Deep learning

7.4. Variational Autoencoder

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Coming back to generating a signal, instead of training an autoencoder and modeling the distribution of Z, we can try an alternative approach:

Impose a distribution for Z and then train a decoder g so that $g(Z)$ matches the training data.

This can be done with a **Variational Autoencoder** (Kingma and Welling, 2013).

We want to train a model $p(X = x \mid Z = z; w)$ such that, with $p(Z = z)$ fixed, for instance to $\mathcal{N}(0, I)$, the marginal

$$p(X = x; w) = \int p(X = x \mid Z = z; w)p(Z = z)dz$$

match the training data, hence maximizes

$$\sum_n \log p(X = x_n; w).$$

This value is sometimes referred to as the (log of the) **model evidence**.

The model for $p(X = x \mid Z = z)$ plays the role of a decoder: Given the latent representation z, it estimates the signal x.

A form that echoes Gaussian mixture models, is to take

$$p(X \mid Z = z; w) = \mathcal{N}(\mu^g(z; w), \text{diag}(\sigma^g(z; w))).$$

where μ^g and σ^g are of same shape as X and are computed by a deep model g.

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$$\begin{aligned} p(X = x) &= \int p(X = x, Z = z; w) dz \\ &= \int \frac{p(X = x, Z = z; w)}{q(Z = z)} q(Z = z) dz \\ &= \mathbb{E}_{z \sim q(Z)} \left[\frac{p(X = x, Z = z; w)}{q(Z = z)} \right]. \end{aligned}$$

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Hence, if we sample one $z \sim q(Z)$, the quantity

$$\frac{p(X = x, Z = z; w)}{q(Z = z)}$$

is an unbiased estimator of $p(X = x; w)$.

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Due to its convexity the log of our unbiased estimator of $p(X = x; w)$ is not an unbiased estimator of $\log p(X = x; w)$.

We can look at that more precisely:

$$
\begin{aligned}
&\mathbb{E}_{z\sim q(Z)}\left[\log \frac{p(X=x,Z=z;w)}{q(Z=z)}\right] \\
&= \mathbb{E}_{z\sim q(Z)}\left[\log \frac{p(Z=z\mid X=x;w)p(X=x;w)}{q(Z=z)}\right] \\
&= \log p(X=x;w) + \mathbb{E}_{z\sim q(Z)}\left[\log \frac{p(Z=z\mid X=x;w)}{q(Z=z)}\right] \\
&= \log p(X=x;w) - \mathbb{D}_{\mathrm{KL}}\left(q(Z)\,\|\,p(Z\mid X=x;w)\right).
\end{aligned}
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\end{aligned}$$

Where

$$\mathbb{D}_{\mathrm{KL}}(a\,\|\,b) = \int a(u)\log\frac{a(u)}{b(u)}du = -\int a(u)\log\frac{b(u)}{a(u)}du$$

is the **Kullback-Leibler divergence.**

This quantity is non-negative, hence the expectation of the log of our estimator is a lower bound of $\log p(X=x;w)$, called the **Evidence Lower Bound** (ELBO).

Hence, to have the model fit the data when we optimize the ELBO, we need a $q(Z)$ that makes $\mathbb{D}_{\mathrm{KL}}\left(q(Z) \,\|\, p(Z \mid X = x; w)\right)$ as small as possible.

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All the derivations remain valid if q is a function of X. The quantity we want to maximize is then

$$\log p(X = x; w) - \mathbb{D}_{\mathrm{KL}}\left(q(Z \mid X = x; w') \,\|\, p(Z \mid X = x; w)\right)$$

and maximizing it will both maximize $\log p(X = x; w)$, and minimize the KL term, hence will bring $q(Z \mid X = x; w')$ close to $p(Z \mid X = x; w)$.

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The role of $q(Z \mid X = x; w')$ is very similar to that of an encoder: Given the signal x, it estimates what z are consistent with the decoding.

We can again use a Gaussian whose parameters are computed by a deep model f

$$q(Z \mid X = x; w') \sim \mathcal{N}(\mu^f(x; w'), \mathrm{diag}(\sigma^f(x; w'))).$$

One last technical point is that we can rewrite the ELBO as

$$\mathbb{E}_{z\sim q(Z|X=x;w')}\left[\log \frac{p(X=x,Z=z;w)}{q(Z=z\mid X=x;w')}\right]$$
$$=\mathbb{E}_{z\sim q(Z|X=x;w')}\left[\log \frac{p(X=x\mid Z=z;w)p(Z=z)}{q(Z=z\mid X=x;w')}\right]$$
$$=\mathbb{E}_{z\sim q(Z|X=x;w')}\left[\log p(X=x\mid Z=z;w)-\log \frac{q(Z=z\mid X=x;w')}{p(Z=z)}\right]$$
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&= \mathbb{E}_{z\sim q(Z|X=x;w')}\left[\log p(X=x\mid Z=z;w) - \log \frac{q(Z=z\mid X=x;w')}{p(Z=z)}\right] \\
&= \mathbb{E}_{z\sim q(Z|X=x;w')}\Big[\log p(X=x\mid Z=z;w)\Big] - \mathbb{D}_{\mathrm{KL}}\left(q(Z\mid X=x;w')\,\|\,p(Z)\right).
\end{aligned}$$

This form allows to take advantage of the closed-form expression of the KL divergence between Gaussians to get a less noisy estimate:

$$\begin{aligned}
&\mathbb{D}_{\mathrm{KL}}\left(\mathcal{N}(\mu_1,\Sigma_1),\mathcal{N}(\mu_2,\Sigma_2)\right) \\
&\qquad = \frac{1}{2}\left[\log\frac{|\Sigma_1|}{|\Sigma_2|} - D + (\mu_1-\mu_2)^\top \Sigma_2^{-1}(\mu_1-\mu_2) + \mathrm{Tr}\left(\Sigma_2^{-1}\Sigma_1\right)\right].
\end{aligned}$$

So the final loss is

$$\mathscr{L}(w, w') = \frac{1}{N} \sum_n \mathbb{D}_{\mathrm{KL}} \left(q(Z \mid X = x_n; w') \,\|\, p(Z) \right) - \log p(X = x_n \mid Z = z_n; w)$$

where $\forall n,\ z_n \sim q(Z \mid X = x_n; w')$.

Minimizing the first term

$$\mathbb{D}_{\mathrm{KL}}\left(q(Z \mid X = x_n; w') \,\|\, p(Z)\right)$$

brings $q(Z \mid X = x_n; w')$ close to $p(Z) = \mathcal{N}(0, I)$.

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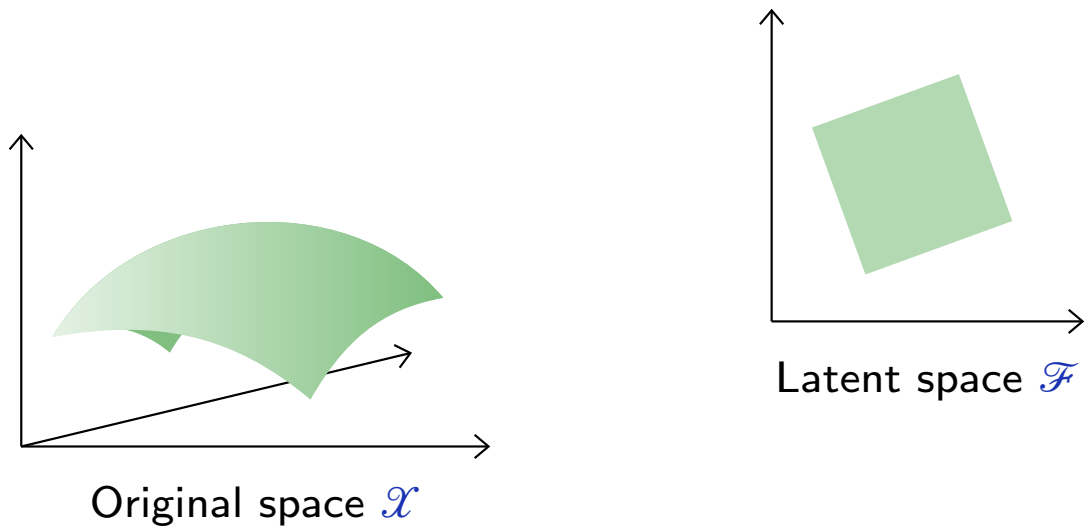

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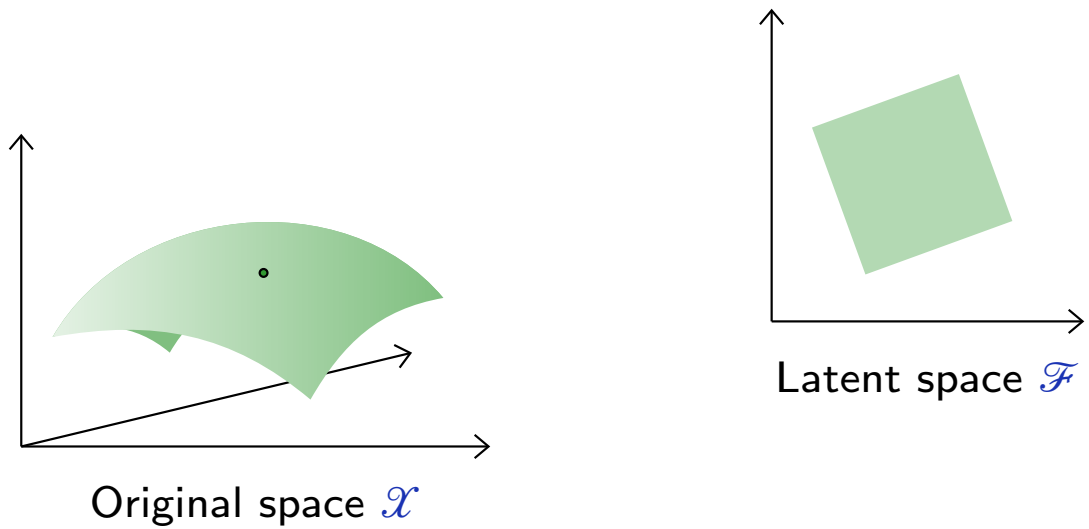

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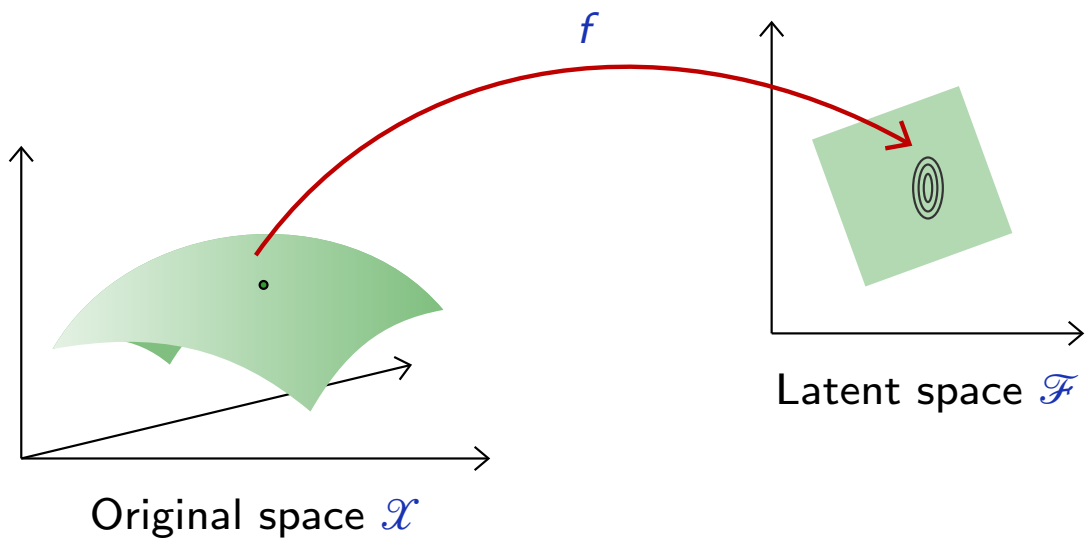

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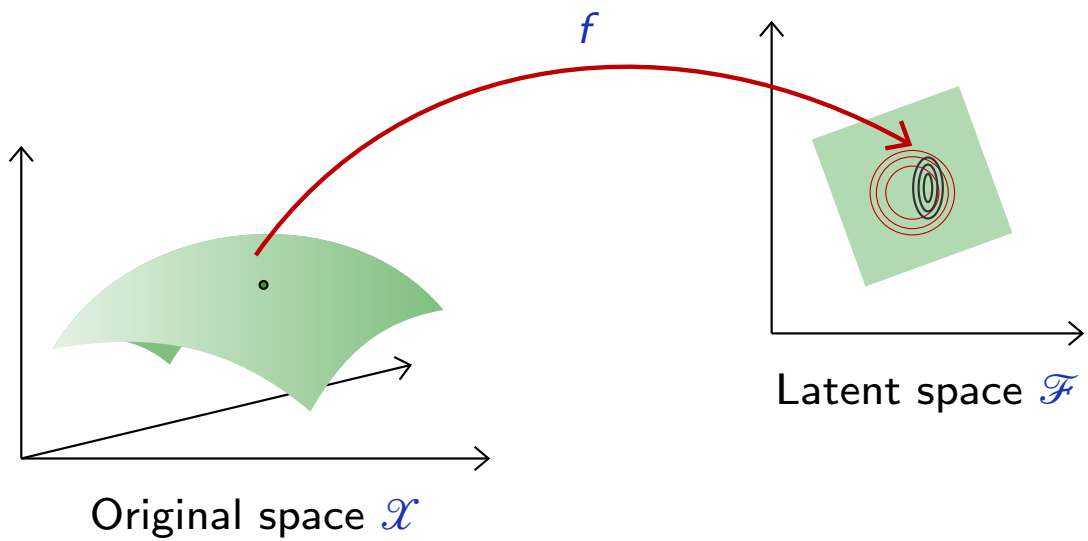

Minimizing the second term for a $z_n \sim q(Z \mid X = x_n; w')$

$$-\log p(X = x_n \mid Z = z_n; w)$$

maximizes the likelihood of the original data point x_n under $p(X \mid Z = z_n; w)$.

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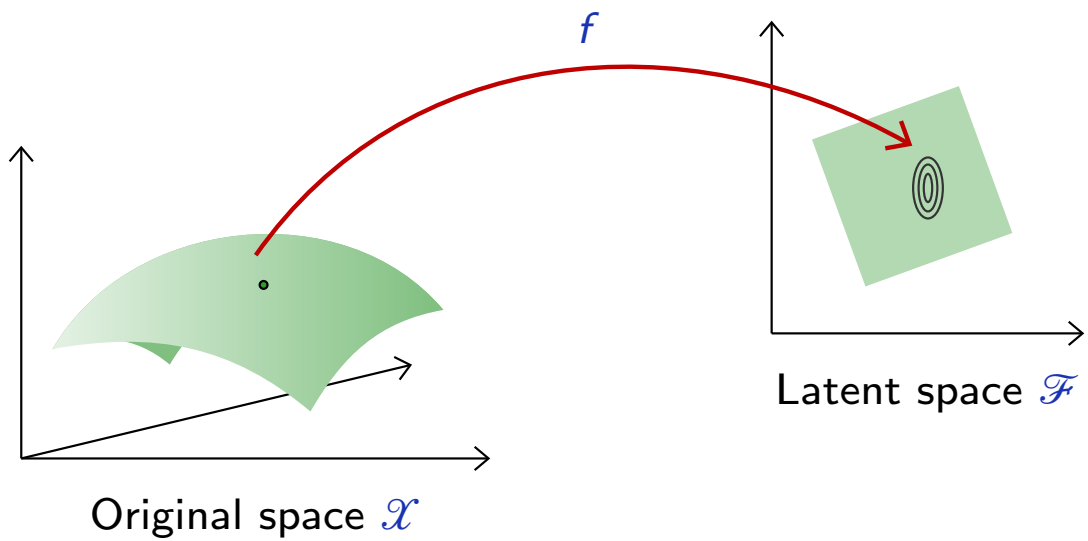

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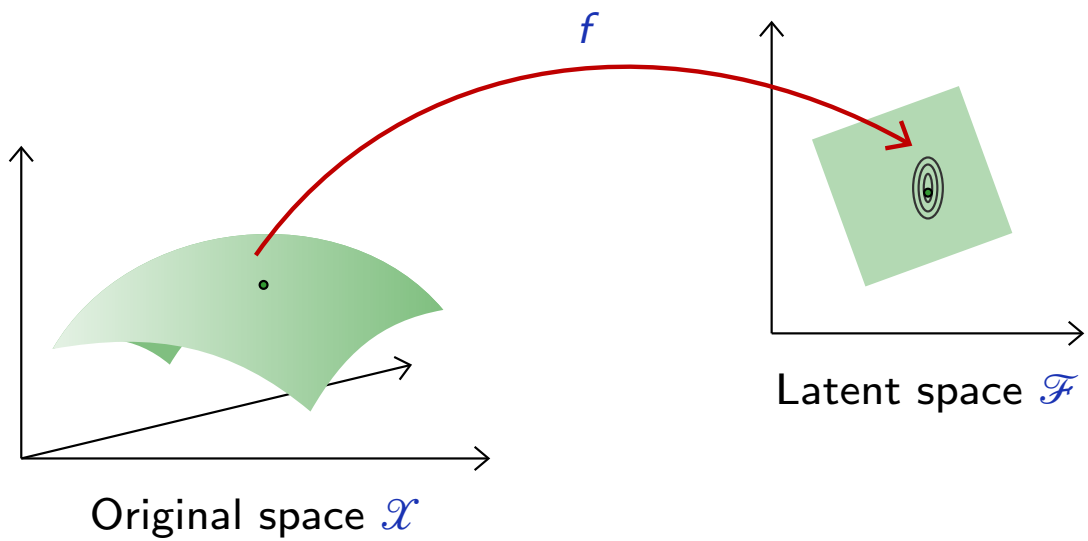

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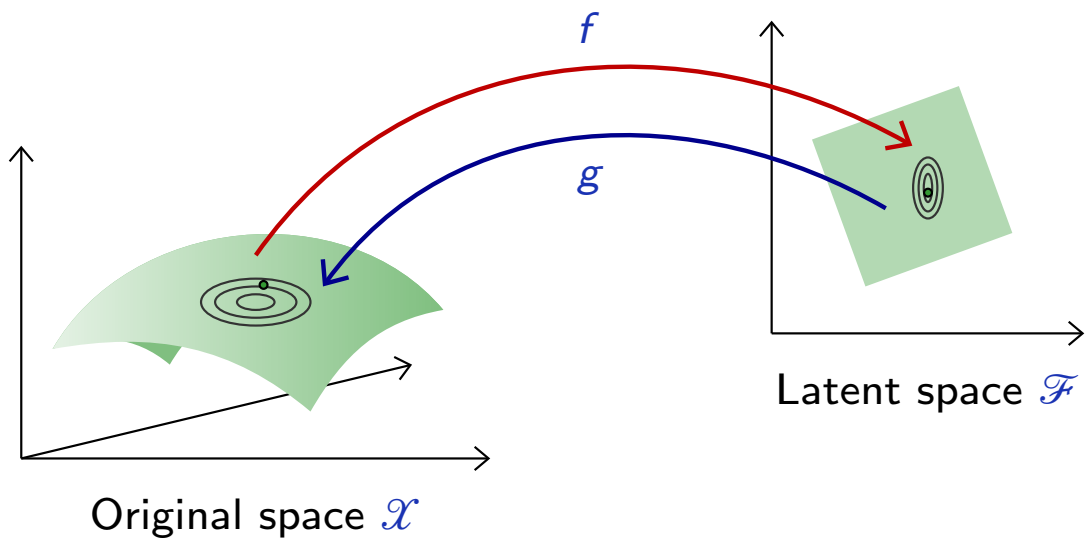


The assumption of independence between the component of $P(X \mid Z = z)$ allows the model to overfit the variance and additionally leads to grainy samples.

We fix this by forcing a variance of 1 during training and 0 during sampling.

```
class VariationalAutoEncoder(nn.Module):
    def __init__(self, nb_channels, latent_dim):
        super().__init__()

        self.encoder = nn.Sequential(
            nn.Conv2d(1, nb_channels, kernel_size=1),
            nn.ReLU(inplace=True),
            nn.Conv2d(nb_channels, nb_channels, kernel_size=5),
            nn.ReLU(inplace=True),
            nn.Conv2d(nb_channels, nb_channels, kernel_size=5),
            nn.ReLU(inplace=True),
            nn.Conv2d(nb_channels, nb_channels, kernel_size=4, stride=2),
            nn.ReLU(inplace=True),
            nn.Conv2d(nb_channels, nb_channels, kernel_size=3, stride=2),
            nn.ReLU(inplace=True),
            nn.Conv2d(nb_channels, 2 * latent_dim, kernel_size=4),
        )

        self.decoder = nn.Sequential(
            nn.ConvTranspose2d(latent_dim, nb_channels, kernel_size=4),
            nn.ReLU(inplace=True),
            nn.ConvTranspose2d(nb_channels, nb_channels, kernel_size=3, stride=2),
            nn.ReLU(inplace=True),
            nn.ConvTranspose2d(nb_channels, nb_channels, kernel_size=4, stride=2),
            nn.ReLU(inplace=True),
            nn.ConvTranspose2d(nb_channels, nb_channels, kernel_size=5),
            nn.ReLU(inplace=True),
            nn.ConvTranspose2d(nb_channels, 1, kernel_size=5),
        )
```

```
def encode(self, x):
    output = self.encoder(x).view(x.size(0), 2, -1)
    mu, log_var = output[:, 0], output[:, 1]
    return mu, log_var

def decode(self, z):
    mu = self.decoder(z.view(z.size(0), -1, 1, 1))
    return mu, mu.new_zeros(mu.size())
```

```
def sample_gaussian(param):
    mean, log_var = param
    std = log_var.mul(0.5).exp()
    return torch.randn(mean.size(), device=mean.device) * std + mean


def log_p_gaussian(x, param):
    mean, log_var, x = param[0].flatten(1), param[1].flatten(1), x.flatten(1)
    var = log_var.exp()
    return -0.5 * (((x - mean).pow(2) / var) + log_var + math.log(2 * math.pi)).sum(1)


def dkl_gaussians(param_a, param_b):
    mean_a, log_var_a = param_a[0].flatten(1), param_a[1].flatten(1)
    mean_b, log_var_b = param_b[0].flatten(1), param_b[1].flatten(1)
    var_a = log_var_a.exp()
    var_b = log_var_b.exp()
    return 0.5 * (
        log_var_b - log_var_a - 1 + (mean_a - mean_b).pow(2) / var_b + var_a / var_b
    ).sum(1)
```

Note in particular the **re-parameterization trick**:

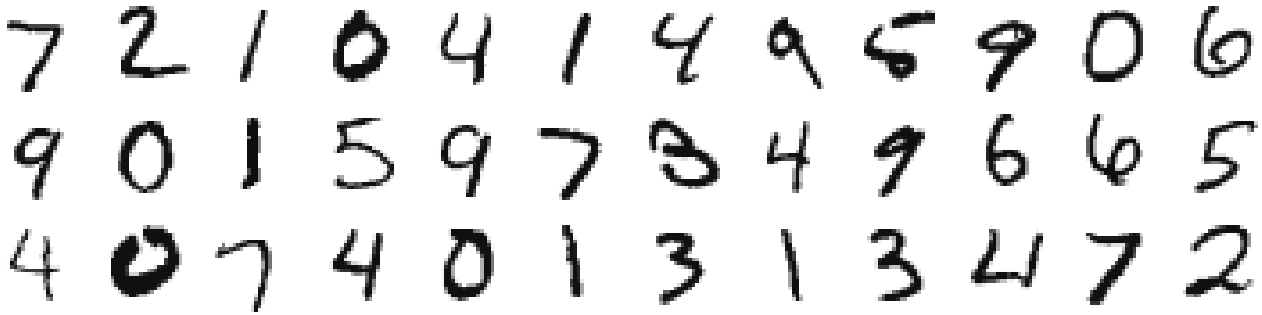
```
def sample_gaussian(param):
    mean, log_var = param
    std = log_var.mul(0.5).exp()
    return torch.randn(mean.size(), device=mean.device) * std + mean
```

Implementing the sampling of z that way allows to compute the gradient w.r.t the density's parameters without any particular property of `randn()`.

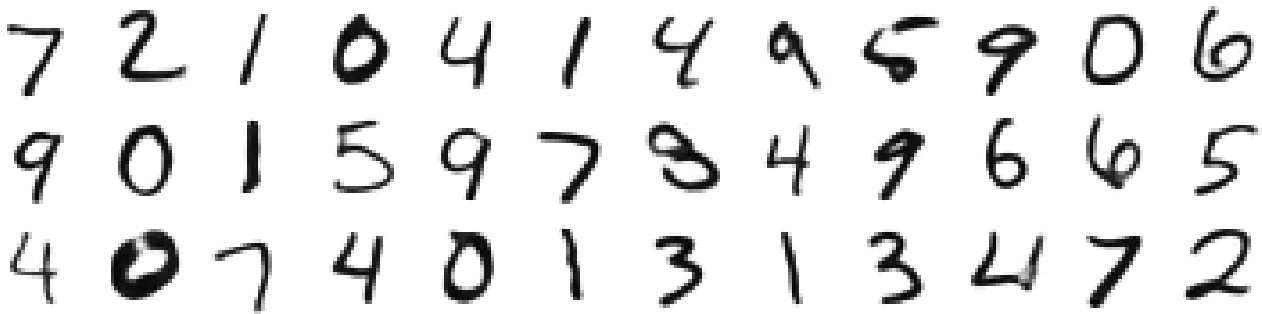
```
for x in train_input.split(args.batch_size):
    param_q_Z_given_x = model.encode(x)
    z = sample_gaussian(param_q_Z_given_x)
    param_p_X_given_z = model.decode(z)
    log_p_x_given_z = log_p_gaussian(x, param_p_X_given_z)

    dkl_q_Z_given_x_from_p_Z = dkl_gaussians(param_q_Z_given_x, param_p_Z)
    loss = -(log_p_x_given_z - dkl_q_Z_given_x_from_p_Z).mean()

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

```
parser.add_argument("--nb_epochs", type=int, default=25)

parser.add_argument("--learning_rate", type=float, default=1e-3)

parser.add_argument("--batch_size", type=int, default=100)

parser.add_argument("--latent_dim", type=int, default=32)

parser.add_argument("--nb_channels", type=int, default=32)
```

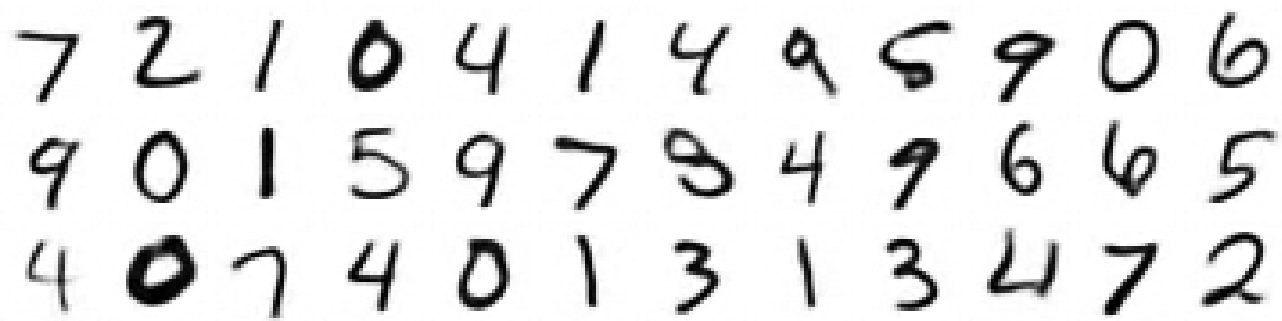
Original



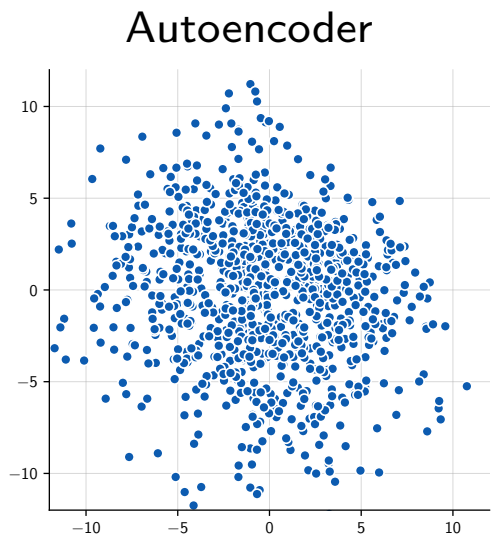
Autoencoder reconstruction ($d = 32$)



Variational Autoencoder reconstruction ($d = 32$)



We can look at two latent features to check that they are Normal for the VAE.



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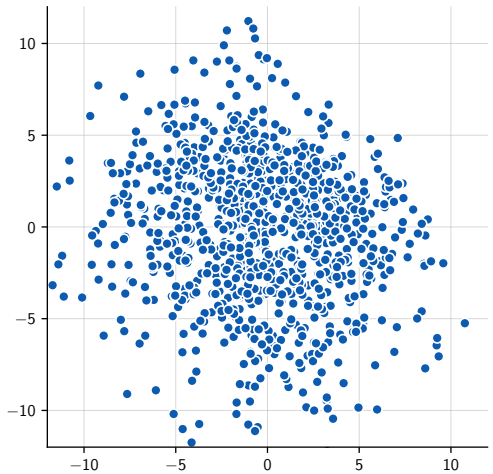
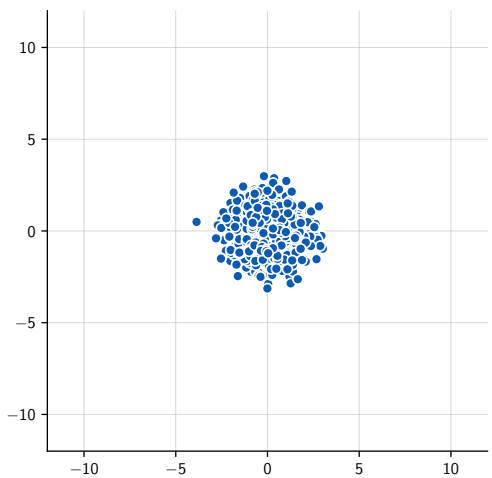
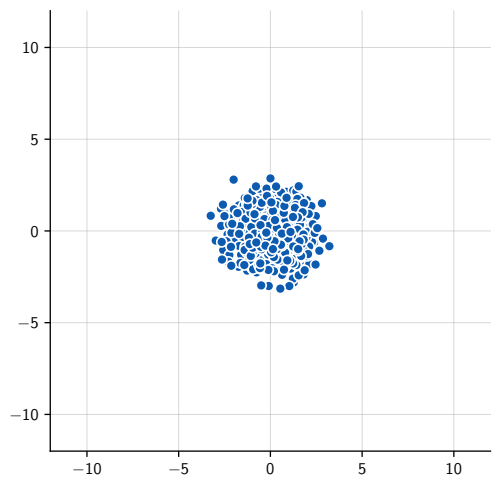
Autoencoder



Variational autoencoder

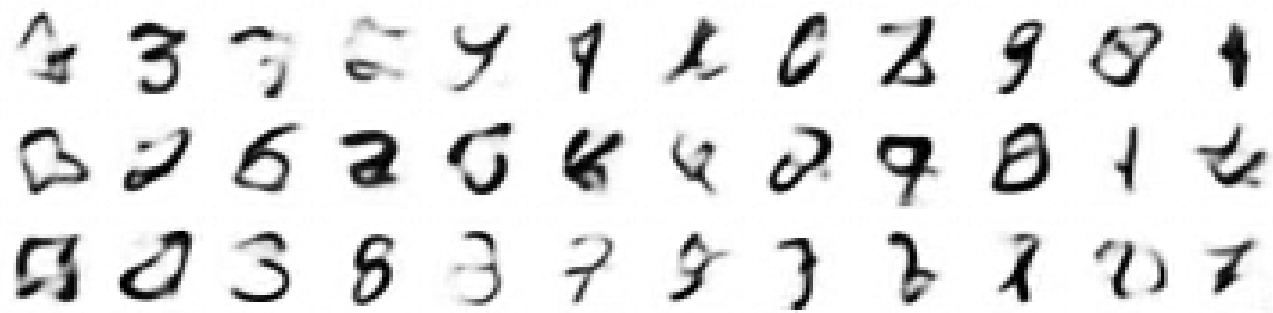


$\mathcal{N}(0,1)$



Autoencoder sampling ($d = 32$)

Variational Autoencoder sampling ($d = 32$)

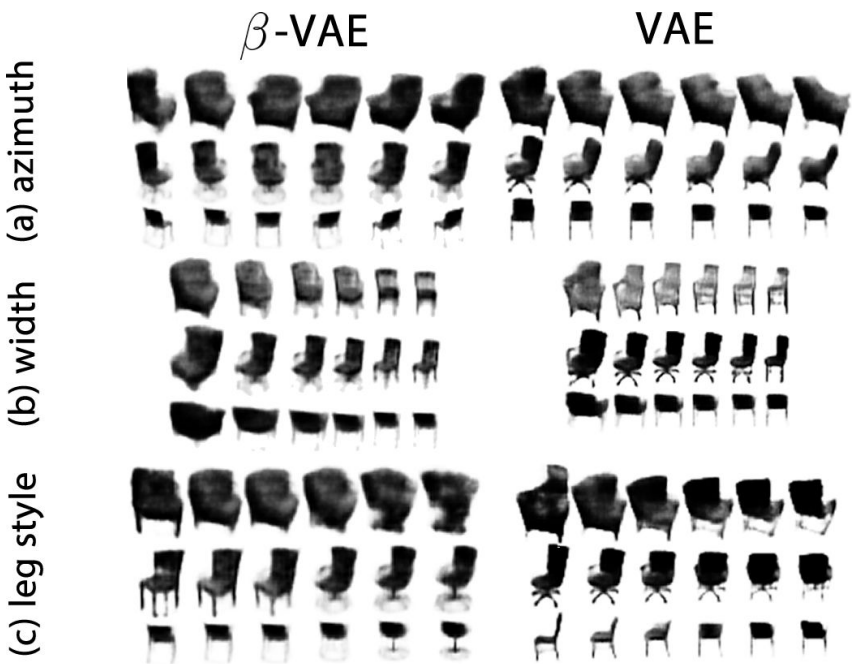


Making the embedding $\sim \mathcal{N}(0, 1)$, often results in "disentangled" representations.

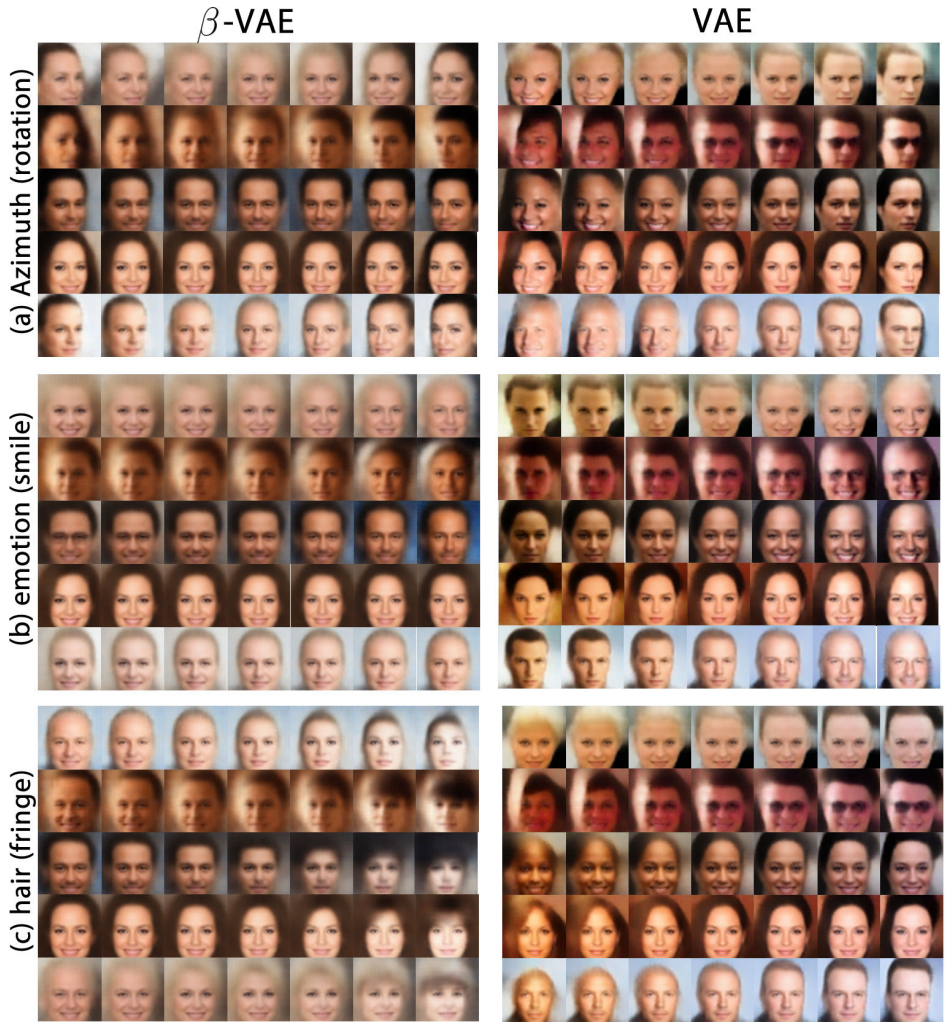
This effect can be reinforced with a greater weight of the KL term

$$\frac{1}{N} \sum_n \beta \, \mathbb{D}_{\mathrm{KL}} \left(q(Z \mid X = x_n; w') \,\|\, p(Z) \right) - \log p(X = x_n \mid Z = z_n; w)$$

resulting in the β-VAE proposed by Higgins et al. (2017).



(Higgins et al., 2017)



(Higgins et al., 2017)

The End

References

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D. P. Kingma and M. Welling. **Auto-encoding variational bayes**. CoRR, abs/1312.6114, 2013.