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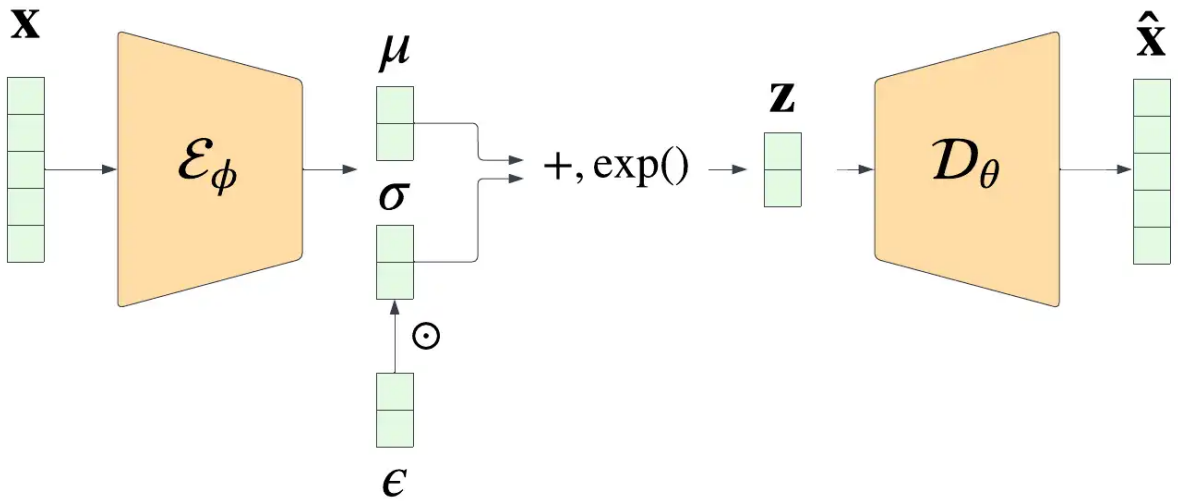

Variational Autoencoder (VAE)

December 31, 2022 31 min read

Here I discuss one of the two most popular classes of generative models for creating images.

Generative models in machine learning are capable of looking at a set of data points (e.g. images), capturing some inner structure in them and producing new data points (e.g. new images), which bear the properties of the training data set.

Since its inception in the late 2013 **Variational Autoencoder (VAE)** has become one of two most popular generative models for producing photorealistic images. A popular alternative is called Generative Adversarial Networks (GANs), they are beyond the scope of this post.

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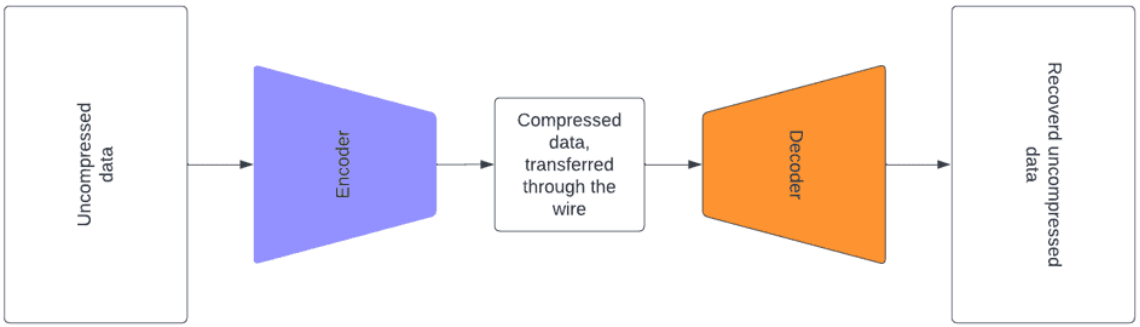
need some background in information theory. For understanding VAE we will also cover some background in Bayesian machine learning.

Information theory: entropy, mutual information and KL-divergence

In 1940-1950 information theorists such as Claude Shannon posed a set of problems, related to finding the most economical ways of data transmission.

Suppose that you have a signal (e.g. long text in English), and you need to transmit it through a channel (e.g. wire) with a severely limited bandwidth. It would be beneficial to compress this signal, using some kind of encoding, before transfering it through the wire, so that we make as good use of our data transfer channel, as possible. The receiving side should decompress the signal after receiving it.



Encoder-decoder architecture. Uncompressed data are passed on input, they are encoded into a compressed representation, which is transferred through the transmission channel (e.g. wire), and decoded by the decoder on the receiving side.

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It is intuitive that if you encode frequent letters with the shortest sequences and non-frequent letters with remaining (longer) sequences, you'll get an optimal encoding. Consider the following example of an alphabet and an optimal encoding:

Letter	Letter code	Frequency	Length of letter code
A	0	0.5	1
B	10	0.25	2
C	110	0.125	3
D	111	0.125	3

Observe that the length of the code of letter A equals to $-\log_2 p(A)$.

If your alphabet has a distribution p, e.g. $p(A) = 0.5$, the optimal encoding of your signal would achieve the minimal length of average text, if $H(p) = \sum_i p_i \log p_i = \mathbb{E}(-\log p) \to \min$.

$H(p)$ is called **entropy**, as previously this function was introduced in physical chemistry by Ludwig Boltzmann to describe a different process.

Now, if you use an encoding with a different distribution of letter codes q to transfer your signal, this encoding would be sub-optimal, as average length of a letter would

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The difference in length between the optimal encoding and sub-optimal encoding is then $D(p,q) = -\sum_i p_i \log q_i - (-\sum_i p_i \log p_i) = -\sum_i p_i \frac{\log q_i}{\log p_i}$.

This quantity is called **Kullback-Liebler divergence**, and for encoding to be optimal it should be minimal. As entropy $H(p) = \sum_i p_i \log p_i$ does not depend on q, it would suffice to optimize $H(p,q) = \sum_i p_i \log q_i$, this quantity is known as **Cross entropy**.

Autoencoders

Inspired by information theory, machine learning practitioners employed the concept of **Autoencoders**.

To the best of my knowledge first publication of autoencoders or autoassociative neural networks was made by Mark Kramer in 1991, where autoencoders were seen as a non-linear dimensionality reduction tool, a non-linear analogue of PCA.

The logic of autoencoder is to train such encoder $\mathcal{E}_\phi$ and decoder $\mathcal{D}_\theta$ neural networks that encoder can compress the high-dimensional input data x to a low-dimensional latent representation z (or h on the image below) and then the decoder is able to reconstruct $\hat{x}$ (or x' on the image below) accurately enough from this latent representation.

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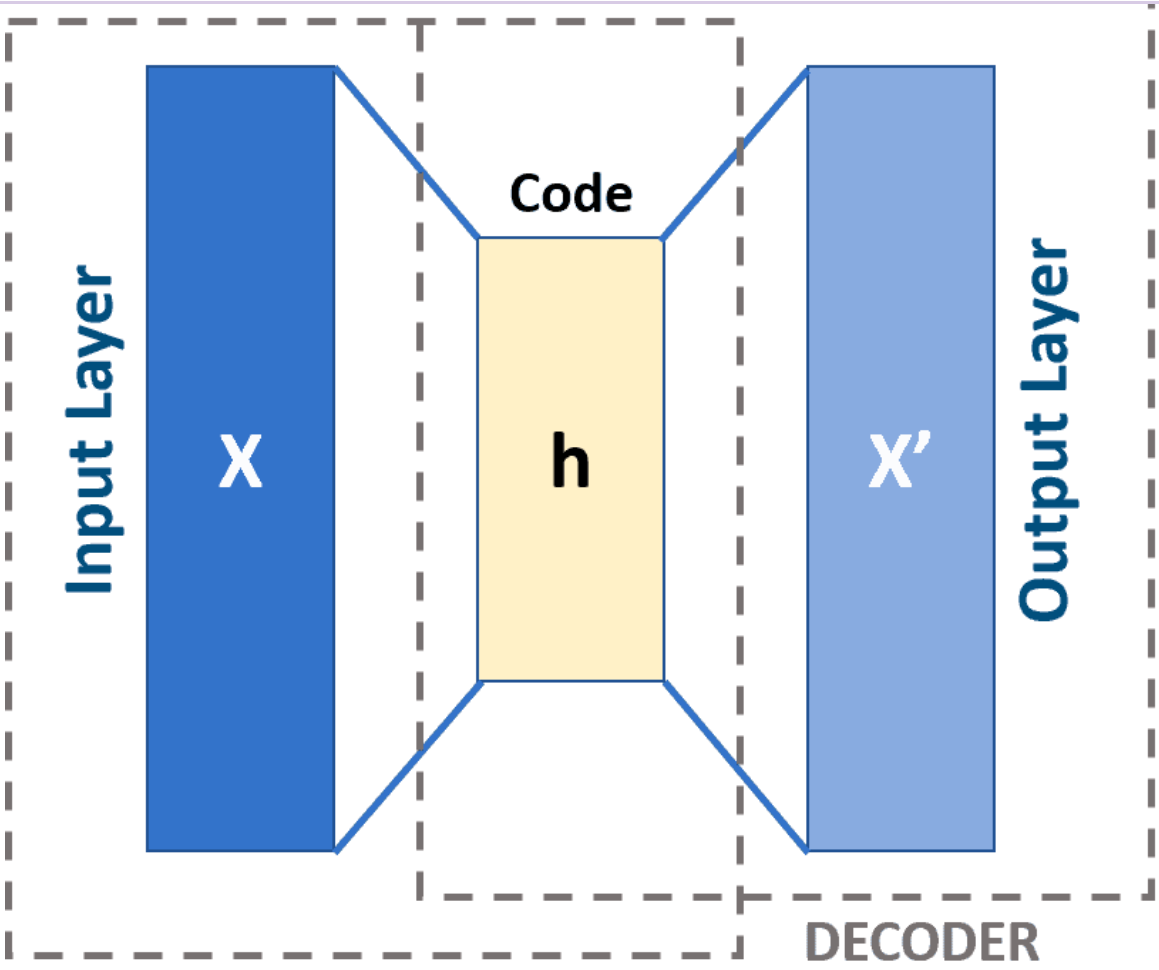

Autoencoder neural network.

This approach was re-used much later, circa 2010, by Yoshua Bengio group. They figured out that autoencoders can be used for other purposes, such as denoising:

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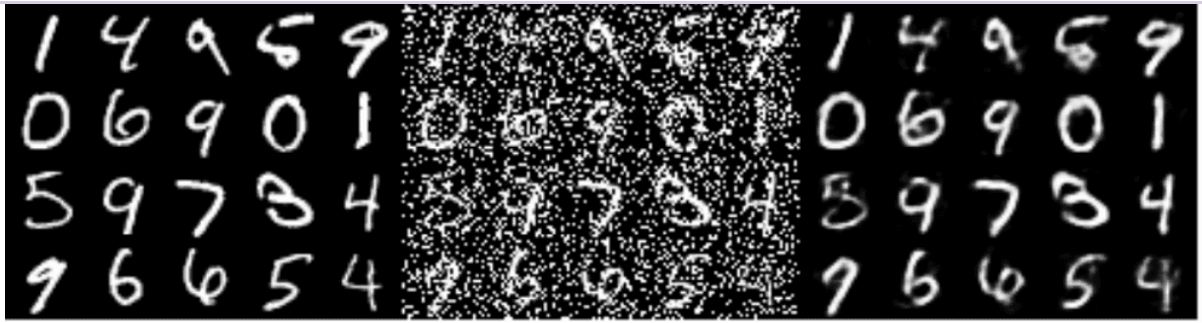

Denoising autoencoder (DAE). Suppose that you had a dataset of hand-written digits (MNIST). Each digit's image is corrupted with white noise and then passed to a Denoising Autoencoder. The purpose of the DAE is to recover the original image as accurately as possible.

Moreover, Bengio borrowed the idea of stacking individual encoders/decoders from Hinton's RBMs and this approach gave rise to stacked denoising autoencoders and, eventually, Diffusion models, but that's a topic for another day.

Holes in the latent space

Now, what happens, if we drop the decoder part, just sample a random point from the encoder latent space and generate an output from it with the decoder? This is supposed to give us an image. Hence, our model would be generative.

However, one of the arising problems is the fact that data points in our training dataset oftentimes do not cover the whole latent space. In the worst-case scenario theoretically our autoencoder could just map all the data points to a straight line, effectively enumerating them.

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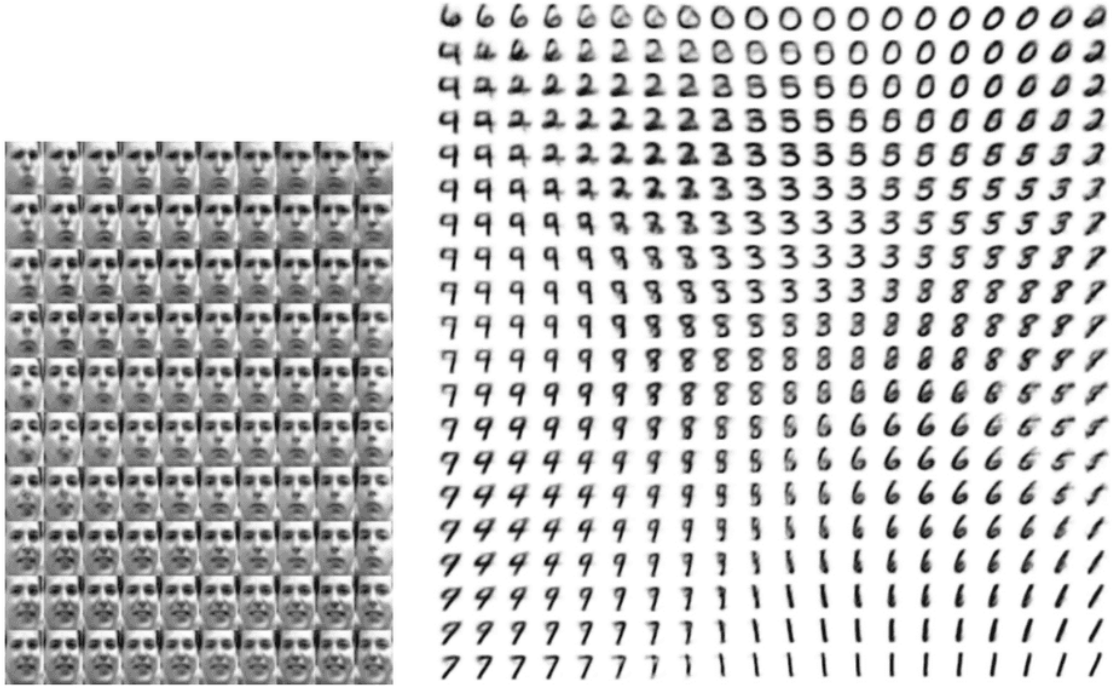
come up with a way to regularize our latent space, so that the whole manifold of images is mapped to the whole latent space, preferably in a smooth way. This is the motivation for VAE.

VAE makes sure that the latent space has a Gaussian distribution, so that by gradually moving from one point of latent space to its neighbour, we get a meaningful gradually changing output:



(a) Learned Frey Face manifold (b) Learned MNIST manifold

Sampling from nearby points of VAE latent space produces similar output images. Illustration from the original paper.

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VAE, devised by Max Welling group in the late 2013, has arguably become the most wide-spread flavour of autoencoders. It maps the data points to a distribution (usually, Gaussian), so that the mapping is smooth and no holes are produced. It is formulated in Bayesian terms.

The idea of this approach starts from the information theory perspective: we want to train such an encoder neural network $\mathcal{E}_\phi$ with parameters ϕ that the Kullback-Liebler divergence between the input image $\mathbf{x}$ and its latent representation $\mathbf{z}$ is minimized: $KL(\mathbf{x}, \mathbf{z}) \rightarrow min$.

This principle is also known as Infomax and was borrowed by Bengio and, later, Welling teams from one of the flavours of Independent Component Analysis (ICA).

Computationally VAE minimizes the divergence using stochastic gradient descent. However, as we'll see later using a regular neural network training approach does not get the job done, as normal gradient estimator has a very high variance and does not converge computationally (we'll see this in a moment).

Hence, training VAE employs a specific computational technique, called doubly-stochastic gradient descent and a special trick, called re-parametrization trick, which we will explore later.

But first we need to understand the language, in which VAE is described, as it is a Bayesian model, and we will have to cover a lot of background in Bayesian ML.

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All hail our lord and saviour Bayes... (meh, just kidding)

Bayes formula

To explain the Bayesian framework, employed by VAE, we have to start with Bayes formula:

$$\underbrace{p(z|x)}_{\text{posterior}} = \frac{\overbrace{p(x|z)}^{\text{evidence}} \cdot \overbrace{p(z)}^{prior}}{\underbrace{p(x)}_{\text{evidence}}}$$

In case of VAE the notation is as follows:

- we have a dataset of images $X = \{\mathbf{x}^{(\mathbf{i})}\}$
- each input image is denoted $\mathbf{x}^{(\mathbf{i})}$
- its latent representation, which is generated by VAE's encoder half, is denoted $\mathbf{z}^{(\mathbf{i})}$
- the weights of encoder network $\mathcal{E}$ are denoted ϕ; Kingma and Welling call them **variational parameters**

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The authors of VAE, D. Kingma and M. Welling, assume that there exists some prior distribution of latent parameters $p(\mathbf{z})$, from which latent representation of each data point is sampled. For each image $\mathbf{x}$ we maximize the posterior $p_\phi(z|x)$.

Variational inference

Direct calculation of posterior $p(\mathbf{z}|\mathbf{x})$ using Bayes formula is impossible, as we need to calculate the probability of evidence $p(x)$, for which the integral $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$ is intractable (i.e. it is not possible to calculate it analytically or computationally in practice).

So we need to come up with a practical way of overcoming this obstacle.

Typically, Bayesians have two solutions for problems like this: one solution is Markov Chain Monte Carlo methods. In this particular case MCMC estimator is time-consuming and gradient, calculated with it, has a high variance, so the model fails to converge.

An alternative approach is Variational Inference approach, which we explain here.

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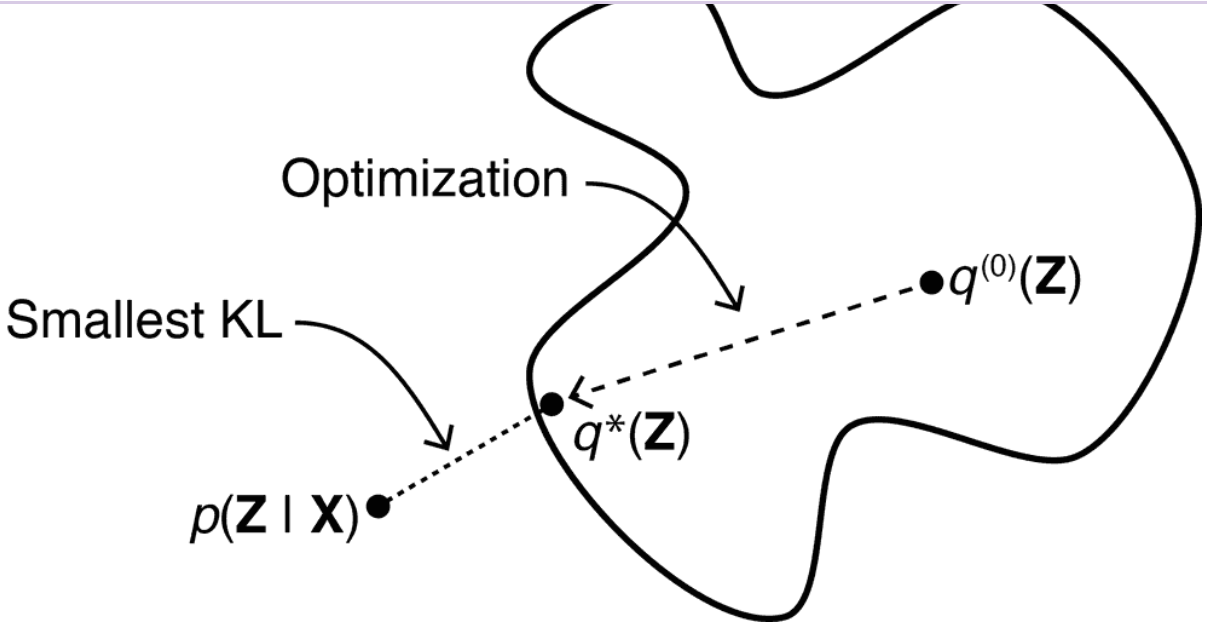

Variational inference. Variational inference aims to approximate the true variational posterior $p(\mathbf{z}|\mathbf{x})$ with the best approximation $q^*(\mathbf{z})$ from a certain class of functions Q. This optimization process minimizes the Kullback-Liebler divergence between the approximation $q(\mathbf{z})$ and true posterior $p(\mathbf{z}|\mathbf{x})$. Image taken from Gregory Gundersen blog post on Variational Inference.

In variational inference we choose a class of functions Q, from which we will try to pick an approximation $q(\mathbf{z})$ (called **guide**) of the posterior $p(\mathbf{z}|\mathbf{x})$, such that Kullback-Liebler divergence between this approximation and true posterior is minimal.

ELBO maximization

Now, we need to come up with a technical way to find this optimal guide $q(\mathbf{z})$ numerically.

integral, and multiplication by 1 terms.

$$\log p(\mathbf{x}) = \int q(\mathbf{z}) \log p(x) d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{z}|\mathbf{x})} d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{x},\mathbf{z}) q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x}) q(\mathbf{z})} d\mathbf{z} =$$

$$= \int q(\mathbf{z}) \log \frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} + \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x})} d\mathbf{z} = \mathcal{L}(q(\mathbf{z})) + KL(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x})).$$

Now we see that log-evidence $\log p(\mathbf{x})$ consists of two non-negative terms. Let us interpret them:

$$\log p(\mathbf{x}) = \underbrace{\mathcal{L}(q(\mathbf{z}))}_{\text{ELBO - Evidence lower bound}} + KL(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}))$$

The first term is called **Evidence Lower BOund (ELBO)**. The second term is our cost function $KL(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}))$, which Variational Inference aims to minimize. As log-evidence $\log p(\mathbf{x})$ is fixed, the greater ELBO gets, the closer in terms of KL divergence guide $q(\mathbf{z})$ approximates the posterior $p(\mathbf{z}|\mathbf{x})$:

$$KL \geq 0 \Rightarrow KL(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x})) \rightarrow \min \Leftrightarrow \mathcal{L}(q(\mathbf{z})) \rightarrow \max$$

Hence, to find the optimal guide $q(\mathbf{z})$, in practice we have to maximize ELBO. Let us break it down further:

$$\mathcal{L}(q(\mathbf{z})) = \int q(\mathbf{z}) \log \frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} =$$

$$= \int q(\mathbf{z}) \log p(\mathbf{x},\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} = \underbrace{\mathbb{E}_{q(\mathbf{z})} \log p(\mathbf{x}|\mathbf{z})}_{\text{Expected log-likelihood}} -$$

$$\underbrace{KL(q(\mathbf{z}) \| p(\mathbf{z}))}_{\text{Regulariser term KL-divergence}}$$

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a regularizer term that guarantees that our guide (i.e. latent space) distribution stays relatively close to the prior $p(\mathbf{z})$, which is usually chosen to be Gaussian.

VAE makes use of ELBO as its loss function for training. It approximates its true gradient with stochastic gradients over mini-batches of data points (e.g. images), so that integrals are replaced with sums.

There is also one nitpick: in VAE our latent representation vector $\mathbf{z}$ is not deterministic, but stochastic. Hence, in order to make the gradient of ELBO differentiable, we'll have to use a special reparametrization trick.

Reparametrization trick

Unlike the normal convolutional neural networks, VAE makes use of **doubly stochastic gradient descent**. Input images are the first source of stochasticity in VAE.

But there is also a second source: in case of VAE the latent representation $\mathbf{z}$ is not just a deterministic low-dimensional vector like in normal autoencoders. Instead, it is a random variable (usually, multivariate gaussian), whose mean μ and variance σ the model aims to learn.

So the mean and variance of $\mathbf{z}$ are deterministic, but then for each data point in the training batch we sample a random point from that distribution, introducing some extra noise.

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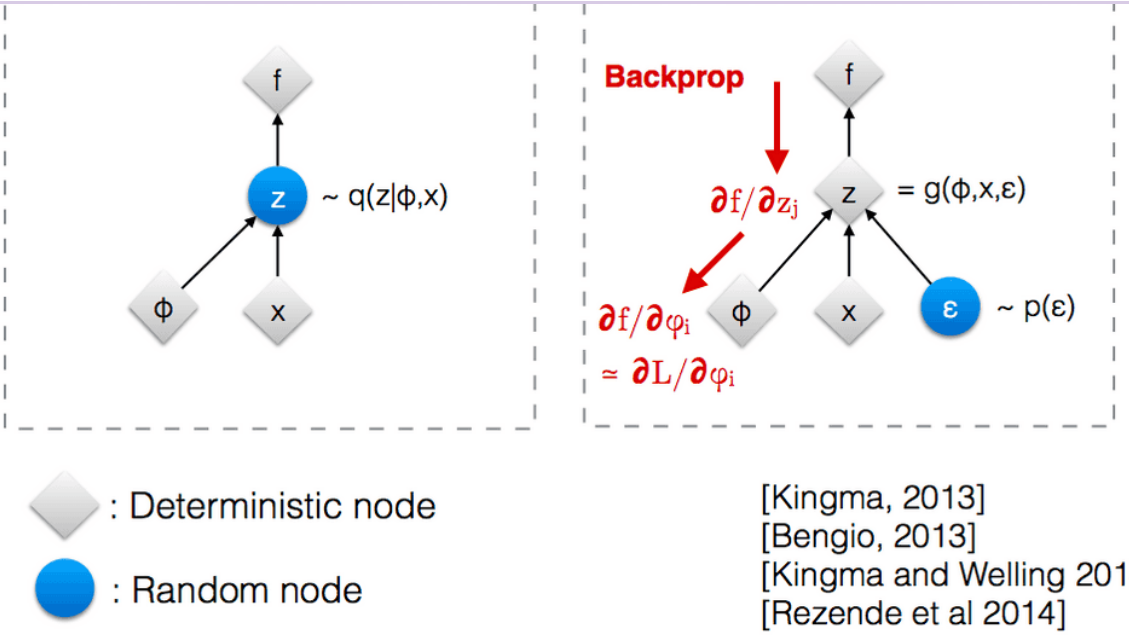

Re-parametrization trick. In VAE our latent representation **z** is a vector-valued random variable, not just a deterministic vector. In order to keep the doubly stochastic gradient differentiable, we keep distribution mean and variance deterministic (on this picture they and other weights of encoder are included into ϕ parameter), but inject randomness through a random variable ϵ

Why doing so?

There are 3 reasons, all technical.

First, as I mentioned previously, it is a practical way to achieve a gradient estimator that would actually converge. MCMC gradient estimator, used normally, would have too big of a variance, and training process fails to converge in practice.

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them deterministic, and inject randomness with a separate variable ϵ, it keeps μ and σ differentiable and lets the model learn them.

Third, the data points in the training set might not cover the whole latent space. Randomness helps to partially mitigate the issue of presense of holes in the latent space.

Practical implementation of loss and its gradients

Ok, now we're done with Bayesian theory. It might by nice for drawing inspiration, but it is "more like guidelines, rather than actual rules". Time to implement our loss and its gradient it in practice. Look at the loss function again:

$$\mathcal{L}(q(\mathbf{z})) = \underbrace{\mathbb{E}_{q(\mathbf{z})} \log p(\mathbf{x}|\mathbf{z})}_{\text{Expected log-likelihood}} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Regulariser term KL-divergence}}$$

First, let us interpret the terms. In case of VAE, our guide $q(\mathbf{z})$ is the output of encoder neural network. As encoder output depends on variational parameters ϕ and input data $\mathbf{x}$, we will denote $q(\mathbf{z})$ in case of VAE $q_\phi(\mathbf{z}|\mathbf{x})$. We are searching for the guide in the form of a multivariate Gaussian: $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \mu, \sigma)$.

Second, $p(\mathbf{x}|\mathbf{z})$ corresponds to reconstruction of image from the latent representation by the decoder, so it is rather $p(\hat{\mathbf{x}}|\mathbf{z})$; the term also depends on the decoder (generative) parameters θ, thus we shall denote it $p_\theta(\hat{\mathbf{x}}|\mathbf{z})$. Possible options for it are Bernoulli MLP and Gaussian MLP errors. I'd go with Gaussian - in that case reconstruction error takes the form of L2 error: $\log p(\mathbf{x}|\hat{\mathbf{x}}) = \log e^{-\frac{(\mathbf{x}-\hat{\mathbf{x}})^2}{2}} = ||\mathbf{x} - \hat{\mathbf{x}}||_2^2$.

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identity matrix of variance: $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$

So, we get:

$$\mathcal{L}(q(\mathbf{z})) = \int\int \log p_\theta(\mathbf{x}|\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} d\mathbf{x} + \int\int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} d\mathbf{z} d\mathbf{x} =$$

$$= \int\int \log p_\theta(\mathbf{x}|\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} d\mathbf{x} + \int\int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{z}) d\mathbf{z} d\mathbf{x} - \int\int q_\phi(\mathbf{z}|\mathbf{x}) \log q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} d\mathbf{x}.$$

Let us work with individual terms:

1. $\int\int \log p_\theta(\mathbf{x}|\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} d\mathbf{x}$ - this term depends on the choice of reconstruction error function. In case of Gaussian posterior it will look like an L2 norm, in case of Bernoulli - like cross-entropy.
2. $\int\int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{z}) d\mathbf{z} d\mathbf{x} = \int \mathcal{N}(\mathbf{z}; \mu, \sigma) \log \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I}) = -\frac{J}{2} \log(2\pi) - \frac{1}{2} \sum_{j=1}^{J} (\mu_j^2 + \sigma_j^2)$
3. $\int\int q_\phi(\mathbf{z}|\mathbf{x}) \log q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} d\mathbf{x} = \int \mathcal{N}(\mathbf{z}; \mu, \sigma) \log \mathcal{N}(\mathbf{z}; \mu, \sigma) = -\frac{J}{2} \log(2\pi) - \frac{1}{2} \sum_{j=1}^{J} (1 + \log \sigma_j^2)$

In practice we are working with finite sets of points and are using Monte-Carlo estimators. Hence, adding the three terms together and replacing integrals with sums we get:

$$\underbrace{\sum_{j=1}}_{\text{regularization term}} \qquad \underbrace{\sum_{l=1}}_{\text{reconstruction quality term}}$$

As I said before, in practice reconstruction quality term takes form of either L2 norm of difference between input and reconstructed image in case of Gaussian posterior $p_\theta(\mathbf{x}|\mathbf{z})$, or cross-entropy in case of multivariate Bernoulli posterior $p_\theta(\mathbf{x}|\mathbf{z})$.

Implementation

There is a nice repository on Github with various flavours of VAE, implemented in PyTorch. I've reproduced it, removing some of the optional abstraction layers.

First, let us define the configuration options for our VAE training:

```
config = {
    'model_params': {
      'name': 'VAE',
      'in_channels': 3,
      'latent_dim': 128
    },

    'data_params': {
      'root_dir': "Data/celeba/",
      'annotations_file_name': "list_eval_partition.csv",
      'annotations_file_name': "list_eval_partition.csv",
      'train_batch_size': 64,
      'val_batch_size':  64,
      'patch_size': 64,
      'num_workers': 4
    },
```

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```
        'LR': 0.005,
        'weight_decay': 0.0,
        'scheduler_gamma': 0.95,
        'kld_weight': 0.00025,
        'manual_seed': 1265
    },

    'trainer_params': {
        # 'gpus': [1],
        'max_epochs': 100
    },

    'logging_params': {
        'save_dir': "logs/",
        'name': "VAE"
    }
}
```

Second, let us set implement the VAE itself.

```
from typing import *
import torch
from torch import nn


class VAE(nn.Module):
    """Vanilla Variational Autoencoder (VAE) implementation.

    Based on: https://github.com/AntixK/PyTorch-VAE.
    """
    def __init__(self, in_channels: int, latent_space_dimension: int
        super(VAE, self).__init__()
```

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```
    self.hidden_layers_channels = [512, 256, 128, 64, 32]
else:
    self.hidden_layers_channels = hidden_layers_channels

hidden_layers_channels_reversed = self.hidden_layers_channel

self.latent_space_dimension = latent_space_dimension

# encoder
# -------
encoder_modules = []
current_in_channels = in_channels
for index, dim in enumerate(self.hidden_layers_channels):
    encoder_modules.append(nn.Sequential(
        nn.Conv2d(in_channels=current_in_channels, out_chanr
        nn.BatchNorm2d(self.hidden_layers_channels[index]),
        nn.ReLU()
    ))
    current_in_channels = dim

self.encoder = nn.Sequential(*encoder_modules)

# latent vector
# -------------

# Each convolutional layer of the encoder downscales the imc
# Hence, by the time we reach latent layer, the image dimens
self.downscaled_image_dimensionality = int(config['data_paran

self.mu = nn.Linear(self.hidden_layers_channels[-1] * (self.
self.log_var = nn.Linear(self.hidden_layers_channels[-1] * (

# decoder
# -------
```

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```
        decoder_modules = []
        current_in_channels = self.hidden_layers_channels[-1]
        for index, dim in enumerate(hidden_layers_channels_reversed)
            decoder_modules.append(nn.Sequential(
                nn.ConvTranspose2d(in_channels=current_in_channels,
                nn.BatchNorm2d(dim),
                nn.ReLU(),

            ))
            current_in_channels = dim
        self.decoder = nn.Sequential(*decoder_modules)

        # output layer
        # ------------
        self.final_layer = nn.Sequential(
            nn.Conv2d(self.hidden_layers_channels[0], out_channels=3
        )


    def encode(self, input: torch.Tensor) -> List[torch.Tensor]:
        """Generates a latent representation vector from an input."'
        result = self.encoder(input)
        result = torch.flatten(result, start_dim=1)

        mu = self.mu(result)
        log_var = self.log_var(result)

        return [mu, log_var]

    def decode(self, latent_vector: torch.Tensor, batch_size: int) -
        """Re-constructs an input from a latent representation."""
        result = self.decoder_input(latent_vector)
        # result = result.view(-1, 512, 2, 2)
        result = result.view(batch_size, self.hidden_layers_channels
```

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```
        result = self.final_layer(result)
        return result

    def reparametrize(self, mu: torch.Tensor, log_var: torch.Tensor)
        """Re-parametrization trick implementation. We sample N(mu,
        std = torch.exp(0.5 * log_var)
        eps = torch.randn_like(std)
        return eps * std + mu

    def forward(self, input: torch.Tensor, **kwargs) -> List[torch.T
        mu, log_var = self.encode(input)
        z = self.reparametrize(mu, log_var)
        batch_size = input.size()[0]
        return [self.decode(z, batch_size), input, mu, log_var]

    def loss_function(self, *args, **kwargs) -> dict:
        """
        VAE loss, consisting of 2 terms, reconstruction term and reg
        KL(N(\mu, \sigma), N(0, 1)) = \log \frac{1}{\sigma} + \frac{
        """
        recons = args[0]
        input = args[1]
        mu = args[2]
        log_var = args[3]

        kld_weight = kwargs['M_N']  # Account for the minibatch samp
        reconstruction_loss = nn.functional.mse_loss(recons, input)

        kld_loss = torch.mean(-0.5 * torch.sum(1 + log_var - mu ** 2

        loss = reconstruction_loss + kld_weight * kld_loss

        return {
            'loss': loss,
```

```
        }

    def sample(self, batch_size: int, current_device: int, **kwargs)
        """Samples a batch of random points (vectors) from the later
        and generates a batch of output images from it."""
        z = torch.randn(batch_size, self.latent_space_dimension)
        z = z.to(current_device)
        samples = self.decode(z, batch_size)

        return samples

    def generate(self, latent_vector: torch.Tensor):
        """Given an input latent space vector, generates an output f
        return self.forward(latent_vector)[0]
```

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We shall train our VAE to synthesize new human faces. I am using CelebA dataset as the basis. For some reason Torchvision wrapper around it failed to load from the Google Drive for me, so I've manually downloaded the dataset from Kaggle and written my own version of it with `kaggle datasets download -d jessicali9530/celeba-dataset` command and unzipped it in `/Data/celeba` folder of my jupyter lab workspace:

```
import os

# from torchvision.datasets import CelebA - failed to load from goog
from torch.utils.data import Dataset
from torchvision import transforms
import pandas as pd
from skimage import io
from PIL import Image
```

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```
    transforms.RandomHorizontalFlip(),
    transforms.CenterCrop(148),
    transforms.Resize(config['data_params']['patch_size']),
    transforms.ToTensor()
])


class CelebADataset(Dataset):
    """A manually-written wrapper around CelebA dataset, downloaded

    Kaggle: https://www.kaggle.com/datasets/jessicali9530/celeba-dat
    Docs: https://pytorch.org/tutorials/beginner/data_loading_tutori

    Download the folder from Kaggle and put it into Data/ folder.
    """
    def __init__(
        self,
        partition_file: str = 'Data/celeba/list_eval_partition.csv',
        root_dir: str = 'Data/celeba/img_align_celeba/img_align_cele
        transform=transform,
        split: str = "train"
    ):
        super(CelebADataset, self).__init__()

        self.partitions = pd.read_csv(partition_file)
        self.root_dir = root_dir
        self.transform = transform
        self.split = split

    def split_to_index(self):
        if self.split == "train":
            split_index = 0
        elif self.split == "validation":
            split_index = 1
```

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```
            else:
                raise ValueError(f"Unknown pratition type: {partition}")

            return split_index

        def __len__(self):
            split_index = self.split_to_index()
            data_in_split = self.partitions[self.partitions['partition']

            return len(data_in_split)

        def __getitem__(self, idx):
            if torch.is_tensor(idx):
                idx = idx.tolist()

            # get index of dataset partition
            split_index = self.split_to_index()

            # fetch the sample, transform it and return the result
            img_name = os.path.join(self.root_dir, self.partitions[self.
            image = Image.open(img_name)

            if self.transform:
                image = self.transform(image)

            return image


    # Load the dataset from file and apply transformations
    celeba_dataset = CelebADataset()
```

Wrap this dataset into a LightningDataModule abstraction:

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```
from torch.utils.data import DataLoader


# Create a torch dataloader for testing purposes
# ----------------------------------------------

if torch.backends.mps.is_available():
    device = torch.device("mps")
elif torch.cuda.is_available():
    device = torch.device("cuda")
else:
    device = torch.device("cpu")

celeba_dataloader = torch.utils.data.DataLoader(
    celeba_dataset,
    batch_size=config['data_params']['train_batch_size'],
    num_workers=0 if device.type == 'cuda' else 2,
    pin_memory=True if device.type == 'cuda' else False,
    shuffle=True
)


# Wrap into LightningDataModule
# -----------------------------

class CelebADataModule(LightningDataModule):
    def __init__(
        self,
        train_batch_size: int = 8,
        val_batch_size: int = 8,
        patch_size: Union[int, Sequence[int]] = (256, 256),
        num_workers: int = 0,
        pin_memory: bool = False,
        **kwargs,
    ):
```

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```
        self.train_batch_size = train_batch_size
        self.val_batch_size = val_batch_size
        self.patch_size = patch_size
        self.num_workers = num_workers
        self.pin_memory = pin_memory

    def setup(self, stage: Optional[str] = None) -> None:
        self.train_dataset = CelebADataset(split='train')
        self.val_dataset = CelebADataset(split='test')

    def train_dataloader(self) -> DataLoader:
        return DataLoader(
            self.train_dataset,
            batch_size=self.train_batch_size,
            num_workers=self.num_workers,
            shuffle=True,
            pin_memory=self.pin_memory,
        )

    def val_dataloader(self) -> DataLoader:
        return DataLoader(
            self.val_dataset,
            batch_size=self.val_batch_size,
            num_workers=self.num_workers,
            shuffle=False,
            pin_memory=self.pin_memory,
        )

    def test_dataloader(self) -> DataLoader:
        return DataLoader(
            self.val_dataset,
            batch_size=144,
            num_workers=self.num_workers,
            shuffle=True,
```

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Almost there. Now we configure our Torch Lightning experiment and trainer. Experiment code:

```
import pytorch_lightning as pl

from torchvision import transforms
import torchvision.utils as vutils
from torchvision.datasets import CelebA
from torch.utils.data import DataLoader


class Experiment(pl.LightningModule):
    def __init__(self, params: dict, model: nn.Module) -> None:
        super(Experiment, self).__init__()
        self.params = params
        self.model = model

    def forward(self, input: torch.Tensor, **kwargs) -> torch.Tensor
        return self.model.forward(input, **kwargs)

    def training_step(self, batch, batch_idx, optimizer_idx=0):
        real_images = batch
        self.curr_device = real_images.device

        results = self.forward(real_images)

        train_loss = self.model.loss_function(
            *results,
            M_N = self.params['kld_weight'], #al_img.shape[0]/ self.
            optimizer_idx=optimizer_idx,
            batch_idx=batch_idx
```

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```
        return train_loss['loss']

    def validaiton_step(self, batch, batch_idx, optimizer_idx=0):
        real_images = batch
        self.curr_device = real_images.device

        results = self.forward(real_images)
        validation_loss = self.model.loss_function(
            *results,
            M_N = 1.0, #real_images.shape[0] / self.num_val_imgs,
            optimizer_idx = optimizer_idx,
            batch_idx = batch_idx
        )

        self.log_dict({f"val_{key}": val.item() for key, val in val_

    def on_validation_end(self) -> None:
        self.sample_images()

    def sample_images(self):
        test_input, test_label = next(iter(self.trainer.datamodule.t

        test_input = test_input.to(self.current_device)
        test_label = test_label.to(self.current_device)

        reconstructions = self.model.generate(test_input, labels=tes

        vutils.save_image(
            reconstructions.data,
            os.path.join(self.logger.log_dir, "Reconstructions", f"r
            normalize=True,
            nrow=12
        )
```

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```
                samples = self.model.sample(144, self.curr_device, label
                vutils.save_image(
                    samples.cpu().data,
                    os.path.join(self.logger.log_dir, "Samples", f"{self
                    normalize=True,
                    nrow=12
                )
            except Warning:
                pass

        def configure_optimizers(self):
            optimizers = []
            schedulers = []

            optimizer = torch.optim.Adam(self.model.parameters(), lr=sel
            optimizers.append(optimizer)

            if self.params['scheduler_gamma'] is not None:
                scheduler = torch.optim.lr_scheduler.ExponentialLR(optim
                schedulers.append(scheduler)

                return optimizers, schedulers
            else:
                return optimizers
```

Now we can finally configure the trainer and run our training procedure:

```
itning import Trainer
tning.loggers import TensorBoardLogger
tning.callbacks import LearningRateMonitor, ModelCheckpoint
allel import DistributedDataParallel as DDP
tning.strategies import DDPStrategy
```

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```
annels=config['model_params']['in_channels'], latent_space_dimension=c
riment(config['exp_params'], model)
rBoardLogger(
g['logging_params']['save_dir'],
odel_params']['name']


ebADataModule()

(
ger,

ateMonitor(),
kpoint(
top_k=2,
th=os.path.join(tb_logger.log_dir , "checkpoints"),
or="val_loss",
last=True


mps", #'cpu', 'cude'

ingle_device', #'ddp_notebook',
ner_params']


ment, datamodule=data_module)
```

Ok, now if we train the model for even a few epochs, it will learn to generate decently looking human faces:

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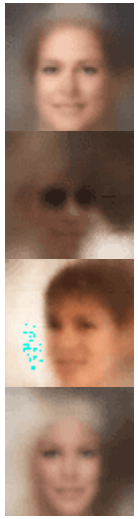
```
samples = model.sample(batch_size=4, current_device=torch.device("cu
for sample in samples:
    transform = T.ToPILImage()
    image = transform(sample)
    image.show()
```



Faces, generated with VAE. Just after 1-5 epochs of training on CelebA dataset we get some decently looking human faces.

Problems and improvements of VAE

Fuzzy results

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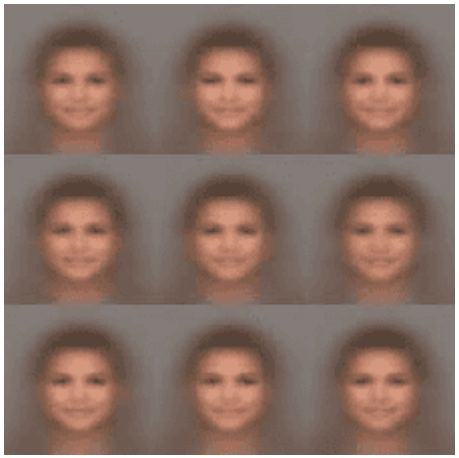

VAE-generated blurred faces.

How to explain this phenomenon? Consider latent space of a VAE, trained to recognized MNIST digits:

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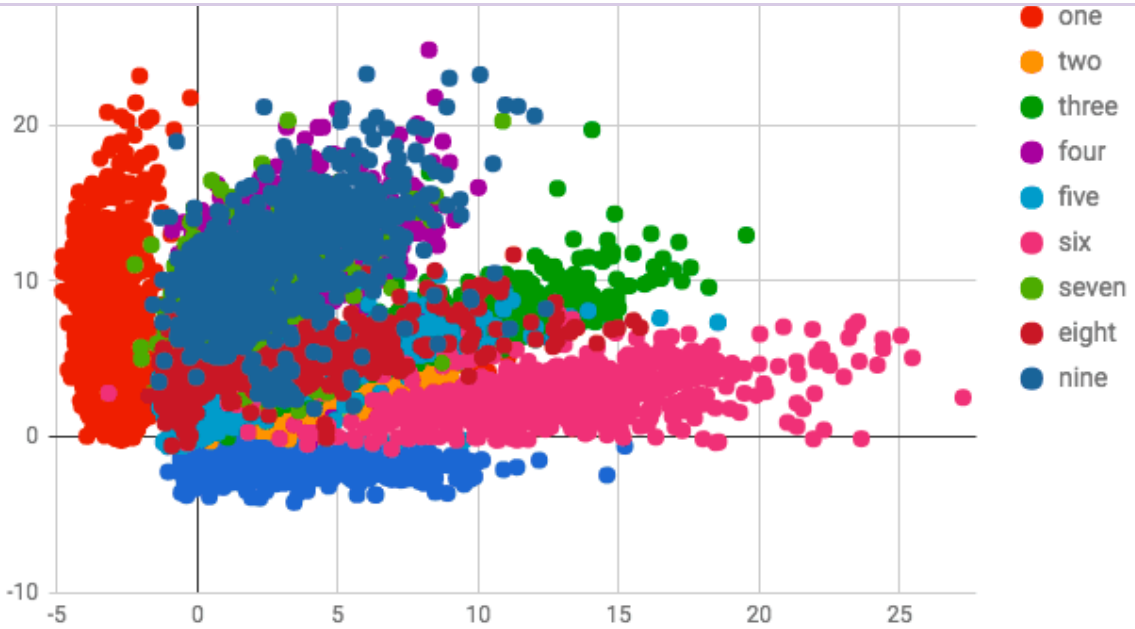

Latent space of VAE, trained to recognize MNIST handwritten digits.

Some classes (e.g. fours and nines) intersect with each other. If you sample a point from a region of latent space, where both fours and nines are frequent, VAE would basically produce a superposition of nine and four. This results in such a blurry image.

Posterior collapse

There are plenty of other issues left with regularization of the latent space of VAE.

For instance, sometimes generative part of VAE almost ignores the input image and generates a very generic image, very dissimilar from the input. Some authors claim that this happens when the regularization term of VAE (that moves prior on **z** closer

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ignored by VAE to a significant extent.

Another reason, possibly contributing to the posterior collapse, is the fact that variance of the Gaussian distribution, used in VAE, is diagonal, while in the real distribution the coordinates might not be independent.

This gave rise to dozens of flavours of VAE, which address these and other issues, such as beta VAE, vector quantization VAE (VQ-VAE) and other, which I won't cover here.

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- https://www.jmlr.org/papers/volume11/vincent10a/vincent10a.pdf - stacked denoising autoencoders by Y.Bengio group
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- https://cedar.buffalo.edu/~srihari/CSE676/14.2%20Denoising%20Autoencoders.pdf - presentation on denoising autoencoders

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- https://gregorygundersen.com/blog/2021/04/16/variational-inference/ - Gregory Gundersen on Variational Inference (VI)
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- https://pyro.ai/examples/svi_part_i.html - implementations of Stochastic VI, VAE etc. in Pyro library
- https://ai.stackexchange.com/questions/8885/why-is-the-variational-auto-encoders-output-blurred-while-gans-output-is-crisp - on blurred outputs of VAE
- https://datascience.stackexchange.com/questions/48962/what-is-posterior-collapse-phenomenon - on posterior collapse
- https://stats.stackexchange.com/questions/347378/variational-autoencoder-why-reconstruction-term-is-same-to-square-loss - on practical aspects of VAE loss
- https://openreview.net/pdf?id=r1xaVLUYuE - Posterior Collapse in VAE paper
- https://www.youtube.com/watch?v=oHtqlRIsXcQ - a talk on Posterior Collapse by the same author as the paper above
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- https://arxiv.org/pdf/1907.06845.pdf - on Bernoulli posterior in VAE
- https://avandekleut.github.io/vae/ - a great blog post on AE and VAE

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← MDS, Isomap, LLE, Spectral embedding

Intro to the Extreme Value Theory and Extreme Value Distribution →

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