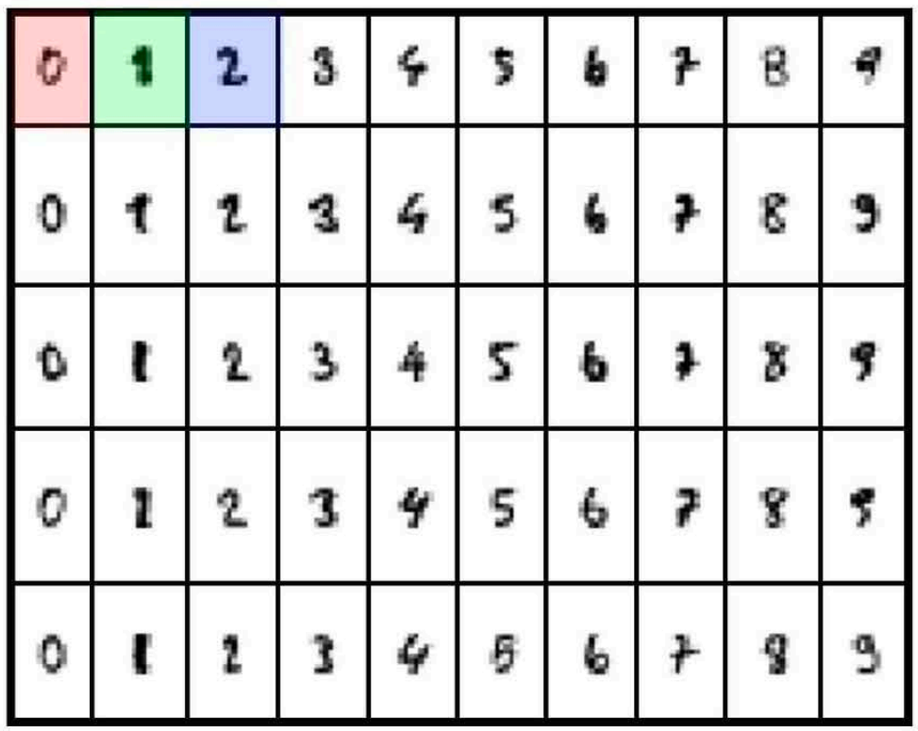
ENM5310: Data-driven modeling and probabilistic scientific computing

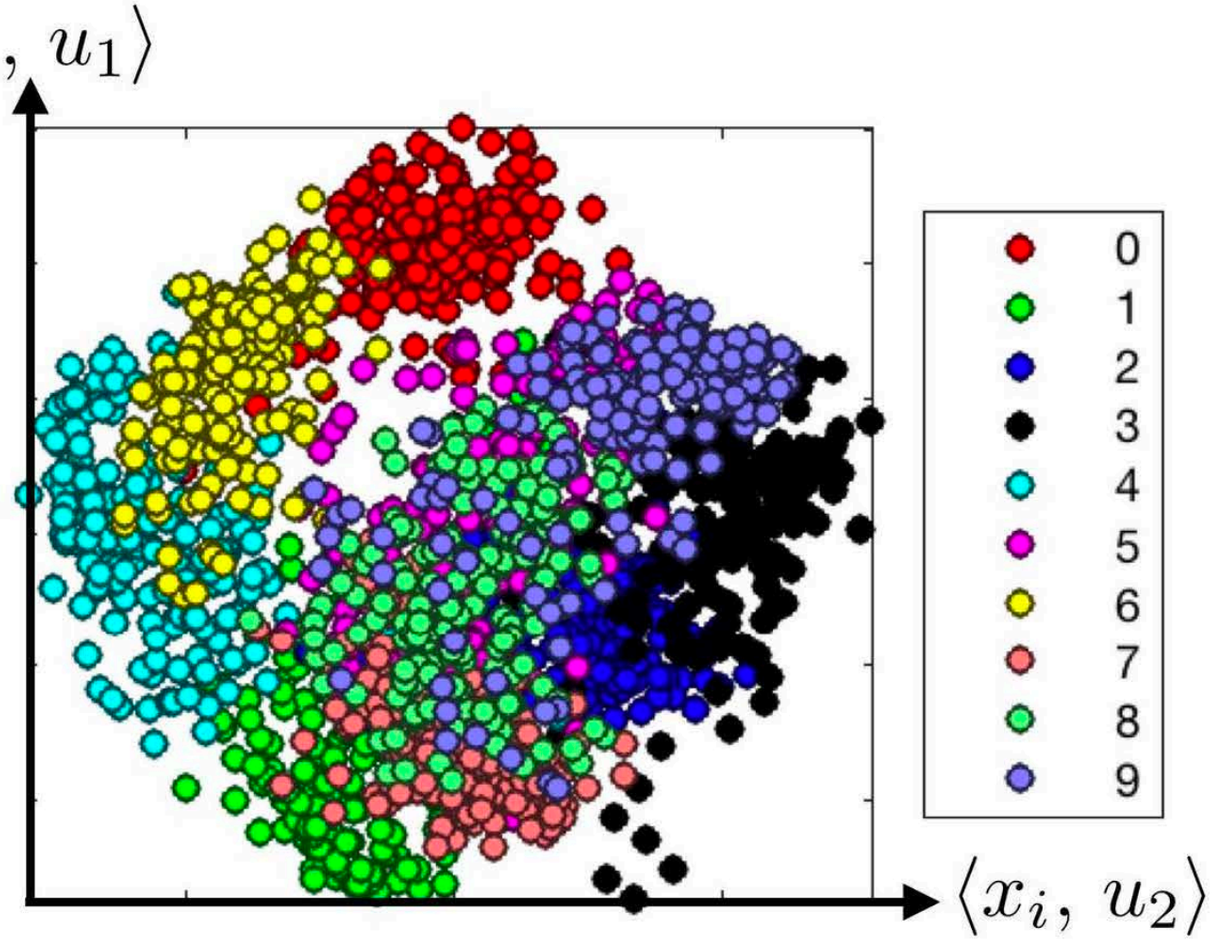
Lecture #22: Variational auto-encoders

Principal component analysis

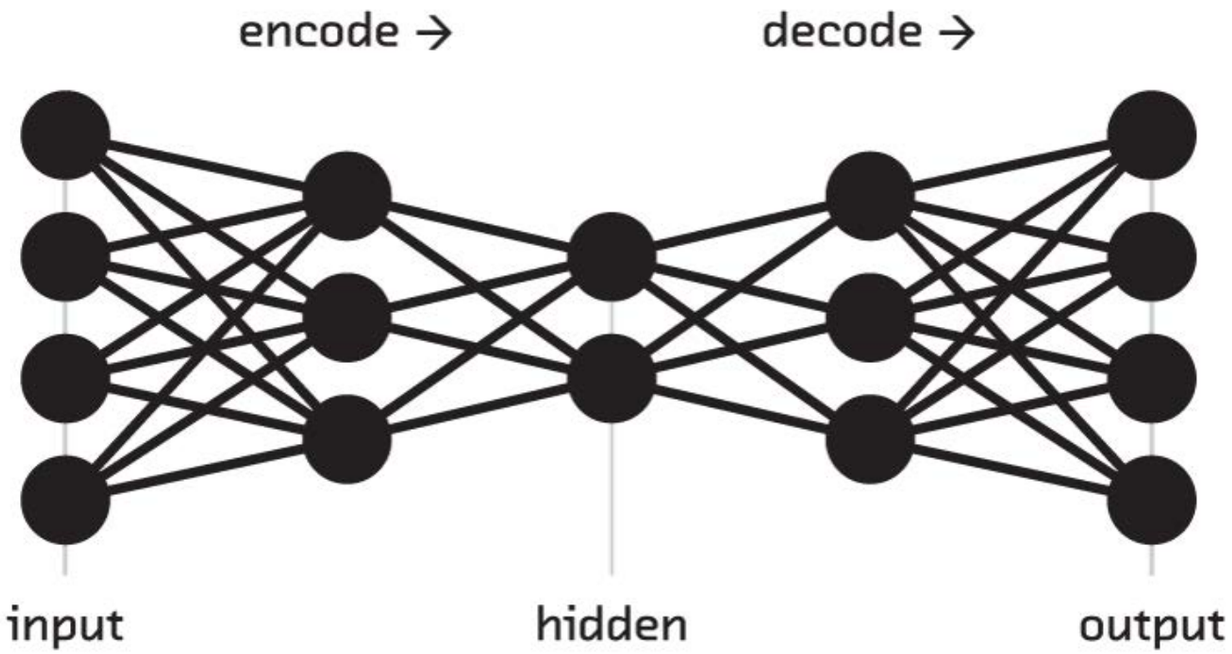
Input data:	$X = (x_i)_{i=1}^n \in \mathbb{R}^{n \times p}, x_i \in \mathbb{R}^p$
Remove mean:	$x_i \leftarrow x_i - \frac{1}{n} \sum_j x_j$
Covariance:	$C \overset{\text{def.}}{=} \frac{1}{n} X^\top X \in \mathbb{R}^{p \times p}$
Eigen-decomposition:	$C = U \operatorname{diag}(\sigma_k^2) U^\top, U = (u_k)_{k=1}^p$

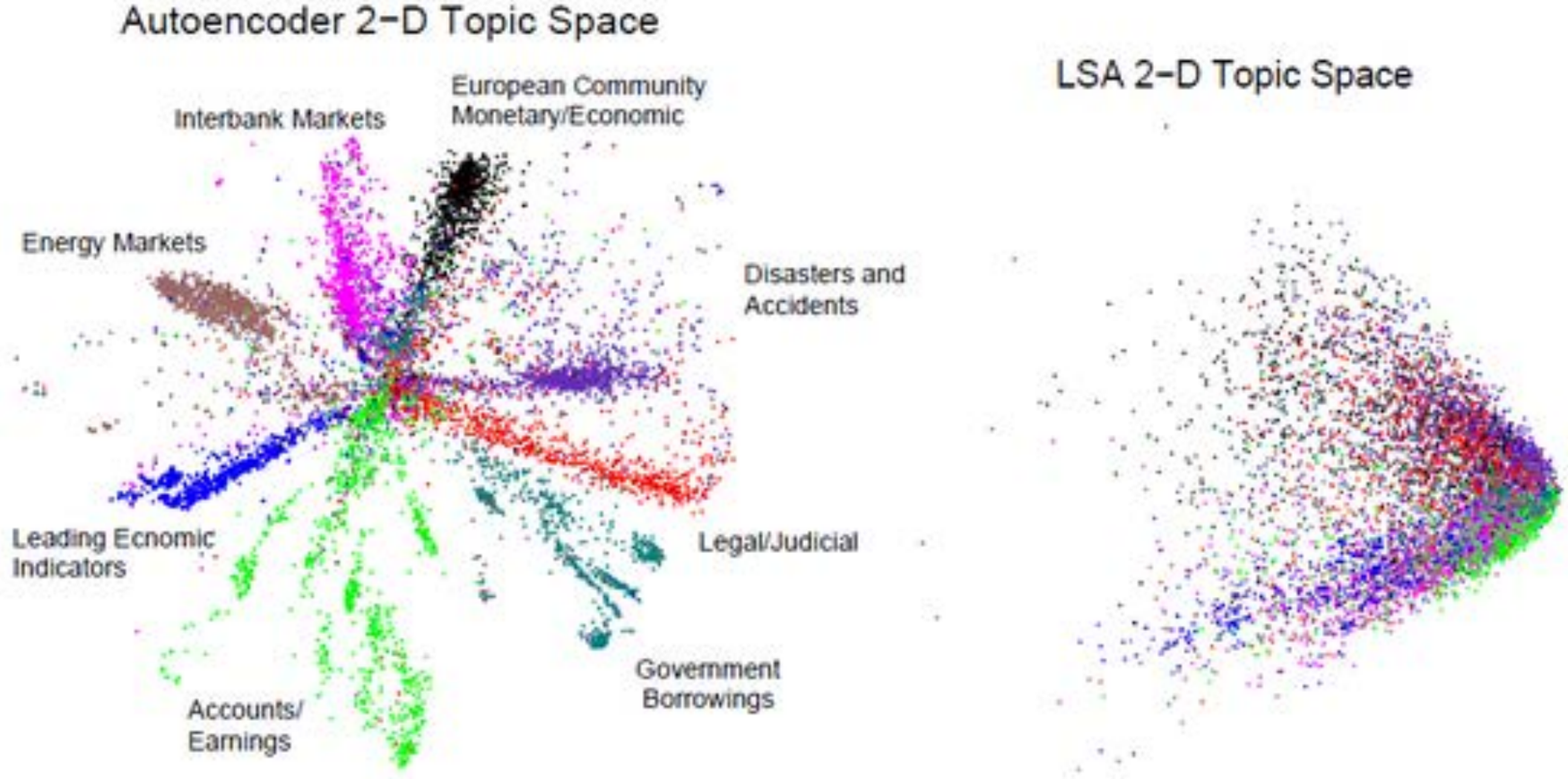
x_1 x_2 x_3





Neural network auto-encoders





Hinton, G. E., & Salakhutdinov, R. R. (2006). Reducing the dimensionality of data with neural networks. science, 313(5786), 504-507.

Tricks of the trade

- Variational bounds
- Density re-parametrizations
- Density ratio estimation
- Variational optimization/evolution strategies
- Adversarial games

Variational bounds

Typical problem:

My loss function $f(\theta)$ is intractable to compute, typically because it involves intractable marginalization. I can't evaluate it let alone minimize it.

Solution:

Let's construct a family of - typically differentiable - upper-bounds:

$$f(\theta) \leq \inf_{\psi} g(\theta, \psi),$$

and solve the optimization problem

$$\theta^*, \psi^* \leftarrow \text{argmin}_{\theta,\psi}\, g(\theta, \psi)$$

instead. Technically, once optimization is finished, you can discard the auxiliary parameter ψ^* - although often turns out to be meaningful and useful in itself, often for approximate inference such as the recognition model of VAEs.

Tricks of the trade:

Jensen's inequality: The mean value of a convex function is never lower than the value of the convex function applied to the mean. Generally appears in some variant of the standard evidence lower bound (ELBO) derivation below:

$$\begin{aligned} -\log p(x) &= -\log \int p(x, y) dy \\ &= -\log \int q(y|x) \frac{p(y, x)}{q(y|x)} dy \\ &\leq -\int q(y|x) \log \frac{p(y, x)}{q(y|x)} dy \end{aligned}$$

http://www.inference.vc/design-patterns/

The re-parametrization trick

One oft-encountered problem is computing the gradient of an expectation of a smooth function *f*:

$$\nabla_\theta \mathbb{E}_{p(z;\theta)}[f(z)] = \nabla_\theta \int p(z;\theta) f(z) dz$$

This is a recurring task in machine learning, needed for posterior computation in variational inference, value function and policy learning in reinforcement learning, derivative pricing in computational finance, and inventory control in operations research, amongst many others. This gradient is often difficult to compute because the integral is typically unknown and the parameters θ, with respect to which we are computing the gradient, are of the distribution $p(z;\theta)$. But where a random variable z appears we can try our random variable reparameterisation trick, which in this case allows us to compute the gradient in a more amenable way:

$$\nabla_\theta \mathbb{E}_{p(z;\theta)}[f(z)] = \mathbb{E}_{p(\epsilon)}[\nabla_\theta f(g(\epsilon,\theta))]$$

http://blog.shakirm.com/2015/10/machine-learning-trick-of-the-day-4-reparameterisation-tricks/

The re-parametrization trick

Let's derive this expression and explore the implications of it for our optimisation problem. One-liners give us a transformation from a distribution $p(\epsilon)$ to another $p(z)$, thus the differential area (mass of the distribution) is invariant under the change of variables. This property implies that:

$$p(z) = \left|\frac{d\epsilon}{dz}\right| p(\epsilon) \implies |p(z)dz| = |p(\epsilon)d\epsilon|$$

Re-expressing the troublesome stochastic optimisation problem using random variate reparameterisation, we find:

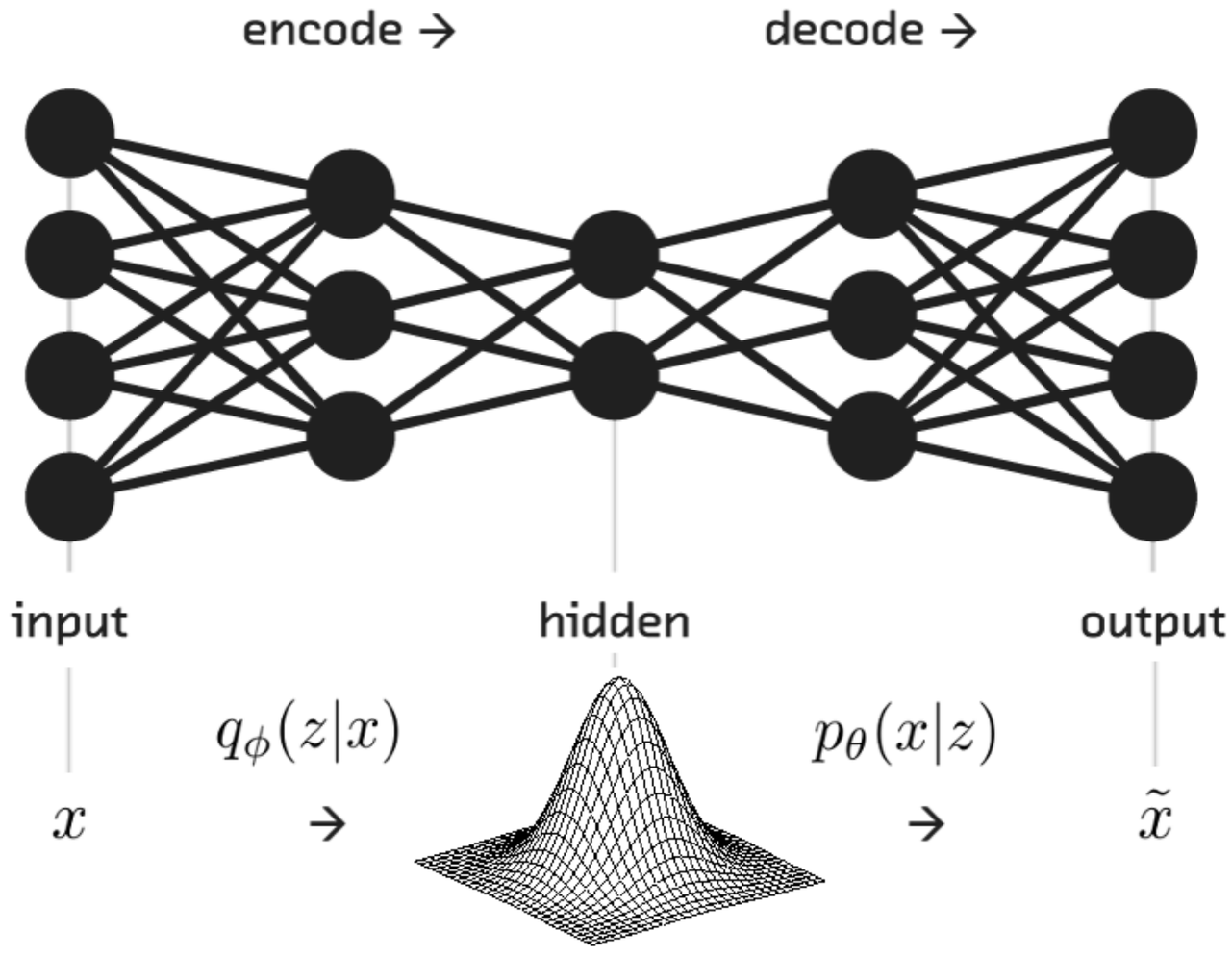
$$\nabla_\theta \mathbb{E}_{p(z;\theta)}[f(z)] = \nabla_\theta \int p(z;\theta) f(z) dz$$

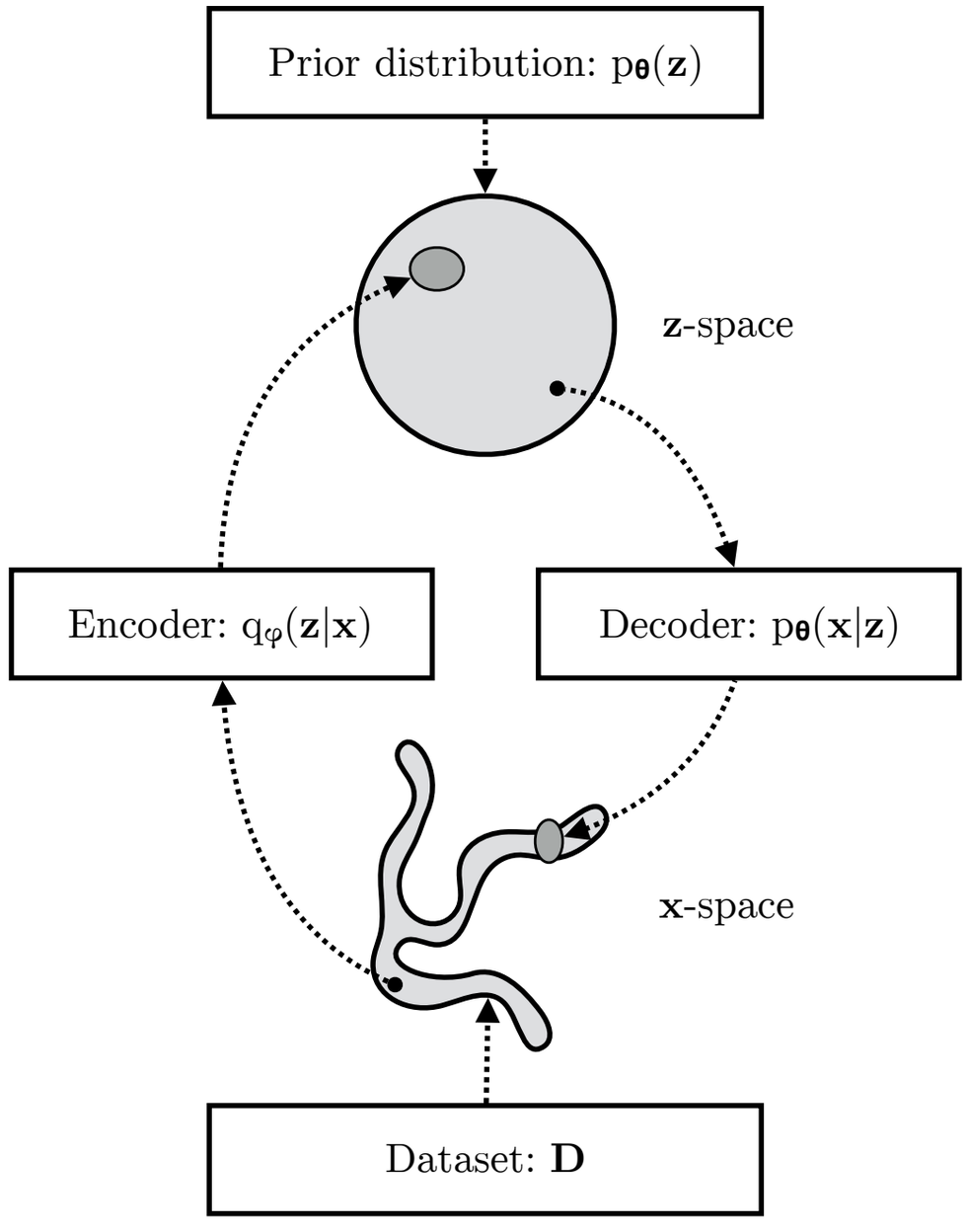
$$= \nabla_\theta \int p(\epsilon) f(z) d\epsilon = \nabla_\theta \int p(\epsilon) f(g(\epsilon,\theta)) d\epsilon$$

$$= \nabla_\theta \mathbb{E}_{p(\epsilon)}[f(g(\epsilon,\theta))] = \mathbb{E}_{p(\epsilon)}[\nabla_\theta f(g(\epsilon,\theta))]$$

http://www.inference.vc/design-patterns/

Variational auto-encoders





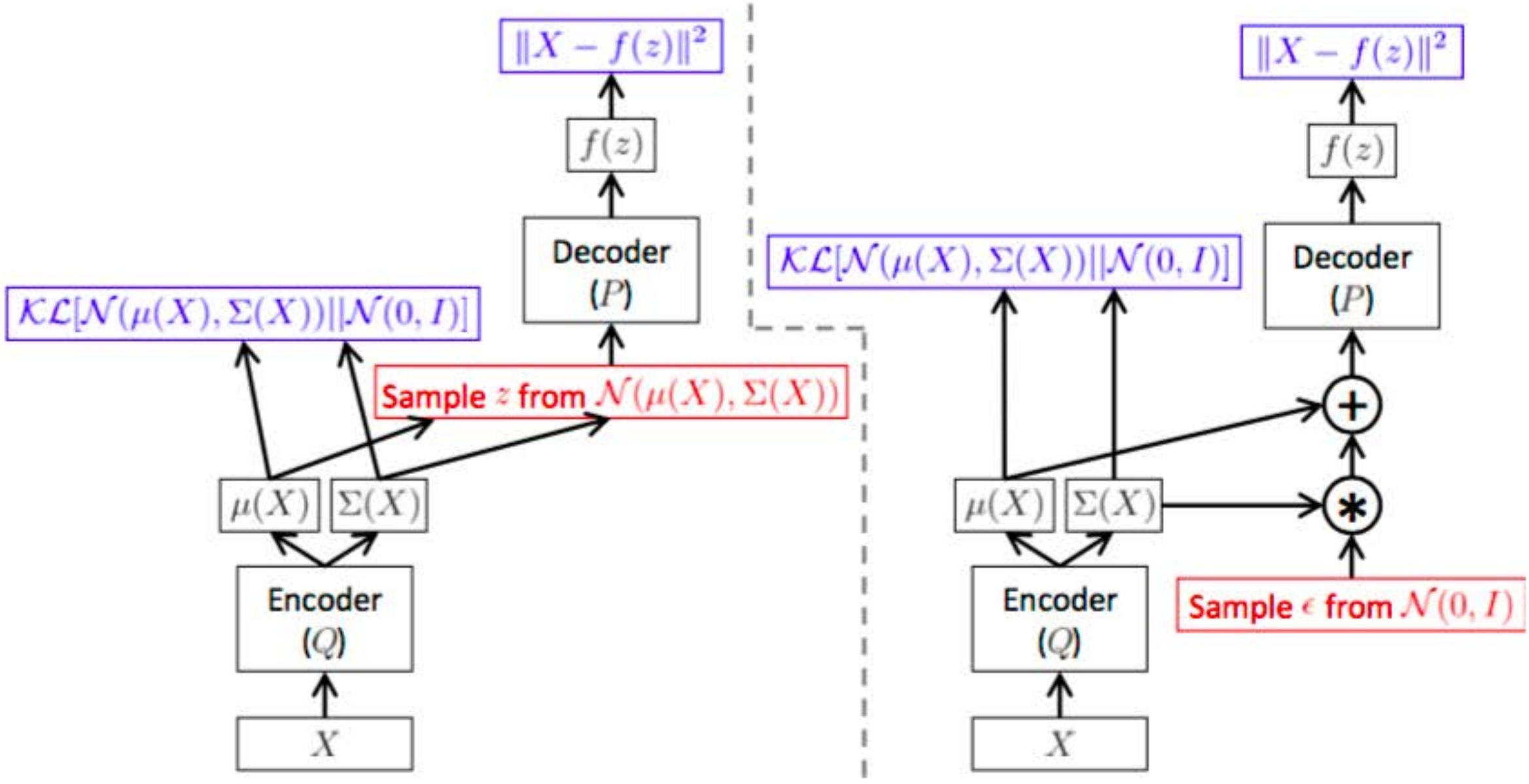
A VAE learns stochastic mappings between the observed **x**-space, whose empirical distribution $q_D(\mathbf{x})$ is typically complicated, and a latent **z**-space, whose distribution can be relatively simple (such as spherical, as in this figure). The generative model learns a joint distribution $p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) = p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p_{\boldsymbol{\theta}}(\mathbf{z})$, factorized into a prior distribution over latent space, $p_{\boldsymbol{\theta}}(\mathbf{z})$, and a stochastic decoder $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$. The stochastic encoder $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$, also called *inference model*, approximates the true but intractable posterior $p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})$ of the generative model.

Kingma, D. P. (2017). Variational inference & deep learning: A new synthesis. (PhD Thesis)

Variational auto-encoders

Before re-parametrization

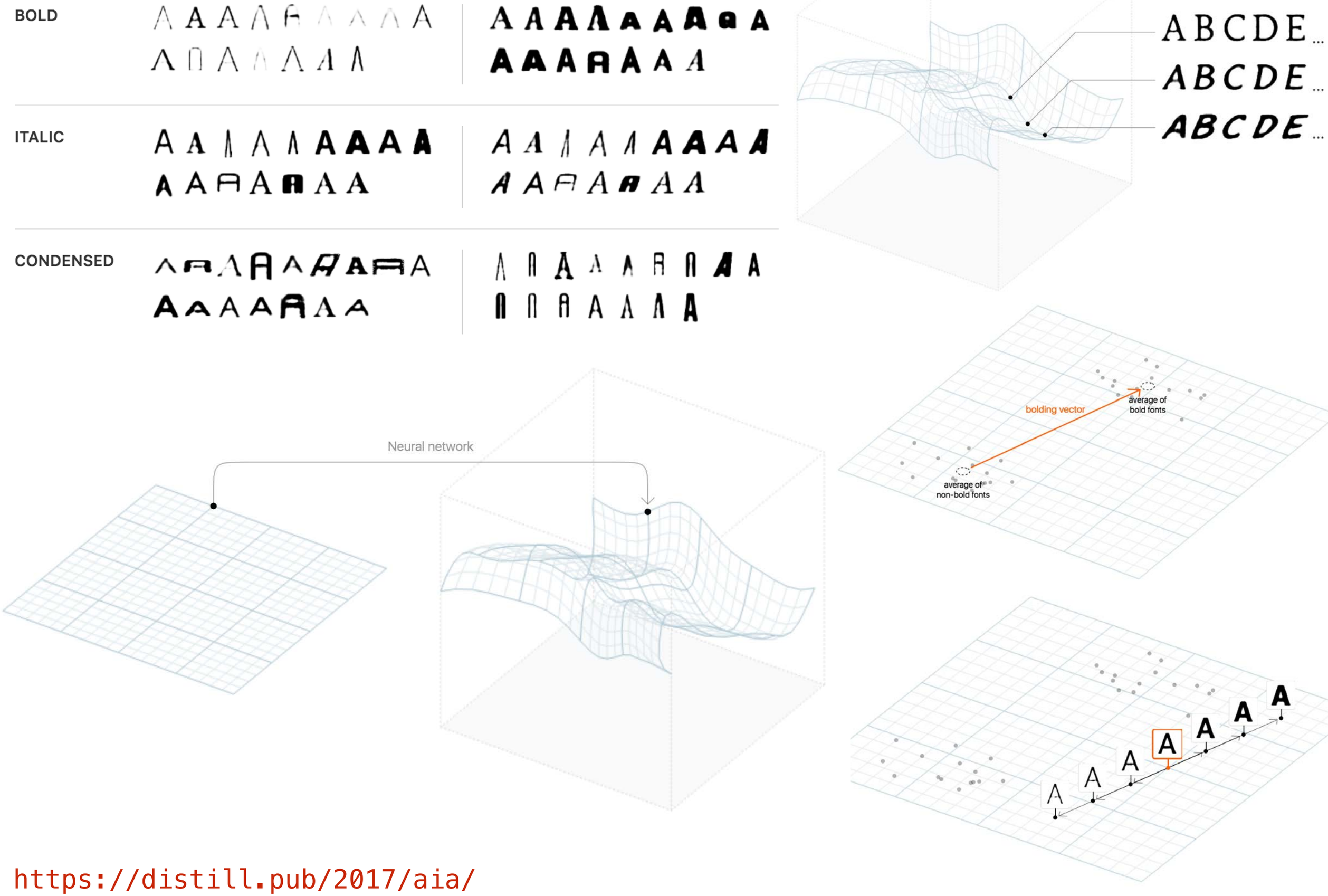
After re-parametrization



Kingma, D. P., & Welling, M. (2013). Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114.

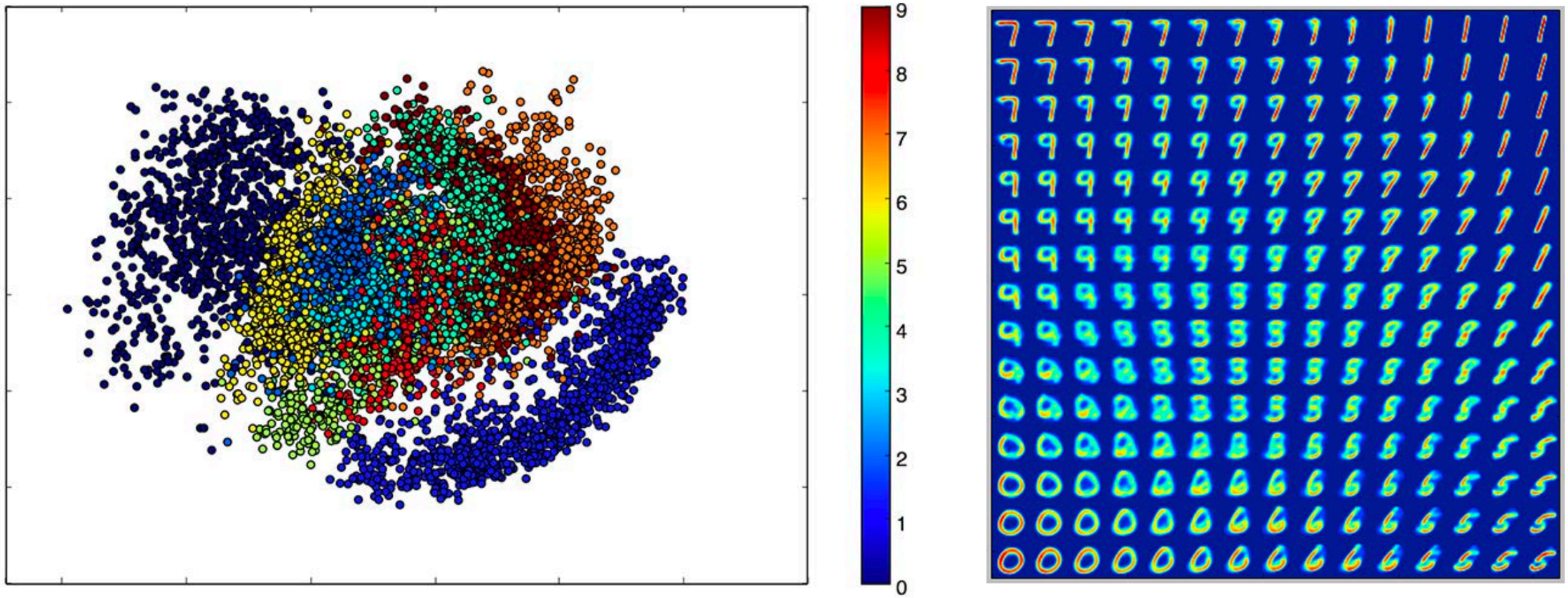
Doersch, C. (2016). Tutorial on variational autoencoders. arXiv preprint arXiv:1606.05908.

Generative models

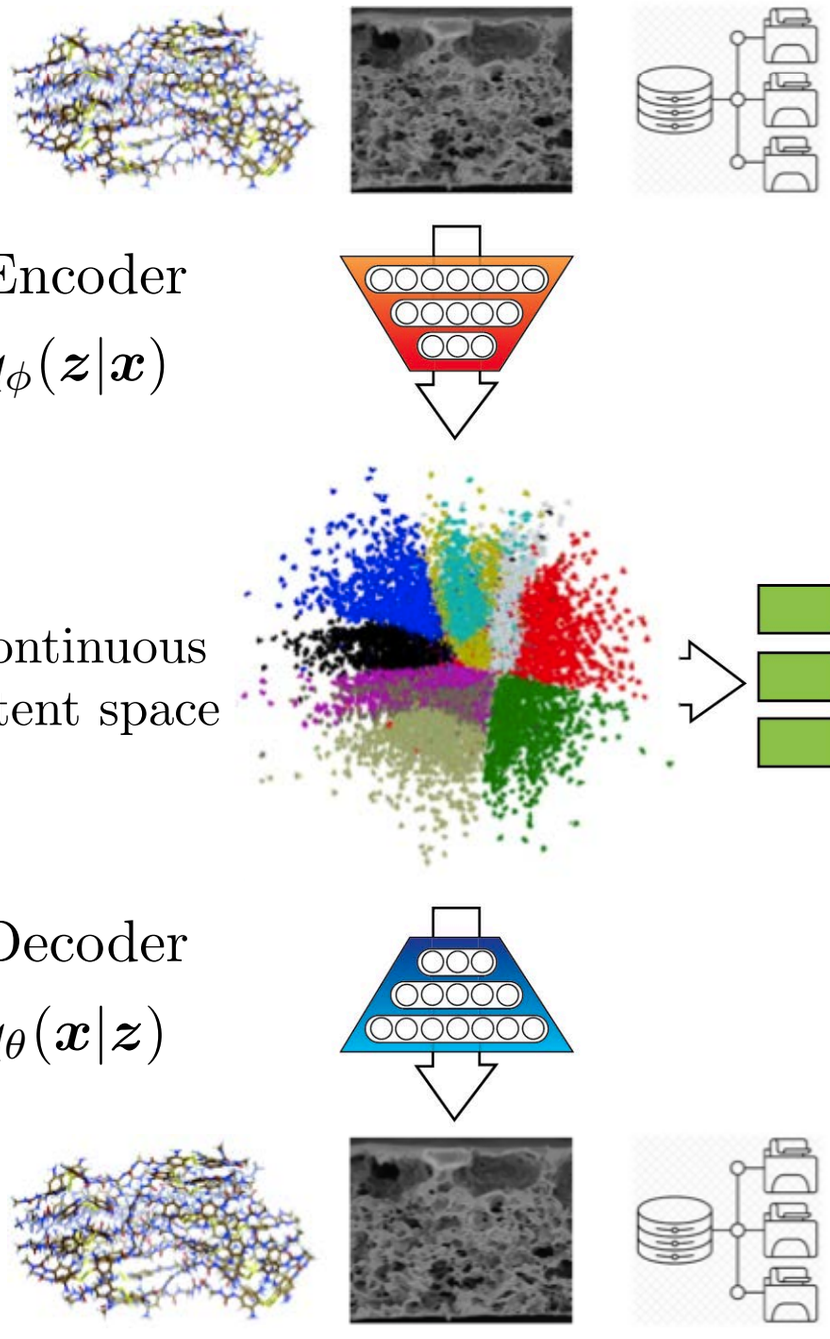


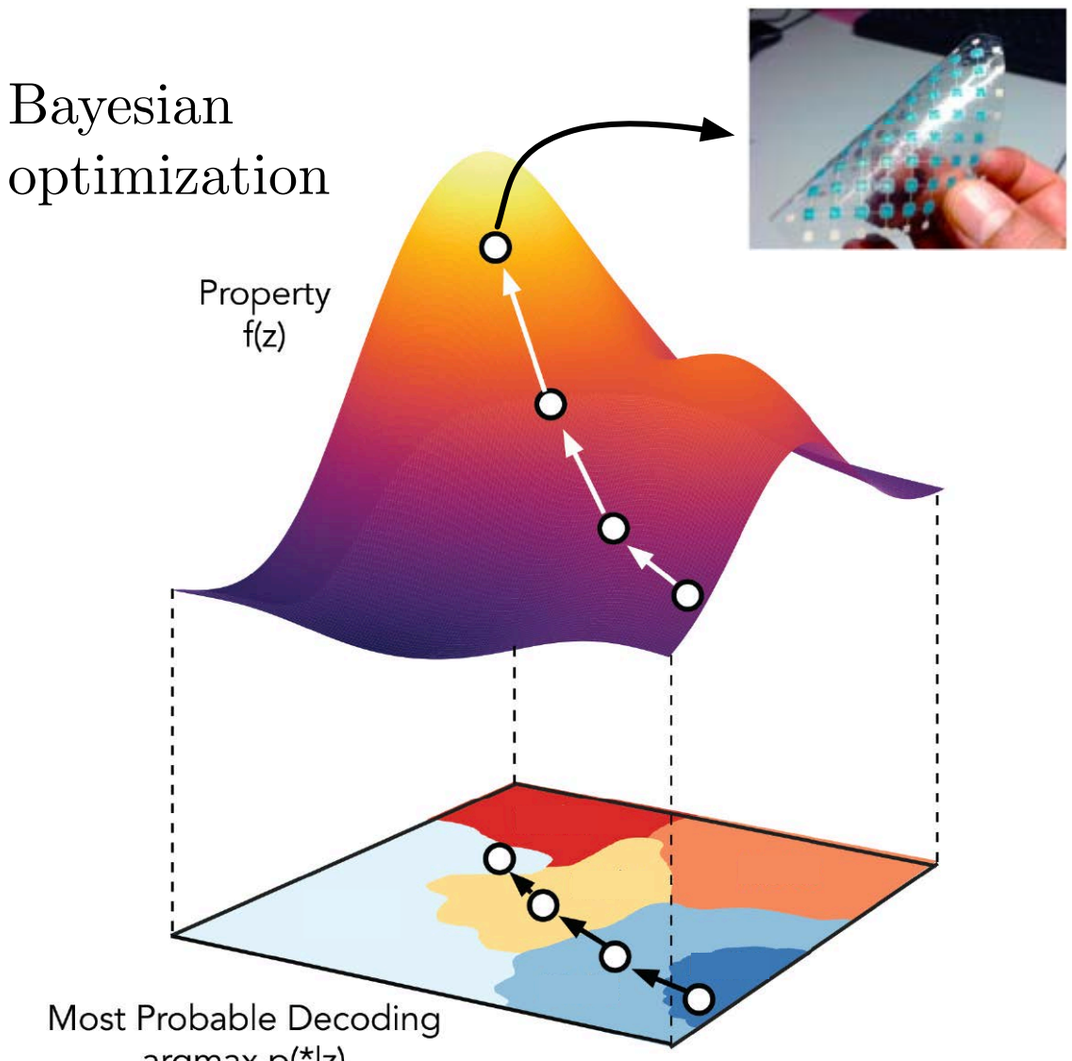
https://distill.pub/2017/aia/

The latent space of hand-written digits



Generative models





Gómez-Bombarelli, R., Wei, J. N., Duvenaud, D., Hernández-Lobato, J. M., Sánchez-Lengeling, B., Sheberla, D., ... & Aspuru-Guzik, A. (2016). Automatic chemical design using a data-driven continuous representation of molecules. ACS Central