Introduction to variational autoencoders

Abstract

Variational autoencoders are interesting generative models, which combine ideas from deep learning with statistical inference. They can be used to learn a low dimensional representation Z of high dimensional data X such as images (of e.g. faces). In contrast to standard auto encoders, X and Z are random variables. It's therefore possible to sample X from the distribution P(X|Z), thus creating e.g. images of faces, MNIST Digits, or speech.

In this talk I will in some detail describe the paper of Kingma and Welling. "*Auto-Encoding Variational Bayes*, *International Conference on Learning Representations." ICLR,* 2014.
arXiv:1312.6114 [stat.ML].

I will also show some code. A TensorFlow notebook can be found at:
https://github.com/oduerr/dl_tutorial/blob/master/tensorflow/vae/vae_demo.ipynb

Introduction to variational autoencoders

Oliver Dürr

Datalab-Lunch Seminar Series

Winterthur, 11 May, 2016

Motivation: Generating Faces

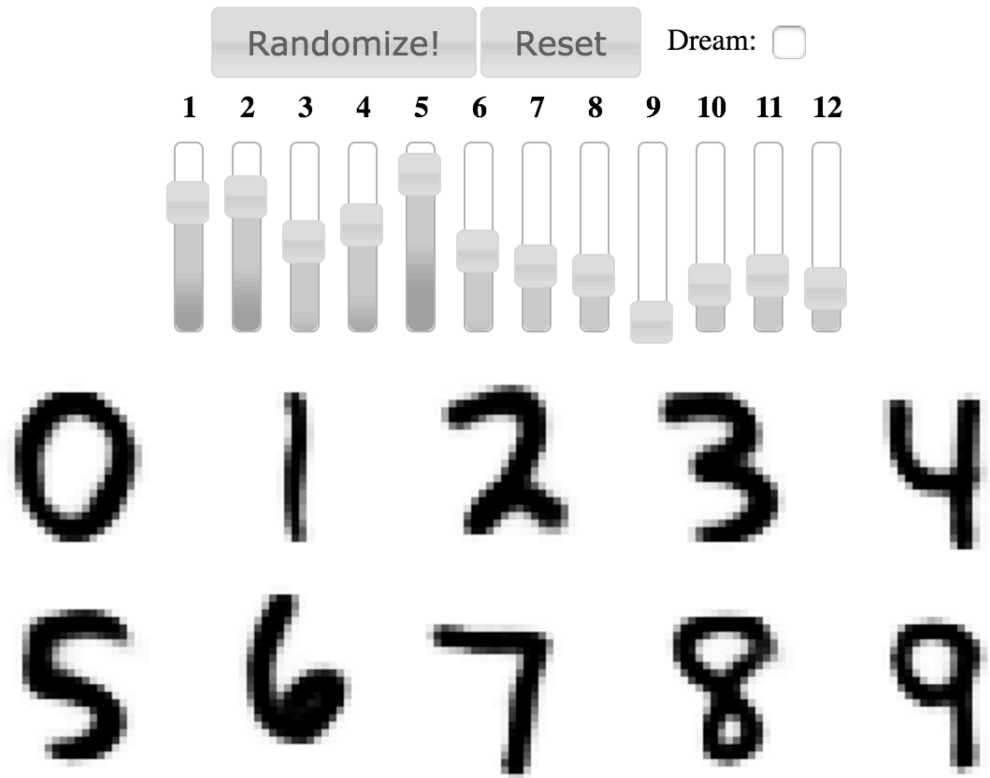
Other examples
- random faces
- MNIST
- Speech

just google vae…

These are not part of the trainingset!

https://www.youtube.com/watch?v=XNZIN7Jh3Sg

Motivation: Generating Hand Written Digits



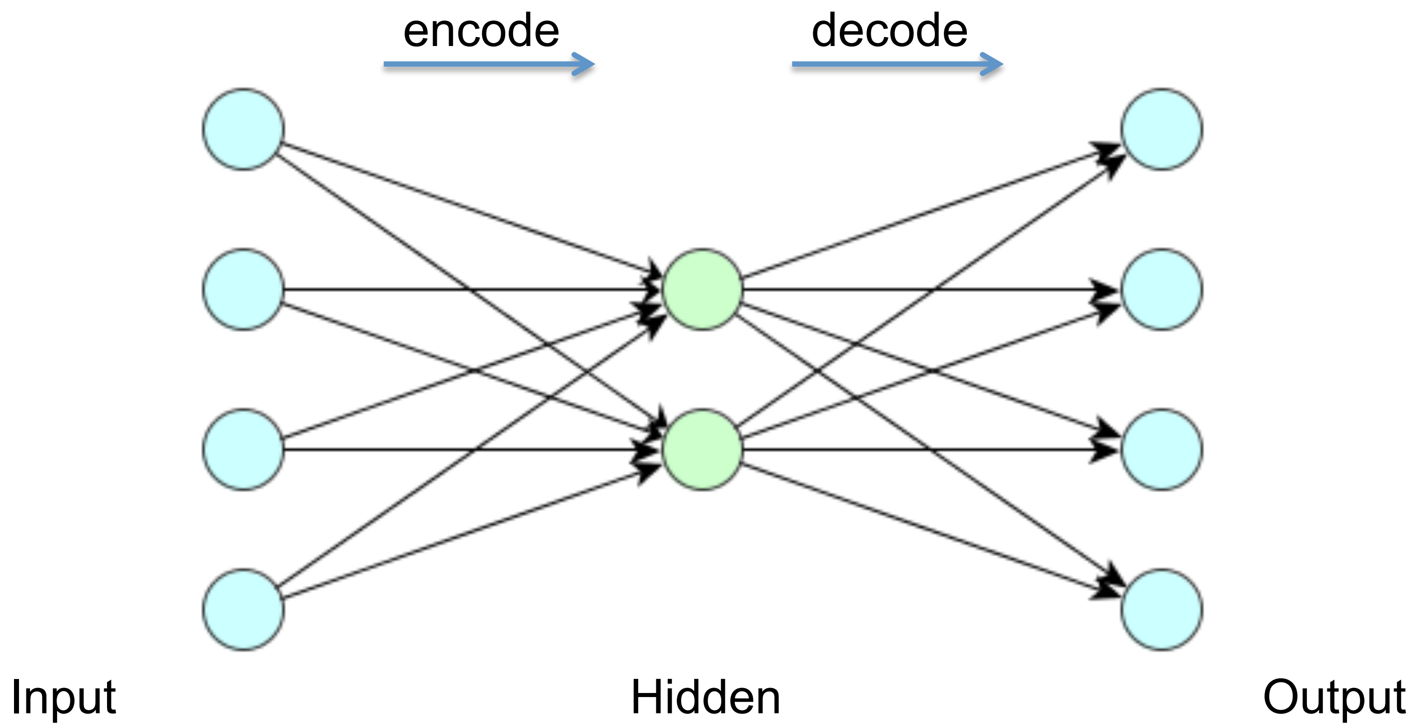
(Latent space) **z**

(Observed space) **x**

http://www.dpkingma.com/sgvb_mnist_demo/demo.html

Idea

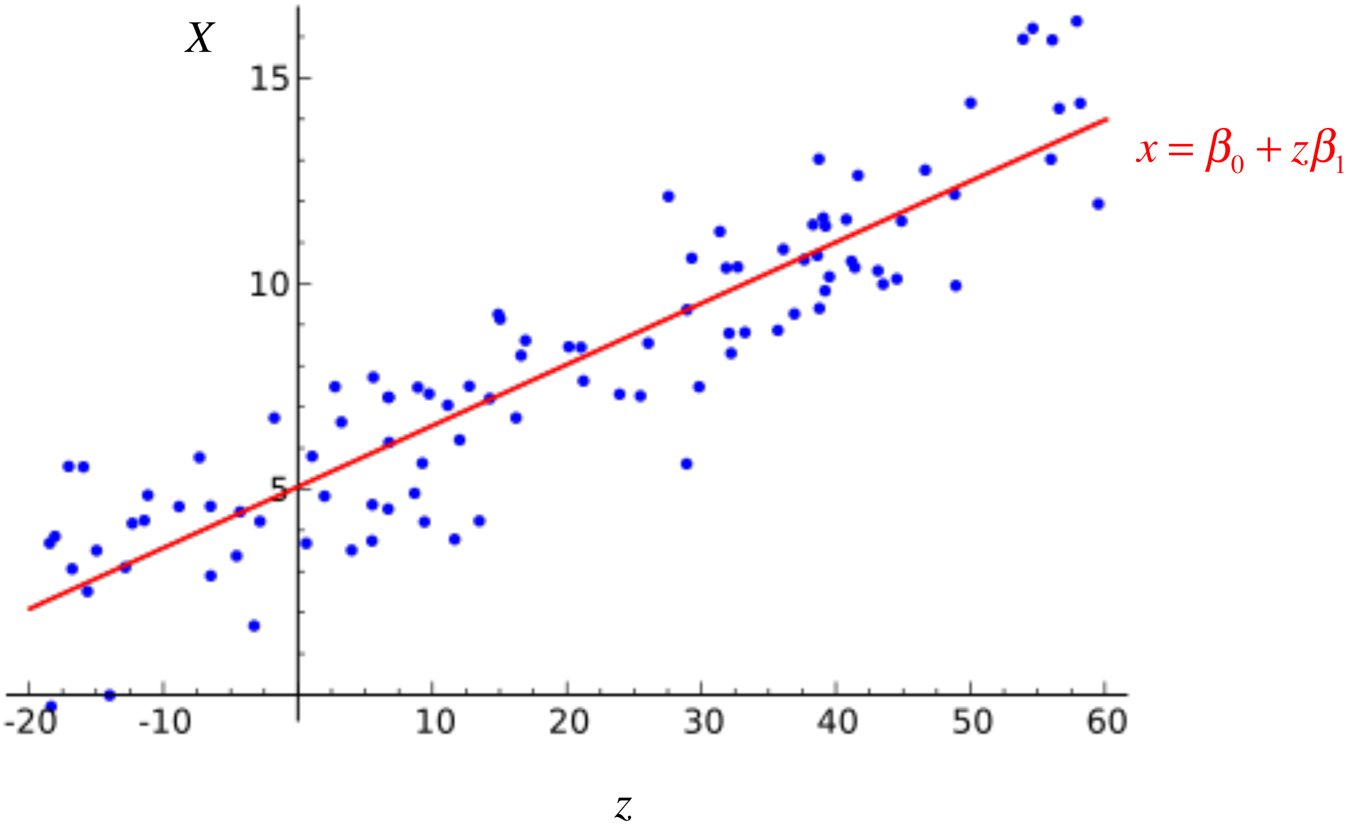
Recap: Auto Encoders ('classical')



A simple autoencoder more see Beates talk on Autoencoders

Recap: Linear Regression

Most people think of linear regression as points and a straight line:



Strange axis names, to be compatible with later notation

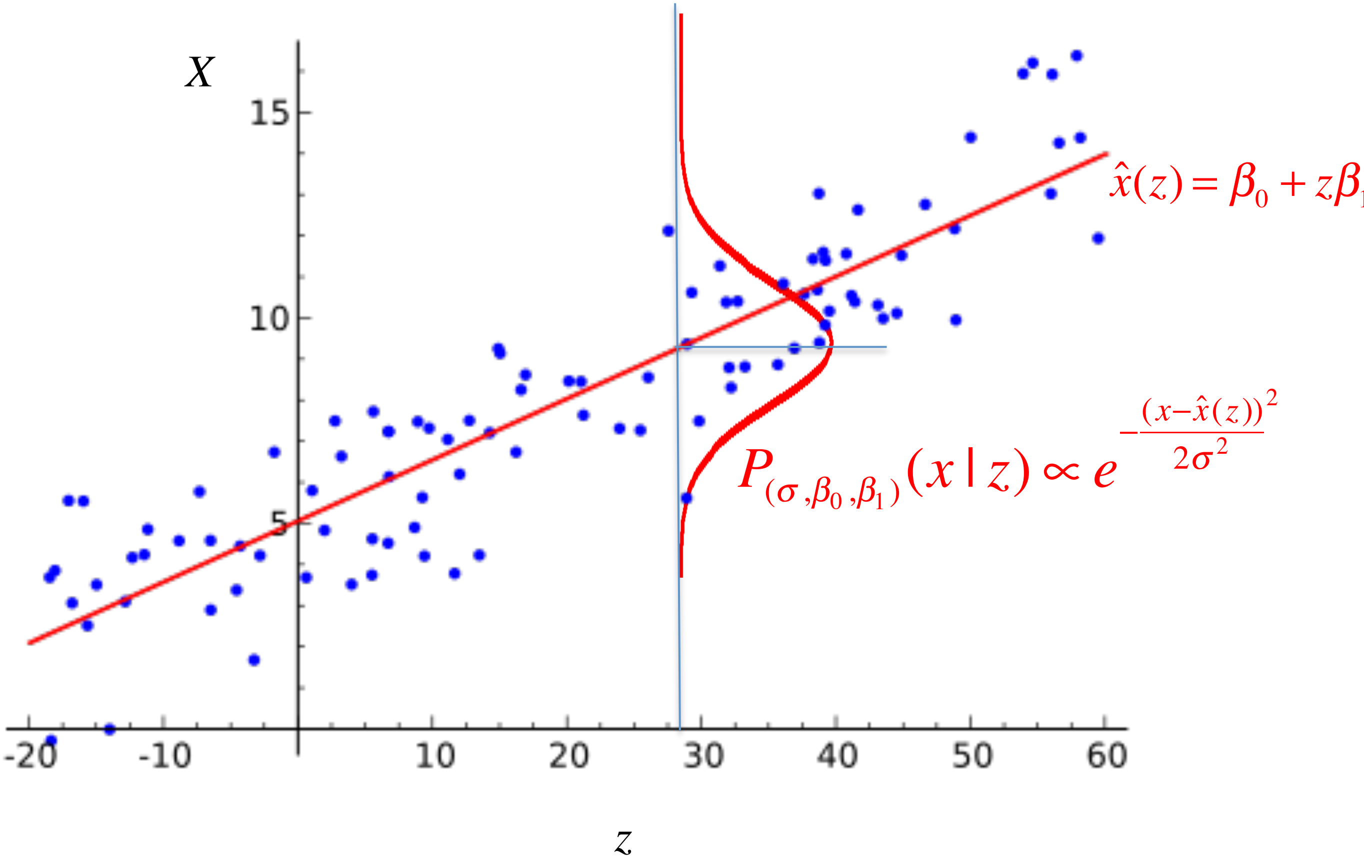
credit: wikipedia

Recap: Linear Regression

Benefits of having an error model:

- How likely is a data point
- Confidence bounds
- Compare models

Statisticians additionally have $P_\theta(X \mid Z)$



Strange axis names, to be compatible with later notation

credit: wikipedia

Recap: Linear Regression (as a graphical model)

Statisticians additionally have $P_\theta(X \mid Z)$

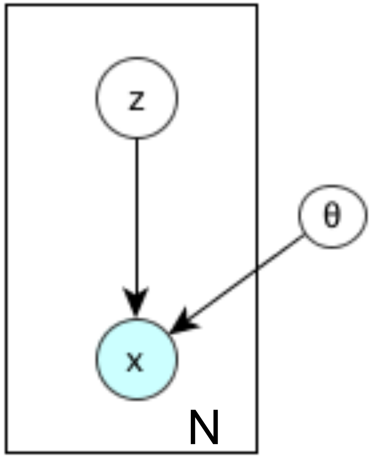
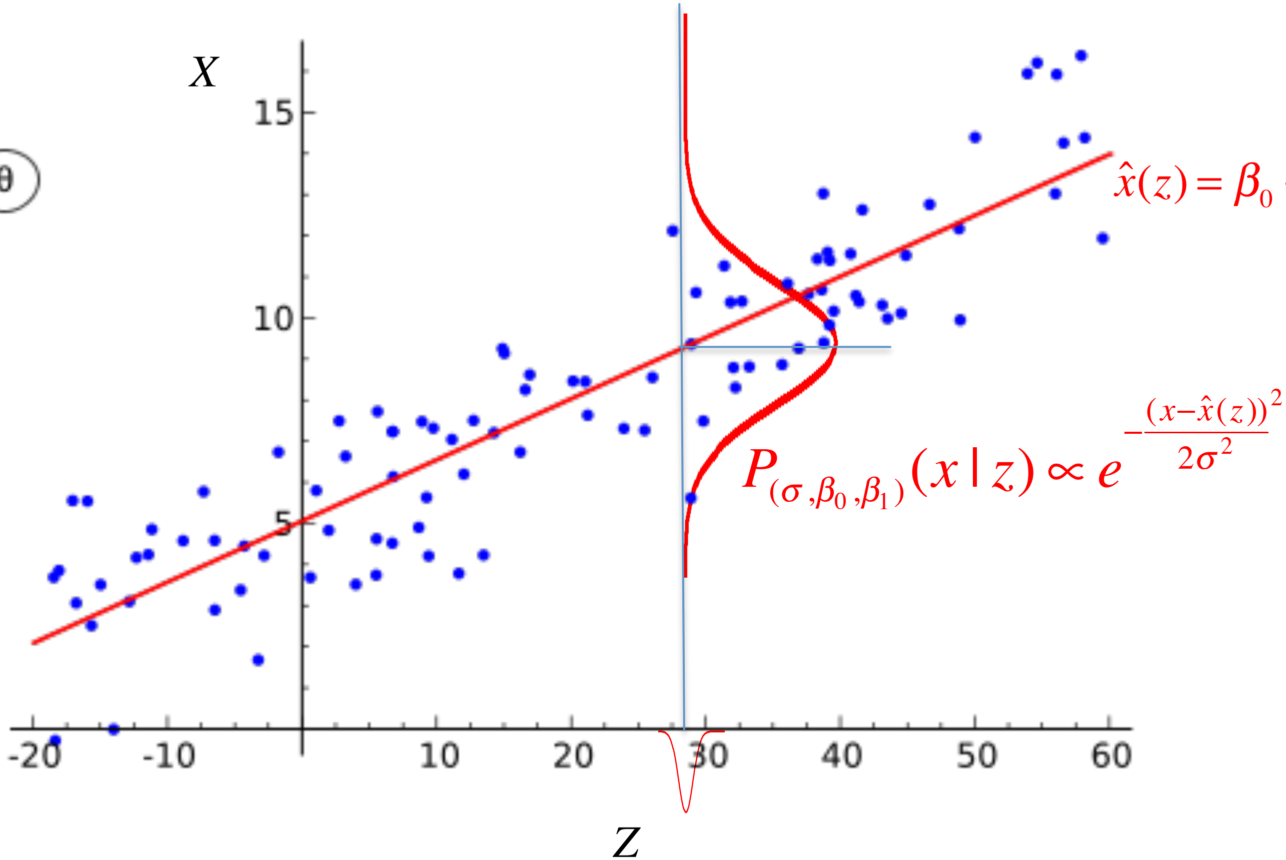


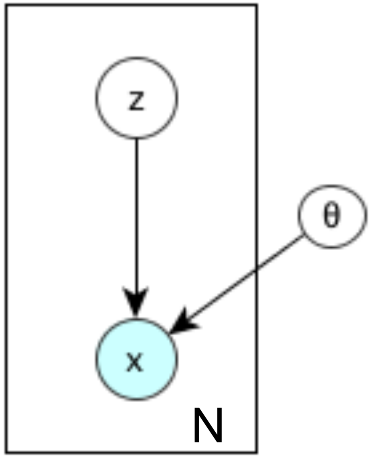
Plate notation of a graphical model to show off

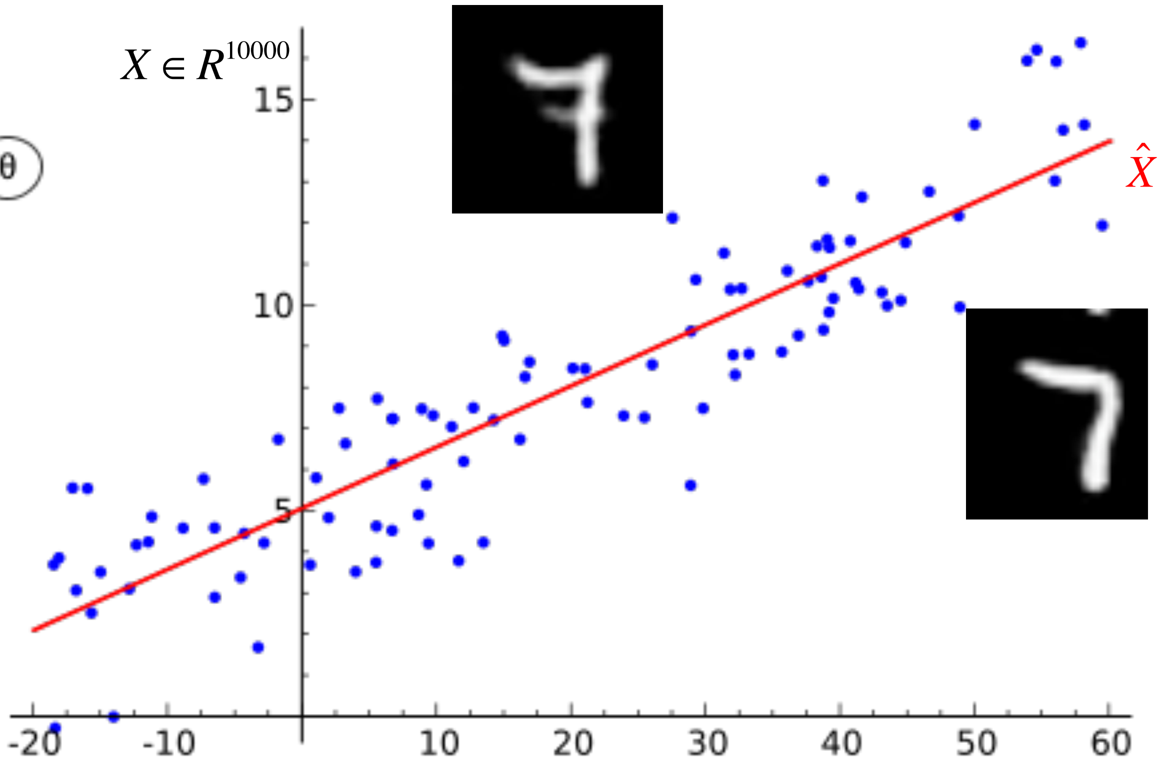


credit: wikipedia

See Beates talk on [Causal inference with graphical models]

Going from R^1 to R^{10000}





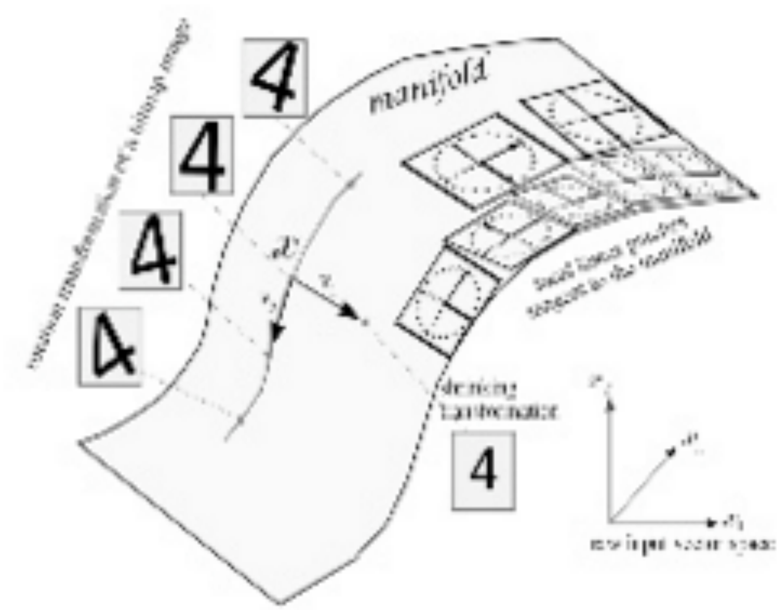
$Z \in R^n$ typically $n = 2,\ldots,50$ "latent space"

Is R^2 "big enough" to create images from R^{100000}?...

credit: wikipedia, digits: https://www.youtube.com/watch?v=hgyB8RegAIQ

Manifold hypothesis

- X high dimensional vector
- Data is concentrated around a low dimensional manifold



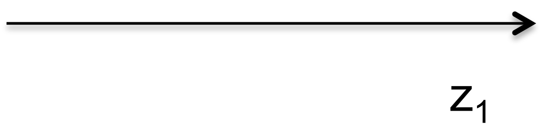
- Hope finding a representation Z of that manifold.

credit: http://www.deeplearningbook.org/

Variational auto encoders (idea of low dim manifold)

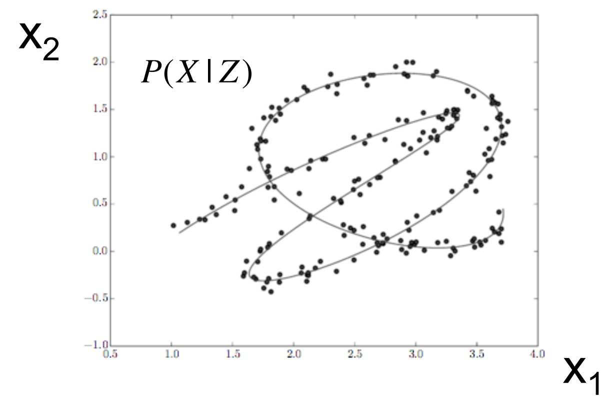
1D

Low Dimensional
representation a line

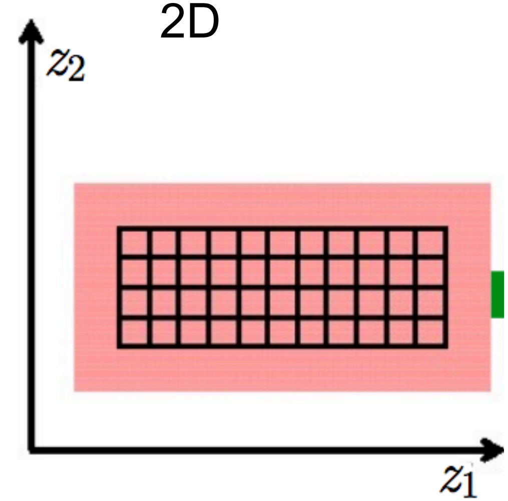


2D

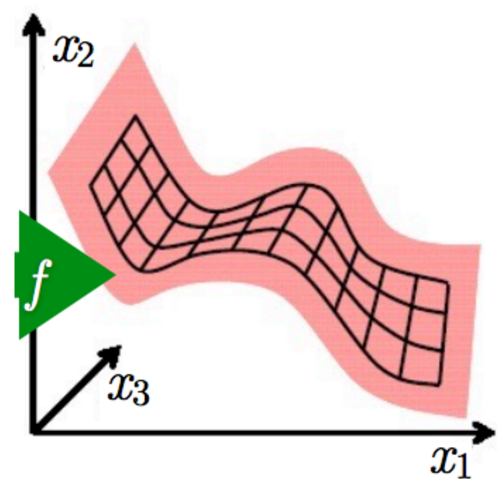
High Dimensional (number of pixels)



2D



3D

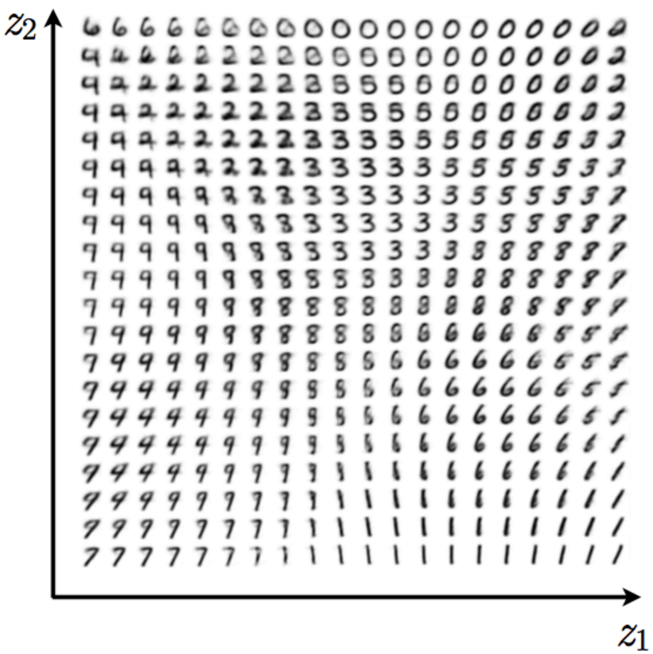


credit: http://www.deeplearningbook.org/

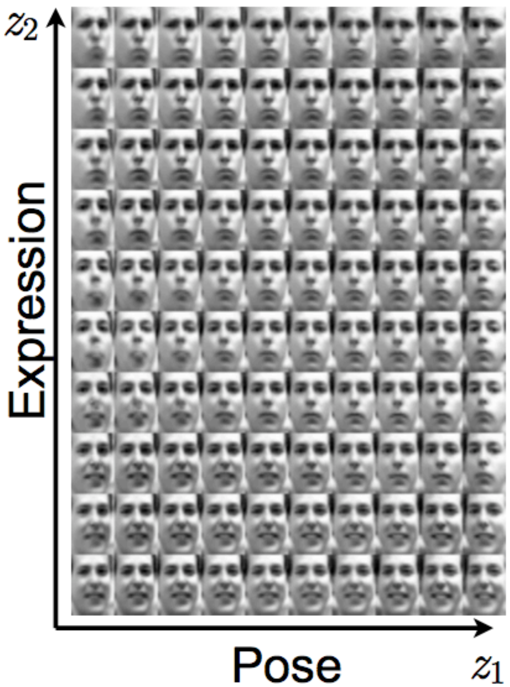
Variational auto encoders (idea of low dim manifold)

Examples of successful unfolding (2D →R^{28x28}, R^{20x26})

MNIST:



Frey Face dataset:



[Frey Face dataset]

2000 pictures of Brendan Frey (20x26)

Kingma and Welling. "*Auto-Encoding Variational Bayes*, *International Conference on Learning Representations.*" *ICLR*, 2014. [arXiv:1312.6114]

How did they do that?

Variational Autoencoders ("history")

Simultaneously discovered by

- Kingma and Welling. "*Auto-Encoding Variational Bayes*, *International Conference on Learning Representations." ICLR,* 2014.
  arXiv:1312.6114 [stat.ML] (20 December 2013, Amsterdam University)
  Talk

- Rezende, Mohamed and Wierstra. "*Stochastic back-propagation and variational inference in deep latent Gaussian models." ICML, 2014*
  arXiv:1401.4082 [stat.ML] (16 January 2014, Google DeepMind)

Alternative approach (for binary distributions)

- *Gregor, Danihelka et all. "Deep autoregressive networks." ICML 2014*
  – Has a more information theoretic ansatz (codings length)
  – Lecture given at *Nando de Freitas ML Course (University of Oxford)* *(a bit hand waving argument but with nice examples)*

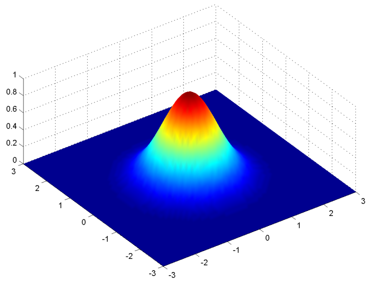
- We focus on the approach as in Kingma, Welling

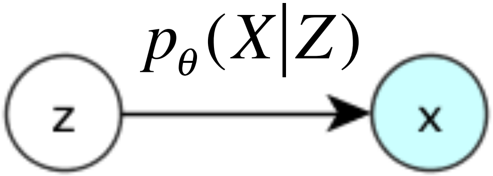
Principle Idea decoder network (graphical model)

- We have a set of N-observations (e.g. images) $\{x^{(1)},x^{(2)},\ldots,x^{(N)}\}$
- Complex model parameterized with θ
- There is a latent space z with

$$z \sim p(z) \quad \text{multivariate Gaussian}$$

$$x|z \sim p_\theta(x|z)$$



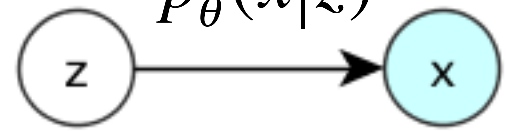


One Example

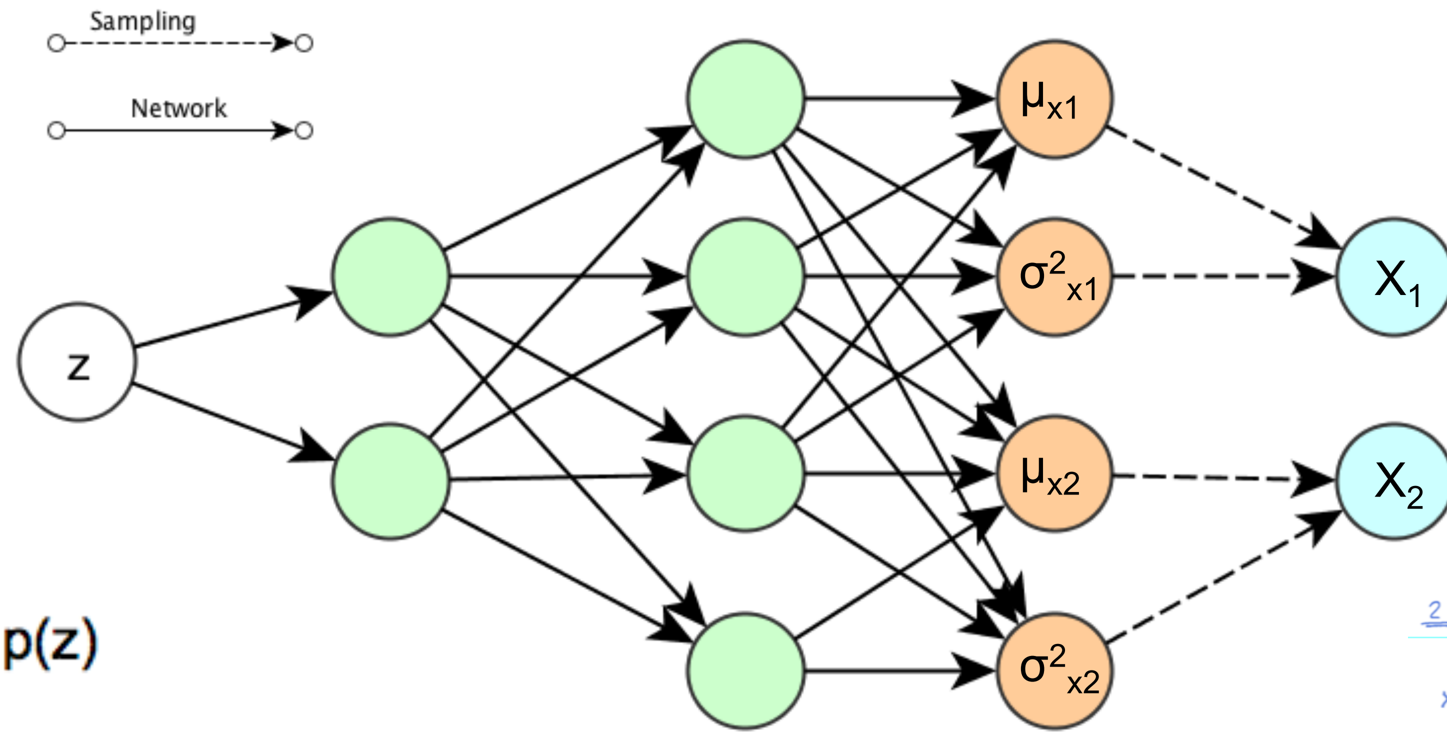
Wish to learn θ from the N training observations $x^{(i)}$ i=1,…,N

The model for the decoder network

$p_\theta(x|z)$



- For illustration z one dimensional x 2D
- Want a complex model of distribution of x given z
- Idea: **NN** + Gaussian (or Bernoulli) here with diagonal covariance Σ



$x|z \sim N(\mu_x, \sigma_x{}^2)$

p(z)

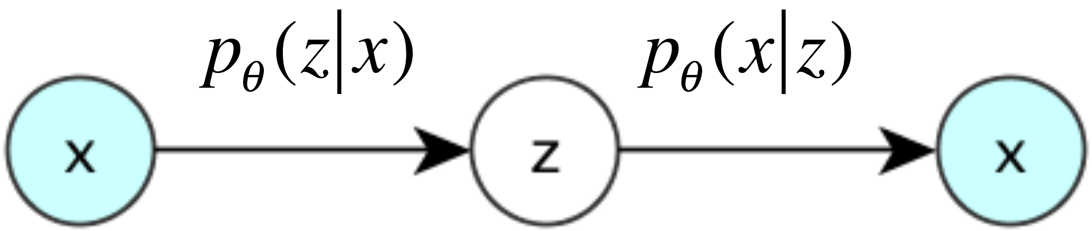
2 D

$P_\theta(x|z)$

$P_\theta(x|z) = N(x; \mu(z), \Sigma)$

$\Sigma_{ij} = \delta_{ij}\, \sigma_i^2(z)$

Training as an autoencoder



Training use maximum likelihood of p(x) given the training data

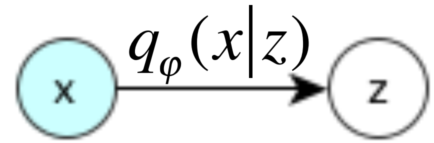
Problem:

$$p_\theta(z|x)$$

Cannot be calculated:

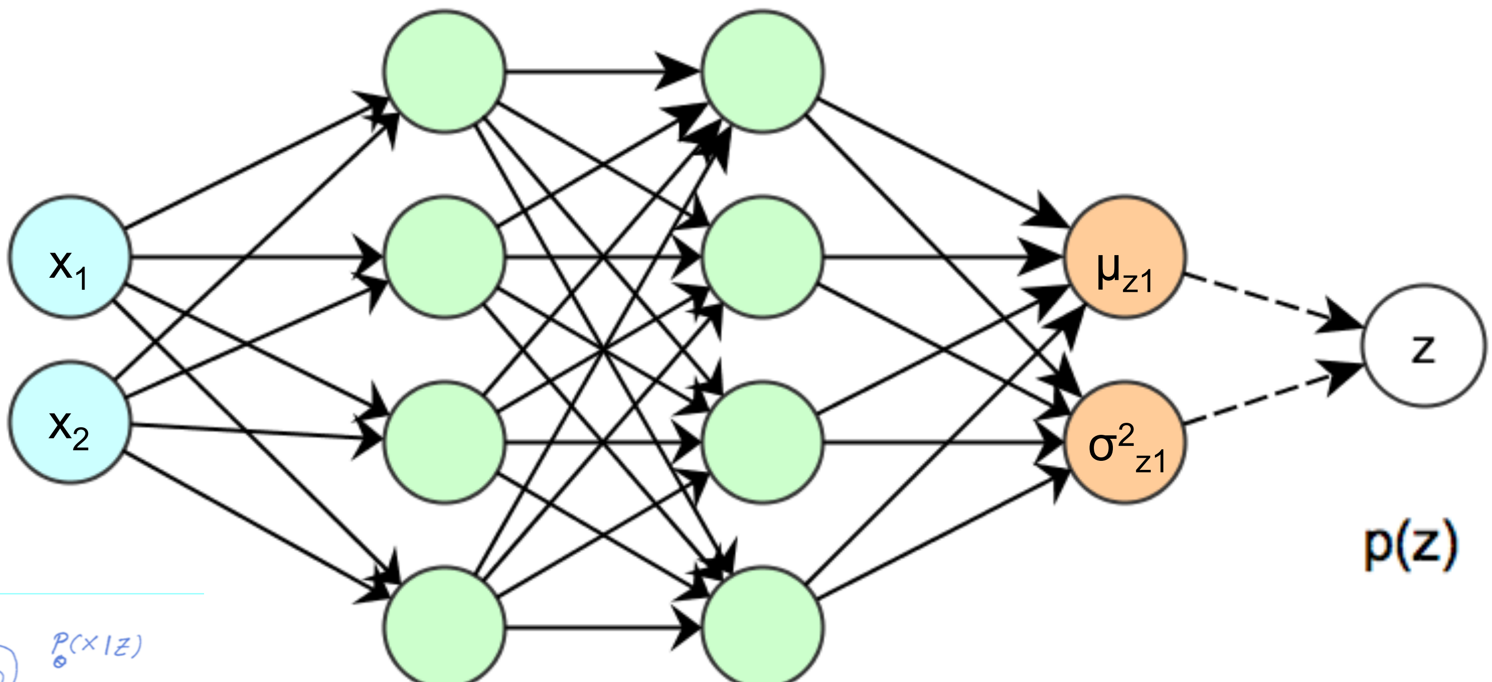
Solution:
- MCMC (too costly)
- Approximate p(z|x) with q(z|x)

The model for the encoder network



- A feed forward NN + Gaussian $\quad q_\phi(z \mid x) = \mathcal{N}(z; \mu_z(x), \sigma_z(x))$

Just a Gaussian, with diagonal covariance.



p(z)

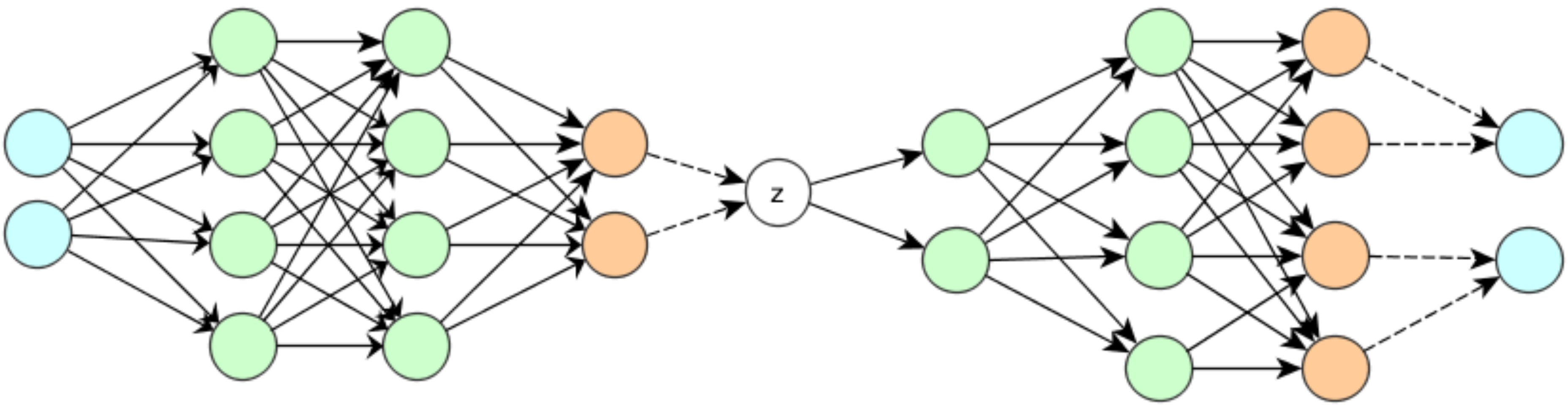
2D

$P_\theta(x|z) = \mathcal{N}(x; \mu(z), \Sigma)$

$\Sigma_{ij} = \delta_{ij}\, \sigma_i^2(z)$

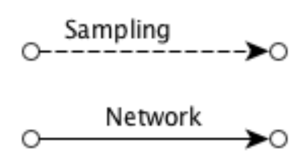
The complete auto-encoder

$q_{\varphi}(x|z)$ $p_{\theta}(x|z)$



Learning the parameters φ and θ via backpropagation

Determining the loss function



Training: Loss Function

- What is (one of the) most beautiful idea in statistics?

- Max-Likelihood, tune Φ, θ to maximize the likelihood

- We maximize the (log) likelihood of a given "image" $x^{(i)}$ of the training set. Later we sum over all training data (using minibatches)

Lower bound of likelihood (mathematical sleight of hand)

Likelihood, for an image $x^{(i)}$ from training set. Writing $x=x^{(i)}$ for short.

$$
\begin{aligned}
L &= \log(p(x)) \\
&= \sum_z q(z|x)\ \log(p(x)) && \text{multiplied with 1} \\
&= \sum_z q(z|x)\ \log\left(\frac{p(z,x)}{p(z|x)}\right) \\
&= \sum_z q(z|x)\ \log\left(\frac{p(z,x)}{q(z|x)}\frac{q(z|x)}{p(z|x)}\right) \\
&= \sum_z q(z|x)\ \log\left(\frac{p(z,x)}{q(z|x)}\right) + \sum_z q(z|x)\ \log\left(\frac{q(z|x)}{p(z|x)}\right) \\
&= L^v + D_{KL}\left(q(z|x) || p(z|x)\right) \\
&\geq L^v
\end{aligned}
$$

D_{KL} KL-Divergence >= 0 depends on how good q(z|x) can approximate p(z|x)

L^v *"lower variational bound of the (log) likelihood"* L^v =L for perfect approximation

Approximate Inference (rewriting L^v)

$$L^v = \sum_z q(z|x)\ \log\left(\frac{p(z,x)}{q(z|x)}\right) \qquad \text{with}\ \ p(z,x) = p(x|z)\,p(z)$$

$$= \sum_z q(z|x)\ \log\left(\frac{p(x|z)p(z)}{q(z|x)}\right)$$

$$= \sum_z q(z|x)\ \log\left(\frac{p(z)}{q(z|x)}\right) + \sum_z q(z|x)\ \log\left(p(x|z)\right)$$

$$= -D_{\mathrm{KL}}\left(q(z|x)||p(z)\right) + \mathbb{E}_{q(z|x)}\left(\log\left(p(x|z)\right)\right) \qquad \text{putting in } x^{(i)} \text{ for } x$$

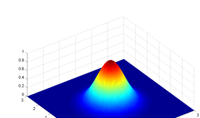
$$= -D_{\mathrm{KL}}\left(q(z|x^{(i)})||p(z)\right) + \mathbb{E}_{q(z|x^{(i)})}\left(\log\left(p(x^{(i)}|z)\right)\right)$$

Regularisation
p(z) is usually a simple prior N(0,1)

Reconstruction quality, log(1) if $x^{(i)}$ gets always reconstructed perfectly (z produces $x^{(i)}$)

Example $x^{(i)}$

$$\xrightarrow{q_\phi(z|x^{(i)})}\ z\ \xrightarrow{p_\theta(x^{(i)}|z)}$$

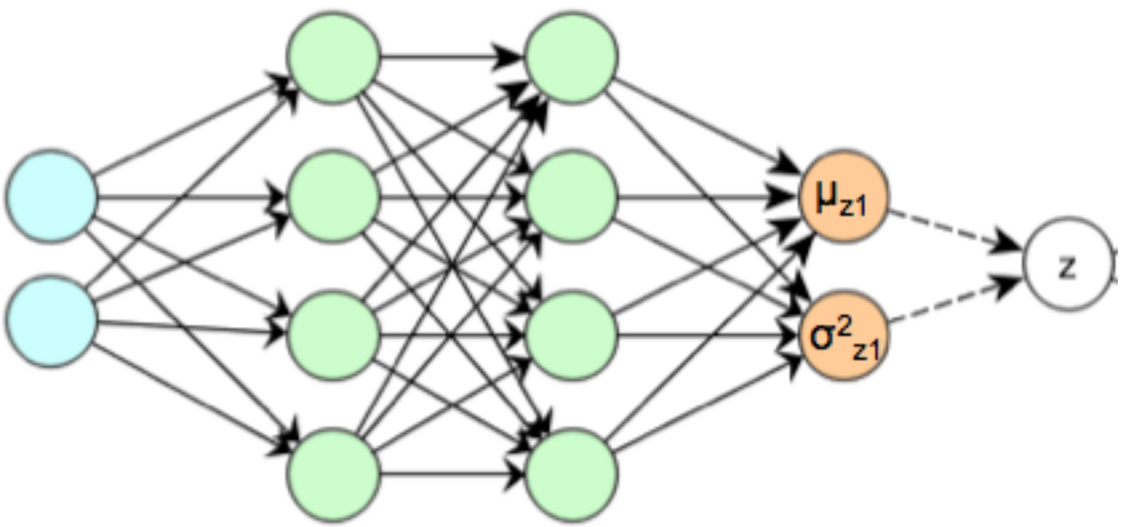


Calculation the regularization $-D_{KL}\left(q(z|x^{(i)})||p(z)\right)$

Use N(0,1) as prior for p(z)

$q(z|x^{(i)})$ is Gaussian with parameters $(\mu^{(i)},\sigma^{(i)})$ determined by NN

$$-D_{KL}\left(q(z|x^{(i)})||p(z)\right) = \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log(\sigma_{z_j}^{(i)^2}) - \mu_{z_j}^{(i)^2} - \sigma_{z_j}^{(i)^2}\right)$$



Sampling to calculate $\mathbb{E}_{q(z|x^{(i)})}\left(\log\left(p(x^{(i)}|z)\right)\right)$

Approximating $\mathbb{E}_{q(z|x^{(i)})}$ with sampling form the distribution $q(z|x^{(i)})$

With $z^{(i,l)}$ $l = 1, 2, \ldots L$ sampled from $z^{(i,l)} \sim q(z|x^{(i)})$

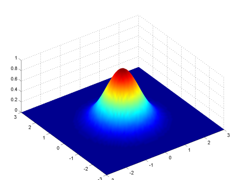
$$L^{v} = -D_{\mathrm{KL}}\left(q(z|x^{(i)})||p(z)\right) + \mathbb{E}_{q(z|x^{(i)})}\left(\log\left(p(x^{(i)}|z)\right)\right)$$

$$L^{v} \approx -D_{\mathrm{KL}}\left(q(z|x^{(i)})||p(z)\right) + \frac{1}{L}\sum_{i=1}^{L}\log\left(p(x^{(i)}|z^{(i,l)})\right)$$

Example $x^{(i)}$

$q_\phi(z|x^{(i)})$

z



$\log(p_\theta(x^{(i)}|z^{(i,1)}))$ where $z^{(i,1)} \sim N(\mu_Z{}^{(i)}, \sigma_Z{}^{2(i)})$

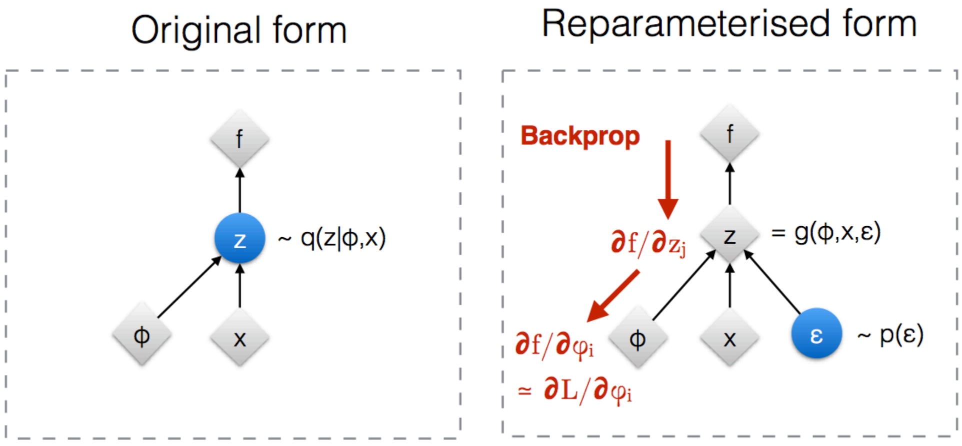
...

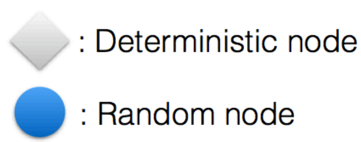
$\log(p_\theta(x^{(i)}|z^{(i,L)}))$ where $z^{(i,L)} \sim N(\mu_Z{}^{(i)}, \sigma_Z{}^{2(i)})$

L is often very small (often just L=1)

One last trick

Backpropagation not possible through random sampling!





[Kingma, 2013]
[Bengio, 2013]
[Kingma and Welling 2014]
[Rezende et al 2014]

Sampling (reparametrization trick)

Cannot back propagate through a random drawn number

$$z^{(i,l)} \sim N(\mu^{(i)}, \sigma^{2(i)})$$

$$z^{(i,l)} = \mu^{(i)} + \sigma^{(i)} \odot \varepsilon_i \quad \varepsilon_i \sim N(0,1)$$

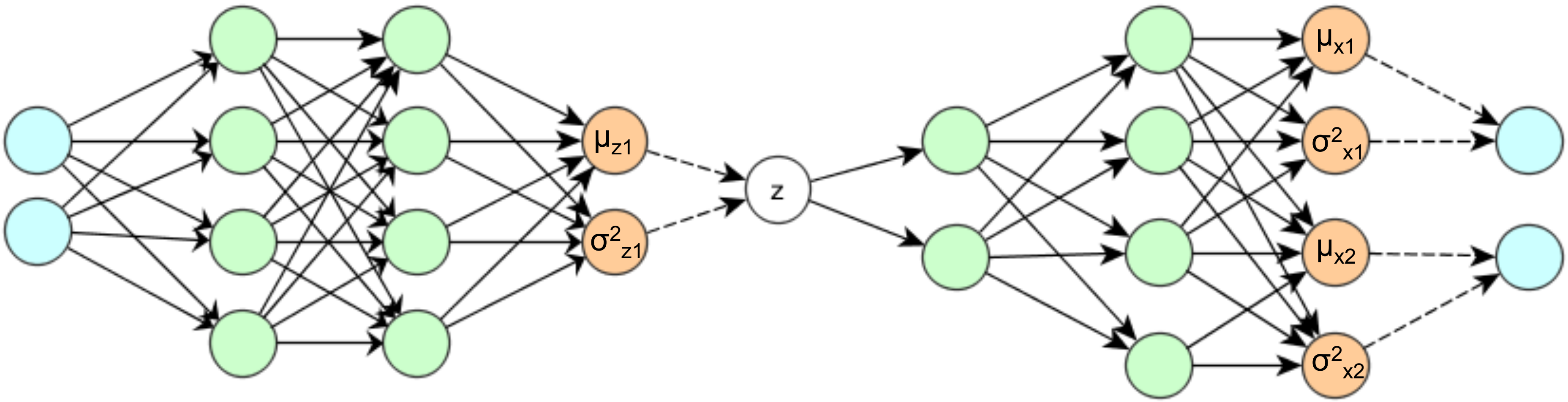
z has the same distribution, but now one can back propagate.

Writing z in this form, results in a deterministic part and noise.

Image from: NIPS Workshop 2015 (Kingma & Welling)

Putting it all together

Prior p(z) ~ N(0,1) and p, q Gaussian, extension to dim(z) > 1 trivial



Cost: Regularisation

$$-D_{KL}\left(q(z|x^{(i)})\|p(z)\right) = \frac{1}{2}\sum_{j=1}^{J}\left(1+\log(\sigma_{z_j}^{(i)^2}) - \mu_{z_j}^{(i)^2} - \sigma_{z_j}^{(i)^2}\right)$$

Cost: Reproduction

$$-\log\left(p(x^{(i)}|z^{(i)})\right) = \sum_{j=1}^{D}\frac{1}{2}\log(\sigma_{x_j}^2) + \frac{(x_j^{(i)}-\mu_{x_j})^2}{2\sigma_{x_j}^2}$$

We use mini batch gradient decent to optimize the cost function over all $x^{(i)}$ in the mini batch

Least Square for constant variance

Use the source Luke

Simple example 2-D distribution

https://github.com/oduerr/dl_tutorial/blob/master/tensorflow/vae/vae_demo-2D.ipynb

Simple MNIST Example

https://github.com/oduerr/dl_tutorial/blob/master/tensorflow/vae/vae_demo.ipynb

Recent developments of VAE

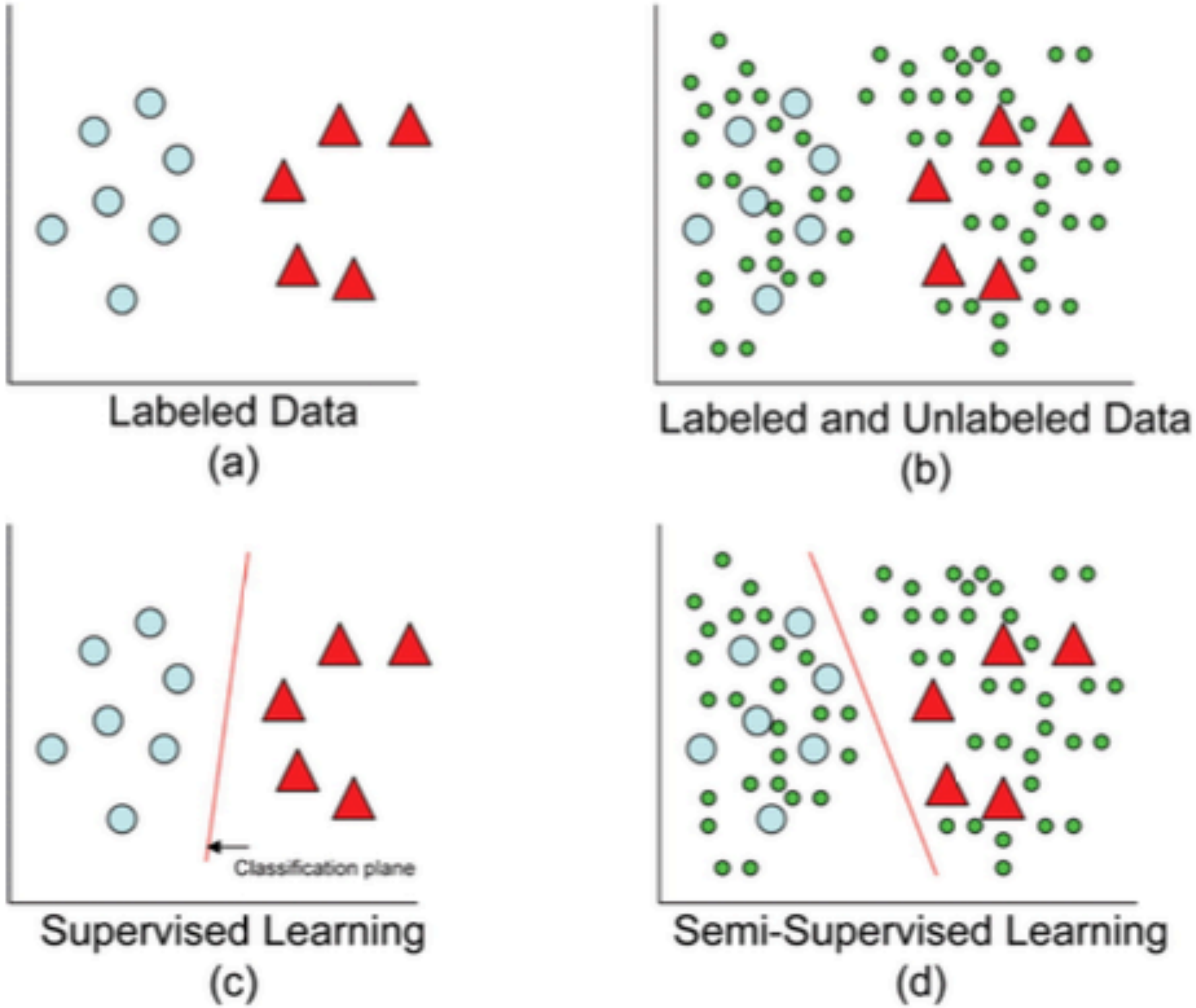
Recent developments in VAE / generative models (subjective overview)

- Authors of VAE Amsterdam University and Google DeepMind teamed up and wrote a paper on semi-supervised learning:
  - Diederik P Kingma, Shakir Mohamed, Danilo Jimenez Rezende, Max Welling. "Semi-supervised learning with deep generative models" (2014)

- Karl Gregor et al. extended the (binary autoencoder) with attention
  - *DRAW: A Recurrent Neural Network For Image Generation* *https://arxiv.org/abs/1502.04623 (2015)*
  - https://www.youtube.com/watch?v=Zt-7MI9eKEo

- Adversial networks as a non-statistical way to generate high dimensional data
  - Play a game:
    - Fist network invents some data ➔P(X) to fool second network
    - Second network tells if first network is a liar.

Semisupervised learning



Slide: Kingma, Rezendem Nohamed, Welling

Semisupervised learning

VAEs are SOTA
on semi-supervised learning on MNIST

That's 10 per class!

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

"Improving Semi-Supervised Learning with Auxiliary Deep Generative Models"

[Maaløe, Sønderby, Sønderby and Winter, 2015]

Thank you, questions?