Variational Auto-Encoders

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Roadmap

1. A reminder on auto-encoders
    a. Basics
    b. Denoising and sparse encoders
    c. Why do we need VAEs ?

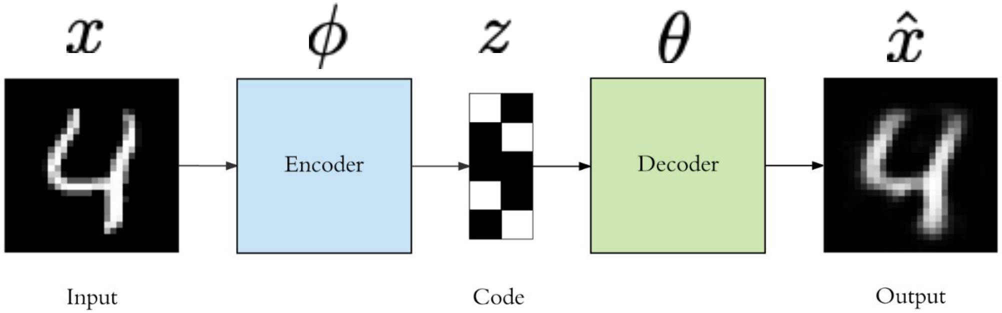
2. Understanding variational auto-encoders
    a. Key ingredients
    b. The reparametrization trich
    c. The underlying math

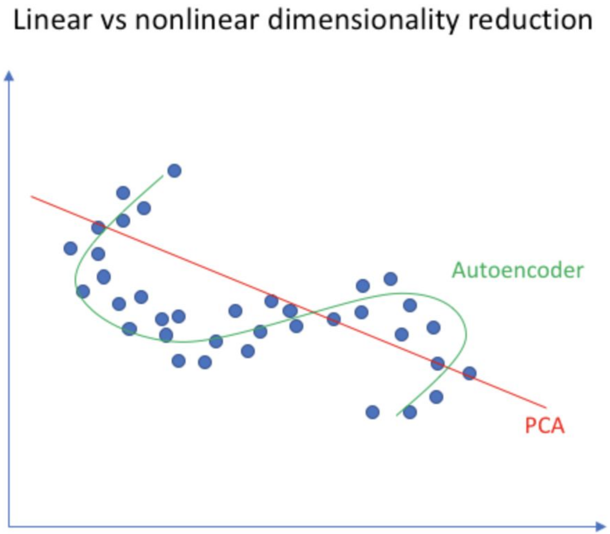
3. Applications and perspectives
    a. Disentanglement
    b. Adding a discrete condition
    c. Applications
    d. Comparison with GANs

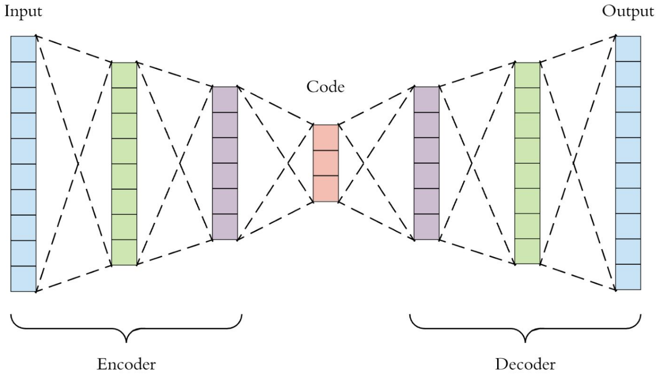
4. Do it yourself in PyTorch
    a. Build a basic denoising encoder
    b. Build a conditional VAE

Auto-Encoders

Basics



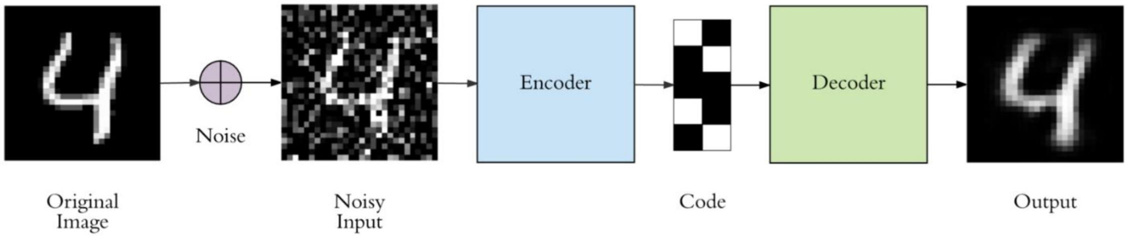


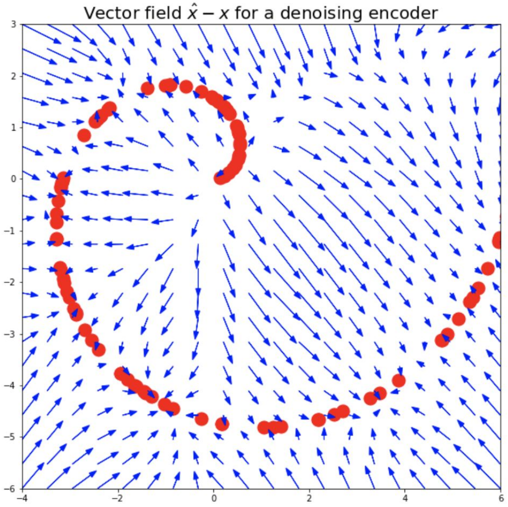


$$\mathcal{L}(x) = \frac{1}{2}\left(x - \theta(\phi(x))\right)^2$$

Denoising and Sparse Auto-Encoders

Denoising :





Sparse : enforces specialization of hidden units

$$\mathcal{L}(x, \hat{x}) + \lambda \sum_i \left| a_i^{(h)} \right|$$

Contractive : enforces that close inputs give close outputs

$$\mathcal{L}(x, \hat{x}) + \lambda \sum_i \left\| \nabla_x a_i^{(h)}(x) \right\|^2$$

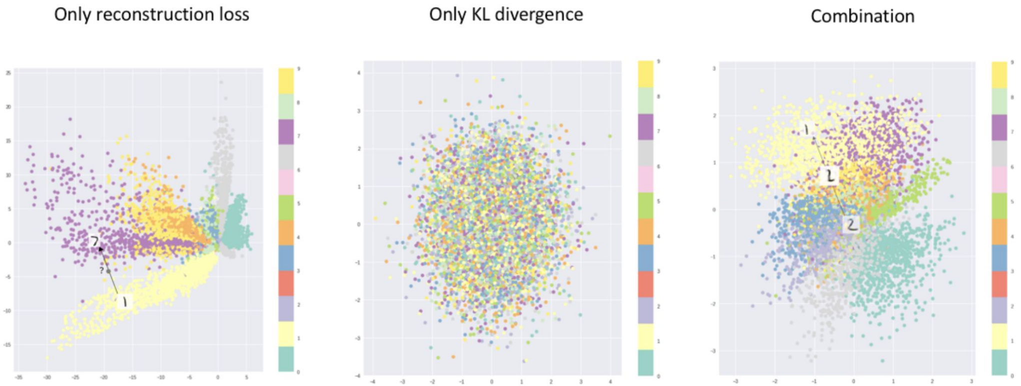
Why do we need VAE ?

VAE's are used as generative models : sample a latent vector, decode and you have a new sample

Q : Why can't we use normal auto-encoders ?
A : If we choose an arbitrary latent vector, we aren't close to any points in the training set and the reconstruction is garbage !

Q : How can we avoid this ?
A : Compactify the latent space !

Q : How can we do this ?
A : Two ingredients :
1. Encode into balls rather than points
2. Bring the balls closer together

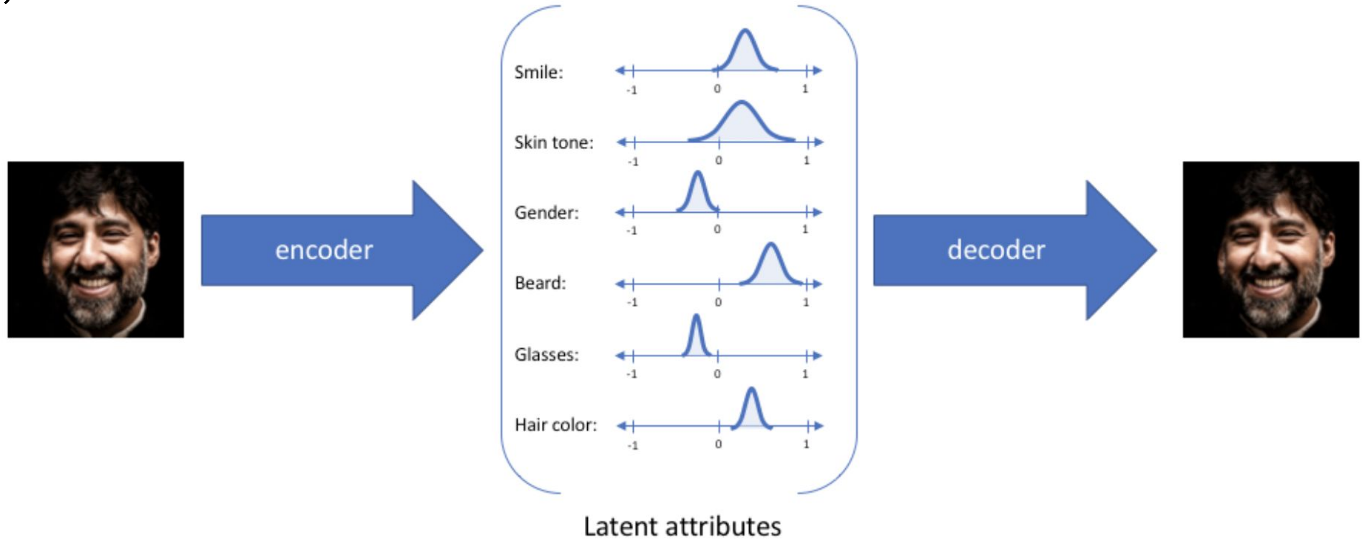


Variational Auto-Encoders

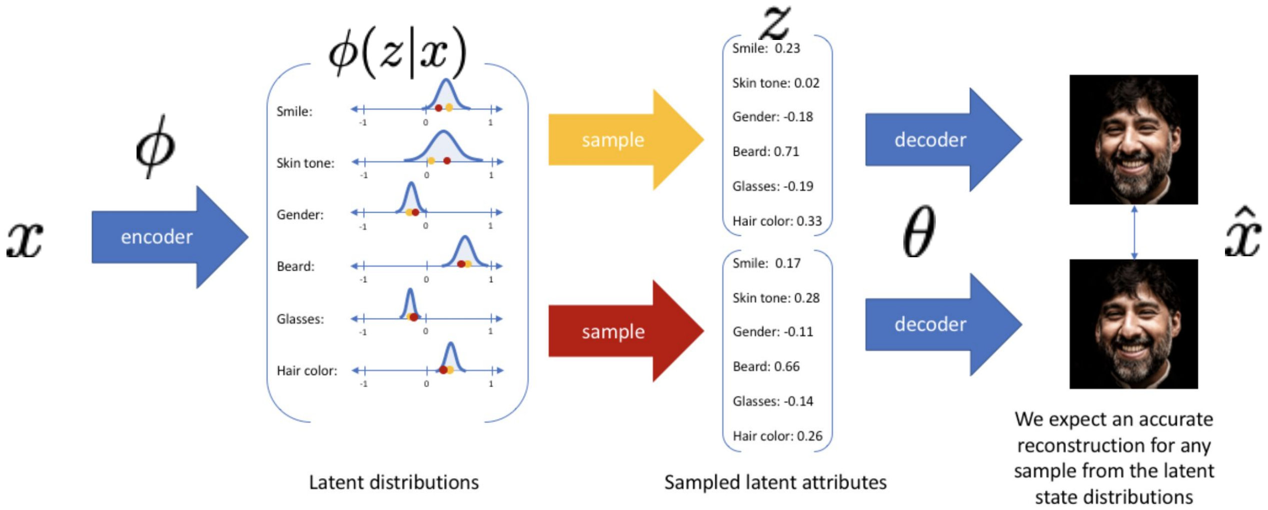
Key Ingredients

Generative models : unsupervised learning, aim to learn the distribution underlying the input data

VAEs : Map the complicated data distribution to a simpler distribution (encoder) we can sample from (Kingma & Welling 2014) to generate images (decoder)



First Ingredient : Encode into Distributions

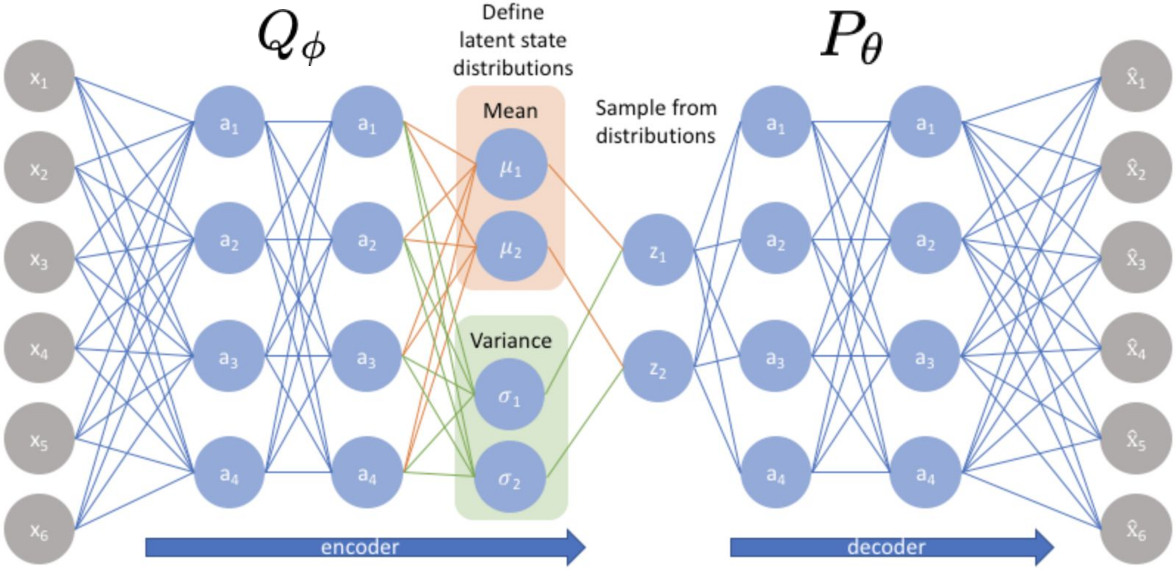


Q : Why encode into distributions rather than deterministic values ?

A1 : This creates balls in latent space
A2 : This ensures that close points in latent space lead to the same reconstruction. This gives "meaning" to the latent space.

Second Ingredient : impose structure

Q : How can I bring the balls together to compactify latent space ?
A : Make sure that Q(z|x) for different x's are close together !



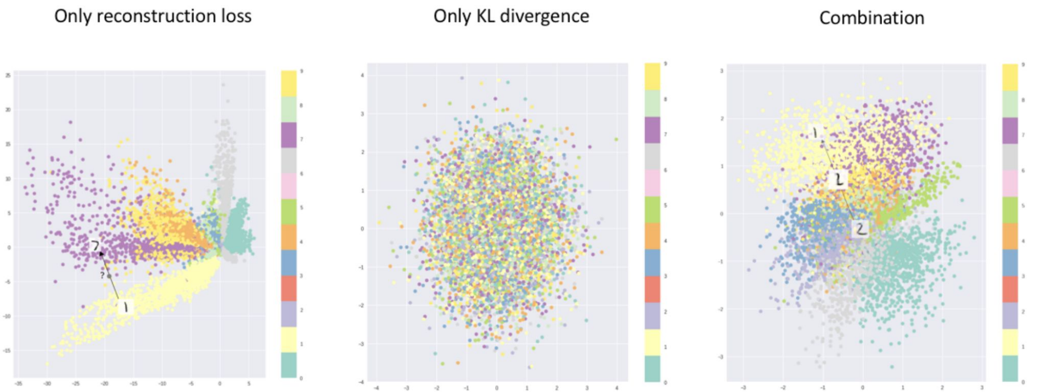
$$z \sim \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$$

Second Ingredient : impose structure

$$\mathcal{L}_{KL} = \mathbb{E}_{x \sim dataset}\left[D_{KL}\{Q_\phi(z|x)||p(z)\}\right], p \sim \mathcal{N}(0,1)$$

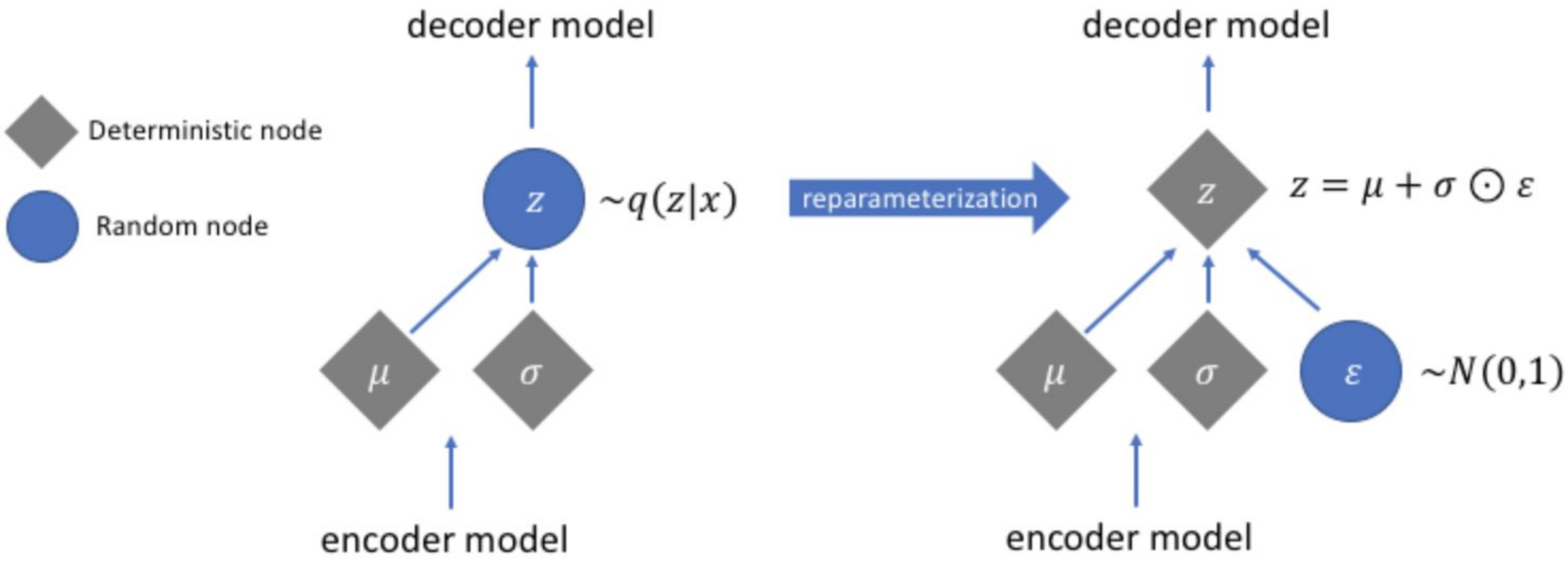
Q : How do we keep the balls close together ?
A : By adding springs the balls which pull them towards the center

Q : How ?
A : KL divergence with N(0,1) prior !



The Reparametrization Trick

Q : How can we backpropagate when one of the nodes is non-deterministic ?
A : Put the random process outside the network !



The Underlying Information Theory

How can we make a latent variable model ?

Choose a nice simple latent distribution $P(z)$, for example $P(z) \sim \mathcal{N}(0, \mathbb{I}_d)$, try to find its mapping to real space, $P(x|z)$, by maximizing the likelihood of observing the dataset under this generative process :

$$\mathcal{L} = \mathbb{E}_{x \sim \mathcal{D}} \log P(x) = \mathbb{E}_{x \sim \mathcal{D}} \log \int_z P(x|z)P(z)dz$$

To do this, we could parametrize $P(x|z)$ by a neural network and perform gradient ascent on $\mathcal{L}$. Problem : we can't calculate the integral in $\mathcal{L}$ for arbitrary $P(x|z)$! We could estimate it with sampling but that would be very inaccurate in high dimension.

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The idea is to circumvent this by introduce another distribution $Q(z)$ and exploit the following lower bound, valid for any $Q(z)$:

$$\mathcal{L} \geq \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}_{z\sim Q} \log P(x|z) - \beta D_{KL}(Q(z)||P(z))\right] = \text{ELBO}$$

This time, we have two things to optimize simultaneously : $Q(z|x)$ (the encoder) and $P(x|z)$ (the decoder) ! Why is this nicer ? Because both terms that appear are tractable

The Underlying Information Theory

$$\mathcal{L} \geq \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}_{z\sim Q}\log P(x|z) - \beta D_{KL}(Q(z)||P(z))\right] = \text{ELBO}$$

- The first term is called the reconstruction loss. Wait, this is silly because we have an intractable integral over z again ! Yes, but this time we have freedom to make $Q(z)$ dependent on x. Whereas before we had to integrate over the whole latent space, here we only have to integrate over a small ball containing values likely to reconstruct x :

$$Q(z|x) \sim \mathcal{N}(\mu(x), \Sigma(x)) \tag{1}$$

If the ball is small enough we can estimate the average just by sampling one point !

The Underlying Information Theory

$$\mathcal{L} \geq \mathbb{E}_{x\sim\mathcal{D}}\left[\mathbb{E}_{z\sim Q}\log P(x|z) - \beta D_{KL}(Q(z)||P(z))\right] = \text{ELBO}$$

- The second term in called the regularization term. Since both $P(z)$ and $Q(z|x)$ are tractable we have an easy analytic formula :

$$\mathcal{D}[\mathcal{N}(\mu(x), \Sigma(x))||\mathcal{N}(0, \mathbb{I}_d)] = \frac{1}{2}\Big(\operatorname{tr}(\Sigma(x)) + (\mu(x))^\top(\mu(x)) - d - \log\det(\Sigma(x))\Big) \tag{2}$$

The Underlying Information Theory

Proof of lower bound :

$$\begin{aligned} D_{KL}(Q(z)||P(z|x)) &= \sum_z Q(z) \log \frac{Q(z)}{P(z|x)} \\ &= \log P(x) + \sum_z Q(z) \log \frac{Q(z)}{P(z)} - \sum_z Q(z) \log P(x|z) \\ &= \log P(x) + \underbrace{D_{KL}(Q(z)||P(z)) - \mathbb{E}_{z\sim Q} \log P(x|z)}_{\text{ELBO}} \end{aligned}$$

$$\begin{aligned} \mathbb{E}_{x\sim\mathcal{D}} \log P(x) &= \mathbb{E}_{x\sim\mathcal{D}} \left[D_{KL}(Q(z)||P(z|x)) + \text{ELBO} \right] \\ &\geq \text{ELBO} \end{aligned}$$

VAEs in Practice

Disentanglement : Beta-Vae

We saw that the objective function is made of a reconstruction and a regularization part.

$$\mathcal{L} = \mathbb{E}_{z \sim Q} \log P(x|z) - \beta D_{KL}(Q(z|x)||P(z))$$

By adding a tuning parameter we can control the tradeoff.

If we increase beta:
- The dimensions of the latent representation are more disentangled
- But the reconstruction loss is less good

Generating Conditionally : CVAEs

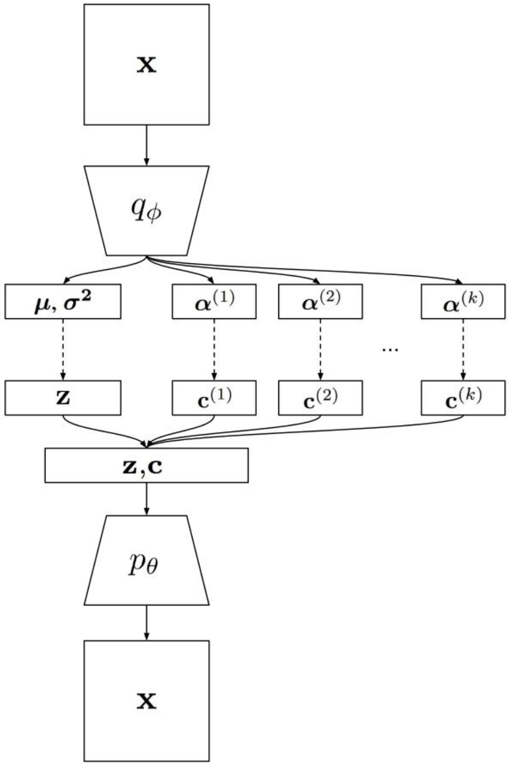
Add a one-hot encoded vector to the latent space and use it as categorical variable, hoping that it will encode discrete features in data (digits in MNIST)

Q : The usual reparametrization trick doesn't work here, because we need to sample discrete values from the distribution ! What can we do ?
A : Gumbel-Max trick

Q : How do I balance the regularization terms for the continuous and discrete parts ?
A : Control the KL divergences independently

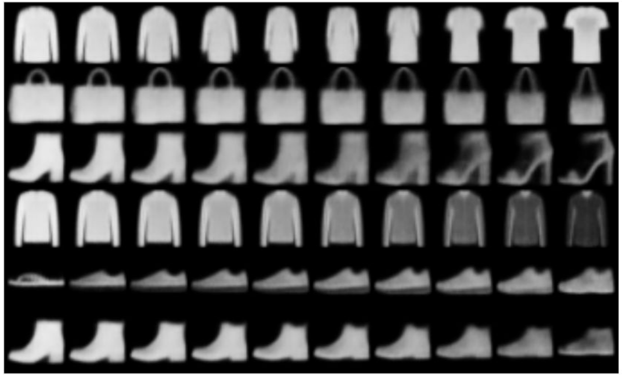
$$\mathcal{L}(\theta, \phi) = \mathbb{E}_{q_\phi(\mathbf{z},\mathbf{c}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z},\mathbf{c})]$$

$$-\gamma|D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))-C_z|-\gamma|D_{KL}(q_\phi(\mathbf{c}|\mathbf{x}) \parallel p(\mathbf{c}))-C_c|$$



Applications

Image generation : Dupont et al. 2018



Text generation : Bowman et al. 2016

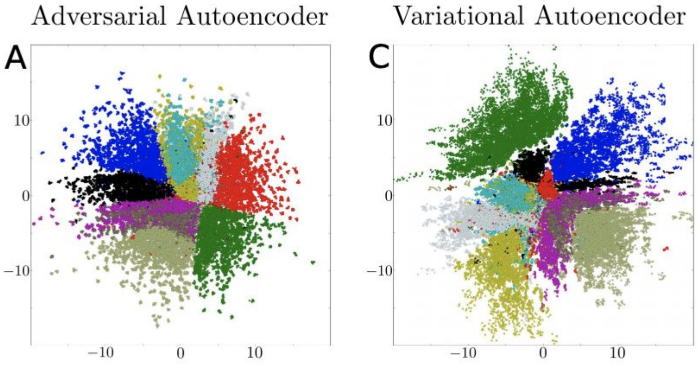
“ i want to talk to you . ”
“i want to be with you . ”
“i do n’t want to be with you . ”
i do n’t want to be with you .
she did n’t want to be with him .

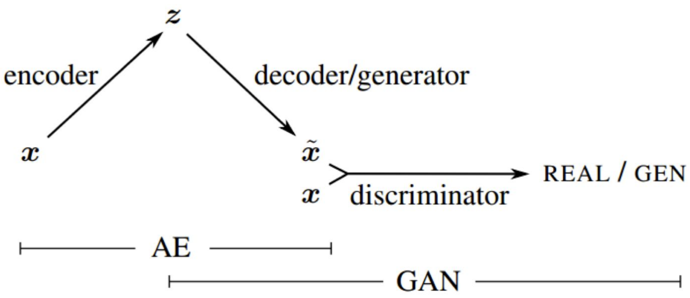
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

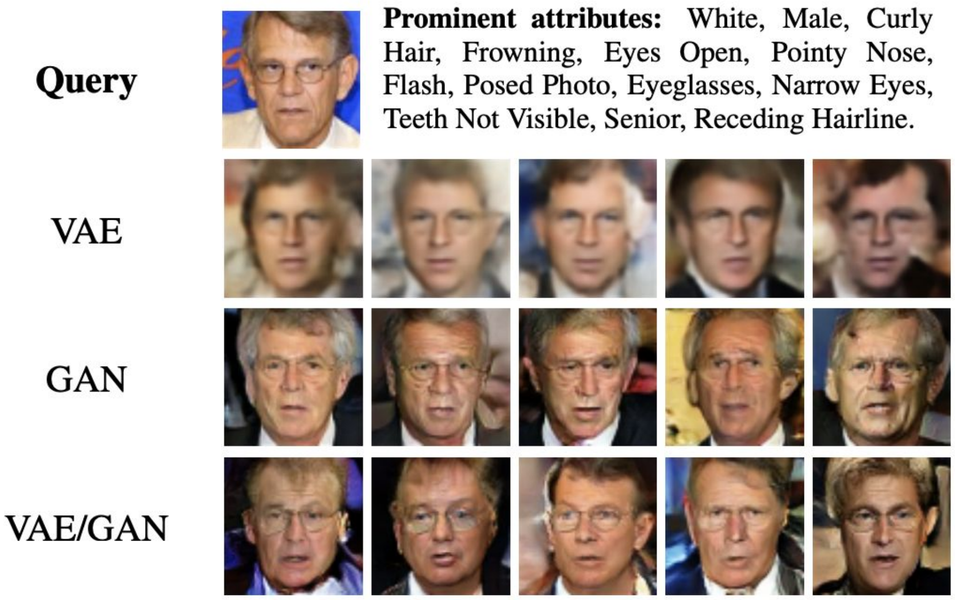
Comparison with GANs

VAE	GAN
Easy metric : reconstruction loss	Metric is hard to interpret
Interpretable and disentangled latent space	Low interpretability
Easy to train	Tedious hyperparameter searching
Noisy generation	Clean generation

Towards a Mix of the Two ?







Do It Yourself
In Pytorch

Auto-Encoder

1. Example: a simple fully-connected auto-encoder

```python
loss_fn = torch.nn.MSELoss()

def train_model(model,loss_fn,data_loader=None,epochs=1,optimizer=None):
    model.train()
    for epoch in range(epochs):
        for batch_idx, (data, _) in enumerate(train_loader):

            data = data.view([-1, 784])
            optimizer.zero_grad()
            output = model(data)
            loss = loss_fn(output, data)
            loss.backward()
            optimizer.step()
            if batch_idx % 50 == 0:
                print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                    epoch, batch_idx * len(data), len(data_loader.dataset),
                    100. * batch_idx / len(data_loader), loss.data.item()))
```

```python
class AutoEncoder(nn.Module):
    def __init__(self, input_dim, encoding_dim):
        super(AutoEncoder, self).__init__()
        self.encoder = nn.Linear(input_dim, encoding_dim)
        self.decoder = nn.Linear(encoding_dim, input_dim)

    def forward(self, x):
        encoded = F.relu(self.encoder(x))
        decoded = self.decoder(encoded)
        return decoded
```

2. DIY: implement a denoising convolutional auto-encoder for MNIST

Variational Auto-Encoder

1. Example: a simple VAE

```
def train(model, data_loader=data_loader,num_epochs=num_epochs):
    for epoch in range(num_epochs):
        for i, (x, _) in enumerate(data_loader):

            # Forward pass
            x = x.to(device).view(-1, image_size)
            x_reconst, mu, log_var = model(x)

            # Compute reconstruction loss and kl divergence
            reconst_loss = F.binary_cross_entropy(x_reconst, x, reduction='sum')
            kl_div = - 0.5 * torch.sum(1 + log_var - mu.pow(2) - log_var.exp())

            # Backprop and optimize
            loss = reconst_loss + kl_div
            optimizer.zero_grad()
            loss.backward()
            optimizer.step()
```

```
class VAE(nn.Module):
    def __init__(self, image_size=784, h_dim=400, z_dim=20):
        super(VAE, self).__init__()
        self.fc1 = nn.Linear(image_size, h_dim)
        self.fc2 = nn.Linear(h_dim, z_dim)
        self.fc3 = nn.Linear(h_dim, z_dim)
        self.fc4 = nn.Linear(z_dim, h_dim)
        self.fc5 = nn.Linear(h_dim, image_size)

    def encode(self, x):
        h = F.relu(self.fc1(x))
        return self.fc2(h), self.fc3(h)

    def reparameterize(self, mu, log_var):
        std = torch.exp(log_var/2)
        eps = torch.randn_like(std)
        return mu + eps * std

    def decode(self, z):
        h = F.relu(self.fc4(z))
        return torch.sigmoid(self.fc5(h))

    def forward(self, x):
        mu, log_var = self.encode(x)
        z = self.reparameterize(mu, log_var)
        x_reconst = self.decode(z)
        return x_reconst, mu, log_var
```

2. DIY: implement a conditional VAE for MNIST

Questions