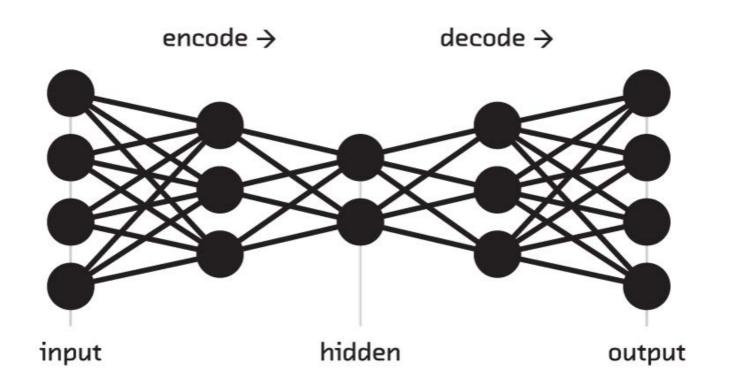
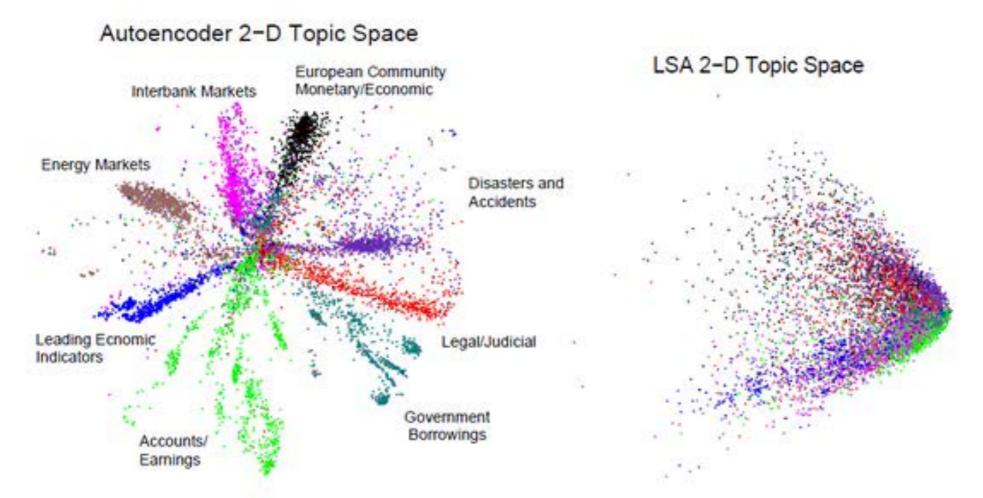
ENM 540: Data-driven modeling and probabilistic scientific computing

Variational auto-encoders



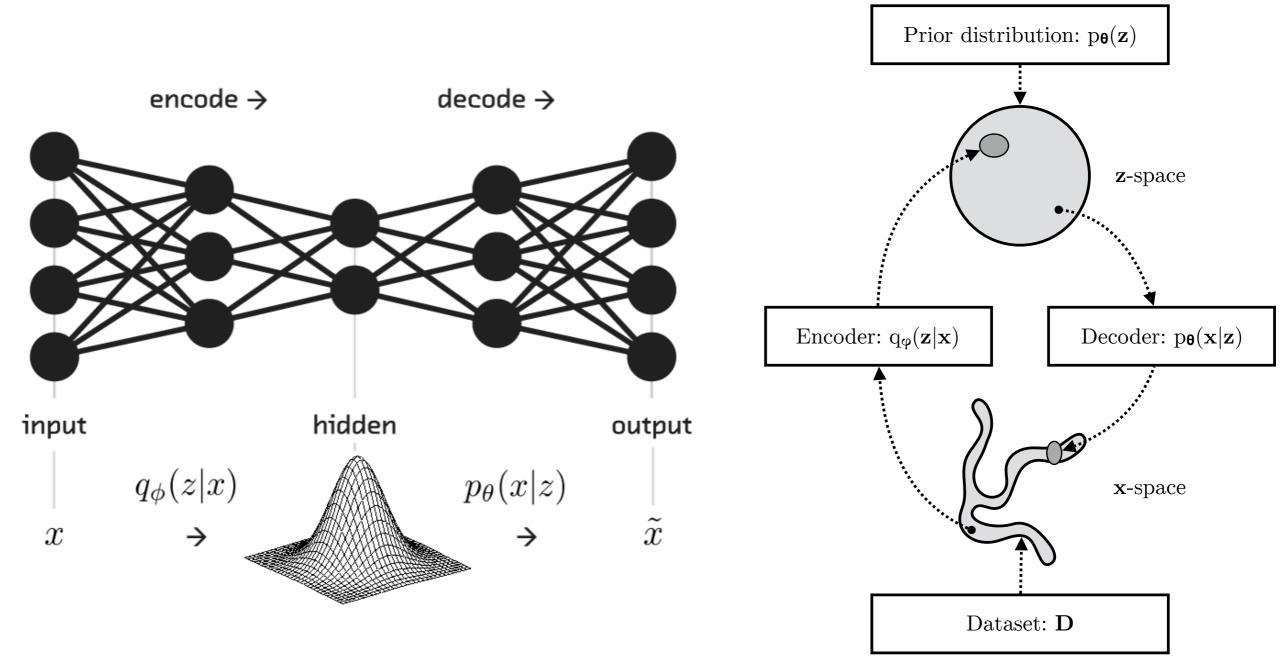
## Neural network auto-encoders





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

## Variational auto-encoders

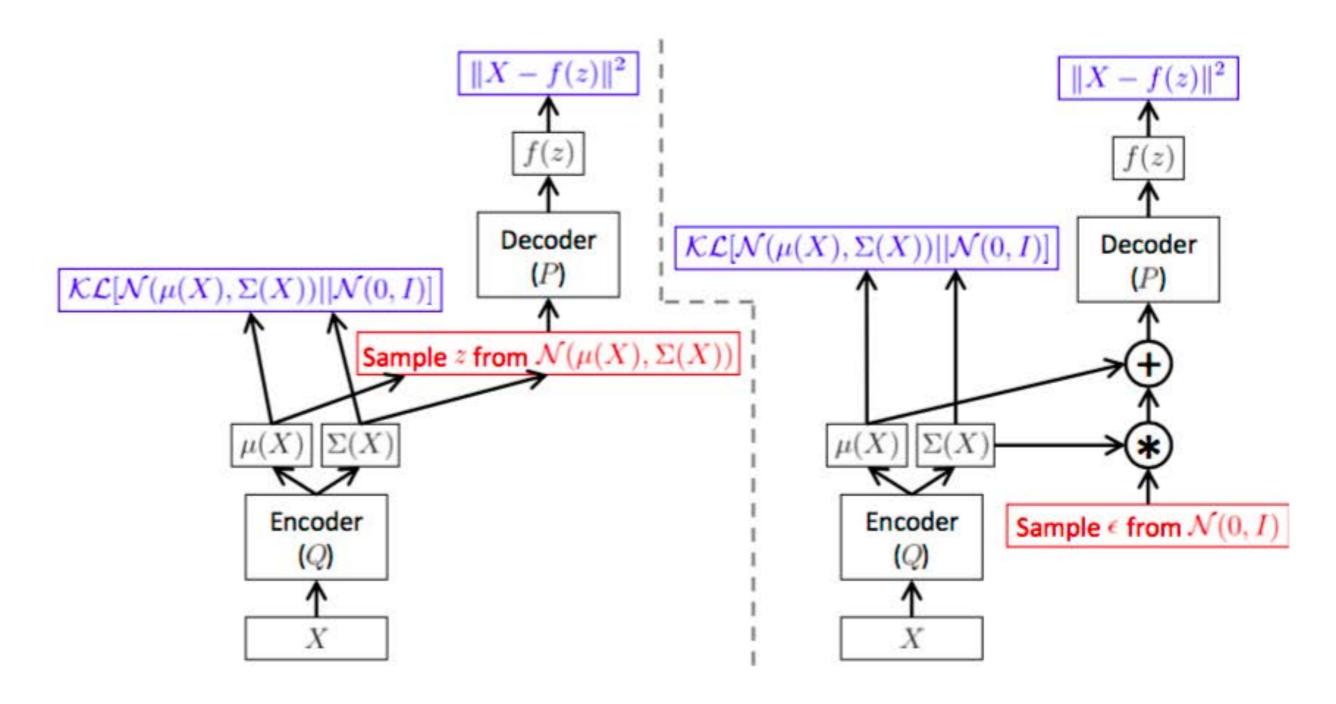


A VAE learns stochastic mappings between the observed  $\mathbf{x}$ -space, whose empirical distribution  $q_D(\mathbf{x})$  is typically complicated, and a latent  $\mathbf{z}$ -space, whose distribution can be relatively simple (such as spherical, as in this figure). The generative model learns a joint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

#### 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

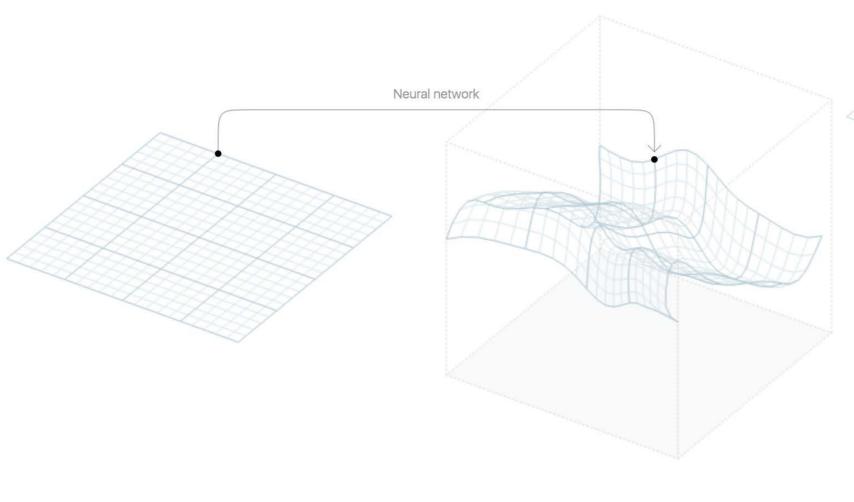
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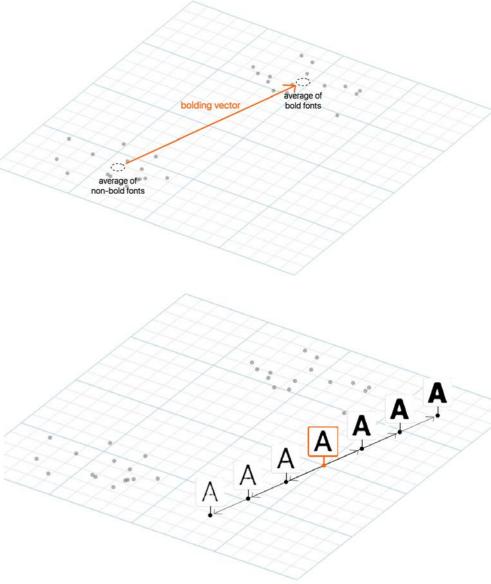
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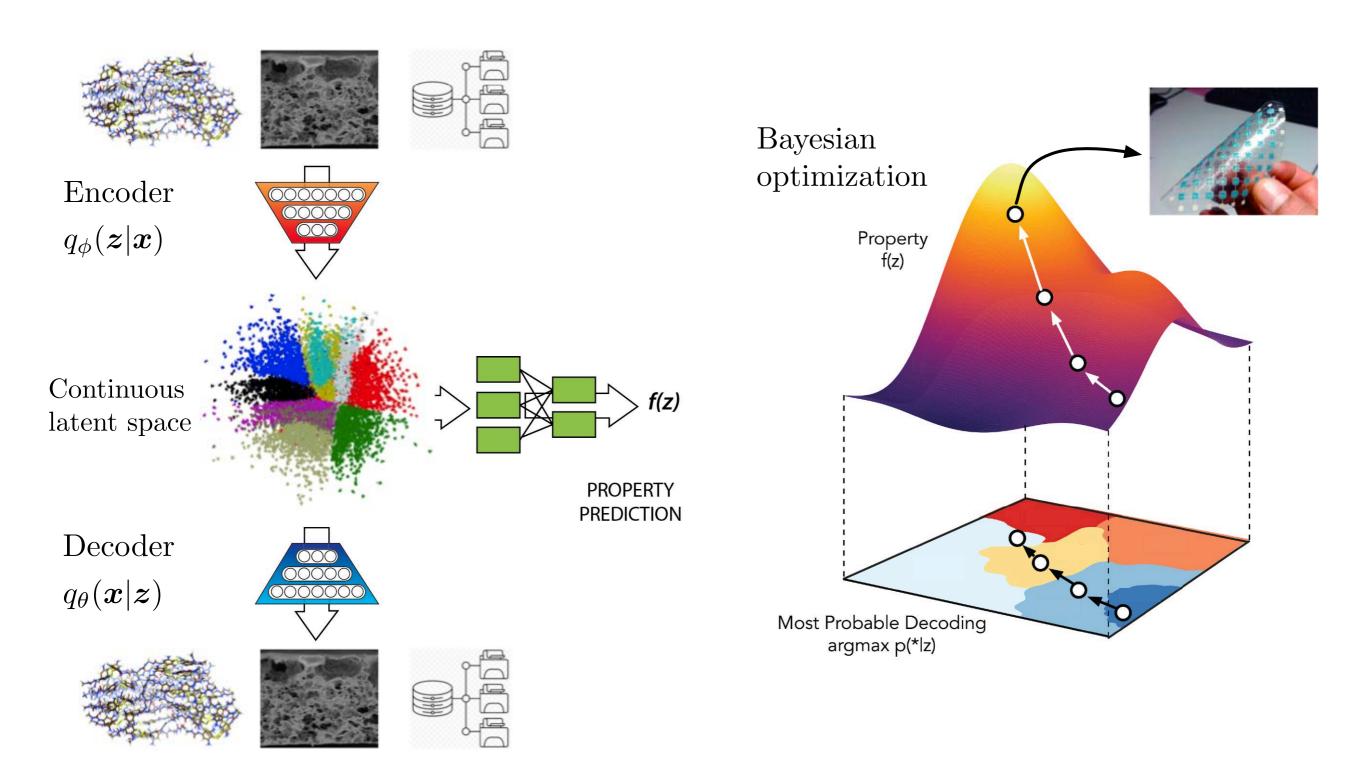
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https://distill.pub/2017/aia/

### 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