Machine Learning

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University of Illinois at Urbana-Champaign, 2018

L22: Variational Auto-Encoders

Goals of this lecture

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- Getting to know Variational Auto-Encoders

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- Understanding generative methods

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- C. Doersch; Tutorial on Variational Autoencoders; arxiv.org/abs/1606.05908

Recap: Maximum likelihood so far?

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Model:

$$p(\boldsymbol{y}|x) = \frac{\exp F(\boldsymbol{y}, x, \boldsymbol{w})/\epsilon}{\sum_{\hat{\boldsymbol{y}}} \exp F(\hat{\boldsymbol{y}}, x, \boldsymbol{w})/\epsilon}$$

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Now and the past few lectures:

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Now and the past few lectures:

How about modeling a distribution $p(x)$ for the data?

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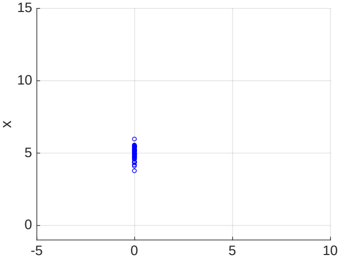
- Fit mean and variance (= parameters θ) of a distribution (e.g., Gaussian)
- Fit parameters θ of a mixture distribution (e.g., mixture of Gaussian, k-means)

Example:



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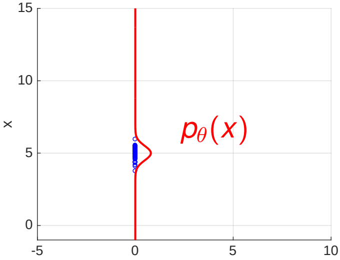

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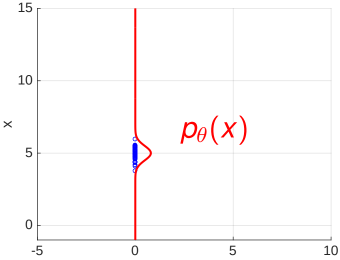

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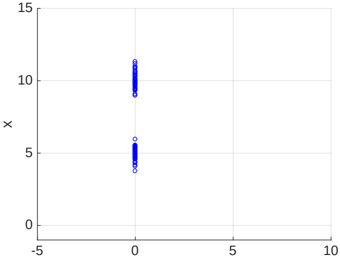

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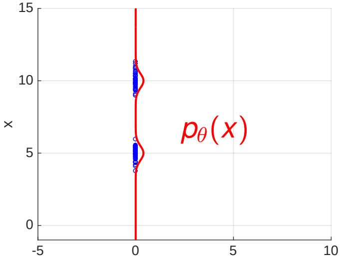

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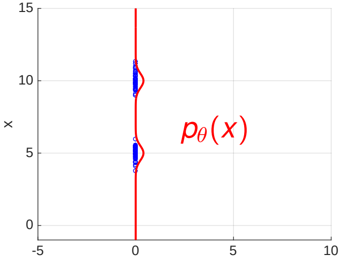

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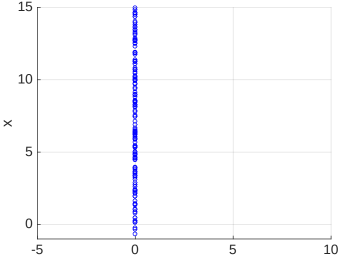

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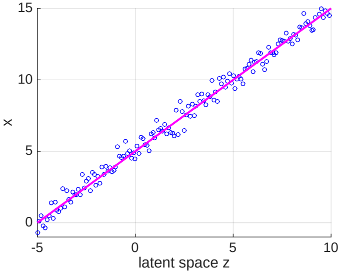

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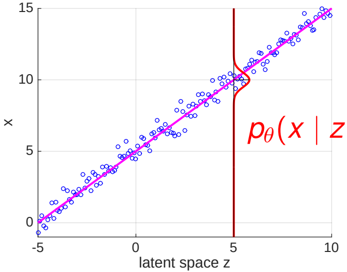

$$p_\theta(x \mid z) \propto \exp\left(-\frac{(x-\mu(z))^2}{2\sigma^2}\right)$$

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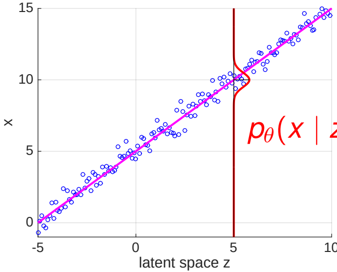

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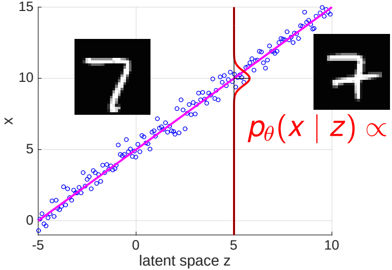
Increasing dimensions:

$x \in \mathbb{R}^{784}$



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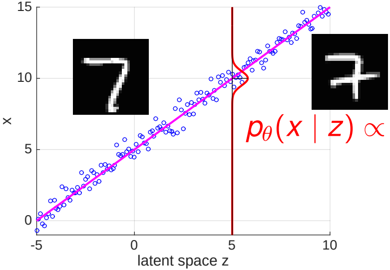

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Manifold hypothesis:

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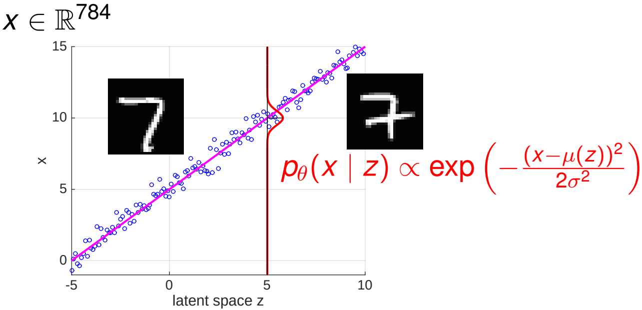

Manifold hypothesis:

- x is a high dimensional vector

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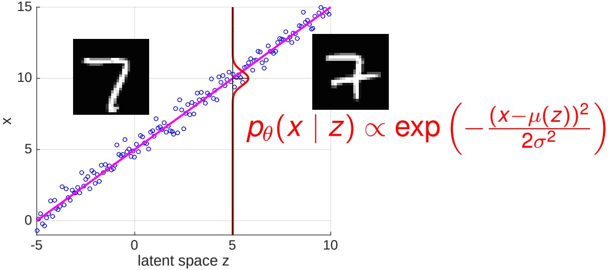

Manifold hypothesis:

- x is a high dimensional vector
- data is concentrated around a low dimensional manifold

Examples of low-dimensional manifolds:

$$z \in [0,1] \quad \rightarrow$$

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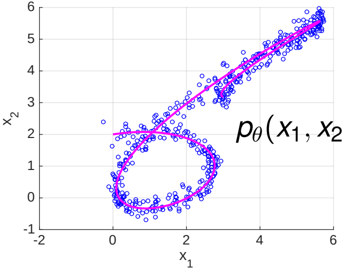

$p_\theta(x_1, x_2|z)$

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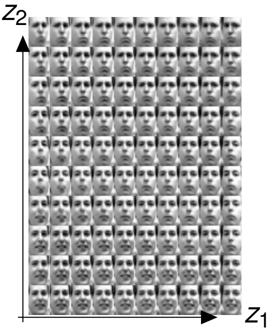

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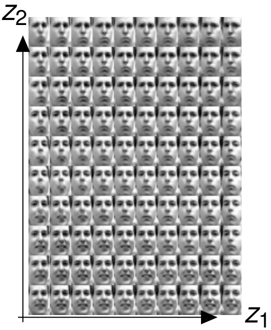

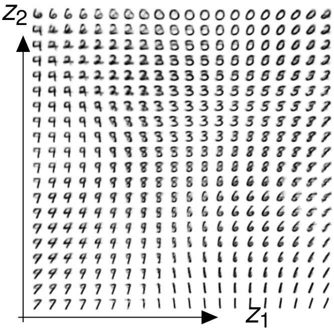

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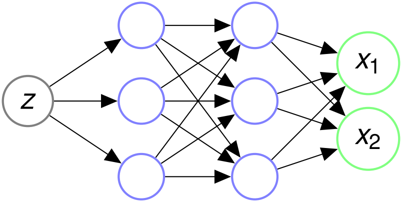

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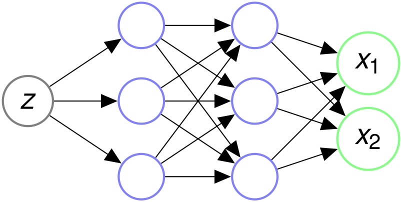

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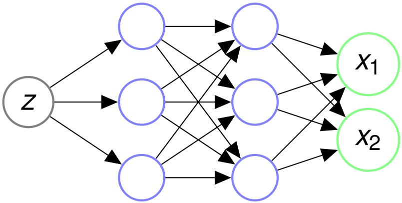

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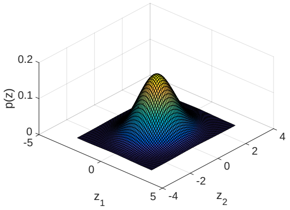

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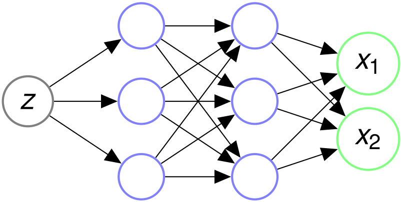

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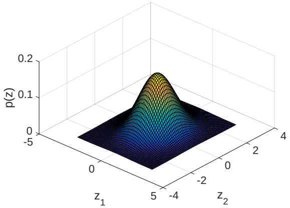

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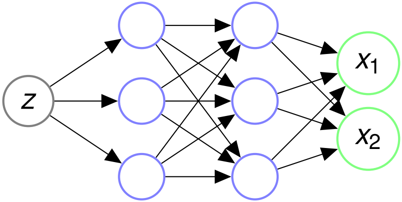

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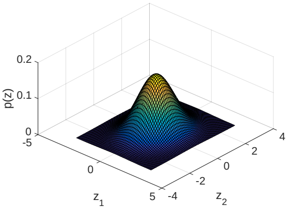

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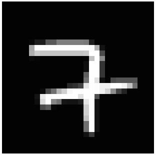

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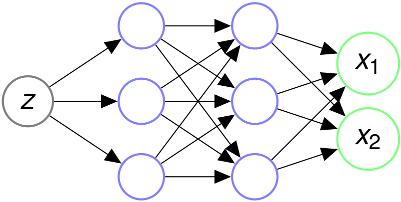

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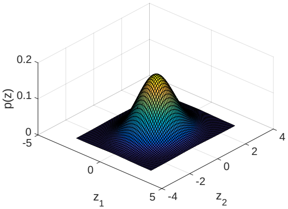

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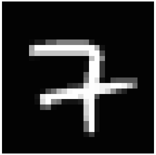
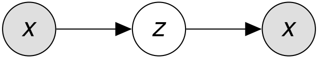


But how to optimize for θ? How do we know which z maps to which x?

Training as an auto-encoder: How about



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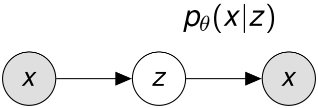

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$$\begin{tikzcd} x \arrow[r, "p_\theta(z|x)"] & z \arrow[r, "p_\theta(x|z)"] & x \end{tikzcd}$$

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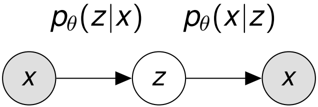

What is $p_\theta(z|x)$?

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- Sampling techniques (generally very costly)

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How to compute normalization constant?

- Sampling techniques (generally very costly)
- Approximate $p_\theta(z|x)$ with $q_\phi(z|x)$ (encoder)

Encoder $q_{\phi}(z|x)$ as a deep net which computes mean and variance:

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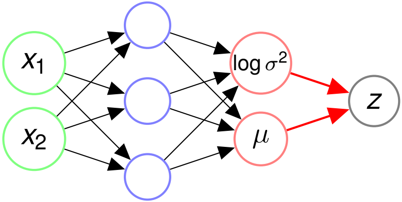
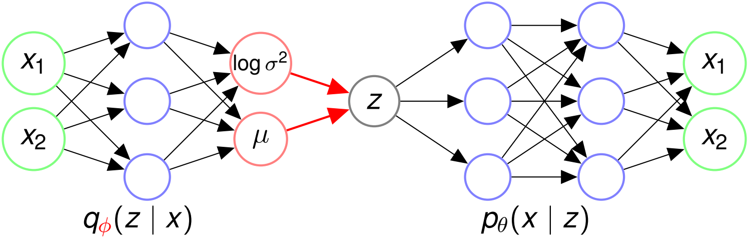


Variational auto-encoder architecture:



Learning parameters θ, ϕ via back-propagation

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$$\begin{aligned}\log p_\theta(x) &= \int_z q_\phi(z|x)\log p_\theta(x)\\ &= \int_z q_\phi(z|x)\log\frac{p_\theta(x,z)}{p_\theta(z|x)}\end{aligned}$$

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&= \int_z q_\phi(z|x) \log \left(\frac{p_\theta(x,z)}{q_\phi(z|x)} \cdot \frac{q_\phi(z|x)}{p_\theta(z|x)} \right)
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&= \int_z q_\phi(z|x) \log \frac{p_\theta(x,z)}{q_\phi(z|x)} + \int_z q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z|x)}
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&= \mathcal{L}(p_\theta, q_\phi) + D_{KL}(q_\phi, p_\theta)
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\end{aligned}
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- Assume $q_\phi(z|x)$ can approximate $p_\theta(z|x)$ well

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$$
\begin{aligned}
\log p_\theta(x) &= \int_z q_\phi(z|x) \log p_\theta(x) \\
&= \int_z q_\phi(z|x) \log \frac{p_\theta(x,z)}{p_\theta(z|x)} \\
&= \int_z q_\phi(z|x) \log \left(\frac{p_\theta(x,z)}{q_\phi(z|x)} \cdot \frac{q_\phi(z|x)}{p_\theta(z|x)} \right) \\
&= \int_z q_\phi(z|x) \log \frac{p_\theta(x,z)}{q_\phi(z|x)} + \int_z q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z|x)} \\
&= \mathcal{L}(p_\theta, q_\phi) + D_{KL}(q_\phi, p_\theta) \\
&\geq \mathcal{L}(p_\theta, q_\phi)
\end{aligned}
$$

- Assume $q_\phi(z|x)$ can approximate $p_\theta(z|x)$ well
- $\mathcal{L}$ is often referred to as empirical lower bound (ELBO)

Approximate Inference:

$$\mathcal{L}(p_\theta, q_\phi) \quad = \quad \int_z q_\phi(z|x) \log \frac{p_\theta(x,z)}{q_\phi(z|x)}$$

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- Reconstruction $\mathbb{E}_{q_\phi}[\log p_\theta(x|z)]$

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$$-D_{KL}(q_\phi, p) = \textbf{Homework}$$

Reconstruction:

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$$\mathbb{E}_{q_\phi}[\log p_\theta(x|z)] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x|z^i) \quad \text{where} \quad z^i \sim \mathcal{N}(z; \mu_\phi(x), \sigma_\phi(x))$$

Variational auto-encoder loss function:

$$\mathcal{L}(p_\theta, q_\phi) \approx -D_{KL}(q_\phi, p) + \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x|z^i)$$

Intuitively:

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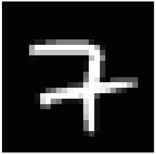 $\rightarrow$

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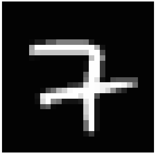 $\rightarrow$ z $\rightarrow$

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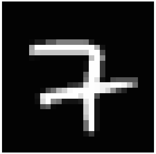

$\rightarrow$ z $\rightarrow$

$\log p_\theta(x|z^1)$

$\vdots$

$\log p_\theta(x|z^N)$

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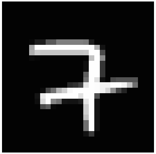
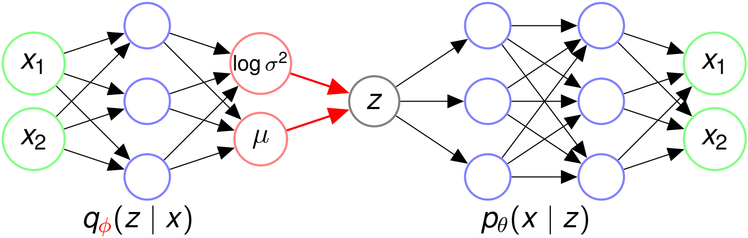


$$\rightarrow \quad z \quad \rightarrow \quad \begin{array}{l} \log p_\theta(x|z^1) \\ \vdots \\ \log p_\theta(x|z^N) \end{array}$$

Typically N small, e.g., N = 1

Where is an issue?



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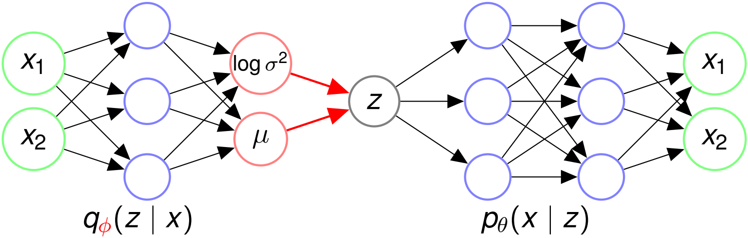

How to backpropagate through the sampling step?

$$z \sim q_{\phi}(z|x) = \mathcal{N}(z; \mu_{\phi}(x), \sigma_{\phi}(x))$$

Reparameterization trick:

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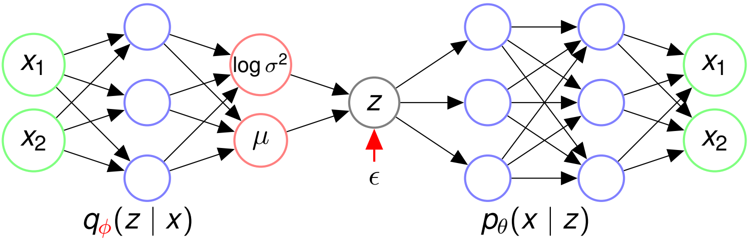
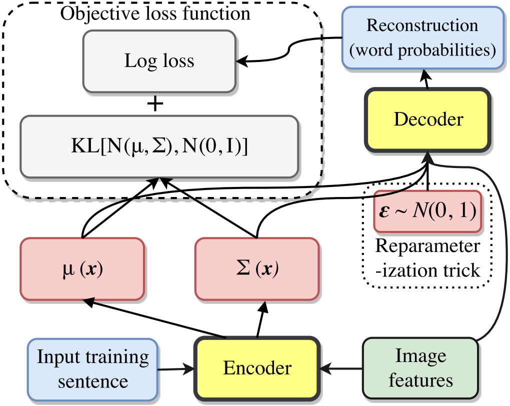
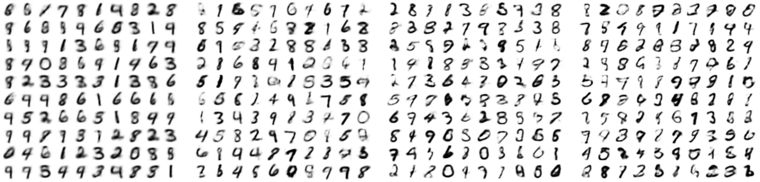


Variational auto-encoder flowchart:



Variational auto-encoder for MNIST digits:



(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Examples of low-dimensional manifolds: ($z \in \mathbb{R}^2$)
Kingma and Welling: "Auto-Encoding Variational Bayes" (ICLR 2014)

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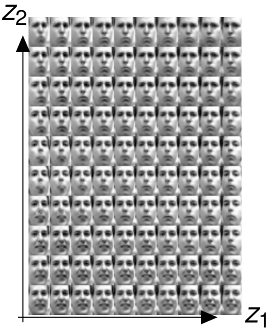

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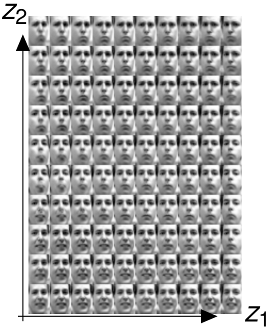
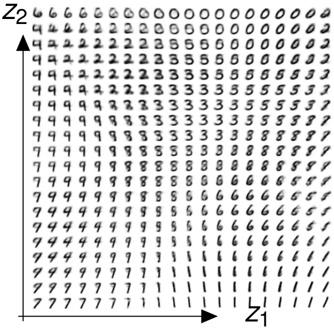
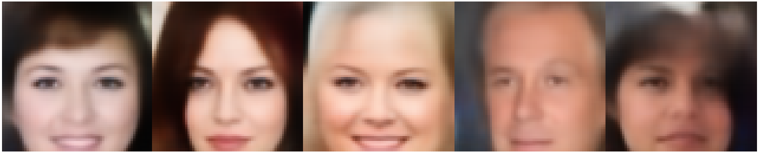




Variational auto-encoder for face generation:



Variational auto-encoder for semi-supervised learning:

Maaloe et al. "Improving Semi-Supervised Learning with Auxiliary Deep Generative Models" (2015)

	100 labels
AtlasRBF (Pitelis et al., 2014)	8.10% ($\pm$0.95)
Deep Generative Model (M1+M2) (Kingma et al., 2014)	3.33% ($\pm$0.14)
Virtual Adversarial (Miyato et al., 2015)	2.12%
Ladder (Rasmus et al., 2015)	1.06% ($\pm$0.37)
Auxiliary Deep Generative Model (1 MC)	2.25% ($\pm$ 0.08)
Auxiliary Deep Generative Model (10 MC)	**0.96% ($\pm$ 0.02)**

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- Why are variational auto-encoder results smooth?

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Next up:

Autoregressive Methods