of the input space.

Note that Autoencoders are *unsupervised*: they don't take labels.

So the encodings they produce stress syntactic similarity, rather than semantic

similarity.

Their use in Transfer Learning depends on the hope that inputs that are syntactically similar also have the same labels.

Denoising

Very much like dimension reduction but with the assumption that

• "less important" features are just random noise that is added to the true example

Autoencoder: Denoising

 $\mathbf{x}^{(i)} + \mathrm{noise}$ $\mathbf{x}^{(i)}$

Generative Artificial Intelligence

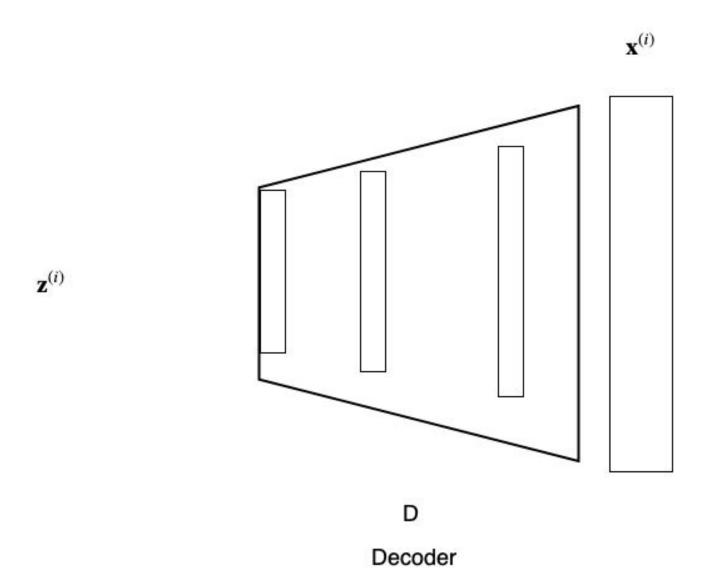
A less obvious use of AE (using the Decoder rather than the Encoder) is to generate examples.

Most of the Machine Learning we have studied thus far is discriminative

- $p(\hat{\mathbf{y}}^{(i)}|\mathbf{x}^{(i)}))$
 - e.g., classifier: discriminate among the possible classes $\mathbf{y^{(i)}}$, given example $\mathbf{x^{(i)}}$

We can use the Decoder on arbitrary z to generate a completely new x:

- $p(\mathbf{x}^{(i')}|\mathbf{z}^{(i')})$ for some i' not in training
- ullet generate a new example $oldsymbol{i'}$, in the domain of ${f x}$, that was not encountered during training



Autoencoder (AE): Details

The task that trains an Autoencoder

- Given input $\mathbf{x^{(i)}}$
- Output of Encoder: $\mathbf{z^{(i)}} = E(\mathbf{x^{(i)}})$
- ullet Output of Decoder: $\mathbf{ ilde{x}^{(i)}} = D(\mathbf{z^{(i)}})$
- "Target": **x**⁽ⁱ⁾

Both the Encoder and Decoder are parameterized (learnable parameters)

• Goal: find the parameters such that

$$ilde{\mathbf{x}}^{(\mathrm{i})} = D(E(\mathbf{x})) pprox \mathbf{x}$$

 $\mathbf{z^{(i)}} = E(\mathbf{x^{(i)}})$ is the latent representation of $\mathbf{x^{(i)}}$.

Loss function

The obvious loss functions compare the original $\mathbf{x^{(i)}}$ and reconstructed $\mathbf{\tilde{x}^{(i)}}$ feature by feature:

Mean Squared Error (MSE)

$$\mathcal{L}^{(\mathrm{i})} = \sum_{j=1}^{|\mathrm{x}|} (\mathrm{x}_j^{(\mathrm{i})} - ilde{\mathrm{x}}_j^{(\mathrm{i})})^2$$

Binary Cross Entropy

For the special case where *each* original feature is in the range $[\mathbf{0},\mathbf{1}]$ (e.g., an image)

$$\mathcal{L}^{(\mathrm{i})} = \sum_{j=1}^{|\mathrm{x}|} \left(\mathrm{x}_j^{(\mathrm{i})} \log(ilde{\mathrm{x}}_j^{(\mathrm{i})}) + (1-\mathrm{x}_j^{(\mathrm{i})}) \log(1- ilde{\mathrm{x}}_j^{(\mathrm{i})})
ight)$$

Variational Autoencoder (VAE): Generative ML

Observe that the Decoder part of the "vanilla" AE $D(\mathbf{z^{(i)}})$

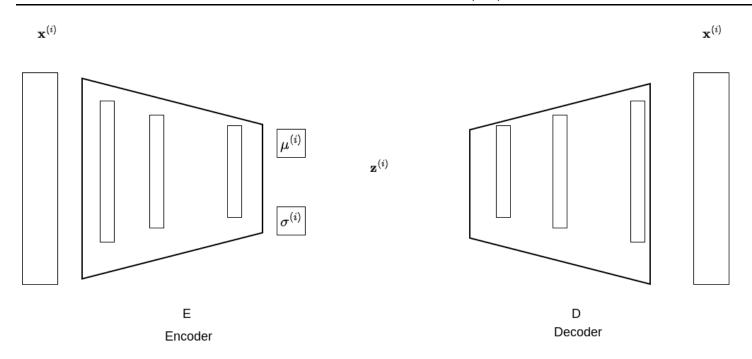
- has been trained to produce "realistic" $ilde{\mathbf{x}}^{(\mathrm{i})}$ only for a $\mathbf{z}^{(\mathrm{i})} = m{E}(\mathbf{x}^{(\mathrm{i})})$
 - i.e., "realistic": appears to come from the distribution of training ${f X}$
- ullet there is no guarantee that $m{D}(\mathbf{z}^{(i')})$ for some $m{i'}$ not in training is realistic

That is: the AE has not been trained to extrapolate beyond the training inputs.

A VAE is able generate outputs

- that could have come from the training distribution from a latent representation $\mathbf{z}^{(i')}$
- but that did not come from X.

Our goal is constructing a Decoder that can extrapolate.



The Decoder will take a *latent vector* ${f z}$ and produce $D({f z})$, just as in a vanilla AE.

The difference is that z will be sampled from a distribution rather than being a unique mapping of a training example.

This will be done by modifying the Encoder

- It will indirectly create $\mathbf{z}^{(i)}$
- It will compute variables $\mu^{(\mathrm{i})}$ and $\sigma^{(\mathrm{i})}$
 - $oldsymbol{z^{(i)}}$ will be *sampled* from a distribution with mean $oldsymbol{\mu^{(i)}}$ and standard deviations $oldsymbol{\sigma^{(i)}}$

As long as ${\bf z}$ is sampled from this distribution, the decoder will produce a "realistic" output.

Note

 μ and σ are

- vectors
- computed values (and hence, functions of x) and not parameters so training learns a function from $x^{(i)}$ to $\mu^{(i)}$ and $\sigma^{(i)}$

To train a VAE:

- ullet pass input $\mathbf{x^{(i)}}$ through the Encoder, producing $oldsymbol{\mu^{(i)}, \sigma^{(i)}}$
 - use $\mu^{(i)}, \sigma^{(i)}$ to sample a latent representation $\mathbf{z}^{(i)}$ from the distribution
- ullet pass the sampled $\mathbf{z^{(i)}}$ through the decoder, producing $oldsymbol{D(\mathbf{z^{(i)}})}$
- ullet measure the reconstruction error $\mathbf{x^{(i)}} m{D(z^{(i)})}$, just as in a vanilla AE
- ullet back propagate the error, updating all weights and μ, σ

Essentially, each input $\mathbf{x^{(i)}}$ has many latent representations (with different probabilities): any sample from the distribution.

Training

Encoder produces

$$E(\mathbf{x}) = q_{\phi}(\mathbf{z}|\mathbf{x}) pprox p_{ heta}(\mathbf{z}|\mathbf{x})$$

We sample from

$$\hat{\mathbf{z}} \sim q_{\phi}(\mathbf{z}|\mathbf{x})$$

Decoder produces

$$D(\hat{\mathbf{z}}) = p_{\theta}(\mathbf{x}|\mathbf{z})$$

Each time (epoch) that we encounter the same training example, we select another random element from the distribution.

So the VAE learns to represent the same example from multiple latents.

Generative

- sample $\hat{\mathbf{z}} \sim \hat{p}(\mathbf{z})$
- ullet use Decoder to produce output $p_{\! heta}(\mathbf{x}|\mathbf{z})$

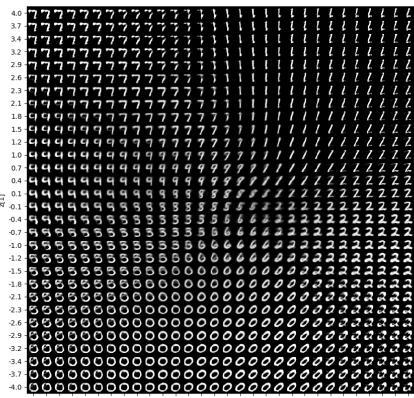
This means we can feed in a z

- that doesn't correspond to any training example
- and perhaps get an output that *resembles* something from the training set, rather than noise.

To give you an idea of the generative nature of the VAE, consider

- Creating latent vectors **z** from scratch
 - not as the output of the Encoder
- Varying these latent vectors systematically and examining the output created by the Decoder

MNIST clustering produced by a VAE



Note that the outputs

- are not instances of any examples
- There was no guarantee that a random z would produce something that looked like a digit!

We may even be able to interpret the elements of z

- **z**₀: control slant?
 - See the bottom row of 0's
- **z**₁: control "verticality"?
 - See right-most column

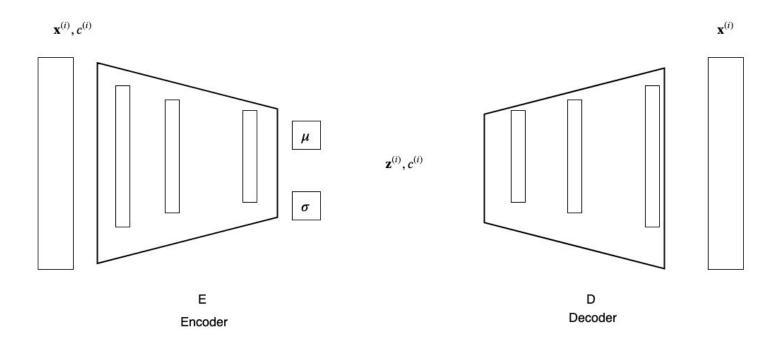
Conditional VAE

Once a VAE is trained, D(z) should produce a realistic output, for any z from the distribution.

However, if the distribution of X includes examples from many classes

- Assuming we have labels as auxilliary information (not used in training)
 - e.g., the 10 digits
- The VAE can't control which class the output will come from

A Conditional VAE allow our generator (Decoder) to control the class c of the output $\tilde{\mathbf{x}}$.



The class label c

- is given as part of training
 - So the Encoder produces a distribution that is conditioned on both ${\bf x}$ and ${m c}$.
- is an additional parameter of the Decoder
 - So the output class can be controlled

$$ilde{\mathbf{x}}^{(\mathrm{i})} = oldsymbol{D}(\mathbf{z}^{(\mathrm{i})}, oldsymbol{c})$$

So now we

- create a latent z
- ullet append a class label c
- and presumably have the decoder produce an output from the desired class.
- ullet The encoding distribution is now conditional on class label c: $q_\phi(z|x,c)$
- ullet So is the decoding distribution $p_{ heta}(x|z,c)$

Again, by restricting the functional form of the prior distribution \hat{p} we can simplify the math.

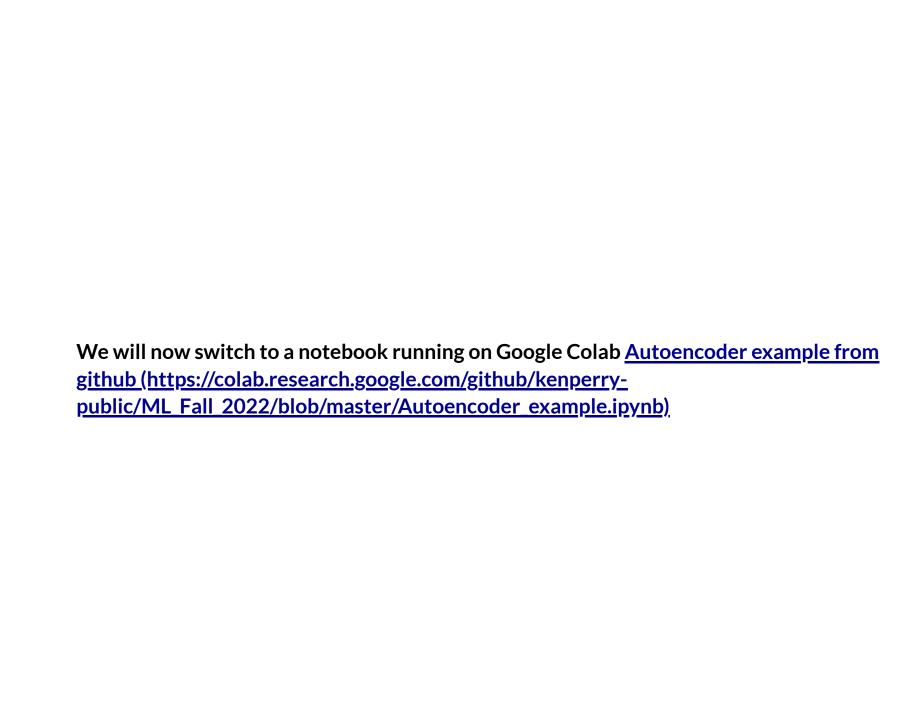
Detour: Autoencoder notebook on Colab

Let's examine some Keras code that implements several types of Autoencoders

- Vanilla
- Denoising
- VAE

We will write our AE's using the Keras Functional API rather than the Sequential model

- We could write the complete AE using the Sequential API
- But
- we want to extract the Encoder and Decoder parts as *separate models*
- we can do this with the Functional API



VAE derivation: Probabilistic formulation

Note: Advanced material

Let's pretend: we don't already know that we will represent ${f z}$ as a function of $\mu_{ heta}({f x})$ and $\sigma_{ heta}({f x})$

this derivation will show why we made that choice

The mathematical derivation of a VAE is quite detailed

- it is interesting but not absolutely necessary to understand
- this is where we define the Loss function

The interested reader is referred to a highly recommended <u>VAE tutorial</u> (<u>https://arxiv.org/pdf/1606.05908.pdf</u>).

We will try to give the essence in the following slides.

TL;DR

- The VAE has a very interesting two part Loss Function
 - Reconstruction Loss, as in the Vanilla AE
 - Divergence Loss
- The Reconstruction Loss is not sufficient
 - Issues of intractability arise
 - The Divergence Loss skirts intractability
 - By constraining the Encoder to produce a tractable distribution

We can state our goal as

- ullet Producing $\hat{f X}^{(i')}$ that comes from the same distribution as training examples f X
- But are non-deterministic
 - lacksquare some $\mathbf{\hat{X}}^{(i')}$ are not exactly equal to $\mathbf{X}^{(\mathbf{i})}$ for any $1 \leq i \leq m$

That is: we want to generate new examples that are similar (but not identical) to the training examples \mathbf{X} .

Let $p(\mathbf{X})$ denote the probability distribution of training examples \mathbf{X} .

Note that $p(\mathbf{X})$ is an *empirical* distribution define by the finite set \mathbf{X}

• We do not have a *closed form* expression for the distribution

One way to conceive of achieving the goal is to condition $p(\mathbf{X})$ on a random variable \mathbf{z} and generate a synthetic example based on the random value $p(\mathbf{X}|\mathbf{z})$

We will use a Neural Network with weights $m{ heta}$ to compute $m{p}_{\! heta}(\mathbf{X}|\mathbf{z})$

VAE derivation: 1

$$\mathbf{ ilde{x}}^{(i)} = \int_{\mathbf{z}} p_{ heta}(\mathbf{x}|\mathbf{z}) q(\mathbf{z})$$

Decoder

Let's try to create an optimization objective function against which we choose our model weights.

We will use Maximum Likelihood as the objective

- Given the weights: how likely is the model to produce the training distribution \mathbf{X} ?
- ullet Recall that the likelihood of the set ${f X}$ is the product of the probabilities that the model produces each ${f x}\in {f X}$
- So the log likehood is the sum of the log probabilities

Since our practice is to minimize Loss (rather than maximize an objective function) we write our loss as (negative of log) likelihood

$$\mathcal{L} = -\log(p(\mathbf{X}))$$

Minimizing \mathcal{L} is equivalent to maximizing likelihood.

Because the generation of \hat{x} depends on a random variable z we marginalize x over z

$$p(\mathbf{x}) = \int_{\mathbf{z} \in Q} p(\mathbf{x}|\mathbf{z}) \; p(\mathbf{z})$$

where random z comes from (as of yet unknown) distribution Q.

That is: there are potentially many (and at least one) random choice that produces approximations of any training example.

We want to train a Neural Network to produce randomized examples that are similar to examples in ${\bf X}.$

This means that, for each example in ${f X}$, we have to sample from ${f p}({f z})$

Some obvious concerns

- ullet It may be very expensive to draw many samples from $oldsymbol{Q}$ for each training $oldsymbol{\mathbf{x}}$
- ullet Moreover: It is likely that that there are many random choices from $oldsymbol{Q}$
 - lacksquare for which the generated $p_{\!\scriptscriptstyleoldsymbol{\Theta}}(\mathbf{x}|\mathbf{z})$
 - lacktriangle is unlike any example in ${f X}$

Let's address these concerns by considering the joint distribution of ${f X}$ and ${f z}$ $p({f x},{f z})$

(from which we can compute $p(\mathbf{z}|\mathbf{x})$ via Bayes formula)

We can improve our sampling by considering only those choices of ${\bf z}$ that could generate ${\bf x}$ and re-write the objective as

$$p(\mathrm{x}) = \int_{\mathrm{z} \in p(\mathrm{z}|\mathrm{x})} \!\! p(\mathrm{x}|\mathrm{z}) \; p(\mathrm{z})$$

The problem is that $p(\mathbf{z}|\mathbf{x})$ is intractable!

- ullet The examples in ${f X}$ are deterministic: they were not produced using a random ${f z}$
 - lacksquare lacksquare is defined as an empirical distribution, i.e., the training examples
 - which weren't conditioned on **z**
 - So we have *no data* on which to infer a joint distribution
- ullet So we don't know the joint distribution $p(\mathbf{x},\mathbf{z})$ or the conditional distribution $p(\mathbf{z}|\mathbf{x})$

The solution is *approximate* the intractable $p(\mathbf{z}|\mathbf{x})$ with a tractable $q_{\Phi}(\mathbf{z}|\mathbf{x})$

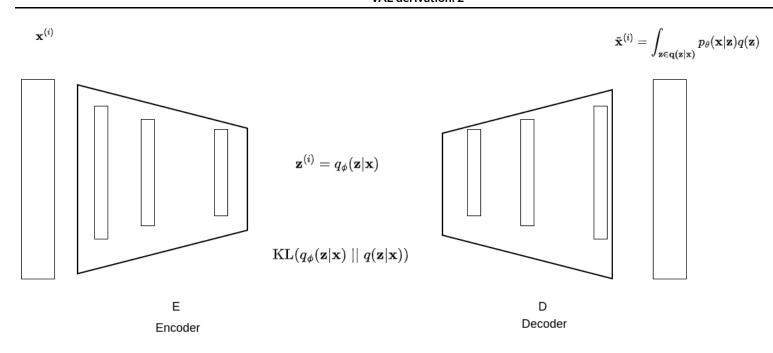
- That is computed by a Neural Network (the "Encoder")
- We will learn this distribution (parameterized by Φ) by training on X.

We need this approximate distribution $q_{\Phi}(\mathbf{z}|\mathbf{x})$ to be as close to the true distribution $p(\mathbf{z}|\mathbf{x})$ as possible.

That is: Using KL divergence as a measure of the difference between two distributions, we want to minimize

$$ext{KL}(q_{\Phi}(ext{z}| ext{x}) \mid\mid p(ext{z}| ext{x}))$$

VAE derivation: 2



Note that prior to the need to approximate $p(\mathbf{z}|\mathbf{x})$, there was only a Decoder in our formulation of a goal of producing $\hat{\mathbf{X}}$ similar to true \mathbf{X} !

The Encoder (i.e., the Neural Network producing $q_{\Phi}(\mathbf{z}|\mathbf{x})$) arose

- ullet Out of the need to compute $p(\mathbf{z}|\mathbf{x})$
- Rather than a priori design considerations

We add the KL divergence to our loss function

$$egin{array}{lll} \mathcal{L} &=& -\log(p_{ heta}(extbf{x})) + ext{KL}(q_{\Phi}(extbf{z}| extbf{x}) \mid\mid p(extbf{z}| extbf{x})) \ &=& \mathcal{L}_R + \mathcal{L}_D \end{array}$$

which now has two objectives

- Reconstruction loss \mathcal{L}_R : maximize the likelihood (by minimizing the negative likelihood)
- Divergence constraint \mathcal{L}_D : $q_\phi(\mathbf{z}|\mathbf{x})$ must be close to $p_\theta(\mathbf{z}|\mathbf{x})$

$$egin{array}{lll} \mathcal{L}_R &=& -\log(p_{ heta}(\mathbf{x})) \ \mathcal{L}_D &=& \mathrm{KL}\left(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}|\mathbf{x})
ight) \end{array}$$

We will show (in the next section: lots of algebra!) that the loss can be re-written as

$$\mathcal{L} = -\mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\log(p_{\Theta}(\mathbf{x}|\mathbf{z}))) + \mathrm{KL}(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}))$$

This is almost identical to our original express for \mathcal{L} except

- Re-write $\log(p_{ heta}(ext{x})) = \mathbb{E}_{z \sim q_{ heta}(ext{z}| ext{x})}(\log(p_{\Theta}(ext{x}| ext{z})))$
- the KL term becomes

$$\mathrm{KL}\left(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z})
ight)$$

rather than the original

$$\mathrm{KL}\left(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}|\mathbf{x})
ight)$$

The purpose of re-writing: replace intractable $p(\mathbf{z}|\mathbf{x})$ with a tractable $p(\mathbf{z})$!

So we can have a Loss function with which we can train!

Advanced: Obtain ${\mathcal L}$ by rewriting ${ m KL}(q_{\Phi}({f z}|{f x}) \mid\mid p({f z}|{f x})$

Let's derive a simpler expression for ${\cal L}$ by manipulating ${
m KL}(q_\Phi({f z}|{f x}) \mid\mid p_\Theta({f z}|{f x}))$:

$$egin{array}{lll} \mathrm{KL}(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}|\mathbf{x})) &=& \sum_{z} q_{\Phi}(\mathbf{z}|\mathbf{x}) (\log(q_{\Phi}(\mathbf{z}|\mathbf{x}) - \log(p(\mathbf{z}|\mathbf{x})) \ &=& \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})} (\log(q_{\Phi}(\mathbf{z}|\mathbf{x}) - \log(p(\mathbf{z}|\mathbf{x}))) \ &=& \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})} (\log(q_{\Phi}(\mathbf{z}|\mathbf{x})) \ &-& (\log(p(\mathbf{x}|\mathbf{z})) + \log(p(\mathbf{z})) - \log(p(\mathbf{x}))) \end{array}$$

$$egin{array}{lll} \mathrm{KL}(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}|\mathbf{x})) &=& \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\ \log(q_{\Phi}(\mathbf{z}|\mathbf{x})) - (\log(p_{\Theta}(\mathbf{x}|\mathbf{z})) + \log(p_{\Theta}(\mathbf{x}|\mathbf{z})) + \log(p_{\Theta}(\mathbf{z}|\mathbf{x})) - & = & \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\ \log(p_{\Theta}(\mathbf{x}|\mathbf{z})) + (\ \log(q_{\Phi}(\mathbf{z}|\mathbf{x})) - & = & -\mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\log(p_{\Theta}(\mathbf{x}|\mathbf{z}))) + \mathrm{KL}(q_{\Phi}(\mathbf{z}|\mathbf{x}) \mid\mid p(\mathbf{z}|\mathbf{x})) + & \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\log(p_{\Theta}(\mathbf{x}|\mathbf{z}))) + & \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\log(p_{\Theta}$$

The key step:

Using Bayes Theorem to re-write

$$\log(q_{\Phi}(\mathbf{z}|\mathbf{x})$$

as

$$\log(p(\mathrm{x}|\mathrm{z})) + \log(p(\mathrm{z})) - \log(p(\mathrm{x}))$$

- ullet This allows us do away with intractable conditional probability $q_{\Phi}(\mathbf{z}|\mathbf{x})$
- In favor of unconditional probability $p(\mathbf{z})$

The LHS cannot be optimized via SGD (recall the tractability issue with $m{p}(\mathbf{z}|\mathbf{x})$).

But the RHS can be made tractable giving a tractable choice of $p(\mathbf{z})$.

Choosing $p(\mathbf{z})$

So what distribution should we use for the prior p(z)?

- It should be differentiable, since we use Gradient Descent for optimization
- It should be tractable with a closed form (such as a normal)
- If we choose $p(\mathbf{z})$ as normal, we can require $q_\phi(\mathbf{z}|\mathbf{x})$ to be normal too
 - The KL divergence between two normals is an easy to compute function of their means and standard deviations.
 - See <u>VAE tutorial (https://arxiv.org/pdf/1606.05908.pdf)</u> Section 2.2

Re-parameterization trick

There is still one impediment to training.

It involves the random choice of $\mathbf{z} \sim q_{\Phi}(\mathbf{z}|\mathbf{x})$ in

$$\mathcal{L}_R = \mathbb{E}_{z \sim q_{\Phi}(\mathbf{z}|\mathbf{x})}(\log(p_{\Theta}(\mathbf{x}|\mathbf{z})))$$

This is not a problem in the forward pass.

But in the backward pass we need to compute

$$rac{\mathcal{L}_R}{\partial \mathbf{\Theta}}$$

How do we back propagte through a random choice?

The "reparameterization trick" redefines the random choice ${\bf z}$ as

$$egin{array}{lll} \mathbf{z} &=& \mu_{ heta}(\mathbf{x}) + \sigma_{ heta}(\mathbf{x}) * \epsilon \ \epsilon &\sim & p(\mathbf{z}) \end{array}$$

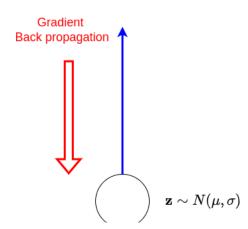
In this formulation, the random variable ϵ appears in a product term

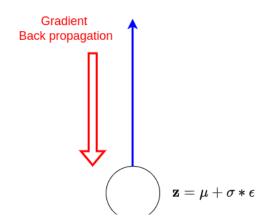
- We can differentiate the product with respect to Θ
- ϵ can be treated as a constant in $\frac{\partial \epsilon}{\partial \Theta}$

The Encoder design is now to produce (trainable parameters) $\mu_{\Theta}, \sigma_{\Theta}$

And z indirectly

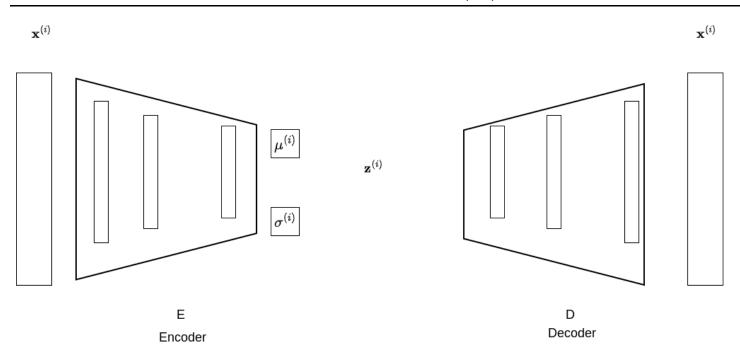
Reparameterization trick





This gets us to the final picture of the VAE:

Variational Autoencoder (VAE)



ELBo (Evidence-based Lower Bound)

By re-writing the Loss, we removed the intractable term $m{p}(\mathbf{z}|\mathbf{x})$

It turns out that even this may not be necessary.

For the truly interested reader:

- The derivation uses a method known as *Variational Inference*. See this <u>blog</u> (https://mbernste.github.io/posts/variational_inference/) for a summary.
- ullet One can show that loss $oldsymbol{\mathcal{L}}$ is equal to -1 times the *ELBo* (Evidence Based Lower Bound)

So if one knows how to maximize the <u>ELBo (https://mbernste.github.io/posts/elbo/)</u>, one can minimize the loss.

Loss function: discussion

Let's examine the role of \mathcal{L}_R and \mathcal{L}_D in the loss function \mathcal{L} .

- What would happen if we dropped \mathcal{L}_D ?
 - We would wind up with a deterministic z and collapse to a vanilla VAE
- What would happen if we dropped \mathcal{L}_R ?
 - ullet the encoding approximation $q_{\Phi}(\mathbf{z}|\mathbf{x})$ would be close to the empirical $p(\mathbf{z}|\mathbf{x})$ in distribution
 - but two variables with the same distribution are not necessarily the same?
 - \circ e.g., get a distribution $m{p}$ by flipping a coin
 - \circ let distribution $m{q}$ be a relabelling of $m{p}$ by changing Heads to Tails and vice-versa
 - \circ $m{p}$ and $m{q}$ are equal in distribution but clearly different

```
In [3]: print("Done")
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Done