Variational Autoencoders

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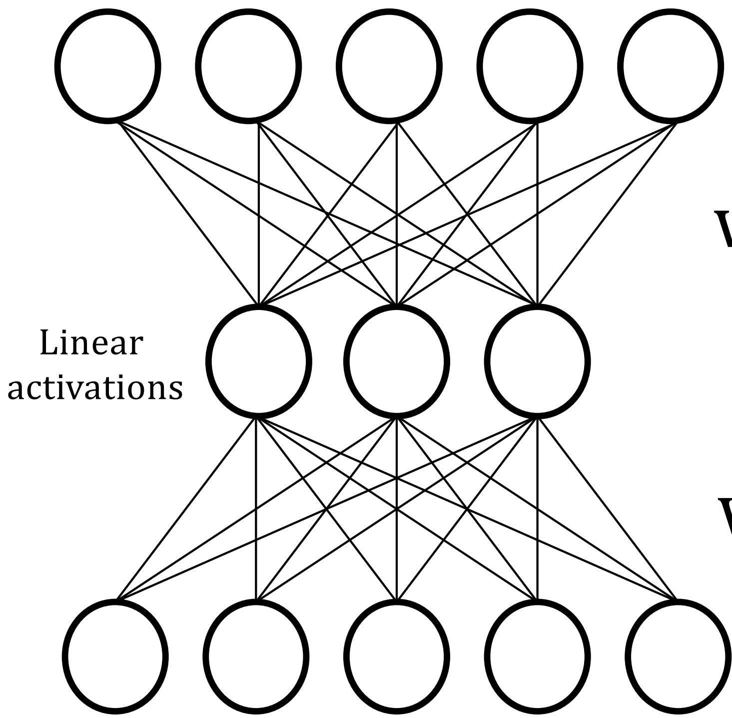
(updated fall 2022)

Reminder about Autoencoders

Simplest Autoencoder: Linear model, 1 hidden layer



output $\tilde{x}$

weights U

weights V

input x

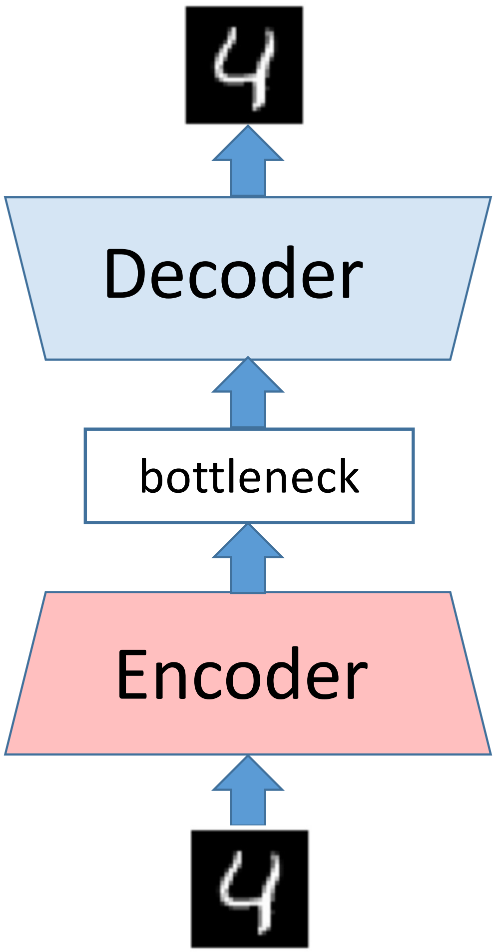
$$\text{loss } \mathcal{L} = \|x - \tilde{x}\|^2$$

$$\tilde{x} = UVx$$

Maps d dimensional input x to k dimensional embedding subspace S

More generally

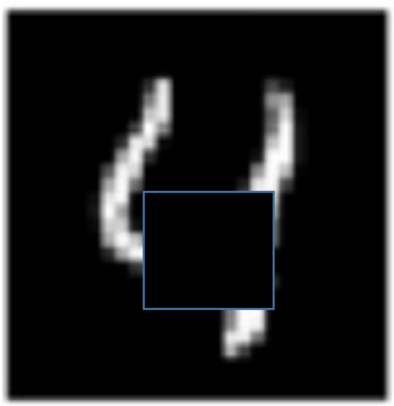
- With multiple layers & nonlinear activations we can map on to a nonlinear embedding space
- We can represent complex data this way and use the encoder as the input to a supervised network
- This lets us learn features from unlabeled data, which is far easier to get than labeled data.



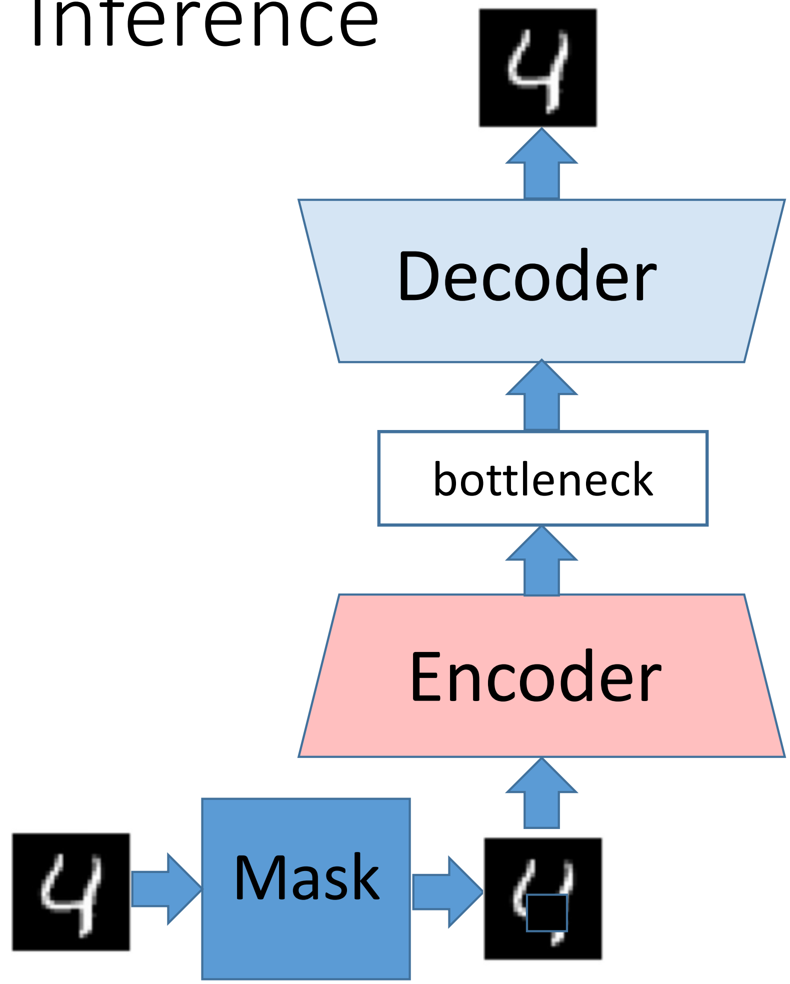
Using autoencoders for generation

Imputation/infill = Masked Inference

- If the "noise" we add is masking out large patches....



- We can train it to fill in blanks.



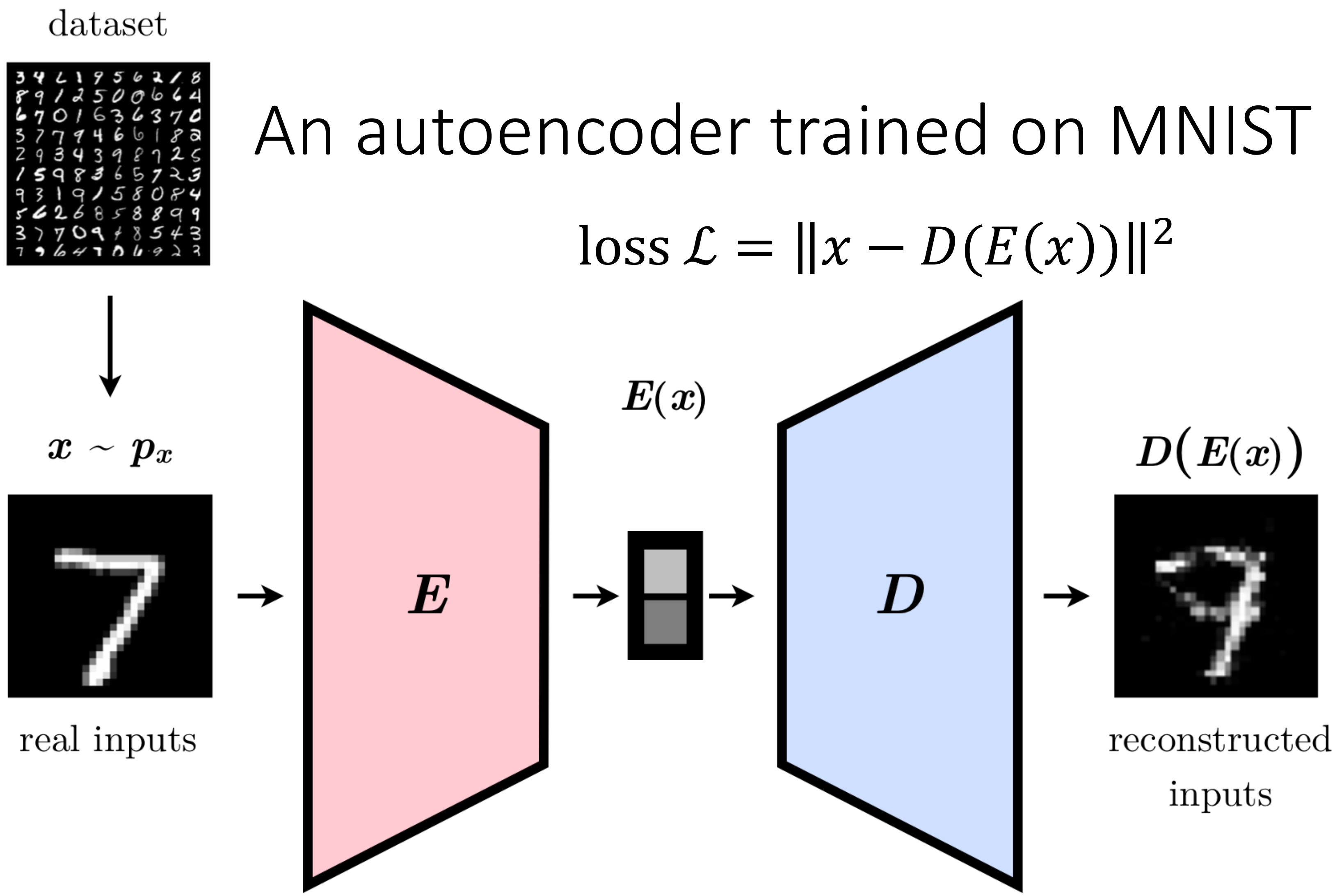
The MNIST dataset

- Famous dataset of handwritten digits
- They trained an autoencoder with a 2-digit

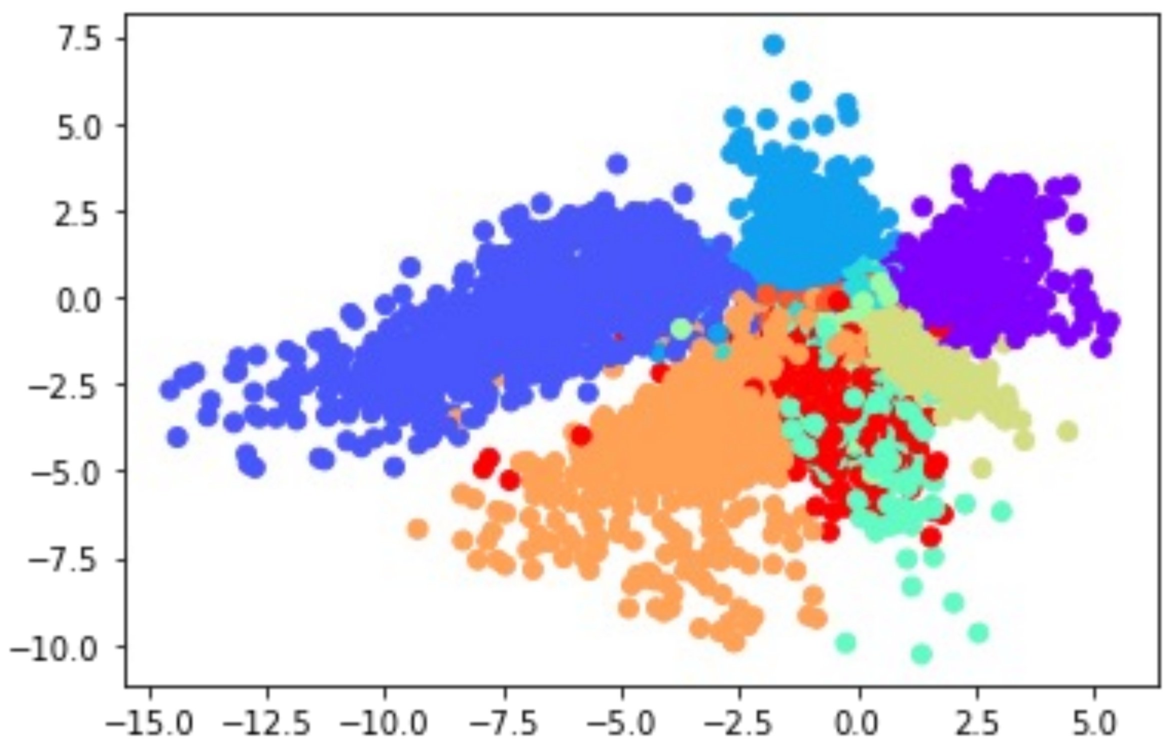
https://emkademy.medium.com/1-first-step-to-generative-deep-learning-with-autoencoders-22bd41e56d18

An autoencoder trained on MNIST

$$\text{loss } \mathcal{L} = \|x - D(E(x))\|^2$$



A 2-D “latent” space of the trained autoencoder

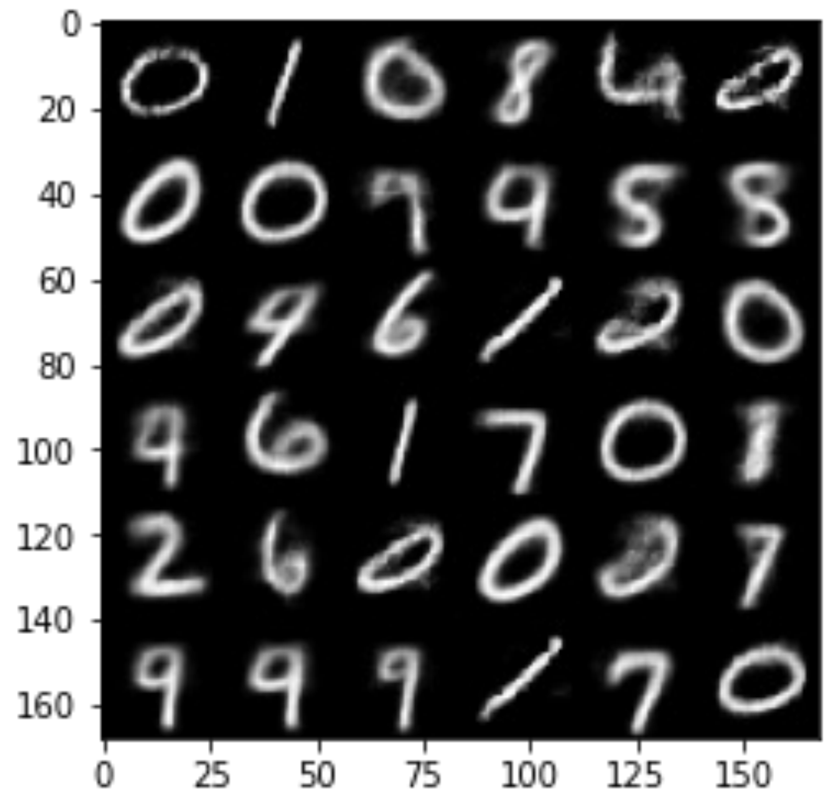


https://emkademy.medium.com/1-first-step-to-generative-deep-learning-with-autoencoders-22bd41e56d18

Generating images from “latent” vectors

- It is difficult to know what will happen when you move in a direction

- There are spots in the space that are…well…weird.



https://emkademy.medium.com/1-first-step-to-generative-deep-learning-with-autoencoders-22bd41e56d18

Variational Autoencoders

Based on (and figures from)

Kingma, Diederik P., and Max Welling. "An introduction to variational autoencoders." Foundations and Trends® in Machine Learning 12.4 (2019): 307-392.

https://arxiv.org/pdf/1906.02691.pdf

…and

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

https://arxiv.org/pdf/1606.05908.pdf

…and

Odaibo, Stephen, " Tutorial: Deriving the Standard Variational Autoencoder (VAE) Loss Function"

https://arxiv.org/pdf/1907.08956.pdf

A Bayesian Autoencoder

- Training goal: recreate the input dataset (just like an autoencoder)
- True objective: a model that will generate things like the training data, but not actually the training data
- Stretch goal: Allow user selection of subclasses (e.g. which MNIST digit) at generation time
- Hope: A smooth, continuous, interpretable latent space for controlling generation.

Some terminology

- If you can directly sample a random variable X and see the outcome x, we call x an **observation**. (e.g. the data our model is trained on)
- If you can't directly sample a random variable Z and see the outcome z, we call Z a **latent variable**.
- We'll typically use those letters with those implications: X is observable, Z is latent.

A simple latent variable model example

- What is the chance I have Covid, if I have a positive Covid test?
- Let Z be the latent variable ”Covid: yes/no”
- Let X be the observable variable “test: positive/negative”

A simple latent variable model example

- P(X) is the unconditioned (aka **prior**) probability of a positive test.

- P(Z) is the **prior** probability of having Covid.

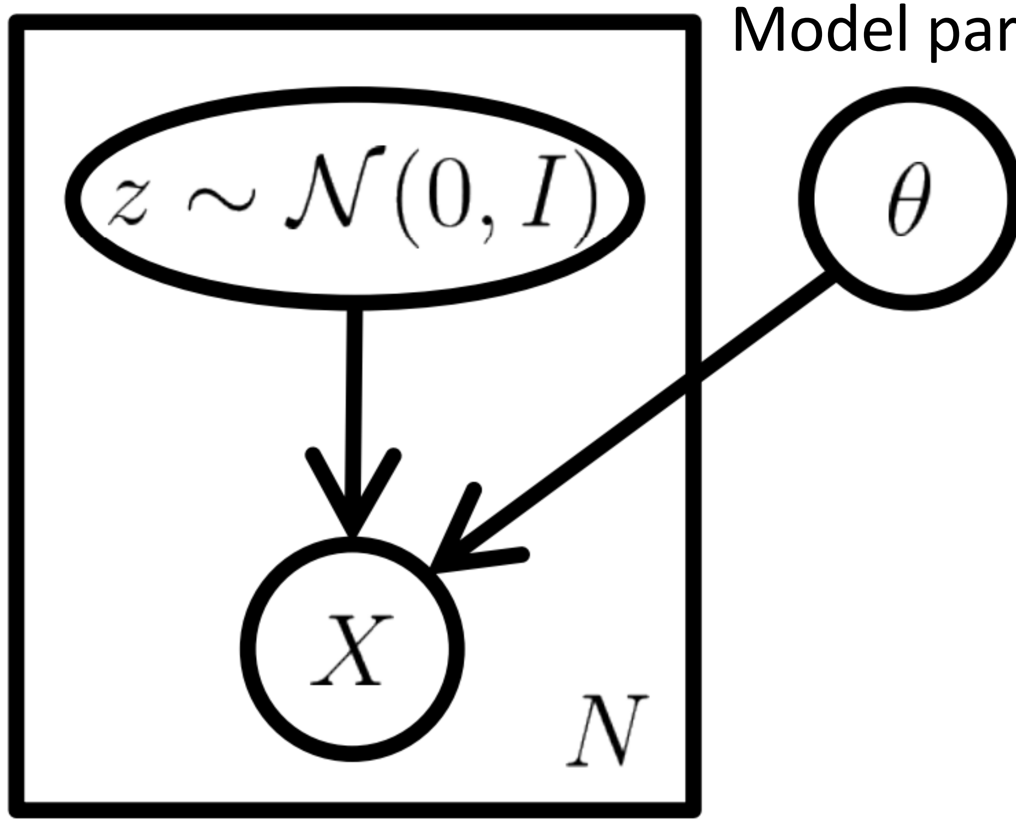
- P(Z|X) is the **posterior** probability of Covid, given the observed outcome.

- P(X|Z) is the probability of a test outcome, given the truth of whether you have Covid. (aka the **likelihood**)

A really simplified overview of a trained VAE

Latent variable(s) drawn from a 0-mean, spherical distribution

Model parameters

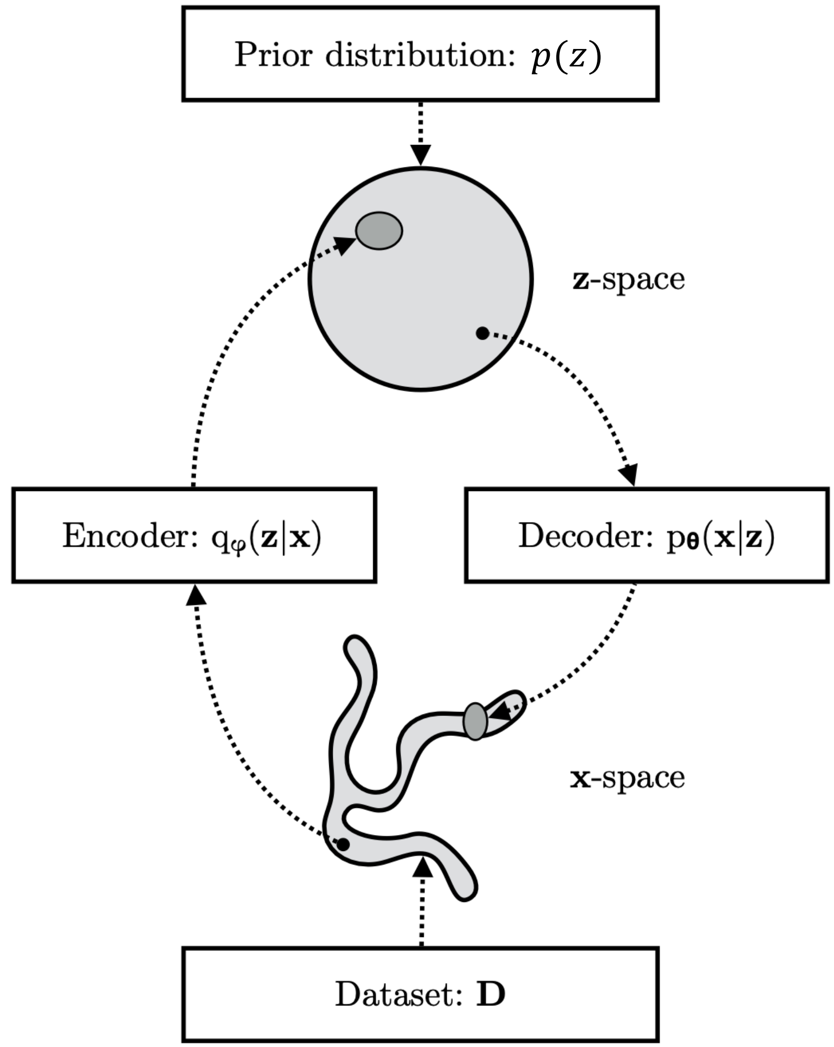


Output examples

Doersch, Carl, “Tutorial on Variational Autoencoders “ (2021)

A more detailed overview

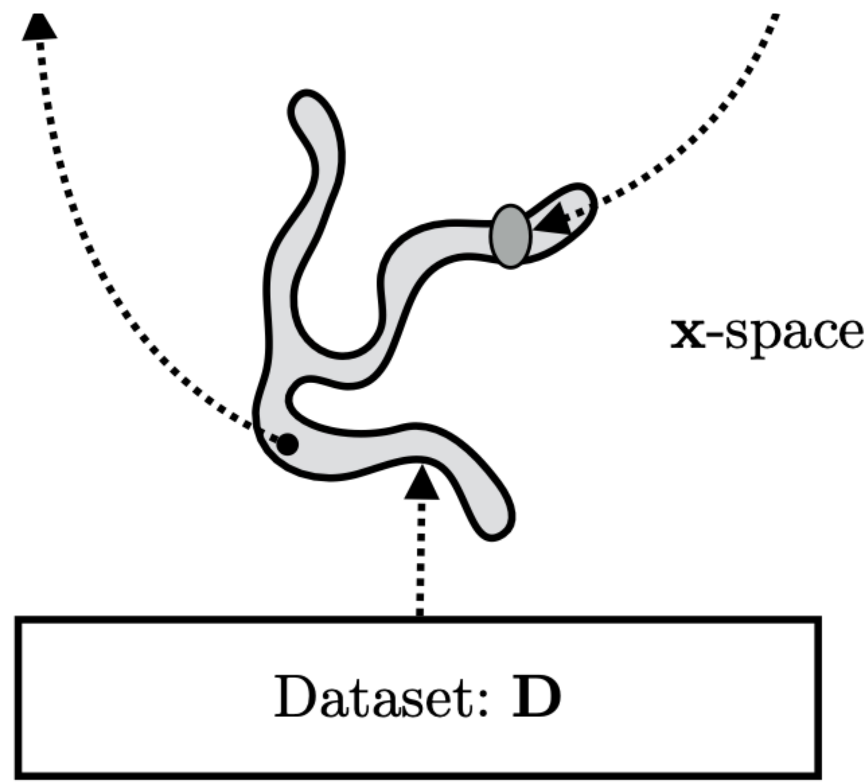
- An encoder/decoder framework
- We train the encoder to encode examples from the dataset as points in the latent space
- We train the decoder to decode points in the latent space into examples in the distribution of the training data



Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

The Evidence distribution $p(\mathbf{x})$

- The Dataset (aka the Evidence) contains examples **x** drawn from the **unknown** distribution p(**x**)
- Examples could be pictures, sounds, whatever.
- If we already had a good estimate of $p(\mathbf{x})$ we wouldn't have to build a VAE. We'd just sample from it.

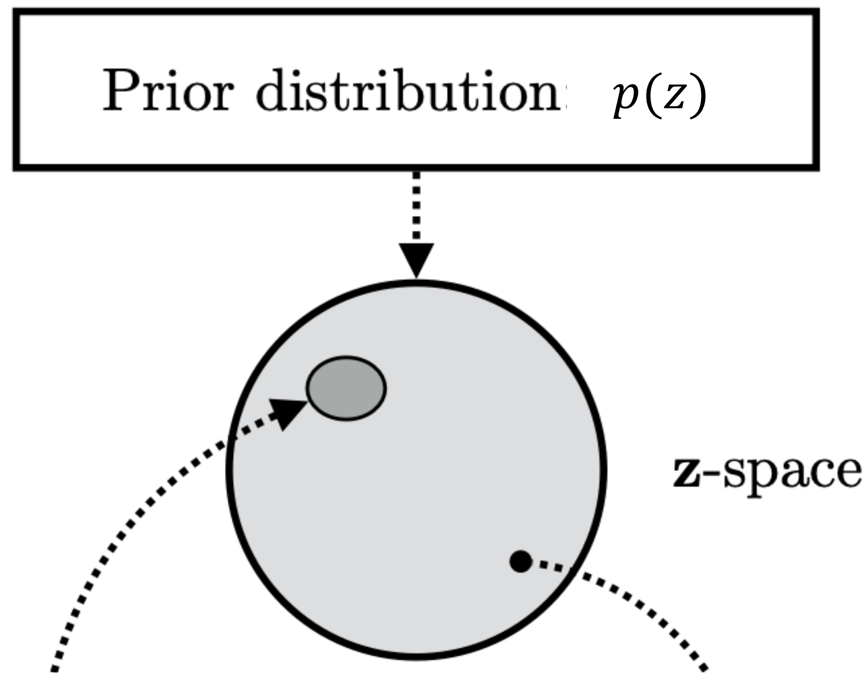


Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

The ”true” latent distribution $p(z)$

- We get to pick what this is.
- To make our lives easier, we’re going to make $p_\theta(z)$ a Normal (Gaussian) distribution.
- This is a parametrized distribution. The mean vector μ and covariance matrix Σ are the parameters θ
- We will later specify $\mu = 0, \Sigma = \mathbf{I}$,the identity matrix. (a spherical, 0-centered distribution)

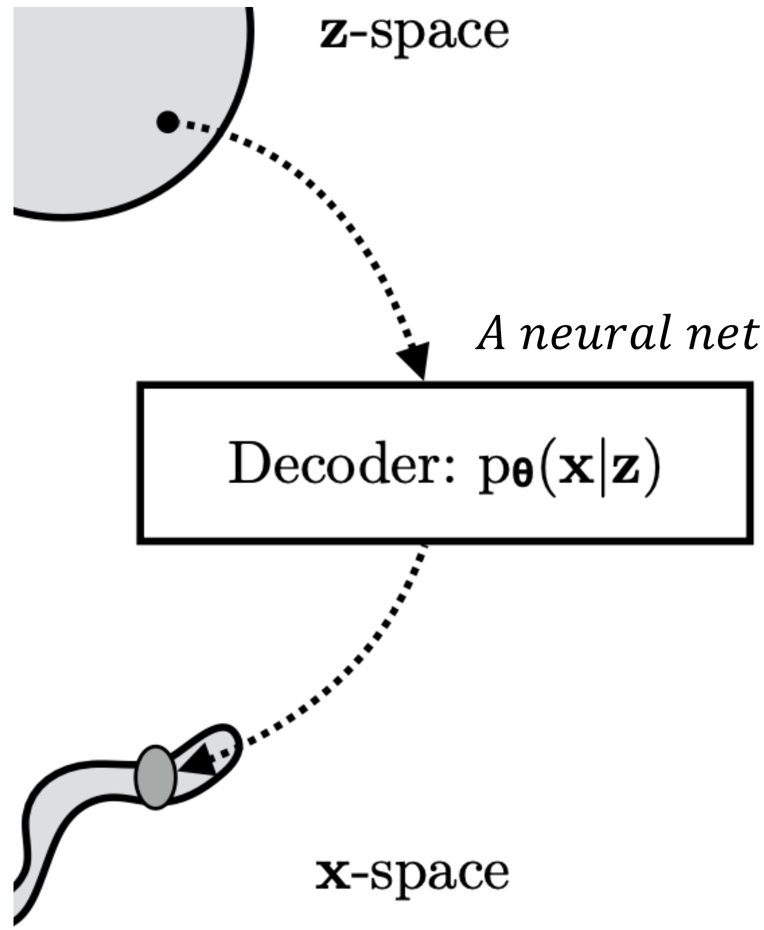
$p(z) = \mathrm{N}(z; 0, \mathrm{I})$



Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

The decoder

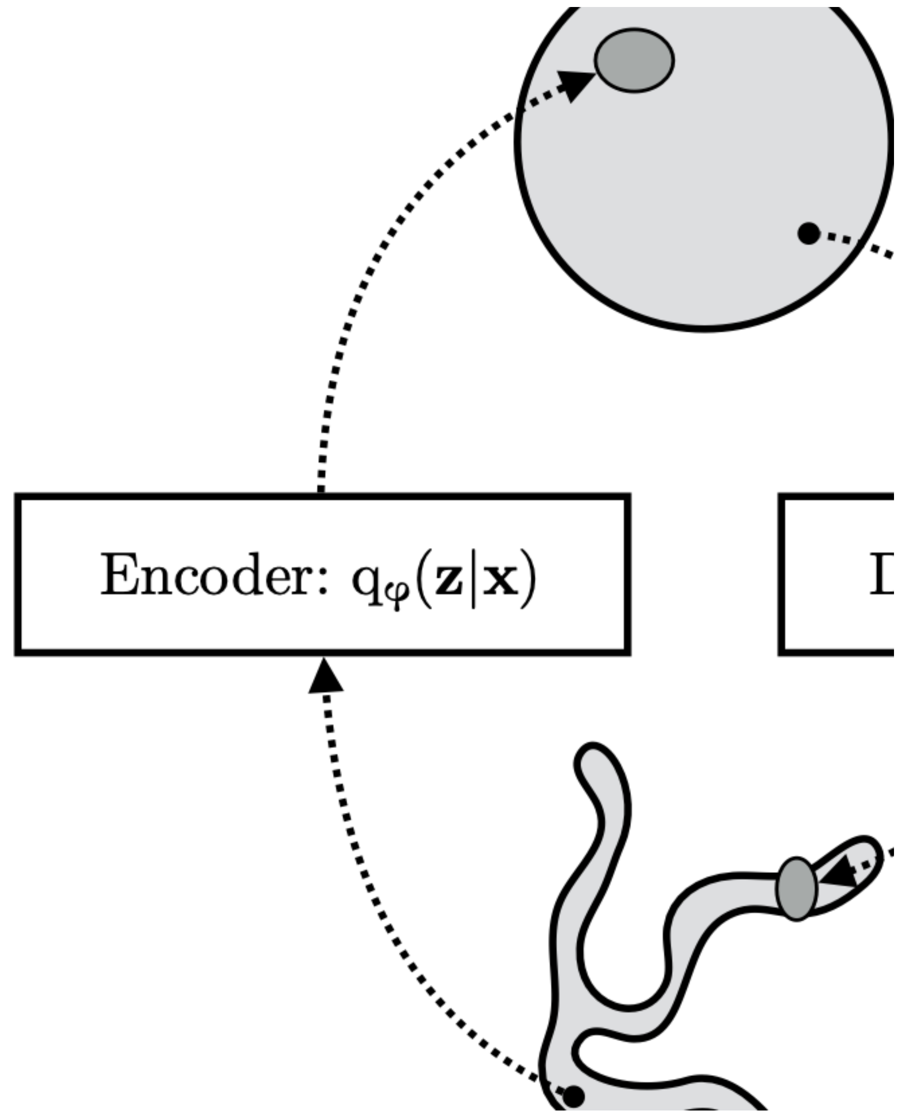
- The Decoder is a neural network with parameters we'll be learning.
- It maps a latent sample z into an example x.
- The Decoder, once trained, will be used to generate new examples.



Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

The Encoder $q_\varphi(\mathbf{z}|\mathbf{x})$

- The Encoder $q_\varphi(\mathbf{z}|\mathbf{x})$ is a neural network we'll be learning the parameters for.
- It approximates $p(\mathbf{z}|\mathbf{x})$, the "true" conditional distribution of the latents, given the data.
- Recall we set the unconditioned distribution $p(\mathbf{z})$ to be a spherical Gaussian,
- $q_\varphi(\mathbf{z}|\mathbf{x})$, therefore, is designed to map example x to a Gaussian distribution for z.



Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

Getting to the math….

- Assume the probability of the evidence x and the latent variables z can be modeled as a joint probability.

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

- We can factorize this like so:

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

- We may specify $p(\mathbf{z})$ before-hand. I.E., as a spherical Gaussian with mean 0.

So…we've got our generative model, right?

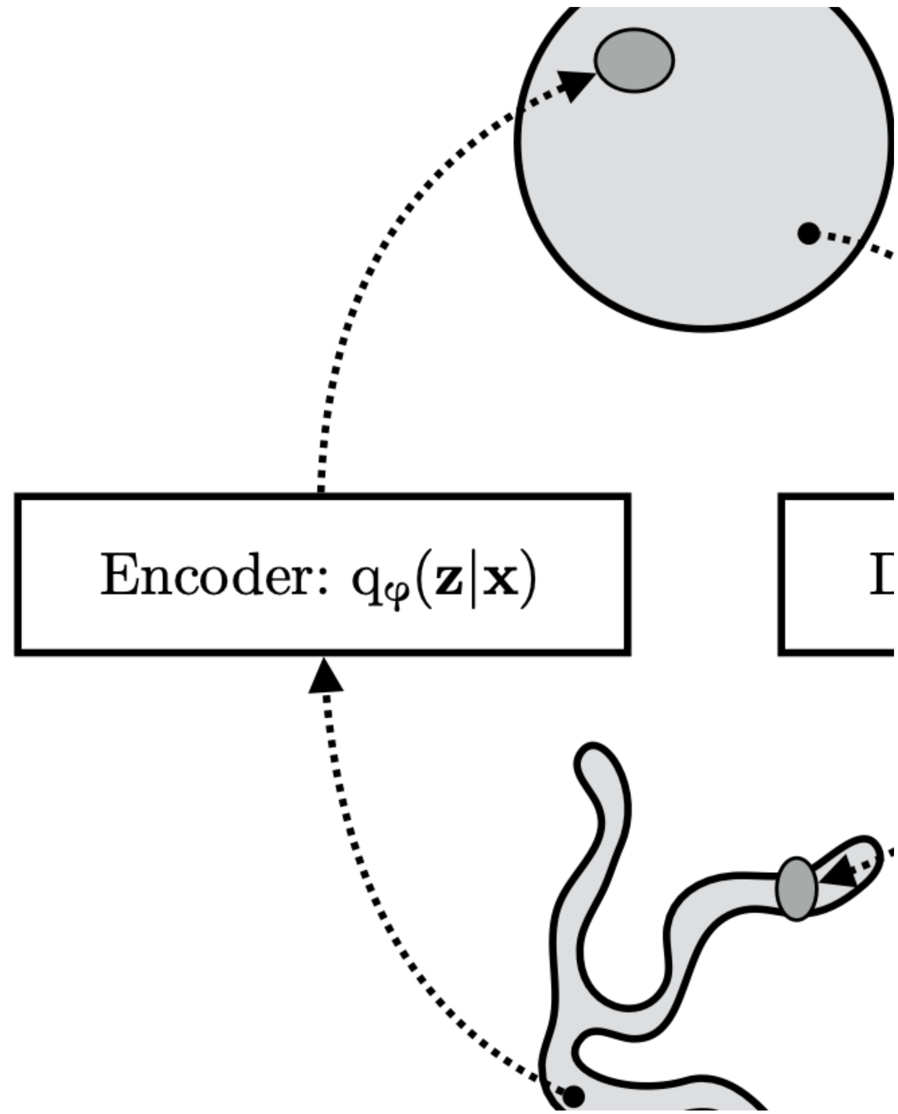
- Just take any neural network and learn a distribution $p(\mathbf{x}|\mathbf{z})$. Done!
- Well…no.
- We could assign random points in an arbitrary spherical distribution to points in the data space…but where is our assurance that nearby points in the distribution of z also produce things in the distribution p(x)?
- That is what the encoder is for.

The Encoder $q_\varphi(\mathbf{z}|\mathbf{x})$

- The Encoder $q_\varphi(\mathbf{z}|\mathbf{x})$ embodies a normal distribution:

$$Q(z|X) = N(z; \mu(\mathrm{X}), \mathrm{diag}(\mathrm{X}))$$

- What the network outputs are means and covariances.
- We then sample a latent vector from this distribution.
- What effect does this have on the z space?



Adapted from Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

What is so hard about this?

Let $\mathbf{x} = \mathrm{x}_1 \ldots \mathrm{x}_{\boldsymbol{n}}$ be a set of observed variables.

Let $\mathbf{z} = \mathrm{z}_1 \ldots \mathrm{z}_{\boldsymbol{m}}$ be a set of latent variables of interest.

We want to infer these latent variables from the evidence. We want to know $p(\mathbf{z}|\mathbf{x})$. If we could do this, we'd have our encoder.

$$p(\mathbf{z}|\mathbf{x}) = \frac{\boldsymbol{p}(\mathbf{z}, \mathbf{x})}{\boldsymbol{p}(\mathbf{x})}$$

How do we learn $p(\mathbf{z}|\mathbf{x})$?

$$p(\mathbf{z}|\mathbf{x}) = \frac{\boldsymbol{p}(\mathbf{z}, \mathbf{x})}{\boldsymbol{p}(\mathbf{x})}$$

When we went the other way, making a decoder from z to x, we dictated the distribution $\boldsymbol{p}(\mathbf{z})$, saying it would be a spherical Gaussian.

If we could already specify the $\boldsymbol{p}(\mathbf{x})$ we want here, we would not need a decoder to generate new examples. We'd just sample directly from the distribution.

So now what?

Idea: Set this up as an estimation problem.

- We want to learn $p(\mathbf{z}|\mathbf{x})$
- Make a family of density functions θ
- Search through θ to find $q^*(\mathbf{z})$, the density function optimizing this equation:

$$q^*(\mathbf{z}) = \underset{q(\mathbf{z}) \in \theta}{\operatorname{argmin}} D_{KL}(q(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}))$$

Here, θ is the set of functions. If those functions were parameterizable (e.g. Gaussians), we could think of θ as being defined by the possible parameter settings.

In the end we'll want to do this…

$$q^*(\mathbf{z}|\mathbf{x}) = \underset{q(\mathbf{z}|\mathbf{x}) \in \theta}{\operatorname{argmin}} D_{KL}(q(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}|\mathbf{x}))$$

Kingma et al. add a dependence on the data in evidence to this formulation. These folks invented the Variational Autoencoder (VAE).

Recall $q(\mathbf{z}|\mathbf{x})$ is learned by our encoder neural net.

Note: we still don't know $p(\mathbf{z}|\mathbf{x})$

So how do we minimize this divergence?

Relation to expected value

$$D_{KL}(Q(z)||P(z|x)) = \sum_{z} Q(z) log\left(\frac{Q(z)}{P(z|x)}\right)$$

$$= \sum_{z} Q(z)(\log Q(z) - \log P(z|x))$$

$$= E_{z\sim Q}[(\log Q(z) - \log P(z|x))]$$

Switching to Doersch's formulation

$$\mathcal{D}\left[Q(z)\|P(z|X)\right] = E_{z\sim Q}\left[\log Q(z) - \log P(z|X)\right]$$

KL Divergence is notated as D[A||B]

Q(z) is our user-defined distribution

P(z|X) is our unknown conditional distribution for z, given the evidence X.

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

Doing some math…

Definition of KL divergence

$$\mathcal{D}[Q(z)||P(z|x)] = E_{z\sim Q}[(\log Q(z) - \log(P(z|x))]$$

Applying Bayes' rule

$$= E_{z\sim Q}\left[\log Q(z) - log\left(\frac{P(x|z)P(z)}{P(x)}\right)\right]$$

Using logarithms

$$= E_{z\sim Q}\left[\log Q(z) - log\big(P(x|z)\big) - \log\big(P(z)\big) + \log\big(P(x)\big)\right]$$

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

Doing some math…

Where we left off

$$= E_{z\sim Q}\left[\log Q(z) - log\left(P(x|z)\right) - \log\left(P(z)\right) + \log\left(P(x)\right)\right]$$

Moving P(x) out of the expectation…since it doesn't depend on z

$$= E_{z\sim Q}\left[\log Q(z) - log\left(P(x|z)\right) - \log\left(P(z)\right)\right] + \log\left(P(x)\right)$$

Remember how we defined KL divergence…

$$= \mathcal{D}[Q(z)||P(z)] + E_{z\sim Q}\left[-\log\left(P(x|z)\right)\right] + \log\left(P(x)\right)$$

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

Doing some math…

Where we left off

$$\mathcal{D}[Q(z)||P(z|x)]$$
$$= \mathcal{D}[Q(z)||P(z)] + E_{z\sim Q}\left[-\log\big(P(x|z)\big)\right] + \log\big(P(x)\big)$$

Negate both sides and move terms

$$\log\big(P(x)\big) - \mathcal{D}[Q(z)||P(z|x)] = E_{z\sim Q}\left[\log\big(P(x|z)\big)\right] - \mathcal{D}[Q(z)||P(z)]$$

Our Q(z) doesn't depend on the evidence x.
Let's rewrite our formula to add that.

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

Conditioning latent generation on evidence

Note that X is fixed, and Q can be *any* distribution, not just a distribution which does a good job mapping X to the z's that can produce X. Since we're interested in inferring $P(X)$, it makes sense to construct a Q which *does* depend on X, and in particular, one which makes $\mathcal{D}\left[Q(z)\|P(z|X)\right]$ small:

$$\log P(X) - \mathcal{D}\left[Q(z|X)\|P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X)\|P(z)\right]$$

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

The left side of this function:

$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]$$

Log P(X) is the log probability of the evidence. We don't know this. If we did, we'd skip all this and sample directly from P(X).

$D[Q(z|X)||P(z|X)]$ is the divergence between $Q(z|X)$, the function our ENCODER will learn for the conditional distribution of the latents z, and the (unknown) real conditional distribution $P(z|x)$.

NOTE: We won't be optimizing this side of the equation.

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The right side of this function:

$$\log P(X) - \mathcal{D}\left[Q(z|X)\|P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X)\|P(z)\right]$$

$E_{z\sim Q}[\log P(X|z)]$ is the expected value of taking a sample our ENCODER made, based on a real example X, and passing that to our DECODER's learned function $P(X|z)$. We want this to equal log *P(X).*

$D[Q(z|X)||P(z)]$ is the divergence between the distribution learned by our ENCODER, Q$(z|X)$, and the "true" unconditioned latent distribution $P(z)$.

We set $\boldsymbol{P(z)}$ before-hand to be $\boldsymbol{N(z; 0, I)}$. That's our choice.

We constrain the learned encoder function Q$(z|X)$ to be a Gaussian with a diagonal covariance matrix.

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

So what are we optimizing?

$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = \boxed{E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]}$$

THIS!

We want what comes out of the decoder: $E_{z\sim Q}[\log P(X|z)]$ to be equal to the X from the data that went into the encoder.

We can measure that with Euclidean distance.

Doersch, Carl, "Tutorial on Variational Autoencoders" (2021)

So what are we optimizing?

$$\log P(X) - \mathcal{D}[Q(z|X) \| P(z|X)] = \boxed{E_{z\sim Q}[\log P(X|z)] - \mathcal{D}[Q(z|X) \| P(z)]}$$

THIS!

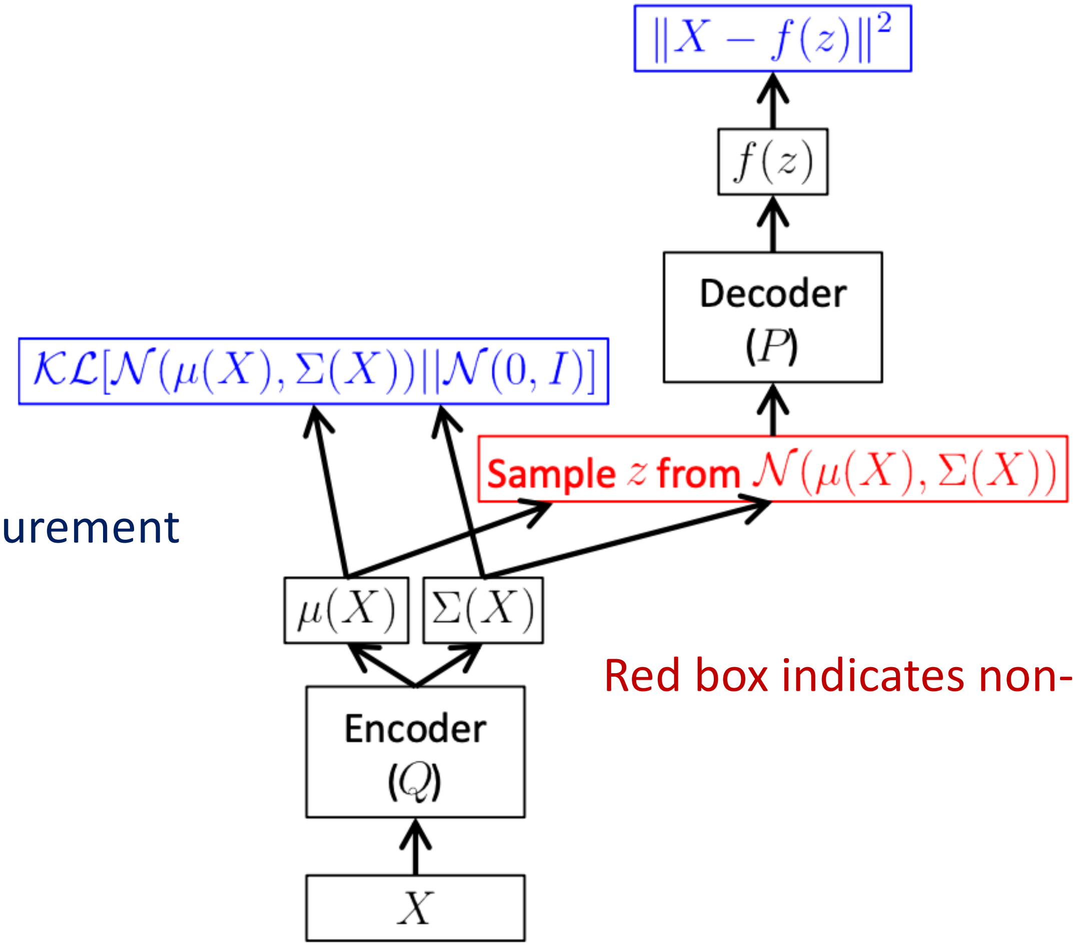
The learned parameters for the encoder's distribution $Q(z|X)$ are the mean vector $\boldsymbol{\mu}$ and the values of the diagonal of our covariance matrix Σ. (Remember, we constrained Σ to be diagonal).

P(z), the distribution we're matching, is $\mathrm{N}(z;0,\mathrm{I})$.

We want $\boldsymbol{\mu}$ to tend to the 0 vector and $\mathrm{tr}(\Sigma)$ trace to tend to D, where D is the dimensionality of the latent space. That pushes Σ towards $\mathbf{I}$.

Doersch, Carl, "Tutorial on Variational Autoencoders " (2021)

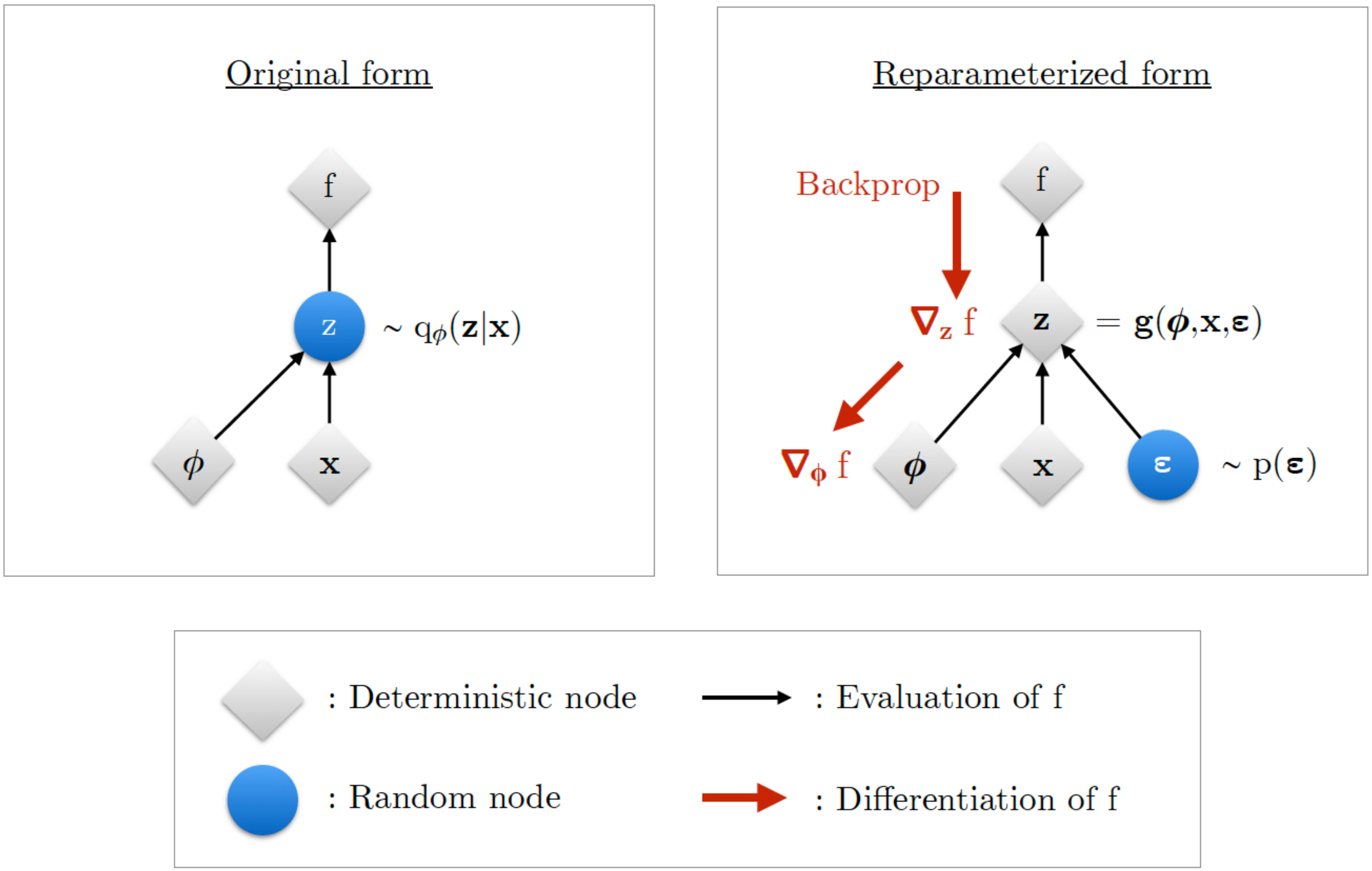
$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right].$$



Blue box indicates loss measurement

Red box indicates non-differentiable

Doersch, Carl, "Tutorial on Variational Autoencoders" (2021)

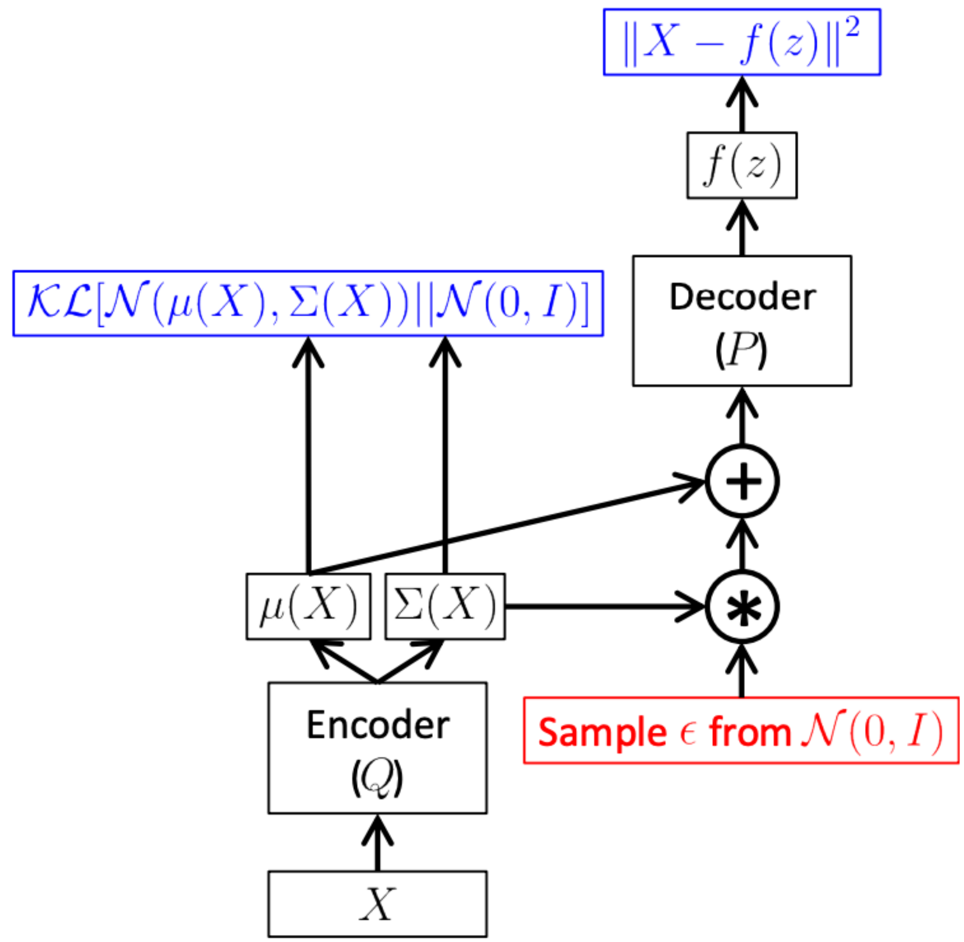


Kingma, D. P., & Welling, M. (2019). An introduction to variational autoencoders.

A graphical view

Blue box indicates loss measurement

Red box indicates non-differentiable



Doersch, Carl, "Tutorial on Variational Autoencoders" (2021)

Where is the “evidence lower bound”?

$$\log P(X) - \mathcal{D}\left[Q(z|X) \| P(z|X)\right] = \boxed{E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]}$$

The ELBO

Rearranging to isolate the log evidence on the left.

$$\log P(X) = E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right] + \mathcal{D}\left[Q(z|X) \| P(z|X)\right]$$

KL divergence is non-negative.

So the ELBO forms a lower bound on the log evidence.

$$\log P(X) \geq E_{z\sim Q}\left[\log P(X|z)\right] - \mathcal{D}\left[Q(z|X) \| P(z)\right]$$

Discussion points

- How do we make these things controllable?
- How do we navigate the latent space?
- What is “disentanglement”?

Adding class conditioning

Why do we want this?

- If I train a VAE on a big dataset of imaged (e.g. CFAR100), I want to be able to use it to generate an image of a particular class (like “dog”)
- Without class conditioning, how could I do this?
- Let’s think about the latent space….

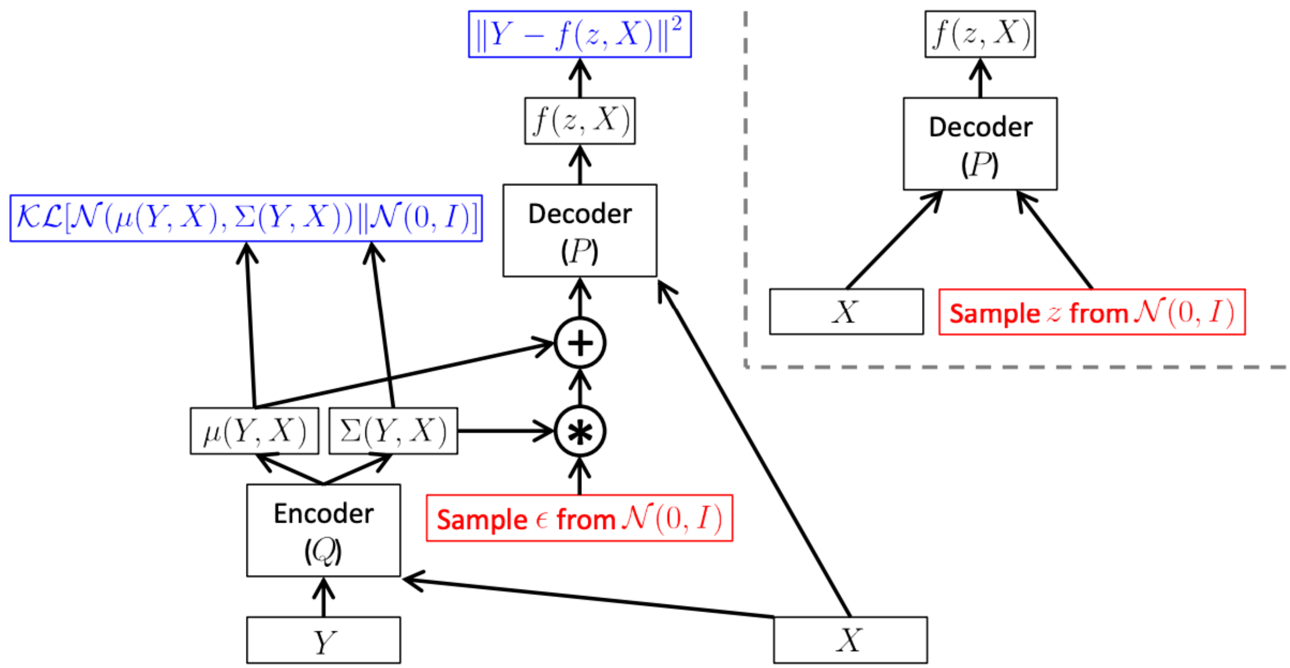


Figure 6: Left: a training-time conditional variational autoencoder implemented as a feedforward neural network, following the same notation as Figure 4. Right: the same model at test time, when we want to sample from $P(Y|X)$.

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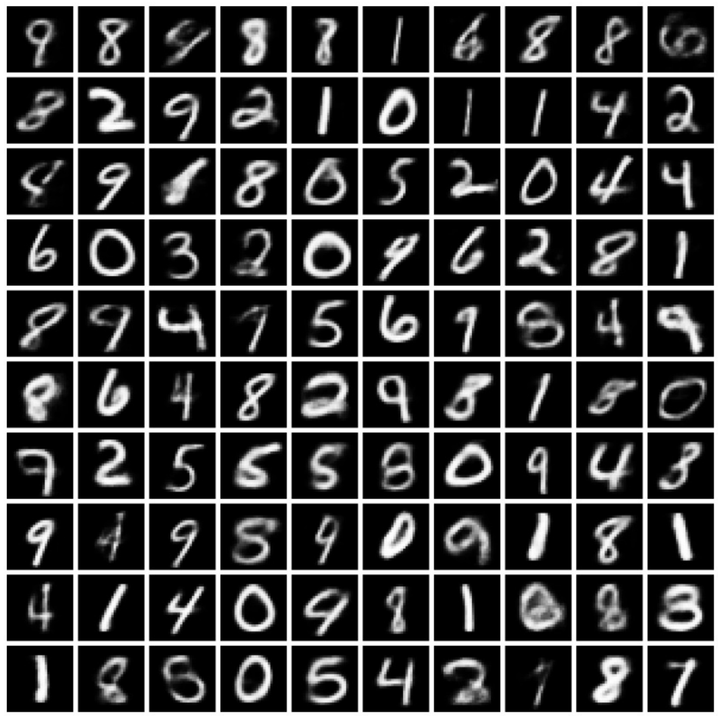
Example output

Unconditioned generation



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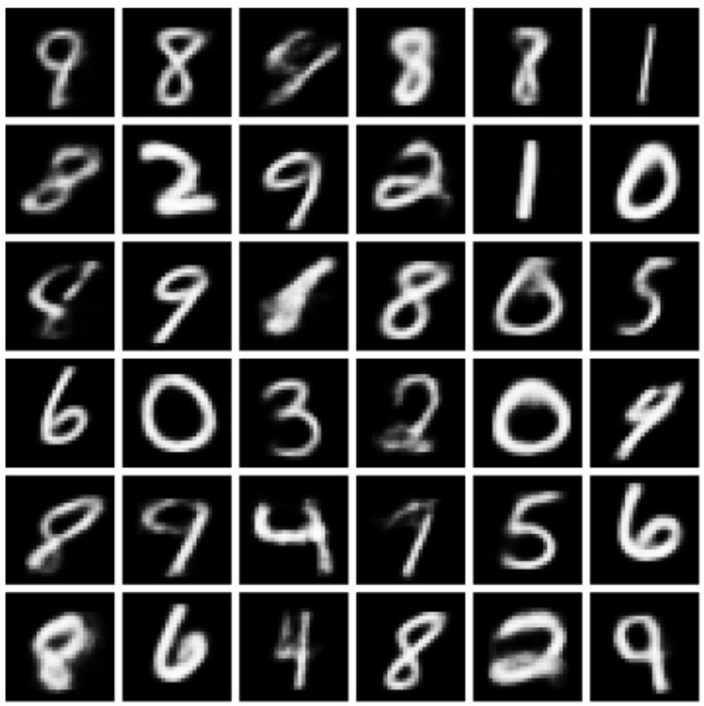
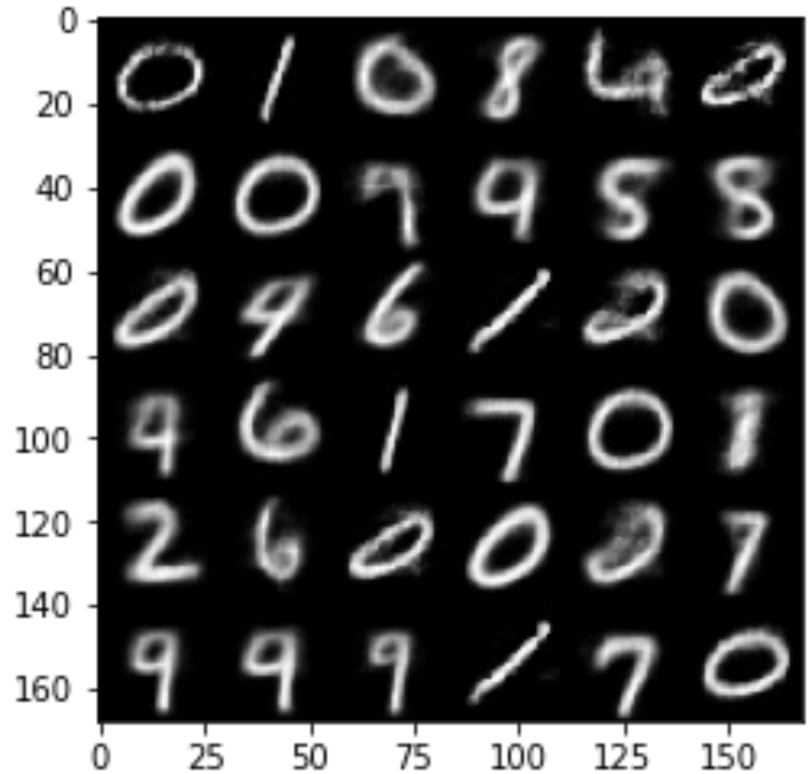
VAE vs Autoencoder: unconditioned output





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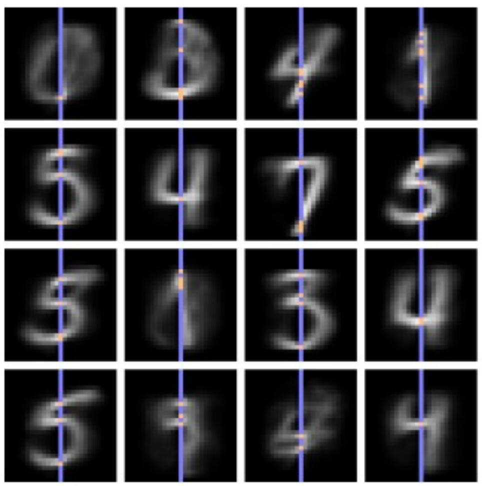
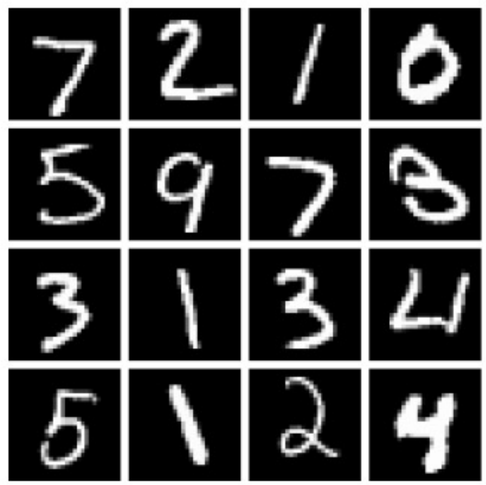
Conditional MNIST generation

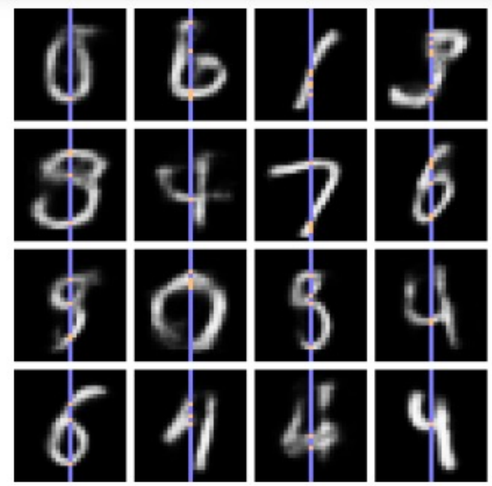
Regressor generation



Ground Truth



CVAE generation



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Kingma’s formulation