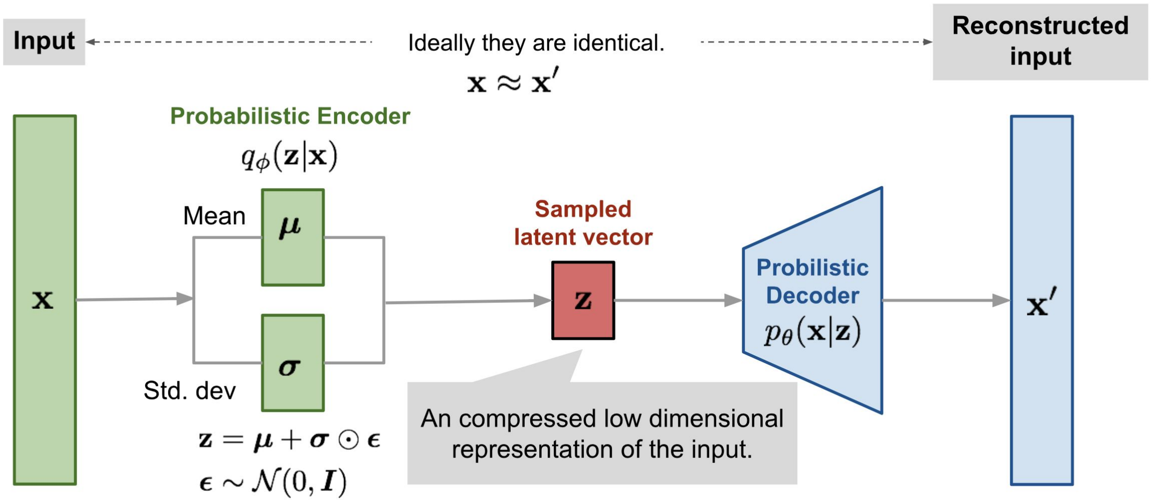
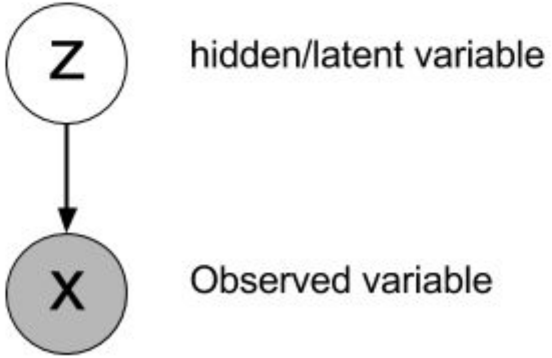
Variational Autoencoders



We understand AE. What is Variational AE?

- Basically a AE, but a generative model
  - The encoder parameterizes a **distribution** and not just a point estimate
    - Hence, **probabilistic non-linear dimensionality reduction**
  - Decoder takes a latent variable, then *generates* an output
- Main hypothesis
  - There is a latent variable *z* which can be used to ge
  - This variable explains the main sources of variation in our data
  - We can incorporate a prior for this *z* as a regularization objective
- What is **variational**? we will cover this soon.



Hidden representation = Latent variable?

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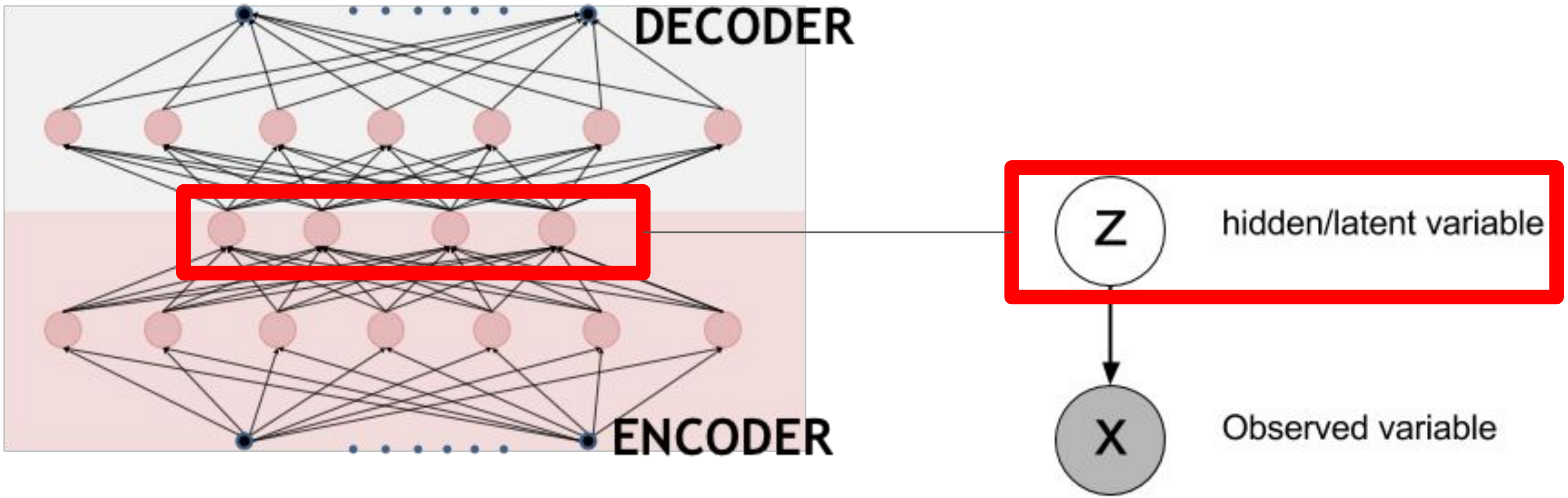
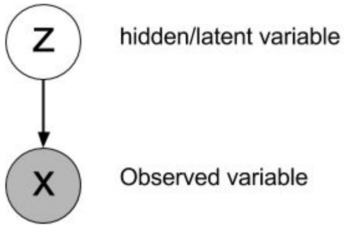


Hidden representation = Latent variable.



- Latent variables
- Hidden representation - a representation that captures the lower dimensional signals that **explain** the data best
  - Data can be explained by a couple of factors of variation
    - E.g. in images - cats/dogs vs book/pen → what if we had a hidden neuron that encoded “has a leg”
    - Or in MNIST → a hidden neuron that encodes “has a loop”
  - Main idea in PCA - project it to a space where only a couple of dimensions explain most of the data

Bayes

Recap of Bayes theorem

Prior $P(z)$: How likely is a certain value of the latent variable z?

Likelihood $P(X|z)$: Given a certain value of z, how likely is a data point? (e.g. image)

Posterior $P(z|X)$: Given a datapoint, what is the probability of a latent variable?

Bayes theorem: $$P(z|X) = \frac{P(X|z)P(z)}{P(X)}$$

https://blog.evjang.com/2016/08/variational-bayes.html

Bayes

Recap of Bayes theorem

Prior $P(z)$: Let's choose this to be a simple distribution - standard Gaussian.

Likelihood $P(X|z)$: Let's call this the decoder part of our network. We can easily parameterize this.

Posterior $P(z|X)$: We **try** to do this in the encoder part of our network.

https://blog.evjang.com/2016/08/variational-bayes.html

Bayes

Bayes theorem: $$P(z|X) = \frac{P(X|z)P(z)}{P(X)}$$

$$P(z|X) = \frac{P(X|z)P(z)}{\boxed{\int_z P(X|z)P(z)dz}} \qquad P(z|X) = \frac{P(X|z)P(z)}{\boxed{\sum_z P(X|z)P(z)}}$$

All values of *z* → All real values!

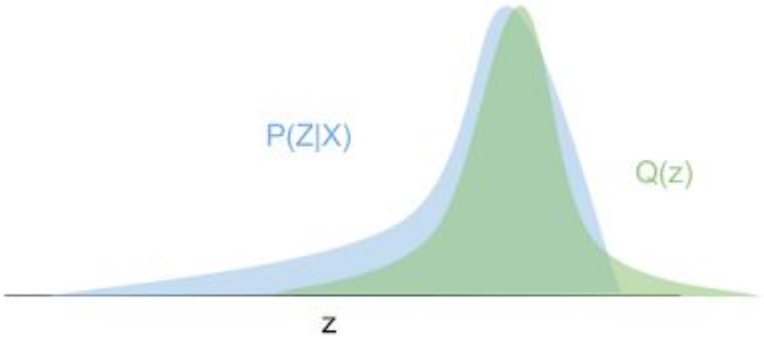
- How is it even possible to compute this integral/sum? It's not, its intractable

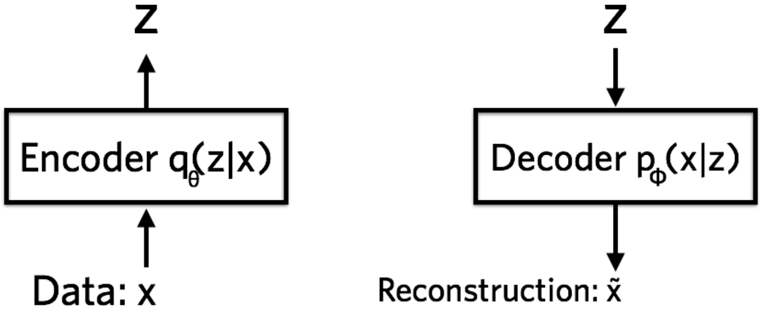
Variational Bayes

We want another distribution to approximate the posterior - which is hard to compute. $Q(Z)$ to approximate $P(Z|X)$

How can we know this distribution is a good approximation?

KL-divergence: $$KL(Q(Z)||P(Z|X)) = \sum_{z \in Z} Q(z|x) \log \frac{Q(z|x)}{P(z|x)}$$





What is KL divergence

A way to measure dissimilarity between two probability distributions, based on information theory.

Consider entropy: $$H(x) = -\sum_x P(x) \log P(x)$$

KL divergence - many, many interpretations

- Number of bits of information lost if we use distribution *q* to represent *p*
- Negative log likelihood that samples generated by distribution *p* has been generated by *q*

Interesting reading here.

Note: KL divergence is always positive!

KL-divergence of variational distribution Q

$$KL(Q_\phi(Z)||P(Z|X)) = \sum_{z \in Z} q_\phi(z|x) \log \frac{q_\phi(z|x)}{p(z|x)}$$

Forward KL

This decomposes through a lot of math (which you can look up [here](#)) to

$$\boxed{\log P(X)} - \underbrace{\boxed{\Big(\mathbb{E}_Q\big[\log P(x|z)\big] - KL(Q(Z|X)||P(Z))\big]\Big)}}_{\mathcal{L}}$$

- Log Likelihood of data (we want to maximize this!)
  - maximizing P(x) ⇒ having some parameterization of the probability distribution our data that best **explains our data**
- This is called the **Variational Lower Bound**

Maximizing the Variational Lower Bound?

Simple rearranging from before, we get

$$P(x) = \mathcal{L} + KL(Q||P)$$

KL-divergence is always > 0 - its like an error term.

Hence $\mathcal{L}$ is the **lower bound.** So… the more you increase $\mathcal{L}$, the better you describe your data, because P(x) increases.

Also, when is this bound **tight?** When Q(z) = P(z|x) and the KL-divergence term is 0 (or close to 0). Thus, the better your Q, the better you are able to train your model.

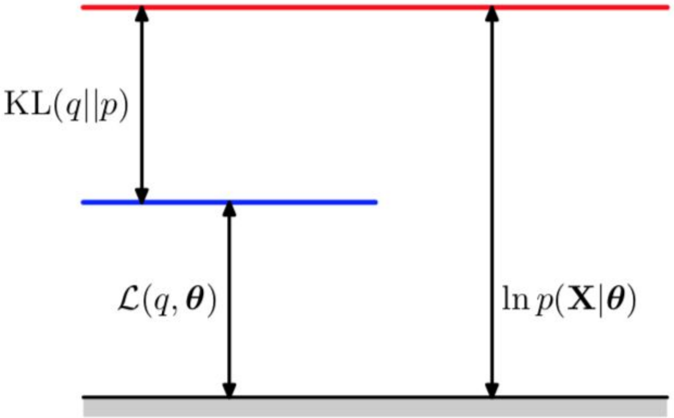
Decomposing the variational lower bound

$$\mathbb{E}_Q\big[\log P(x|z)\big] - KL(Q(Z|X)||P(Z))$$

(negative) Reconstruction Error Regularization

- Reconstruction Error:
  - In traditional autoencoders we use L2 loss
  - With binary data, here, it turns out to Binary Cross Entropy loss
  - What about real valued data? We can say P(x | z) is a Gaussian distribution.
- Regularization term:
  - You don't want the latent variable values to be all over the place
  - Basically, without this term, this is as good as a normal AE.
  - Centered around 0 is a good place to start
    - However, this does not always work well. What if the latent structure of the data was actually a circle (or hypersphere in higher dimensions)?
    - We need to consider other priors

EM … looks familiar?



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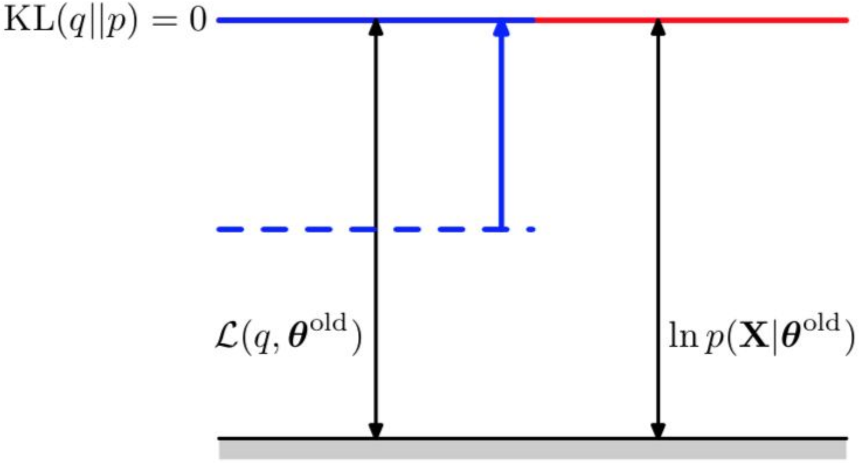
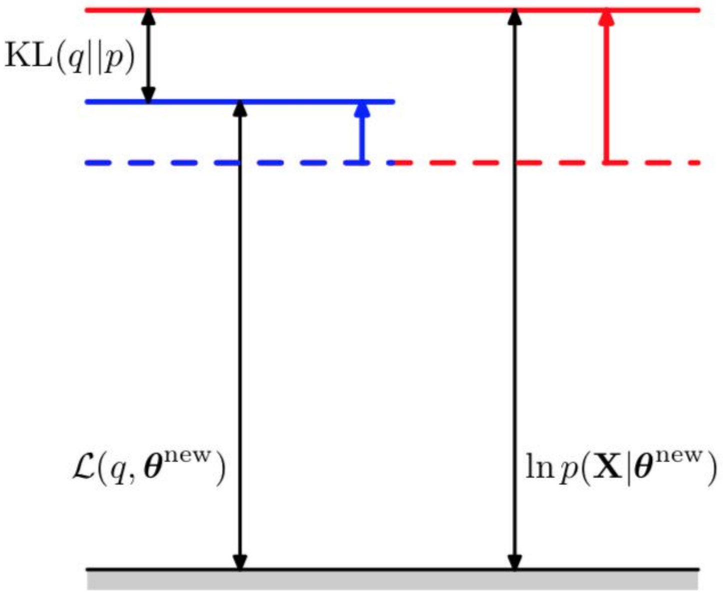


EM … looks familiar?



How do we actually train it?

We want to maximize the variational lower bound.

$$\mathbb{E}_Q\big[\log P(x|z)\big] - KL(Q(Z)||P(Z))$$

Which means the negative of this is our loss function.

$KL(Q(Z)||P(Z))$ is just a deterministic function (Gaussian Q, Gaussian prior for P)

$\mathbb{E}_Q\big[\log P(x|z)\big]$ can be computed *empirically*. That is, sample a bunch of z values, calculate log P(x|z) using those sampled z, and take an average. In the paper, the authors just take 1 sample.

But how is sampling differentiable?

Reparameterization trick

Sampling from a distribution $\mathcal{N}(\mu, \sigma^2)$ itself is not a differentiable operation.

But, due to the nice properties of Gaussian distributions, we can first sample

$\epsilon \sim \mathcal{N}(0,1)$

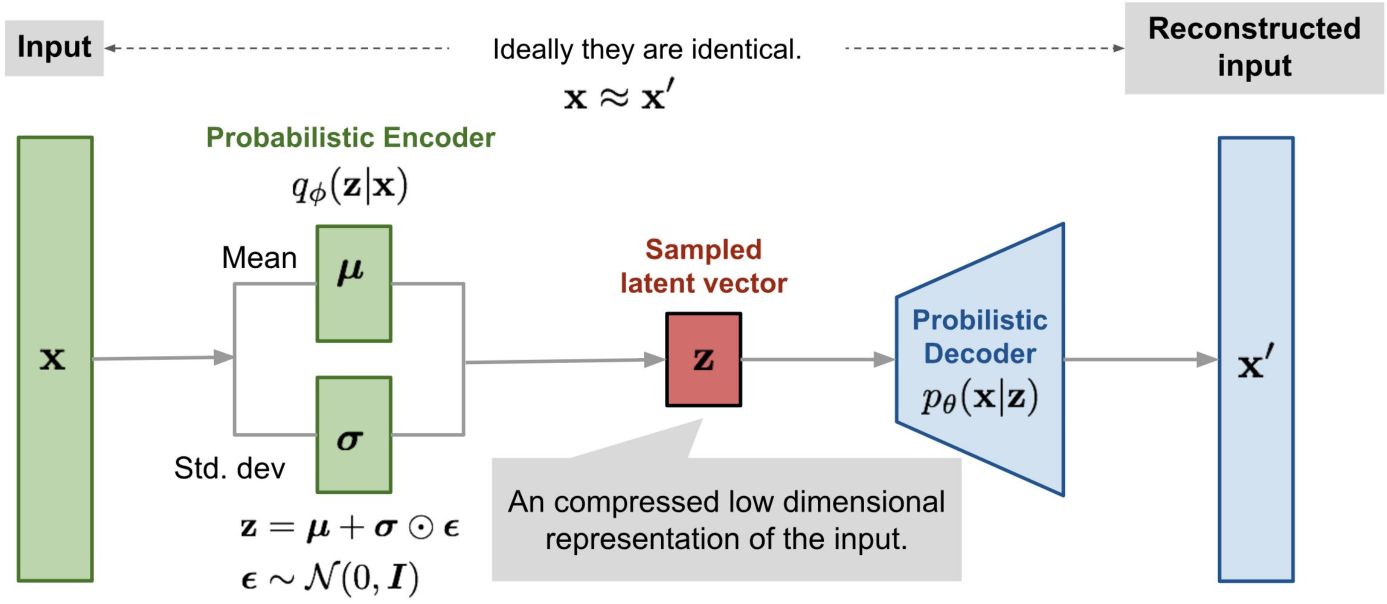
Then we can *transform* it to the *z* that we need using this $z = g(\epsilon) = \mu + \epsilon \circ \sigma$

Then, this $\mathbb{E}_{z\sim\mathcal{N}(\mu,\sigma^2)}\left[f(z)\right]$ and $\mathbb{E}_{\epsilon\sim\mathcal{N}(0,1)}\left[f(g(\epsilon))\right]$ are equivalent.

Addition, element-wise multiplication are all differentiable operations - and epsilon can be sampled agnostic of the actual mean and variance. Then epsilons are just 'inputs' to a network.

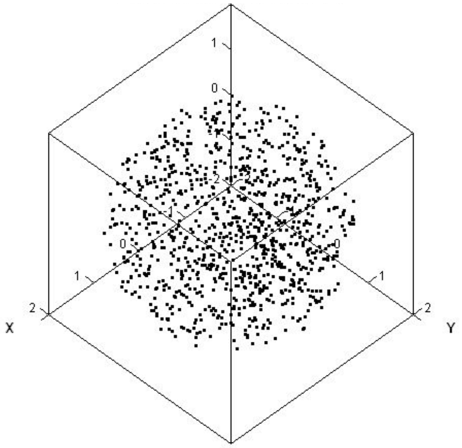
The reparameterization trick is helpful in [many other places] too.

VAE, the full picture



Effect of prior

The KL Divergence term is a strong prior for latent variable values which says the latent values lie in a hypersphere.



What if this is not true? For example, what if we generated samples using latent variables that are distributed like a disc?

(a) Original (b) Autoencoder (c) $\mathcal{N}$-VAE (d) $\mathcal{N}$-VAE, $\beta = 0.1$ (e) $\mathcal{S}$-VAE

https://arxiv.org/pdf/1804.00891.pdf

How do we force latent representations to be more meaningful?

An interesting approach is to *disentangle* latent variables.

Disentagling - each latent variable should capture different information from another.

Think of PCA - each projection is orthogonal to others.

β-VAE

- Main idea is to give an even stronger prior
  - This forces the posterior $Q(z|x)$ to be highly factorized (diagonal covariance)
  - Diagonal covariance → latent dimensions are uncorrelated

Main concepts to remember

- VAEs consist of two tractable distributions (should be easy to compute)
  - P(z) prior of latent variable
  - P(x|z) likelihood given latent variable
- We can train VAEs using back-prop because of reparameterization trick
- VAEs are very very similar to EM.
- We can make VAEs better by obtaining tighter definitions of the lower bound
  - Importance Weighted Autoencoders are an improvement.
- Choosing a good prior matters
  - Also, weighting prior differently gives different disentaglement results.