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

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

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].
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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 the convexity of the $\log$, 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:

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

Where

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

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

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

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

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

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

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

So the final loss is

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

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

Minimizing the first term

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

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

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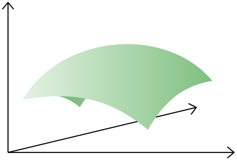

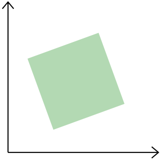

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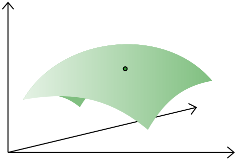
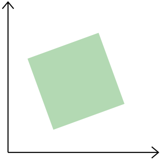


Original space $\mathscr{X}$



Latent space $\mathscr{F}$

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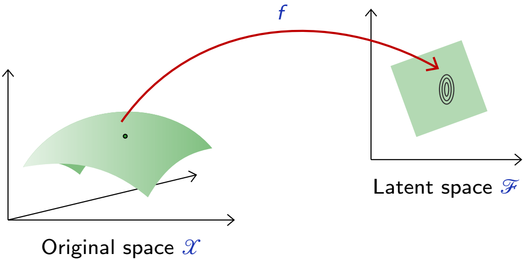

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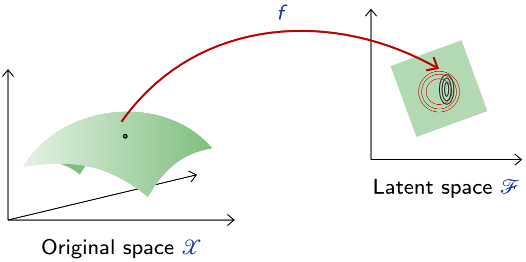

Minimizing the second term for a $z_n \sim q(Z \mid X = x_n; w')$

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

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

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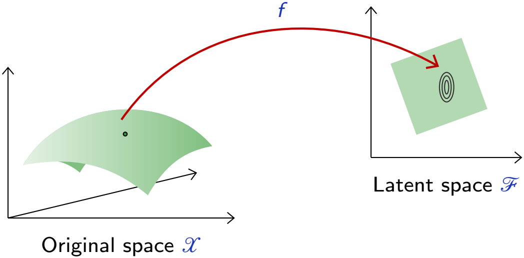

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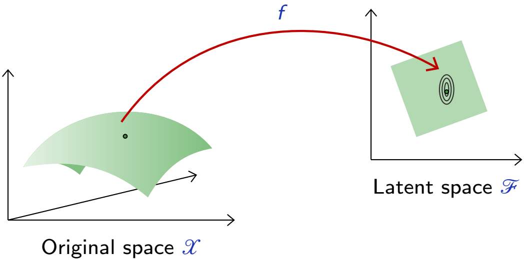

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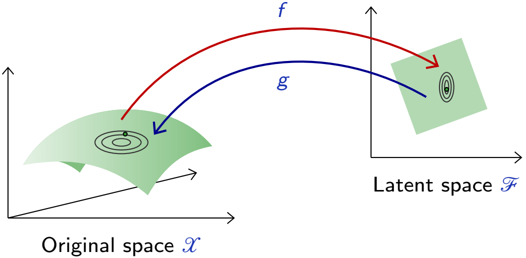


The assumption of independence between the component of $P(X \mid Z = z)$ allows the model to overfit the variance and additionally leads to grainy samples.

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())
```

```python
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**:

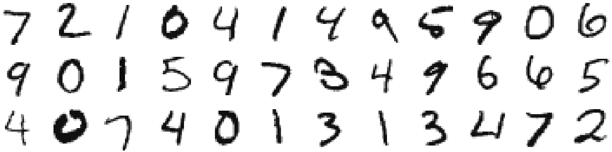
```
def sample_gaussian(param):
    mean, log_var = param
    std = log_var.mul(0.5).exp()
    return torch.randn(mean.size(), device=mean.device) * std + mean
```

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()`.

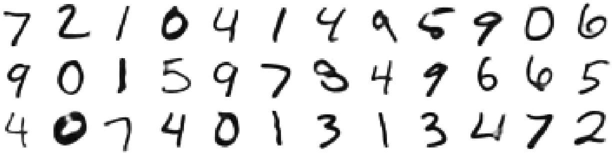
```
for x in train_input.split(args.batch_size):
    param_q_Z_given_x = model.encode(x)
    z = sample_gaussian(param_q_Z_given_x)
    param_p_X_given_z = model.decode(z)
    log_p_x_given_z = log_p_gaussian(x, param_p_X_given_z)

    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)
```

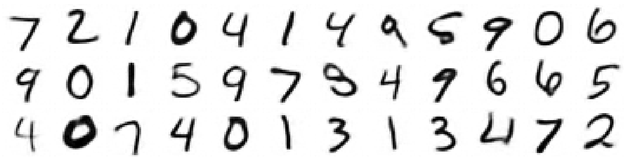
Original



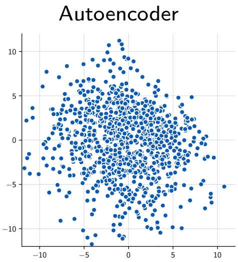
Autoencoder reconstruction ($d = 32$)



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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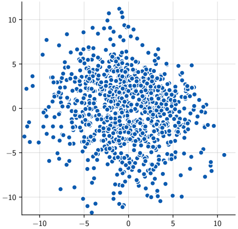
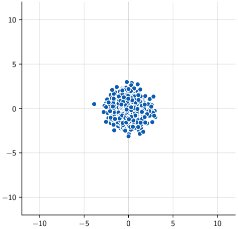
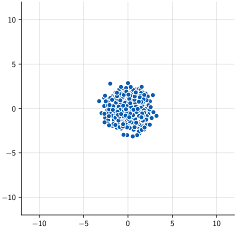
Autoencoder



Variational autoencoder

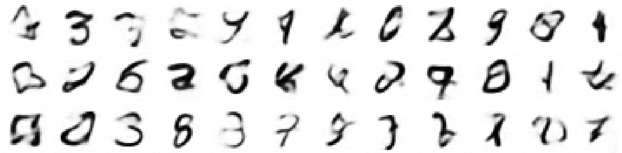


$\mathscr{N}(0,1)$



Autoencoder sampling ($d = 32$)

Variational Autoencoder sampling ($d = 32$)

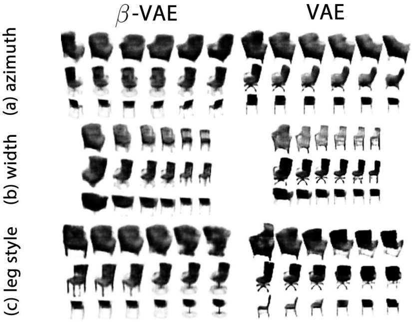


Making the embedding $\sim \mathscr{N}(0, 1)$, often results in "disentangled" representations.

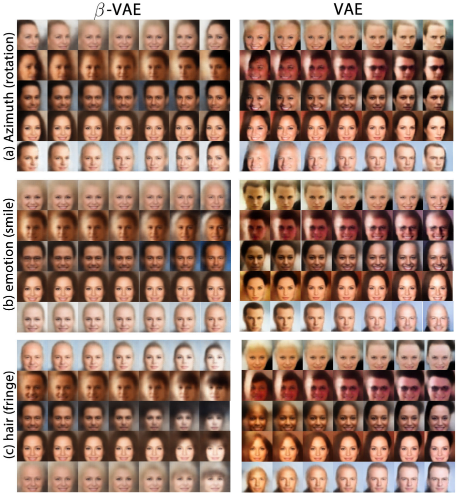
This effect can be reinforced with a greater weight of the KL term

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

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



(Higgins et al., 2017)



(Higgins et al., 2017)

The End

References

I. Higgins, L. Matthey, A. Pal, C. Burgess, X. Glorot, M. Botvinick, S. Mohamed, and A. Lerchner. **beta-vae: Learning basic visual concepts with a constrained variational framework**. In International Conference on Learning Representations (ICLR), 2017.

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