EE-559 – Deep learning

9.3. Denoising and variational autoencoders

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https://fleuret.org/ee559/

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Denoising Autoencoders

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Let X be a sample, $Z = f(X; \theta)$ its latent representation, and $q(x, z)$ the distribution of (X, Z).

We have

$$\begin{aligned}
\operatorname*{argmax}_{\theta} \ \mathbb{I}(X, Z) &= \operatorname*{argmax}_{\theta} \ \mathbb{H}(X) - \mathbb{H}(X \mid Z) \\
&= \operatorname*{argmax}_{\theta} \ -\mathbb{H}(X \mid Z) \\
&= \operatorname*{argmax}_{\theta} \ \mathbb{E}_{q(X,Z)}\Big[\log q(X \mid Z)\Big].
\end{aligned}$$

However, there is no expression of $q(X \mid Z)$ in any reasonable setup.

Give $(X, Z) \sim q_\theta$, for any distribution p we have

$$\mathbb{E}_{q(X,Z)}\Big[\log q(X \mid Z)\Big] \geq \mathbb{E}_{q(X,Z)}\Big[\log p(X \mid Z)\Big].$$

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So we can in particular try to find a "good p", so that the left term is a good approximation of the right one.

If we consider the following model for p

$$p(\cdot \mid Z = z) = \mathcal{N}(g(z; \eta), \sigma)$$

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If optimizing η makes the bound tight, the final loss is the reconstruction error

$$\operatorname*{argmax}_{\theta} \ \mathbb{I}(X,Z) \ \simeq \ \operatorname*{argmin}_{\theta}\left(\min_{\eta} \ \frac{1}{N}\sum_{n=1}^{N}\|x_n - g(f(x_n);\eta)\|^2\right).$$

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This abstract view of the encoder as "maximizing information" justifies its use to build generic encoding layers.

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In their work, Vincent et al. propose to degrade the signal with noise before feeding it to the encoder, but to keep the MSE to the original signal.

This makes the encoder retain information about structures beyond local noise.

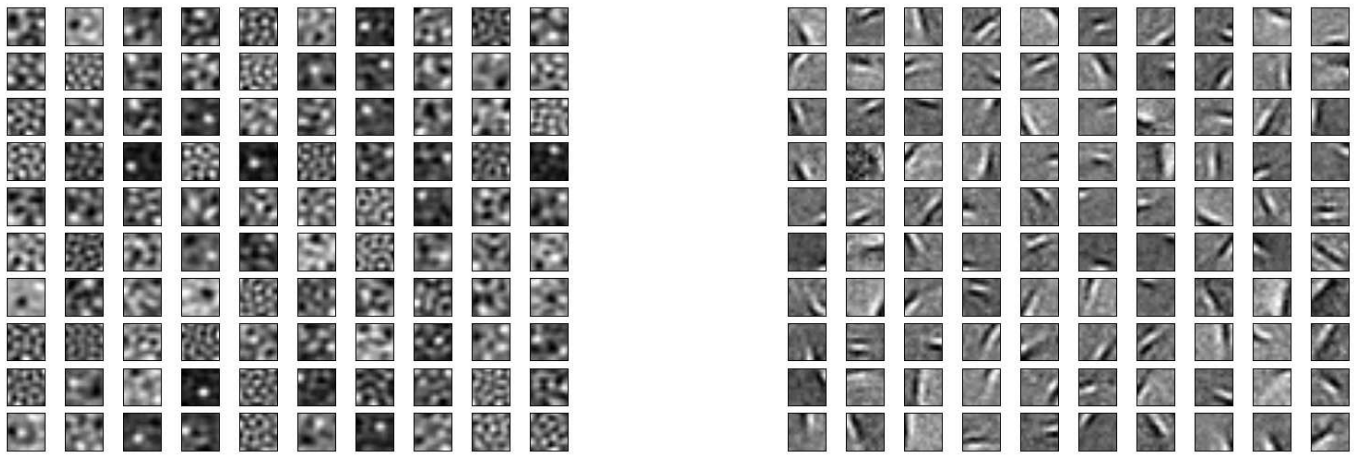

Figure 6: Weight decay vs. Gaussian noise. We show typical filters learnt from natural image patches in the over-complete case (200 hidden units). *Left:* regular autoencoder with weight decay. We tried a wide range of weight-decay values and learning rates: filters never appeared to capture a more interesting structure than what is shown here. Note that some local blob detectors are recovered compared to using no weight decay at all (Figure 5 right). *Right:* a denoising autoencoder with additive Gaussian noise ($\sigma = 0.5$) learns Gabor-like local oriented edge detectors. Clearly the filters learnt are qualitatively very different in the two cases.

(Vincent et al., 2010)

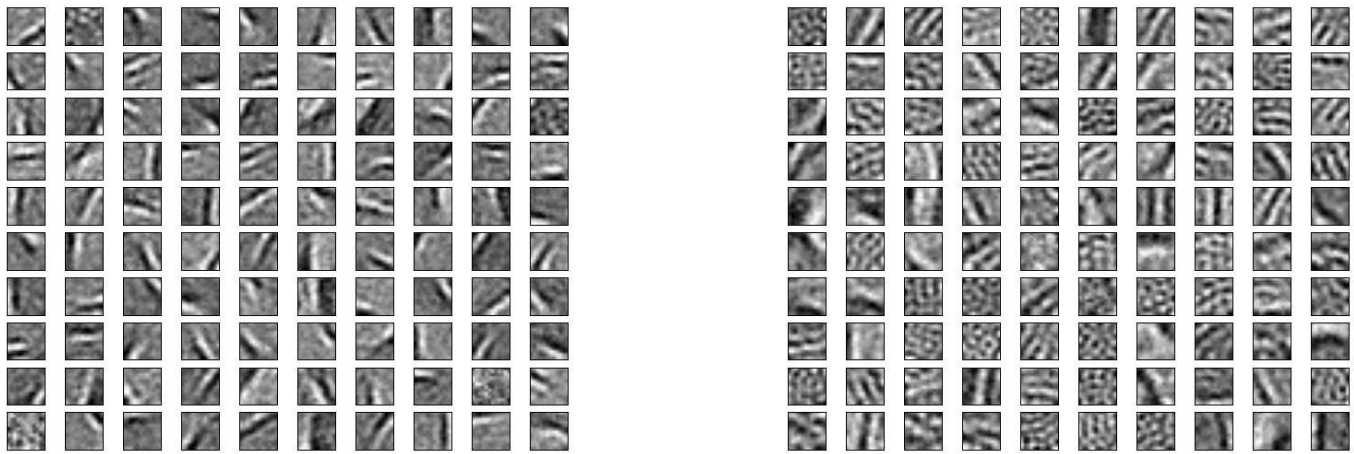

Figure 7: Filters obtained on natural image patches by denoising autoencoders using other noise types. *Left:* with 10% salt-and-pepper noise, we obtain oriented Gabor-like filters. They appear slightly less localized than when using Gaussian noise (contrast with Figure 6 right). *Right:* with 55% zero-masking noise we obtain filters that look like oriented gratings. For the three considered noise types, denoising training appears to learn filters that capture meaningful natural image statistics structure.

(Vincent et al., 2010)

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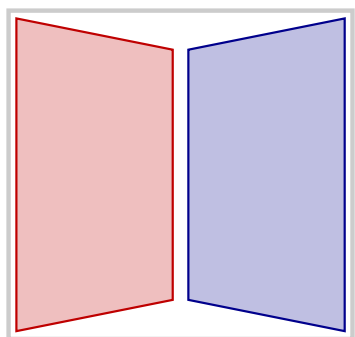

Autoencoder

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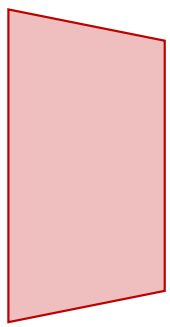

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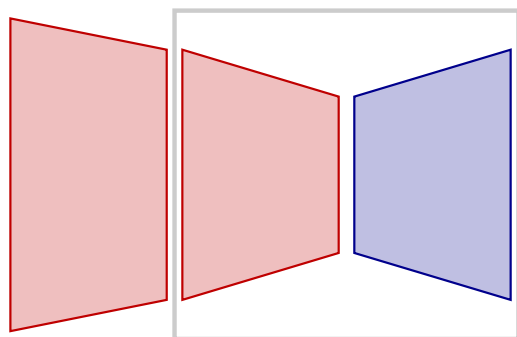

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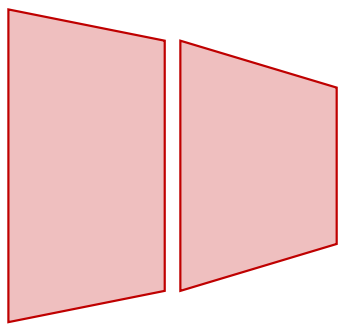

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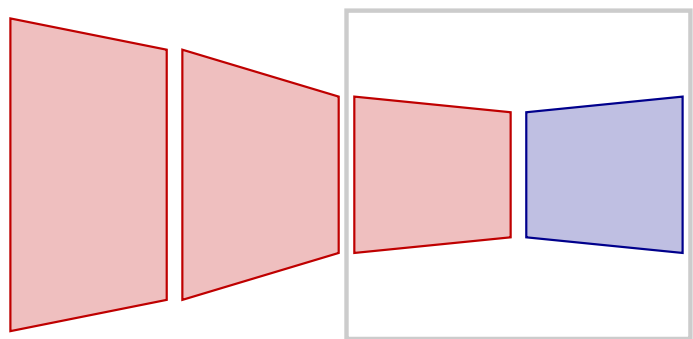

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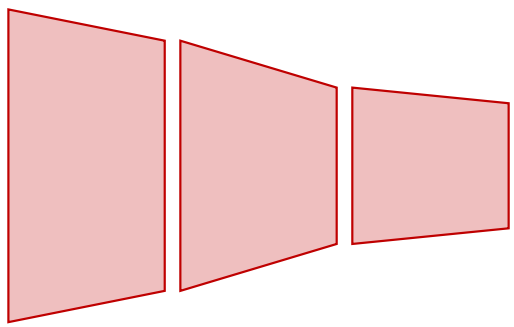

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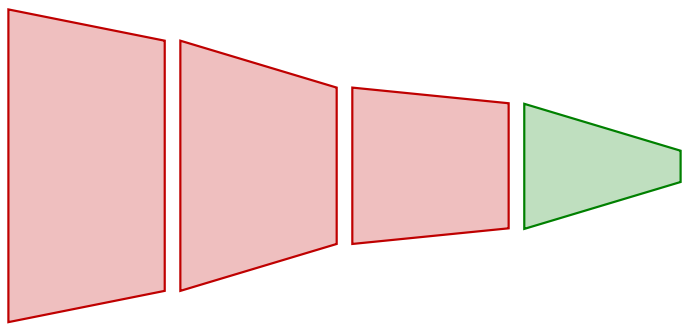

A final classifying layer is added and the full structure can be fine-tuned.

Data Set	SVM_{rbf}	DBN-1	SAE-3	DBN-3	SDAE-3 (ν)
MNIST	**1.40**$\pm$0.23	**1.21**$\pm$0.21	**1.40**$\pm$0.23	**1.24**$\pm$0.22	**1.28**$\pm$0.22 (25%)
basic	**3.03**$\pm$0.15	3.94$\pm$0.17	3.46$\pm$0.16	3.11$\pm$0.15	**2.84**$\pm$0.15 (10%)
rot	11.11$\pm$0.28	14.69$\pm$0.31	10.30$\pm$0.27	10.30$\pm$0.27	**9.53**$\pm$0.26 (25%)
bg-rand	14.58$\pm$0.31	9.80$\pm$0.26	11.28$\pm$0.28	**6.73**$\pm$0.22	10.30$\pm$0.27 (40%)
bg-img	22.61$\pm$0.37	**16.15**$\pm$0.32	23.00$\pm$0.37	**16.31**$\pm$0.32	**16.68**$\pm$0.33 (25%)
bg-img-rot	55.18$\pm$0.44	52.21$\pm$0.44	51.93$\pm$0.44	47.39$\pm$0.44	**43.76**$\pm$0.43 (25%)
rect	**2.15**$\pm$0.13	4.71$\pm$0.19	2.41$\pm$0.13	2.60$\pm$0.14	**1.99**$\pm$0.12 (10%)
rect-img	24.04$\pm$0.37	23.69$\pm$0.37	24.05$\pm$0.37	22.50$\pm$0.37	**21.59**$\pm$0.36 (25%)
convex	19.13$\pm$0.34	19.92$\pm$0.35	**18.41**$\pm$0.34	**18.63**$\pm$0.34	**19.06**$\pm$0.34 (10%)
tzanetakis	**14.41**$\pm$2.18	18.07$\pm$1.31	**16.15**$\pm$1.95	18.38$\pm$1.64	**16.02**$\pm$1.04(0.05)

(Vincent et al., 2010)

Variational Autoencoders

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.

We consider the following two distributions:

- q is the distribution on $\mathscr{X} \times \mathbb{R}^d$ of a pair (X, Z) composed of a sample X taken from the data distribution and the output of the encoder on it,

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- p is the distribution on $\mathcal{X} \times \mathbb{R}^d$ of a pair (X, Z) composed of an encoding state $Z \sim \mathcal{N}(0, I)$ and the output of the decoder g on it.

We should ideally look for the g that maximizes the log-likelihood

$$\frac{1}{N} \sum_n \log p(x_n) = \hat{\mathbb{E}}_{q(X)} \Big[\log p(X) \Big].$$

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$$\frac{1}{N} \sum_n \log p(x_n) = \hat{\mathbb{E}}_{q(X)} \Big[\log p(X) \Big].$$

However, while we can sample z and compute $g(z)$, we cannot compute $p(x)$ for a given x, and even less compute its derivatives.

The **Variational Autoencoder** proposed by Kingma and Welling (2013) relies on a tractable approximation of this log-likelihood.

Note that their framework involves **stochastic** encoder f, and decoder g, whose outputs depend on both their inputs and additional randomness.

Remember that $q(X)$ is the data distribution, and $q(Z \mid X = x)$ is the distribution of the latent encoding $f(x)$. We want to maximize

$$\mathbb{E}_{q(X)}\Big[\log p(X)\Big],$$

or equivalently minimize

$$\begin{aligned}\mathbb{E}_{q(X)}\Big[\log q(X) - \log p(X)\Big] &= \mathbb{D}_{\mathrm{KL}}(q(X) \,\|\, p(X)) \\ &\leq \mathbb{D}_{\mathrm{KL}}(q(X,Z) \,\|\, p(X,Z))\,.\end{aligned}$$

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We will minimize this latter bound, that can be rewritten as

$$\begin{aligned}&\mathbb{D}_{\mathrm{KL}}(q(X,Z) \,\|\, p(X,Z)) = \\ &\qquad \mathbb{E}_{q(X)}\Big[\mathbb{D}_{\mathrm{KL}}(q(Z \mid X) \,\|\, p(Z))\Big] - \mathbb{E}_{q(X,Z)}\Big[\log p(X \mid Z)\Big] + \mathbb{H}(q(X)).\end{aligned}$$

Kingma and Welling use Gaussians with diagonal covariance for both $q(Z \mid X)$ and $p(X \mid Z)$:

- the encoder maps a data point from the signal space $\mathbb{R}^c$ to [the parameters of] a Gaussian in the latent space $\mathbb{R}^d$

$$f : \mathbb{R}^c \to \mathbb{R}^{2d}$$
$$x \mapsto \left(\mu_1^f, \ldots, \mu_d^f, \sigma_1^f, \ldots, \sigma_d^f\right),$$

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$$\begin{aligned} f : \mathbb{R}^c &\to \mathbb{R}^{2d} \\ x &\mapsto \left(\mu_1^f, \ldots, \mu_d^f, \sigma_1^f, \ldots, \sigma_d^f\right), \end{aligned}$$

- the decoder maps a latent value from $\mathbb{R}^d$ to [the parameters of] a Gaussian in the signal space $\mathbb{R}^c$

$$\begin{aligned} g : \mathbb{R}^d &\to \mathbb{R}^{2c} \\ z &\mapsto \left(\mu_1^g, \ldots, \mu_c^g, \sigma_1^g, \ldots, \sigma_c^g\right). \end{aligned}$$

We have to minimize

$$\mathscr{L} = \hat{\mathbb{E}}_{q(X)}\Big[\mathbb{D}_{\mathsf{KL}}\left(q(Z \mid X) \,\|\, p(Z)\right)\Big] - \hat{\mathbb{E}}_{q(X,Z)}\Big[\log p(X \mid Z)\Big].$$

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The first term is the average of

$$\mathbb{D}_{\mathsf{KL}}\left(q(Z \mid X = x) \,\|\, p(Z)\right) = -\frac{1}{2}\sum_{d}\left(1 + 2\log\sigma_d^f(x) - \Big(\mu_d^f(x)\Big)^2 - \Big(\sigma_d^f(x)\Big)^2\right).$$

over the x_ns.

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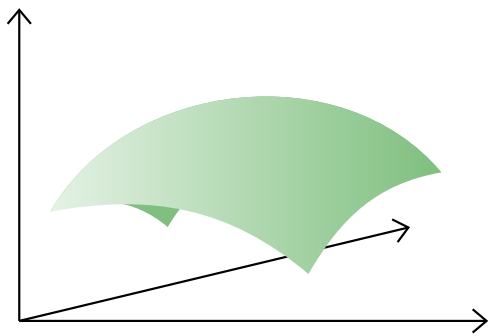
The second term of $\mathscr{L}$ is the average of

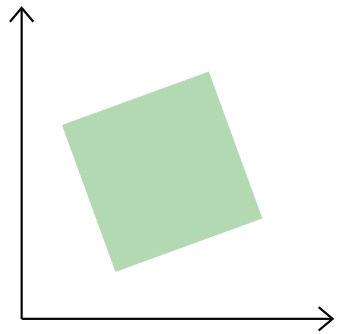
$$-\log p(X = x \mid Z = z) = \frac{1}{2}\sum_{d}\left(\log 2\pi + 2\log\sigma_d^g(z) + \frac{(x_d - \mu_d^g(z))^2}{\left(\sigma_d^g(z)\right)^2}\right)$$

over the x_n, with one z_n sampled for each (could be more)

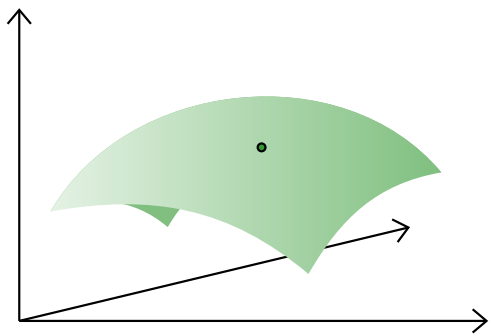
$$z_n \sim \mathcal{N}\left(\mu^f(x_n), \sigma^f(x_n)\right), \quad n = 1, \ldots, N.$$



Original space $\mathscr{X}$



Latent space $\mathscr{F}$



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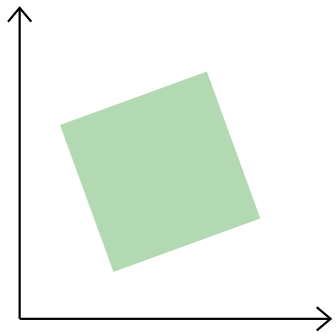

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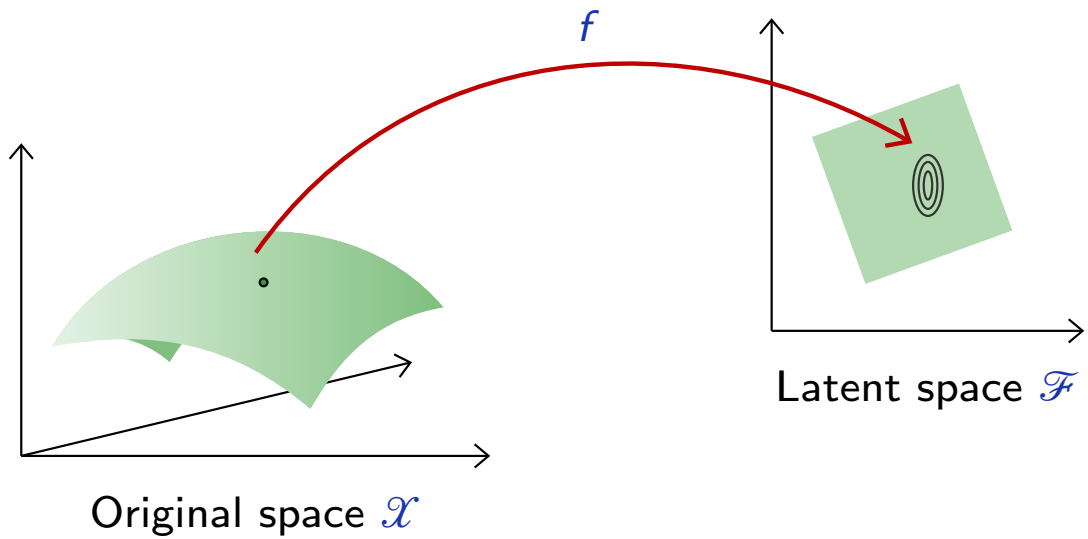
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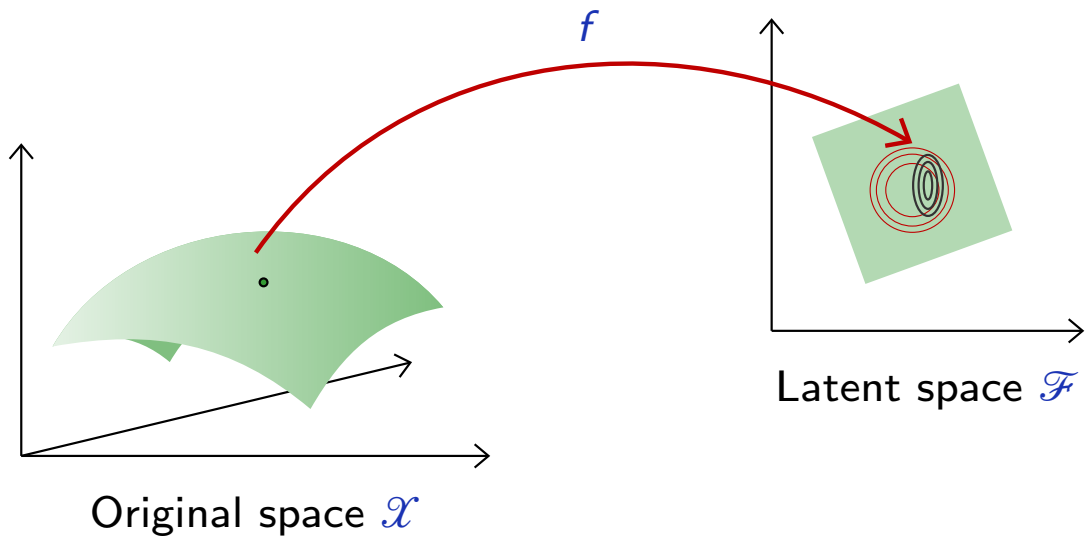
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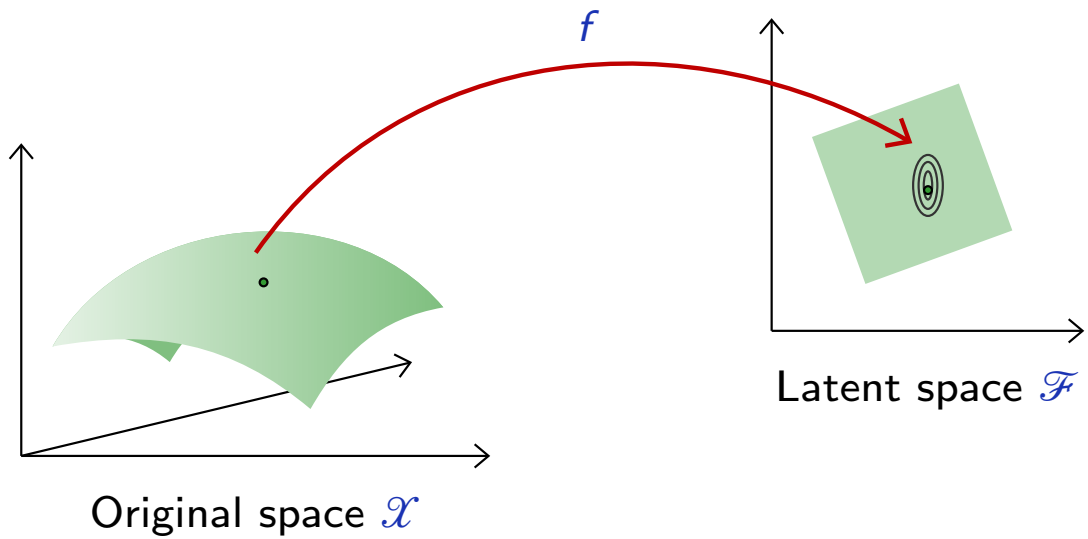
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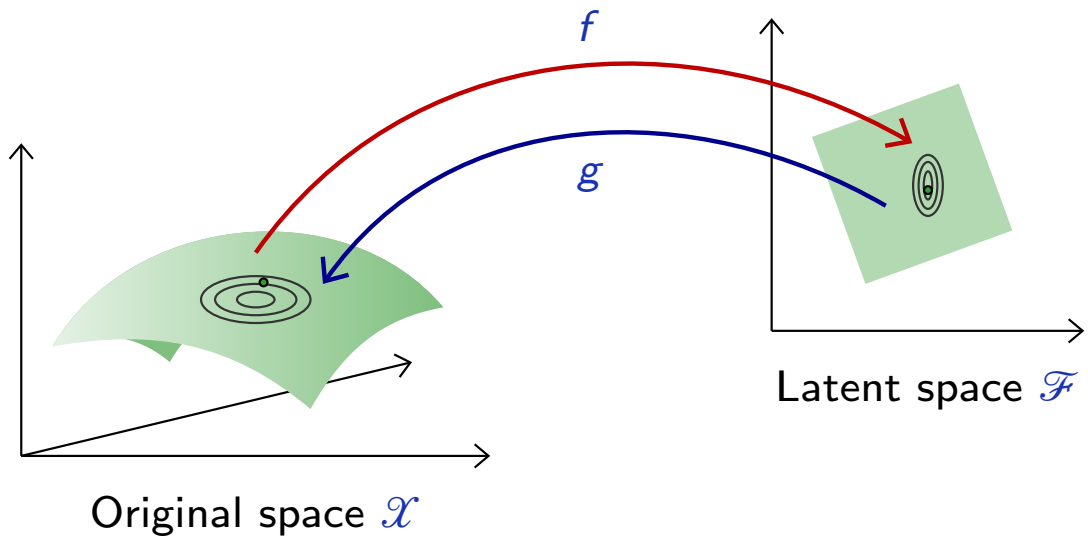
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Regarding implementation: the encoder now maps to twice the number of dimensions, which corresponds to the μ^fs and $\log\left((\sigma^f)^2\right)$s.

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Also, as in Kingma and Welling (2013), **we use a fixed variance of 1 for the decoder.** So it outputs the μ^gs alone, and its dimension remains unchanged.

The first term of the loss is the average of

$$\mathbb{D}_{\mathrm{KL}}\left(q(Z \mid X = x) \,\|\, p(Z)\right) = -\frac{1}{2}\sum_{d}\left(1 + 2\log\sigma_d^f(x) - \left(\mu_d^f(x)\right)^2 - \left(\sigma_d^f(x)\right)^2\right).$$

over the x_n.

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over the x_n.

This can be implemented as

```
param_f = model.encode(input)
mu_f, logvar_f = param_f.split(param_f.size(1)//2, 1)

kl = - 0.5 * (1 + logvar_f - mu_f.pow(2) - logvar_f.exp())
kl_loss = kl.sum() / input.size(0)
```

Since we use a constant variance of 1 for the decoder, the second term of $\mathscr{L}$ becomes the average of

$$-\log p(X = x \mid Z = z) = \frac{1}{2} \sum_{d} (x_d - \mu_d^g(z))^2 + \text{cst}$$

over the x_n, with one z_n sampled for each, *i.e.*

$$z_n \sim \mathcal{N}\left(\mu^f(x_n), \sigma^f(x_n)\right), \quad n = 1, \ldots, N.$$

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This can be implemented as

```
std_f = torch.exp(0.5 * logvar_f)
z = torch.empty_like(mu_f).normal_() * std_f + mu_f
output = model.decode(z)

fit = 0.5 * (output - input).pow(2)
fit_loss = fit.sum() / input.size(0)
```

We had for the standard autoencoder

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z = model.encode(input)
output = model.decode(z)
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z = model.encode(input)
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loss = 0.5 * (output - input).pow(2).sum() / input.size(0)
```

and putting everything together we get for the VAE

```
param_f = model.encode(input)
mu_f, logvar_f = param_f.split(param_f.size(1)//2, 1)

kl = - 0.5 * (1 + logvar_f - mu_f.pow(2) - logvar_f.exp())
kl_loss = kl.sum() / input.size(0)

std_f = torch.exp(0.5 * logvar_f)
z = torch.empty_like(mu_f).normal_() * std_f + mu_f
output = model.decode(z)

fit = 0.5 * (output - input).pow(2)
fit_loss = fit.sum() / input.size(0)

loss = kl_loss + fit_loss
```

We had for the standard autoencoder

```
z = model.encode(input)
output = model.decode(z)
loss = 0.5 * (output - input).pow(2).sum() / input.size(0)
```

and putting everything together we get for the VAE

```
param_f = model.encode(input)
mu_f, logvar_f = param_f.split(param_f.size(1)//2, 1)

kl = - 0.5 * (1 + logvar_f - mu_f.pow(2) - logvar_f.exp())
kl_loss = kl.sum() / input.size(0)

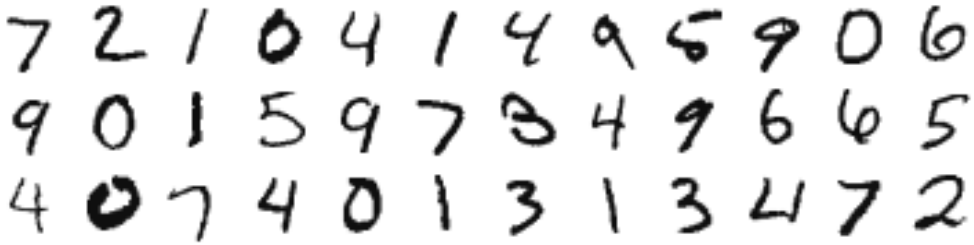
std_f = torch.exp(0.5 * logvar_f)
z = torch.empty_like(mu_f).normal_() * std_f + mu_f
output = model.decode(z)

fit = 0.5 * (output - input).pow(2)
fit_loss = fit.sum() / input.size(0)

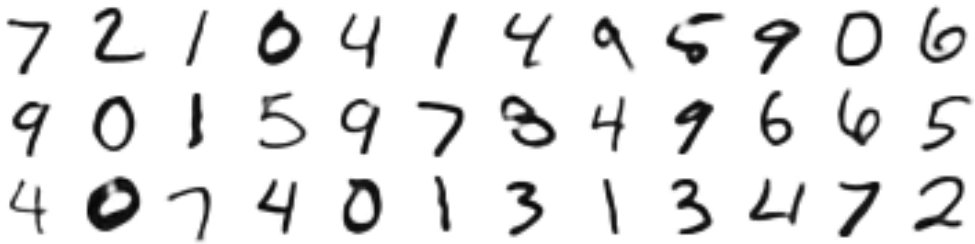
loss = kl_loss + fit_loss
```

During inference we do not sample, and instead use μ^f and μ^g as prediction.

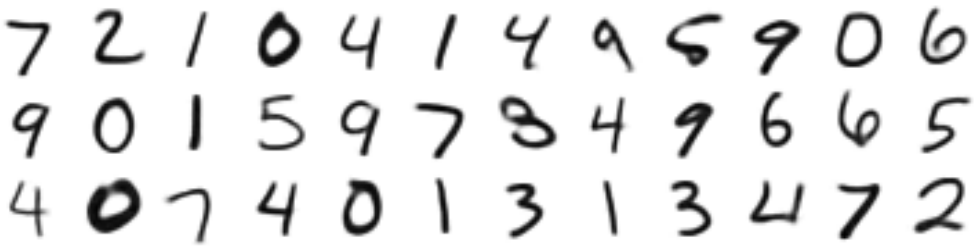
Original



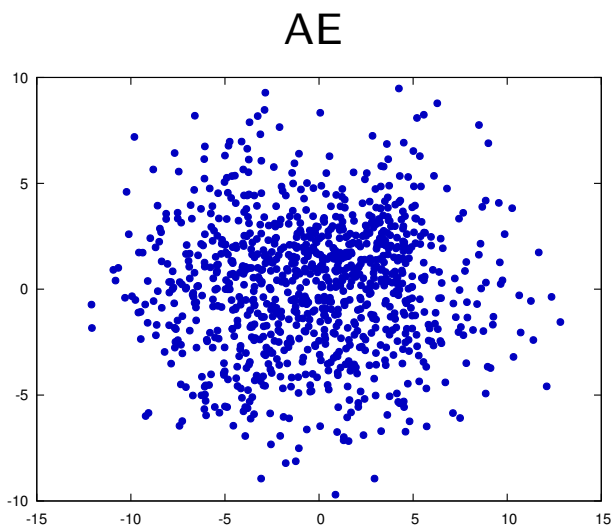
Autoencoder reconstruction ($d = 32$)



Variational Autoencoder reconstruction ($d = 32$)

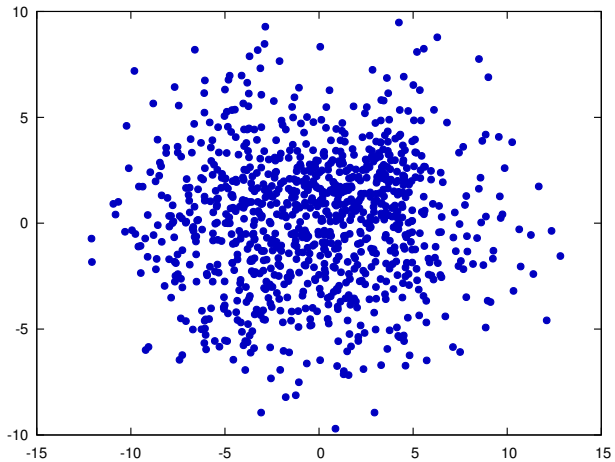


We can look at two latent features to check that they are Normal for the VAE.

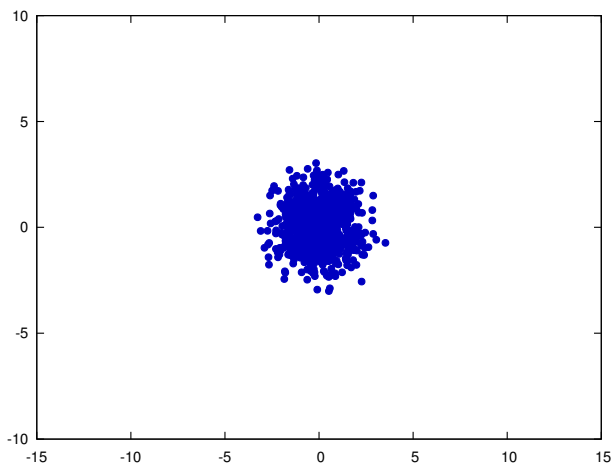


We can look at two latent features to check that they are Normal for the VAE.

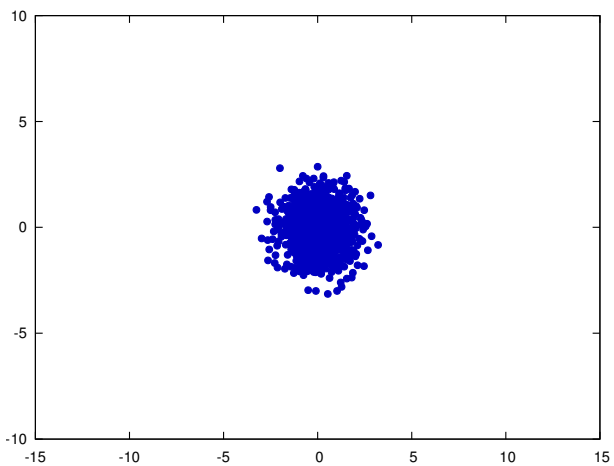
AE



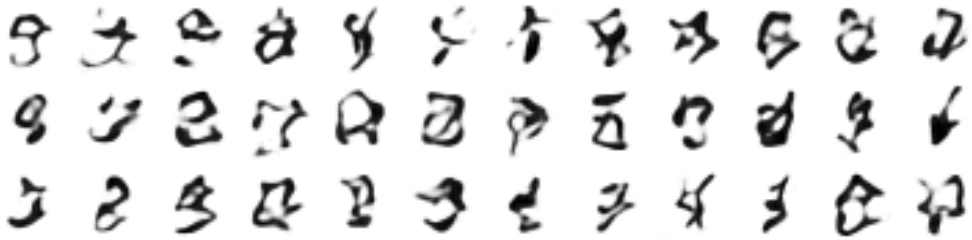
VAE



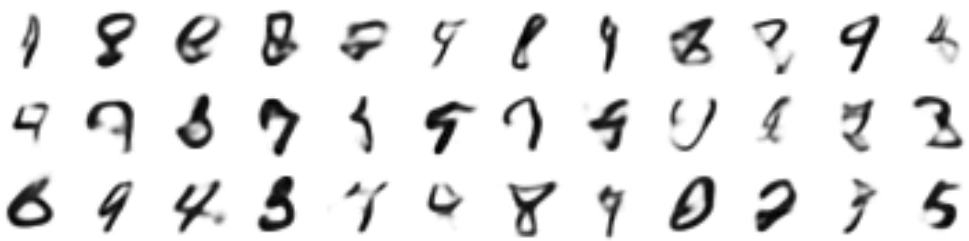
$\mathcal{N}(0, 1)$



Autoencoder sampling ($d = 32$)



Variational Autoencoder sampling ($d = 32$)



The end

References

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P. Vincent, H. Larochelle, I. Lajoie, Y. Bengio, and P.-A. Manzagol. Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion. *Journal of Machine Learning Research (JMLR)*, 11:3371–3408, 2010.