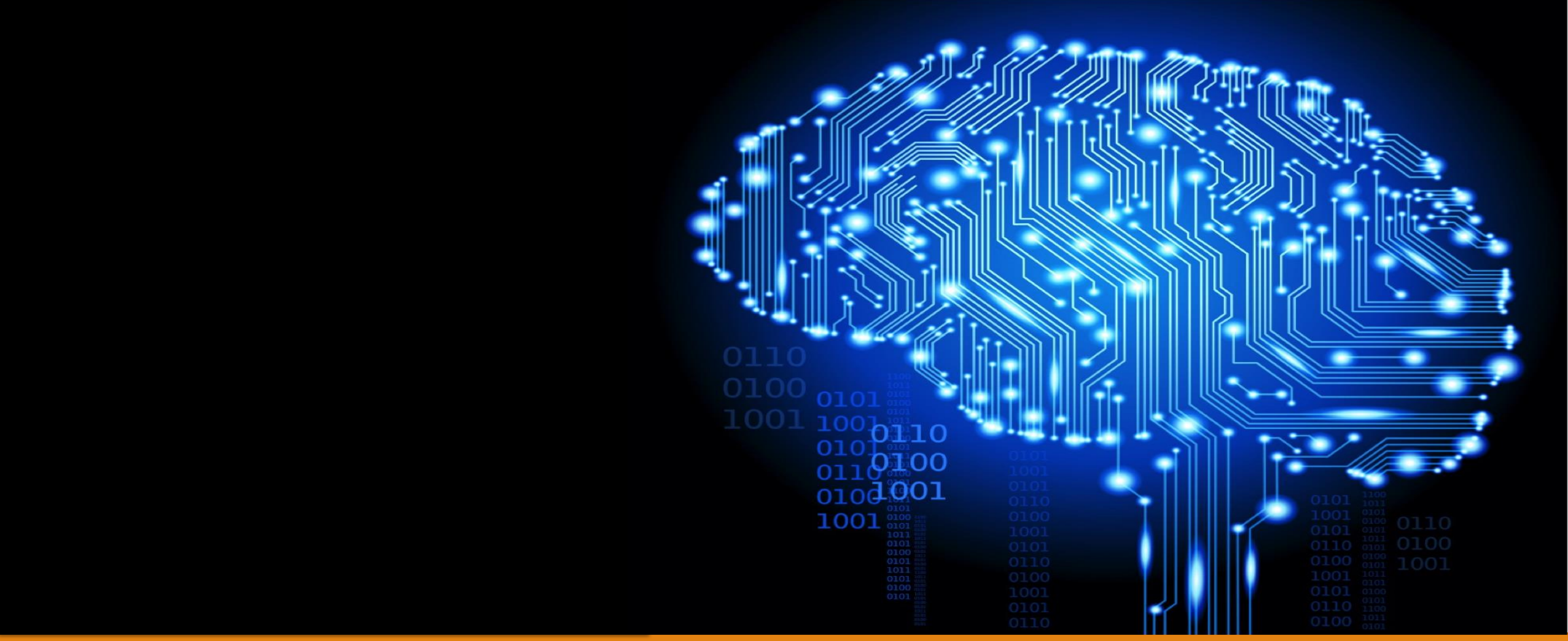


Lecture 8: Deep Generative Models

Efstratios Gavves

Lecture overview

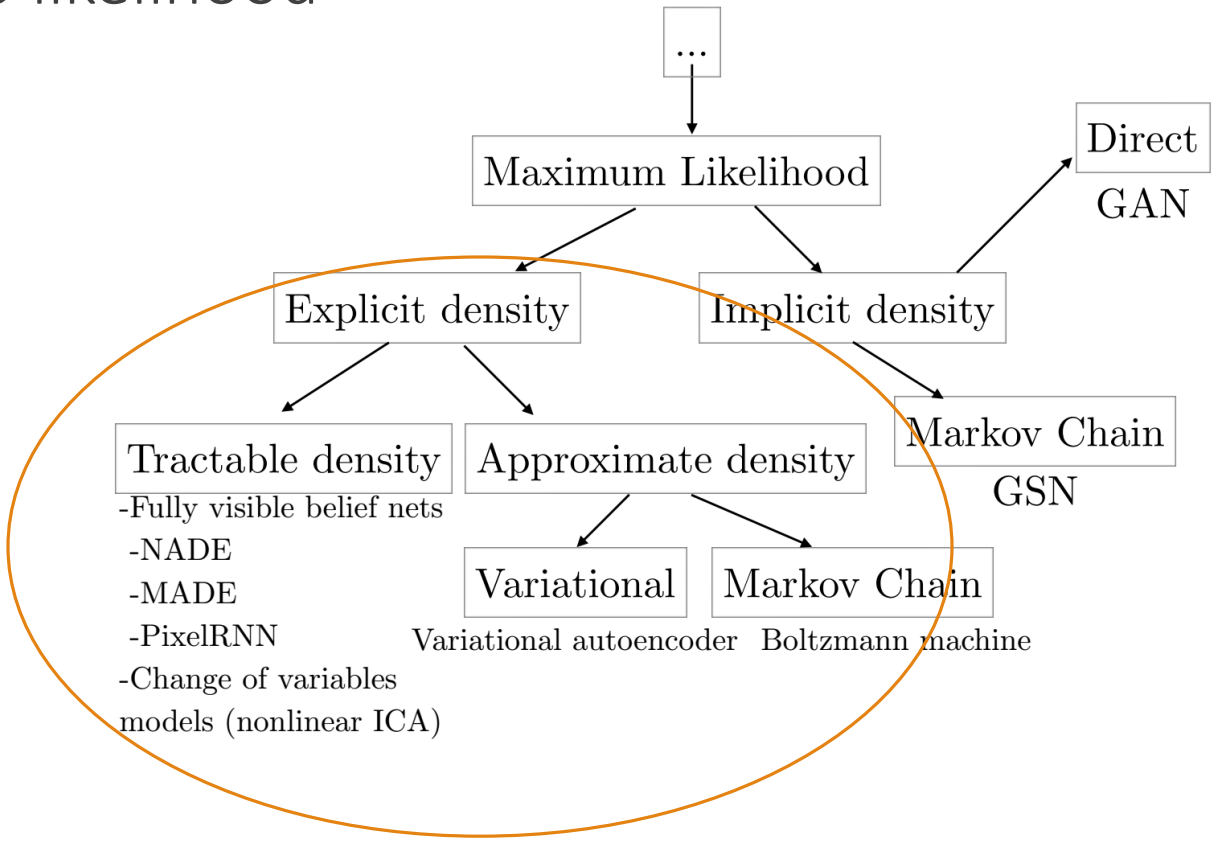
- Early Generative Models
- Restricted Boltzmann Machines
- Deep Boltzmann Machines
- Deep Belief Network
- Contrastive Divergence
- Gentle intro to Bayesian Modelling and Variational Inference
- Variational Autoencoders
- Normalizing Flows

Explicit density models

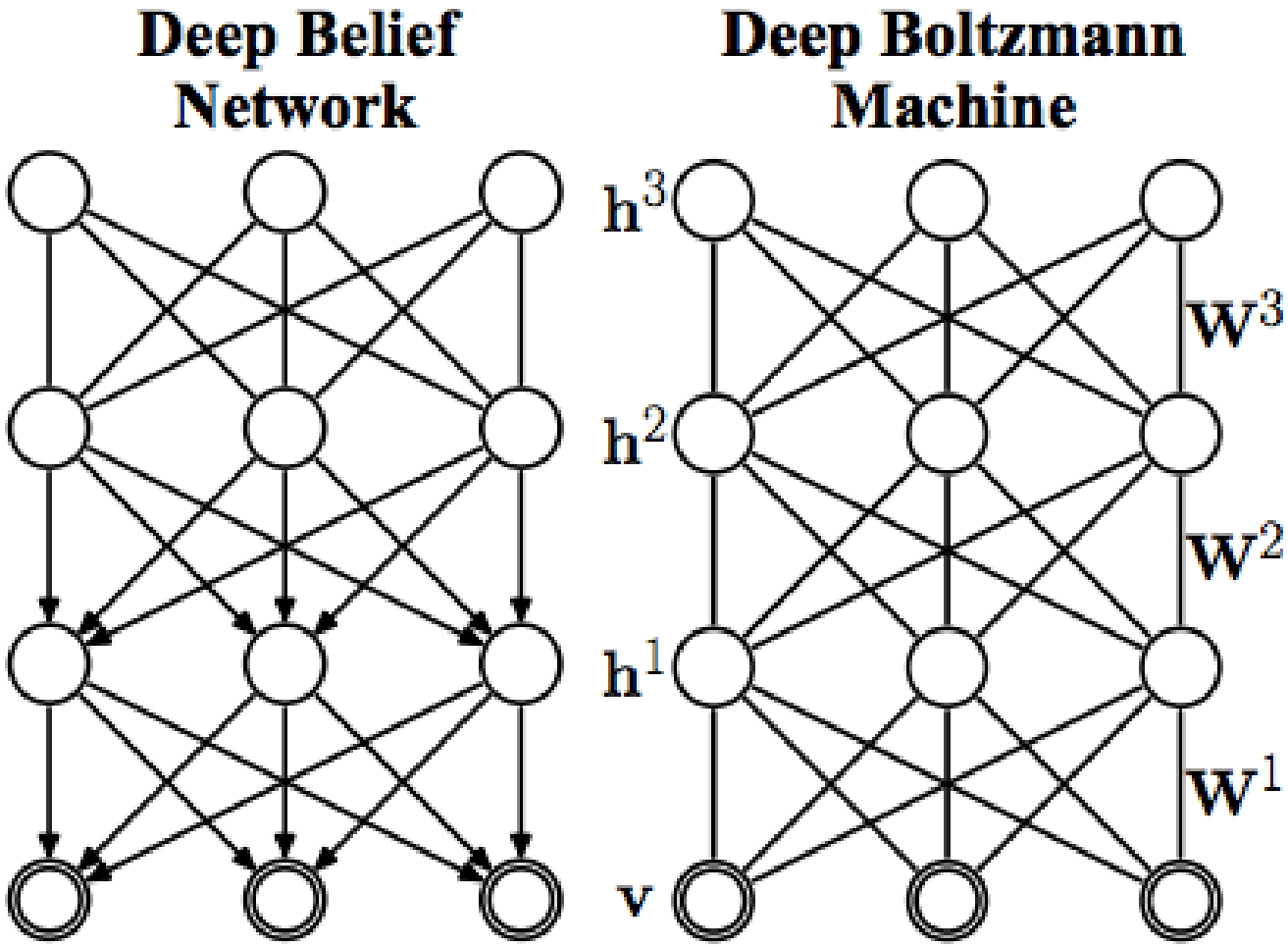
- Plug in the model density function to likelihood
- Then maximize the likelihood

Problems

- Design complex enough model that meets data complexity
- At the same time, make sure model is computationally tractable
- More details in the next lecture



Restricted Boltzmann Machines
Deep Boltzmann Machines
Deep Belief Nets



How to define a generative model?

- We can define an explicit density function over all possible relations ψ_c between the input variables x_c

$$p(x) = \prod_c \psi_c (x_c)$$

- Quite inefficient → think of all possible relations between $256 \times 256 = 65K$ input variables
  - Not just pairwise

- Solution: Define an energy function to model these relations

Boltzmann Distribution

- First, define an energy function $-E(x)$ that models the joint distribution

$$p(x) = \frac{1}{Z}\exp(-E(x))$$

- Z is a normalizing constant that makes sure $p(x)$ is a pdf: $\int p(x) = 1$

$$Z = \sum_{x} \exp(-E(x))$$

Why Boltzmann?

- Well understood in physics, mathematics and mechanics
- A Boltzmann distribution (also called Gibbs distribution) is a probability distribution, probability measure, or frequency distribution of particles in a system over various possible states
- The distribution is expressed in the form

$$F(state) \propto \exp(-\frac{E}{kT})$$

- E is the state energy, k is the Boltzmann constant, T is the thermodynamic temperature

https://en.wikipedia.org/wiki/Boltzmann_distribution

Problem with Boltzmann Distribution?

Problem with Boltzmann Distribution?

- Initially, thought of in the context of binary variables x
- Assuming binary variables x the normalizing constant has very high computational complexity
- For n-dimensional x we must enumerate all possible 2^n operations for Z
- Clearly, gets out of hand for any decent n
- Solution: Consider only pairwise relations

Boltzmann Machines

- The energy function becomes

$$E(x) = -x^T W x - b^T x$$

- x is considered binary

- $x^T W x$ captures correlations between input variables

- $b^T x$ captures the model prior
  - The energy that each of the input variable contributes itself

Problem with Boltzmann Machines?

Problem with Boltzmann Machines?

- Still too complex and high-dimensional
- If x has $256 \times 256 = 65536$ dimensions
- The pairwise relations need a huge W: 4.2 billion dimensions

- **Just for connecting two layers!**

- Solution: Consider latent variables for model correlations

Restricted Boltzmann Machines

- Restrict the model energy function further to a bottleneck over latents h

$$E(x) = -x^T W h - b^T x - c^T h$$

Restricted Boltzmann Machines

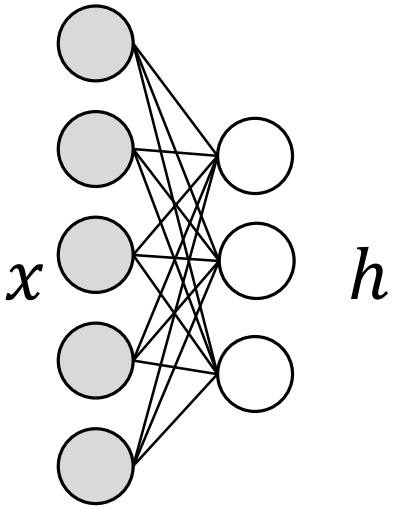
- $E(x) = -x^T W h - b^T x - c^T h$
- The $x^T W h$ models correlations between x and the latent activations via the parameter matrix W
- The $b^T x, c^T h$ model the priors
- Restricted Boltzmann Machines (RBM) assume $\mathbf{x}, h$ to be binary

Restricted Boltzmann Machines

- Energy function: $E(x) = -x^T W h - b^T x - c^T h$

$$p(x) = \frac{1}{Z} \sum_h \exp(-E(x,h))$$

  - Not in the form $\propto \exp(x)/Z$ because of the $\sum$



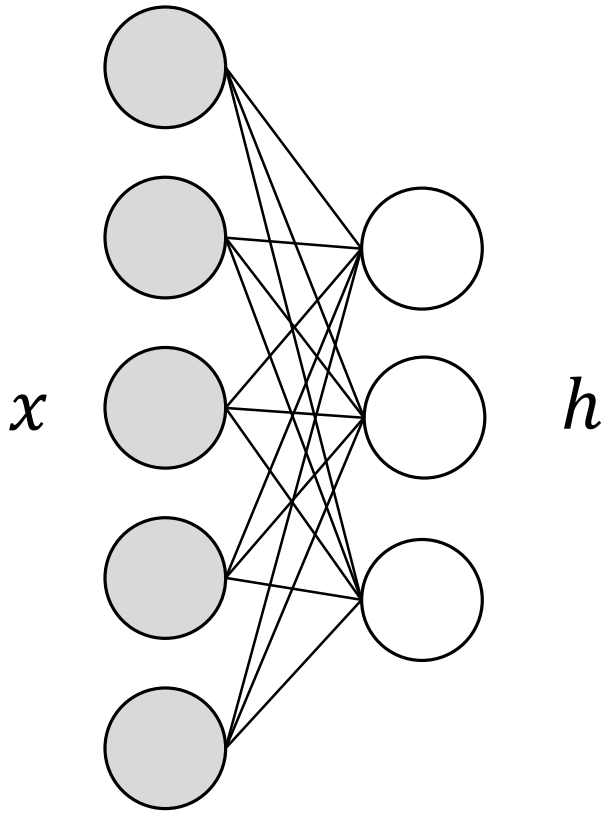
- Free energy function: $F(x) = -b^T x - \sum_i \log \sum_{h_i} \exp(h_i(c_i + W_i x))$

$$p(x) = \frac{1}{Z} \exp(-F(x))$$

$$Z = \sum_x \exp(-F(x))$$

Restricted Boltzmann Machines

- The $F(x)$ defines a bipartite graph with undirected connections
  - Information flows forward and backward



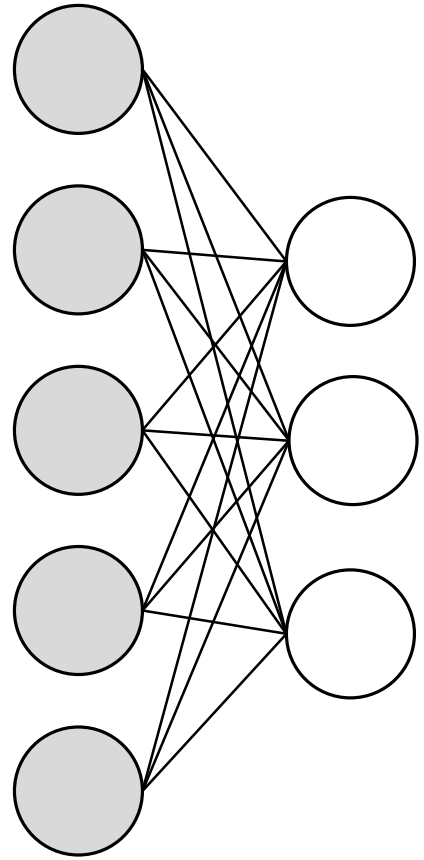
Restricted Boltzmann Machines

- The hidden units h_j are independent to each other conditioned on the visible units

$$p(h|x) = \prod_j p(h_j|x, \theta)$$

- The visible units x_i are independent to each other conditioned on the hidden units

$$p(x|h) = \prod_i p(x_i|h, \theta)$$



Training RBMs

- The conditional probabilities are defined as sigmoids

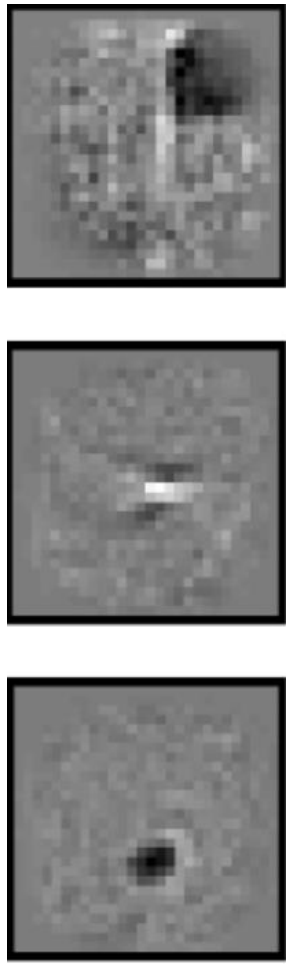
$$p(h_j|x,\theta) = \sigma(W_{.j}x + b_j)$$
$$p(x_i|h,\theta) = \sigma(W_{.i}x + c_i)$$

- Maximize log-likelihood

$$\mathcal{L}(\theta) = \frac{1}{\mathrm{N}}\sum_n \log p(x_n|\theta)$$

and

$$p(x) = \frac{1}{Z}\exp(-F(x))$$



Hidden unit (features)

Training RBMs

- Let's take the gradients

$$\frac{\partial \log p(x_n|\theta)}{\partial \theta} = -\frac{\partial F(x_n)}{\partial \theta} - \frac{\partial \log Z}{\partial \theta}$$
$$= -\sum_h p(h|x_n,\theta)\frac{\partial E(x_n|h,\theta)}{\partial \theta} + \sum_{\tilde{x},h} p(\tilde{x},h|\theta)\frac{\partial E(\tilde{x},h|\theta)}{\partial \theta}$$

Hidden unit (features)

Training RBMs

- Let's take the gradients

$$\frac{\partial \log p(x_n|\theta)}{\partial \theta} = -\frac{\partial F(x_n)}{\partial \theta} - \frac{\partial \log Z}{\partial \theta}$$

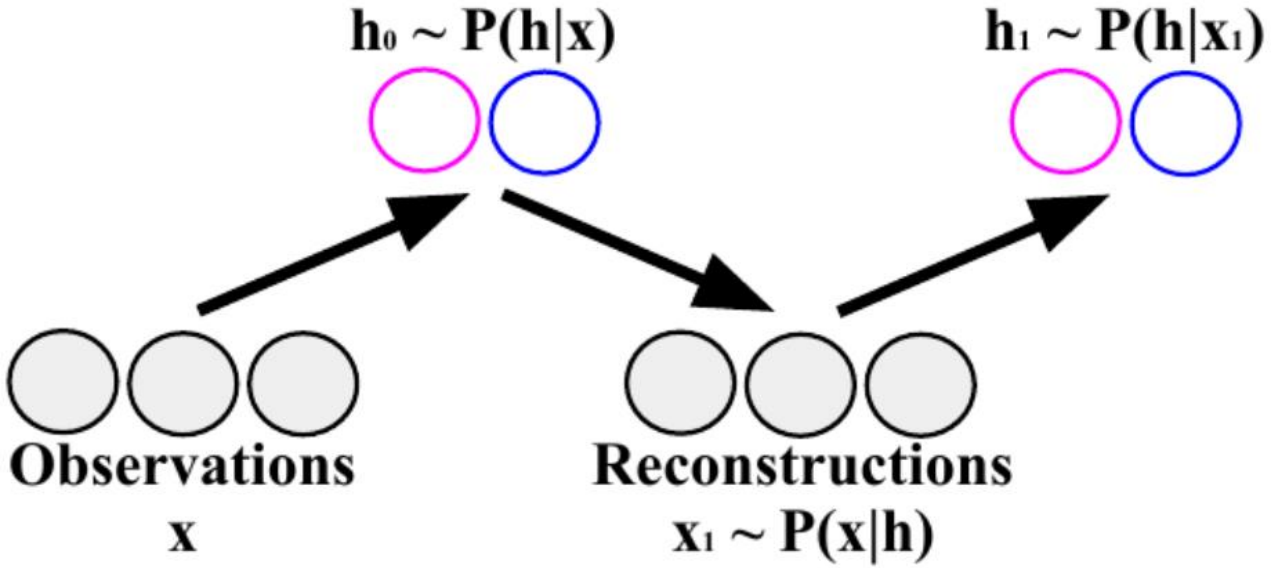
$$= -\sum_h p(h|x_n,\theta)\frac{\partial E(x_n|h,\theta)}{\partial \theta} + \sum_{\tilde{x},h} p(\tilde{x},h|\theta)\frac{\partial E(\tilde{x},h|\theta)}{\partial \theta}$$

- Easy because we just substitute in the definitions the x_n and sum over h
- Hard because you need to sum over both $\tilde{x}, h$ which can be huge
  - It requires approximate inference, *e.g.,* MCMC

Training RBMs with Contrastive Divergence

- Approximate the gradient with Contrastive Divergence
- Specifically, apply Gibbs sampler for k steps and approximate the gradient

$$\frac{\partial \log p(x_n|\theta)}{\partial \theta} = -\frac{\partial E(x_n, h_0|\theta)}{\partial \theta} - \frac{\partial E(x_k, h_k|\theta)}{\partial \theta}$$



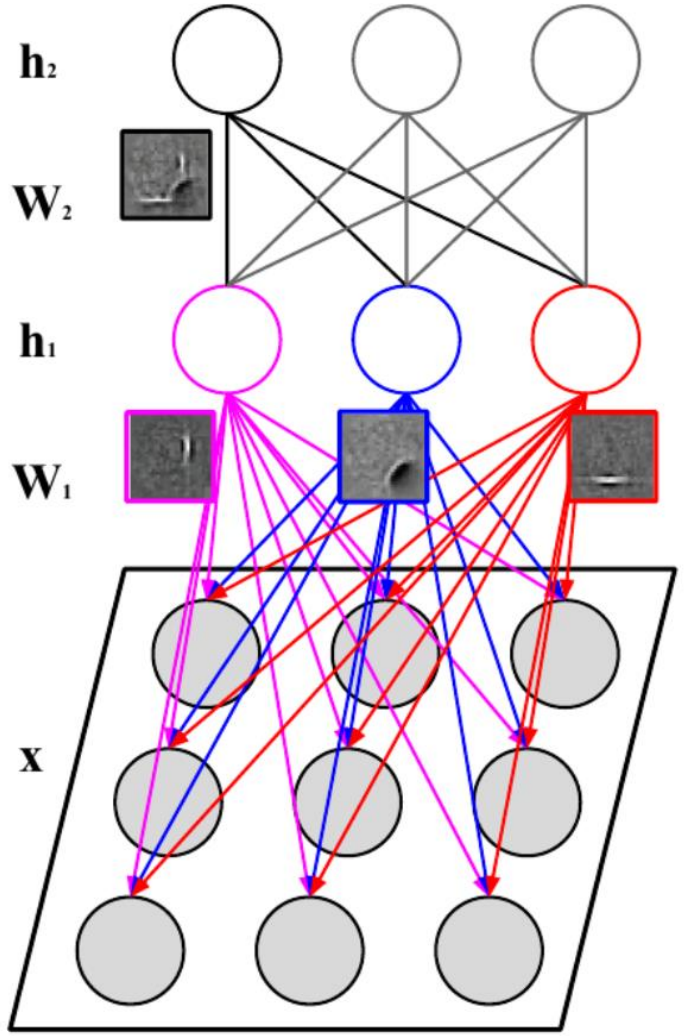
Hinton, *Training Products of Experts by Minimizing Contrastive Divergence*, Neural Computation, 2002

Deep Belief Network

- RBMs are just one layer
- Use RBM as a building block
- Stack multiple RBMs one on top of the other

$$p(x, h_1, h_2) = p(x|h_1) \cdot p(h_1|h_2)$$

- Deep Belief Networks (DBN) are directed models
  - The layers are densely connected and have a single forward flow
  - This is because the RBM is directional, $p(x_i|h, \theta) = \sigma(W_{.i}x + c_i)$, namely the input argument has only variable only from below

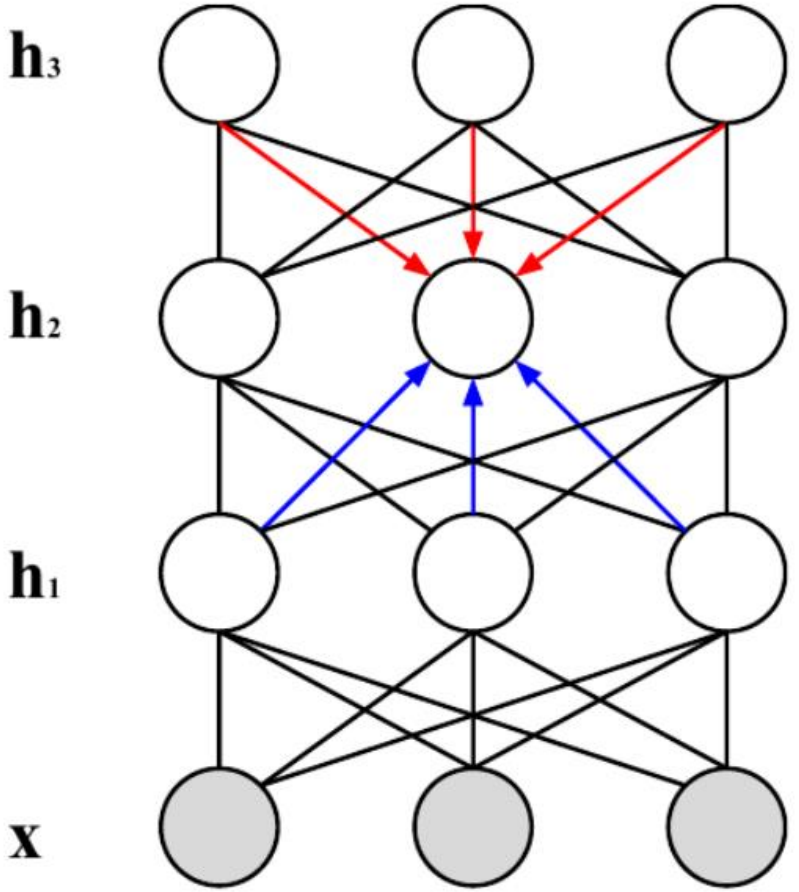


Deep Boltzmann Machines

- Stacking layers again, but now with connection from the above and from the below layers
- Since it's a Boltzmann machine, we need an energy function

$$E(x, h_1, h_2|\theta) = x^T W_1 h_1 + h_1^T W_2 h_2 + h_2^T W_3 h_3$$

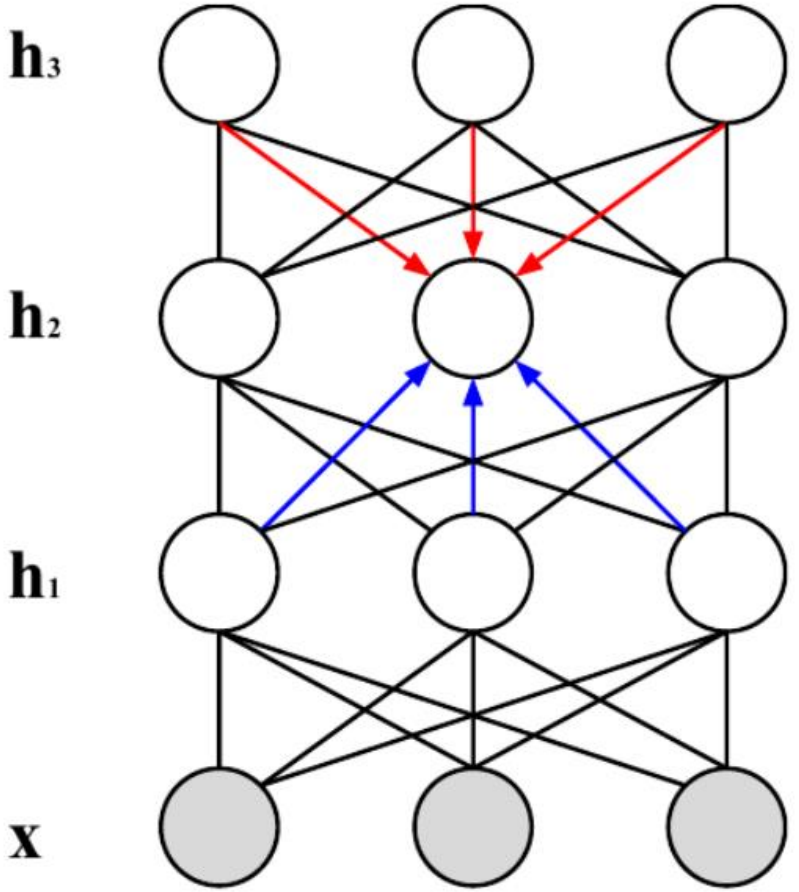
$$p\left(h_2^k \middle| h_1, h_3\right) = \sigma\left(\sum_j W_1^{jk} h_1^j + \sum_l W_3^{kl} h_3^k\right)$$



Deep Boltzmann Machines

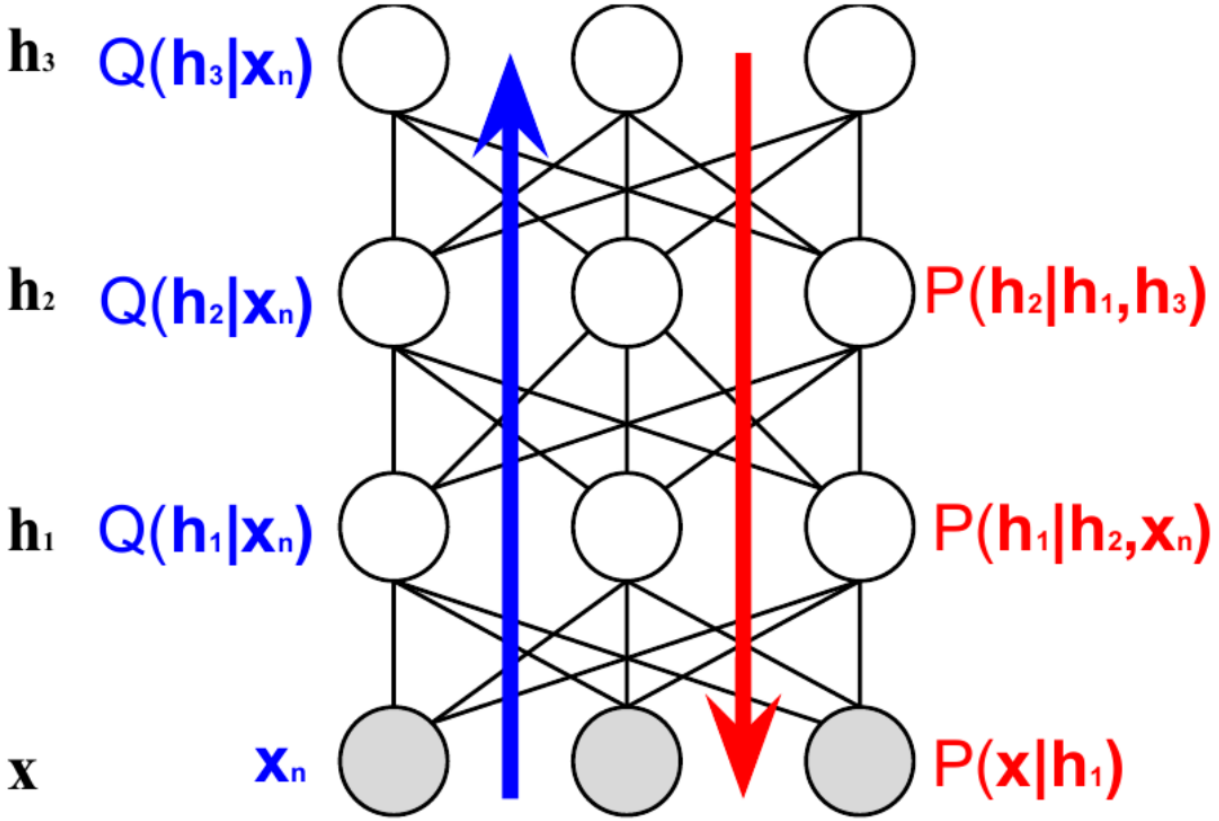
- Schematically similar to Deep Belief Networks
- But, Deep Boltzmann Machines (DBM) are undirected models
  - Belong to the Markov Random Field family
- So, two types of relationships: bottom-up and up-bottom

$$p\left(h_2^k \middle| h_1, h_3\right) = \sigma\left(\sum_j W_1^{jk} h_1^j + \sum_l W_3^{kl} h_3^k\right)$$

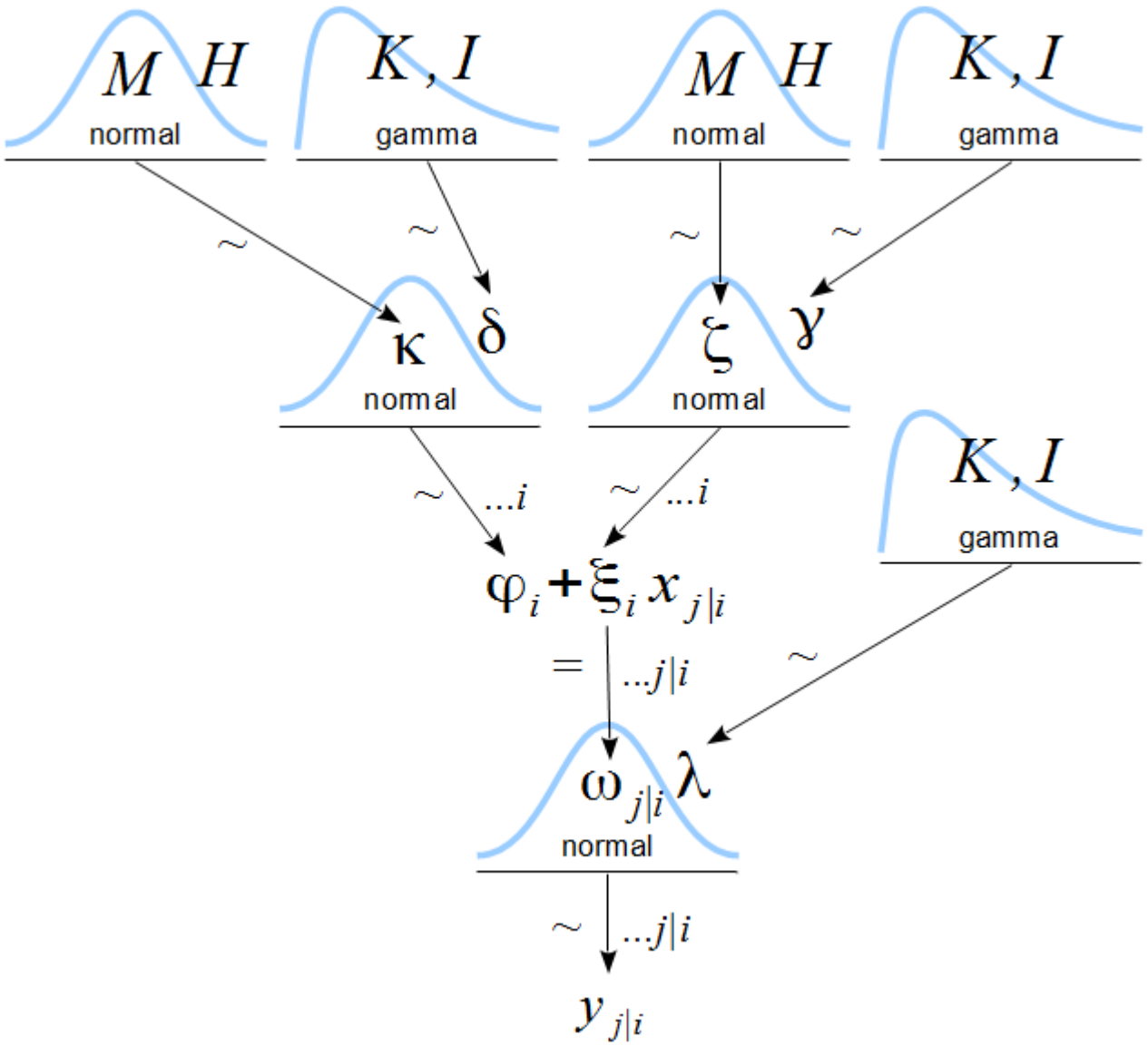


Training Deep Boltzmann Machines

- Computing gradients is intractable
- Instead, variational methods (mean-field) or sampling methods are used



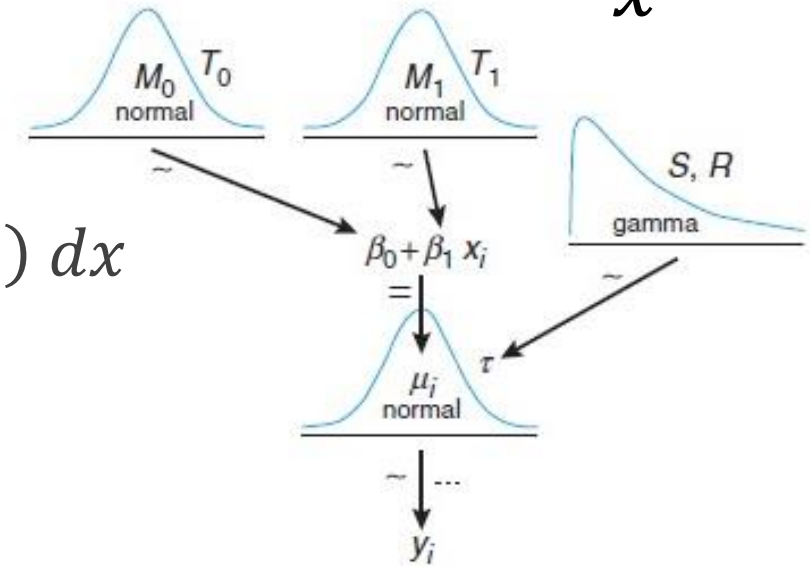
Variational Inference



Some (probabilistic) terminology

- Observed variables x
- Latent variables θ
  - Both unobservable model parameters w and unobservable model activations z
  - $\theta = \{w, z\}$
- Joint probability density function (pdf): $p(x, \theta)$
- Marginal pdf: $p(x) = \int_\theta p(x, \theta)\, d\theta$
- Prior pdf → marginal over input: $p(\theta) = \int_x p(x, \theta)\, dx$
  - Usually a user defined pdf
- Posterior pdf: $p(\theta|x)$
- Likelihood pdf: $p(x|\theta)$

x



Bayesian Terminology

- Posterior pdf

$$p(\theta|x) = \leftarrow \text{Conditional probability}$$

$$= \frac{p(x,\theta)}{p(x)} \leftarrow \text{Bayes Rule}$$

$$= \frac{p(x|\theta)\,p(\theta)}{p(x)} \leftarrow \text{Marginal probability}$$

$$= \frac{p(x|\theta)\,p(\theta)}{\int_{\theta'} p(x,\theta')\;d\theta'} \leftarrow p(x) \text{ is constant}$$

$$\propto p(x|\theta)\,p(\theta)$$

- Posterior Predictive pdf

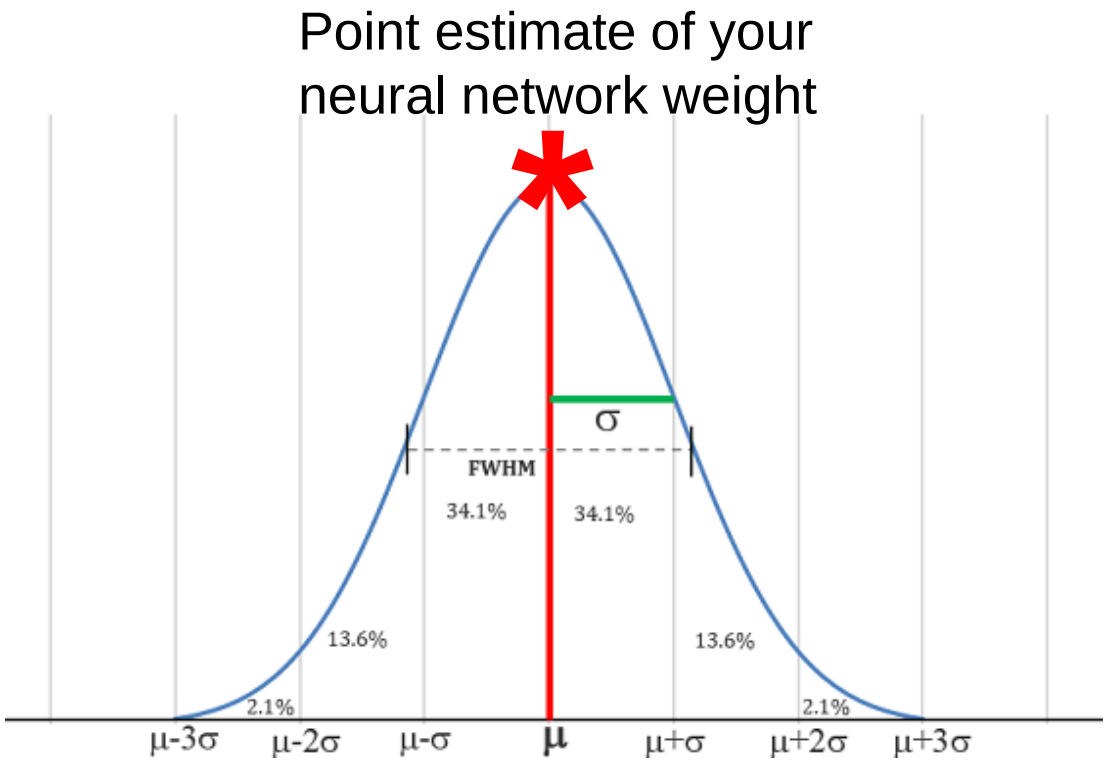
$$p(y_{new}|y) = \int_{\theta} p(y_{new}|\theta)\,p(\theta|y)\,d\theta$$

Bayesian Terminology

- Conjugate priors
  - when posterior and prior belong to the same family, so the joint pdf is easy to compute
- Point estimate approximations of latent variables
  - instead of computing a distribution over all possible values for the variable
  - compute one point only
  - e.g. the most likely (maximum likelihood or max a posteriori estimate)

$$\theta^* = \arg_\theta \max p(x|\theta)p(\theta) \quad (MAP)$$
$$\theta^* = \arg_\theta \max p(x|\theta) \quad (MLE)$$

  - Quite good when the posterior distribution is peaky (low variance)



Bayesian Modelling

- Estimate the posterior density $p(\theta|x)$ for your training data x
- To do so, need to define the prior $p(\theta)$ and likelihood $p(x|\theta)$ distributions
- Once the $p(\theta|x)$ density is estimated, Bayesian Inference is possible
  - $p(\theta|x)$ is a (density) function, not just a single number (point estimate)

- But how to estimate the posterior density?
  - Markov Chain Monte Carlo (MCMC) → Simulation-like estimation
  - Variational Inference → Turn estimation to optimization

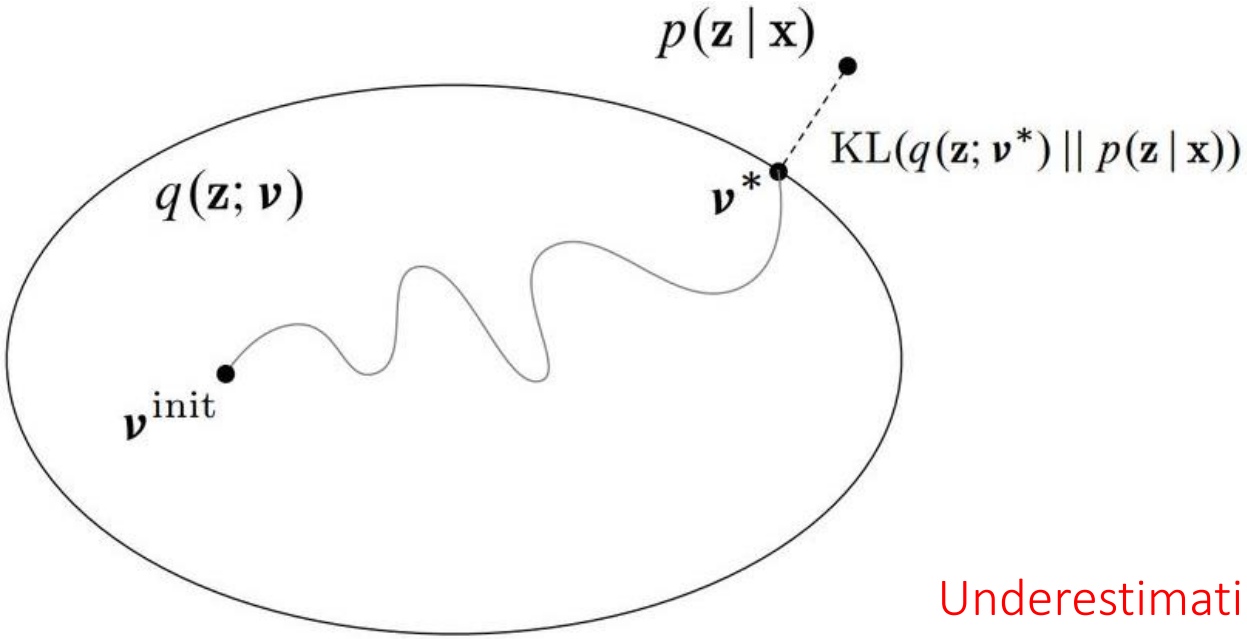
Variational Inference

- Estimating the true posterior $p(\theta|x)$is not always possible
  - especially for complicated models like neural networks
- Variational Inference assumes another function $q(\theta|\varphi)$ with which we want to approximate the true posterior $p(\theta|x)$
  - $q(\theta|\varphi)$ is the approximate posterior
  - Note that the approximate posterior does not depend on the observable variables x
- We approximate by minimizing the **reverse** KL-divergence w.r.t. φ

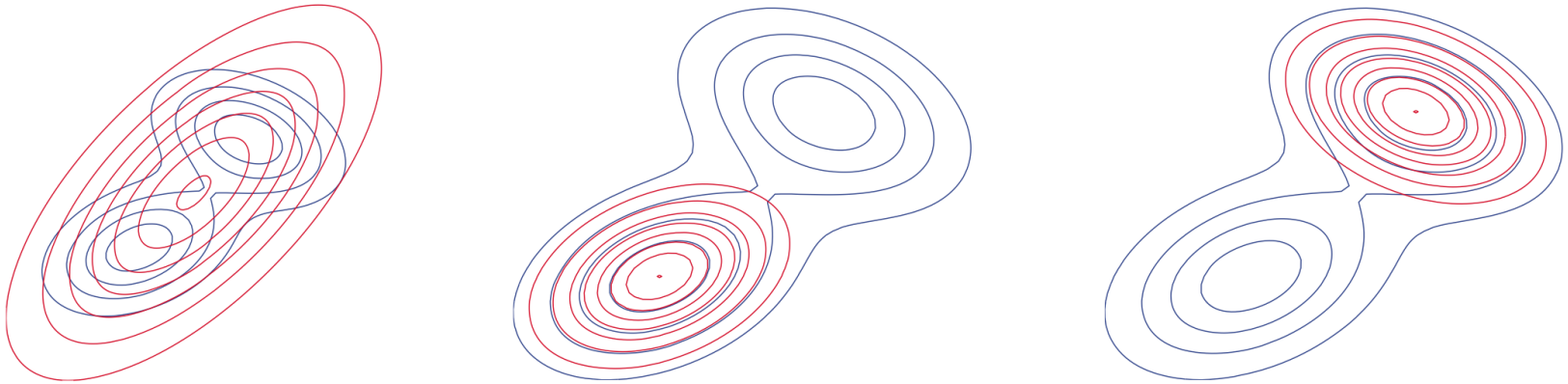
$$\varphi^* = \arg\min_{\varphi} KL(q(\theta|\varphi)||p(\theta|x))$$

- Turn inference into optimization

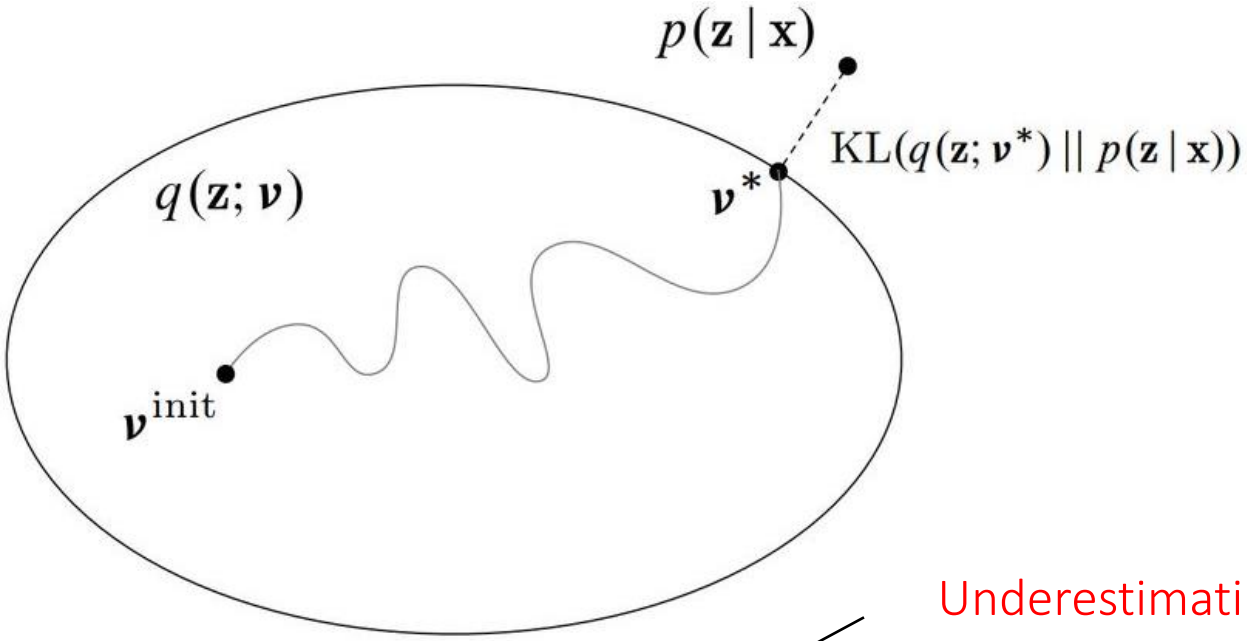
Variational Inference (graphically)



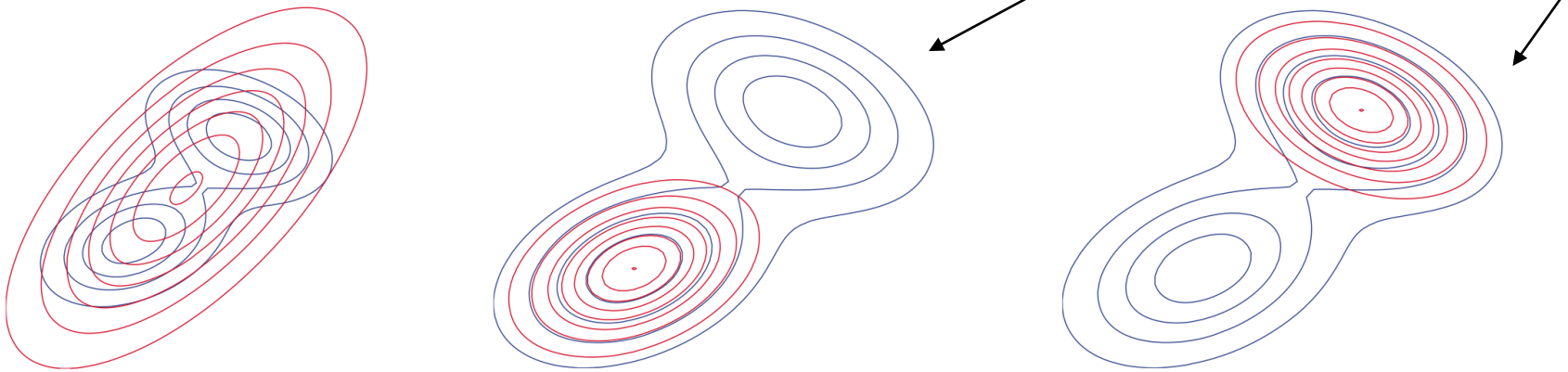
Underestimating variance. Why?



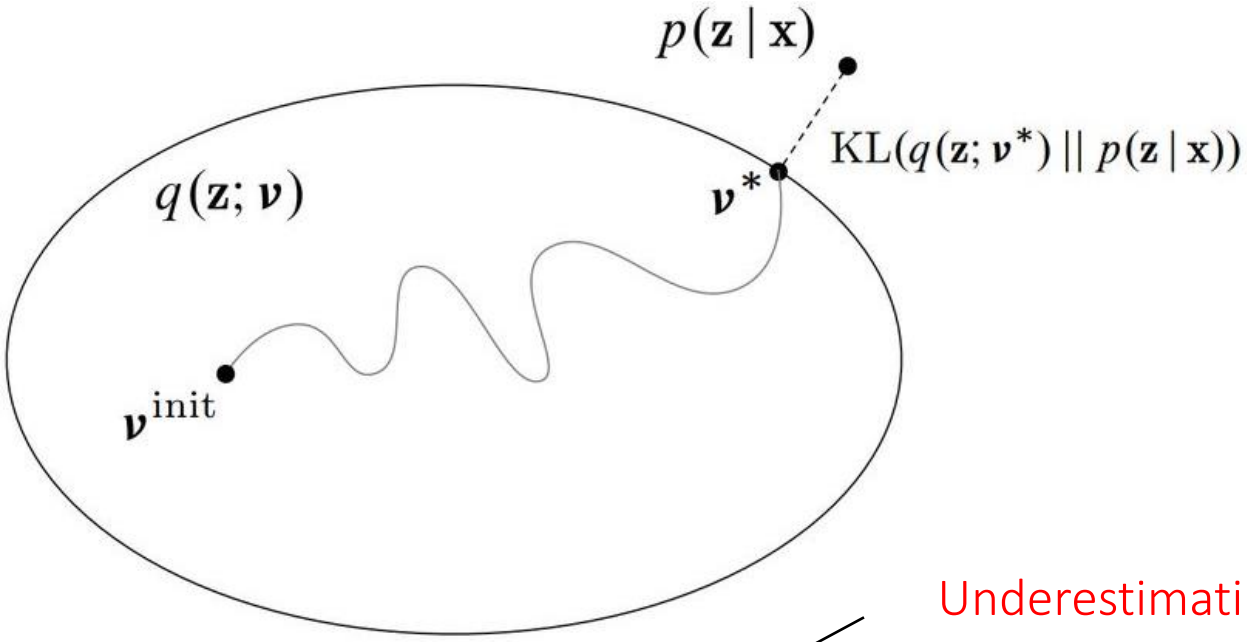
Variational Inference (graphically)



Underestimating variance. Why?

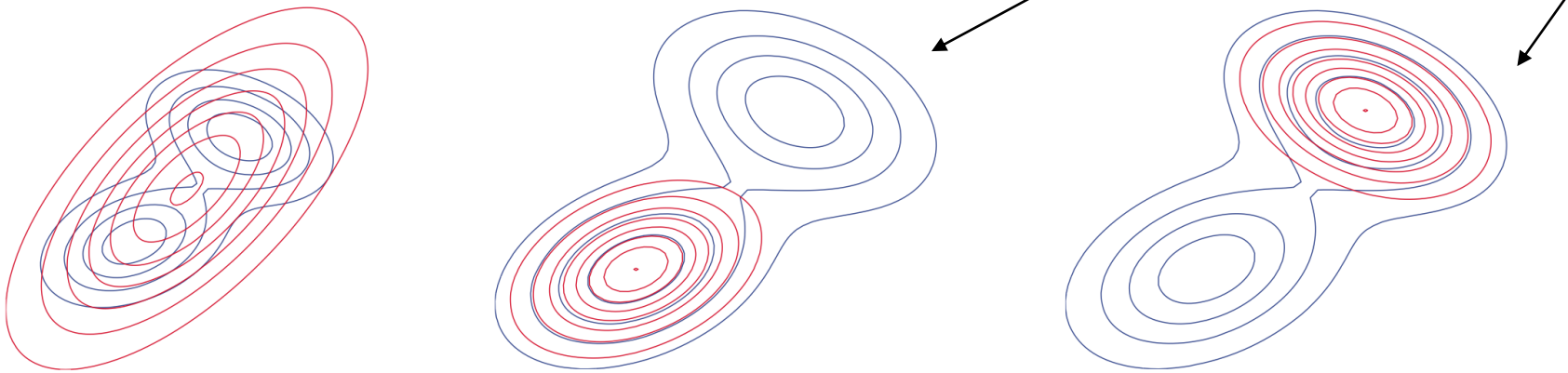


Variational Inference (graphically)

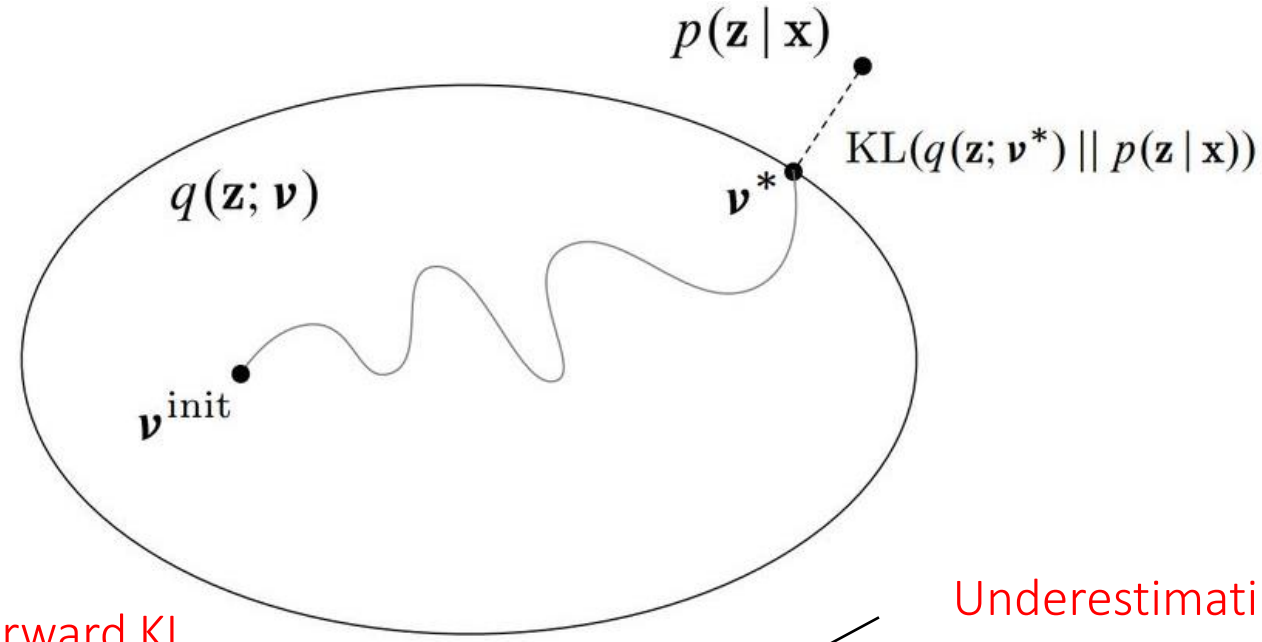


How to overestimate variance?

Underestimating variance. Why?

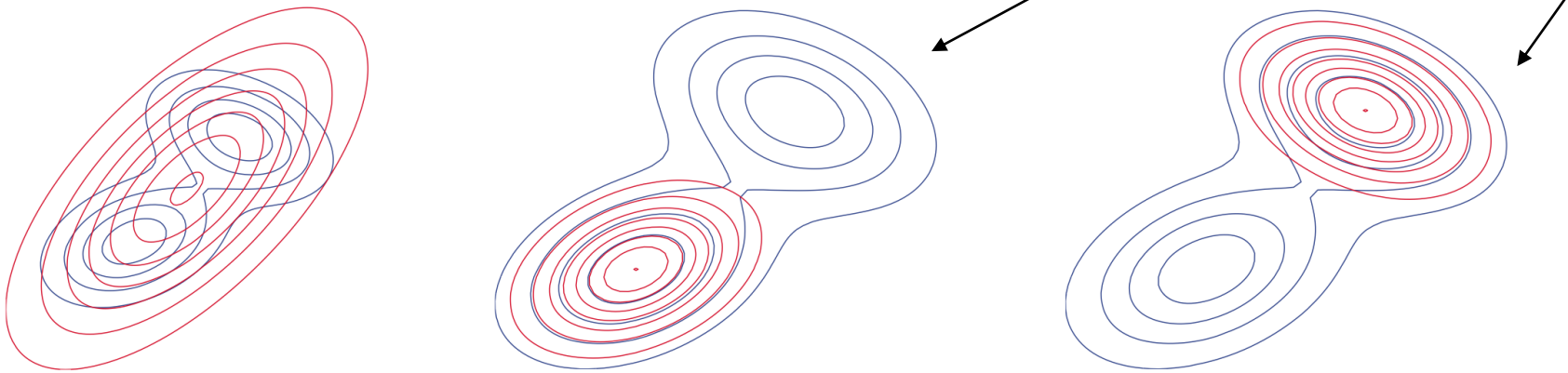


Variational Inference (graphically)



How to overestimate variance? Forward KL

Underestimating variance. Why?



Variational Inference - Evidence Lower Bound (ELBO)

- Given latent variables θ and the approximate posterior

$$q_\varphi(\theta) = q(\theta|\varphi)$$

- What about the log marginal $\log p(x)$?

Variational Inference - Evidence Lower Bound (ELBO)

- Given latent variables θ and the approximate posterior

$$q_\varphi(\theta) = q(\theta|\varphi)$$

- We want to maximize the marginal $p(x)$ (or the log marginal $\log p(x)$

$$\log p(x) \geq \mathbb{E}_{q_\varphi(\theta)}\left[\log \frac{p(x,\theta)}{q_\varphi(\theta)}\right]$$

Evidence Lower Bound (ELBO): Derivations

Evidence Lower Bound (ELBO): Derivations

- Given latent variables θ and the approximate posterior

$$q_\varphi(\theta) = q(\theta|\varphi)$$

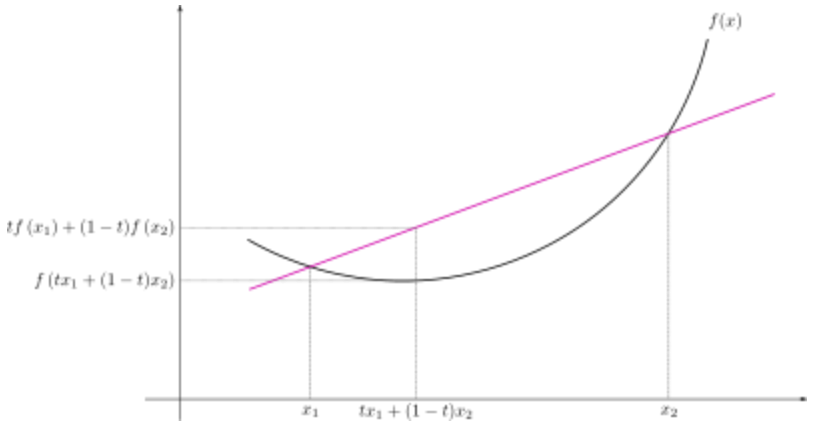
- The log marginal is

$$\log p(x) = \log \int_\theta p(x,\theta)\, d\theta$$

$$= \log \int_\theta p(x,\theta) \frac{q_\varphi(\theta)}{q_\varphi(\theta)}\, d\theta$$

$$= \log \mathbb{E}_{q_\varphi(\theta)} \left[\frac{p(x,\theta)}{q_\varphi(\theta)} \right]$$

$$\geq \mathbb{E}_{q_\varphi(\theta)} \left[\log \frac{p(x,\theta)}{q_\varphi(\theta)} \right]$$



Jensen Inequality

- $\varphi\big(\mathbb{E}([x])\big) \leq \mathbb{E}[\varphi(x)]$

for convex φ

- $\log$ is convave

ELBO: A second derivation

$$
\begin{aligned}
KL\left[q(Z)\|p(Z|X)\right] &= \int_Z q(Z)\log\frac{q(Z)}{p(Z|X)} \\
&= -\int_Z q(Z)\log\frac{p(Z|X)}{q(Z)} \\
&= -\left(\int_Z q(Z)\log\frac{p(X,Z)}{q(Z)} - \int_Z q(Z)\log p(X)\right) \\
&= -\int_Z q(Z)\log\frac{p(X,Z)}{q(Z)} + \log p(X)\int_Z q(Z) \\
&= -L + \log p(X)
\end{aligned}
$$

ELBO: Formulation 1

$$
\begin{aligned}
&\geq \mathbb{E}_{q_\varphi(\theta)}\left[\log \frac{p(x,\theta)}{q_\varphi(\theta)}\right] \\
&= \mathbb{E}_{q_\varphi(\theta)}[\log p(x|\theta)] + \mathbb{E}_{q_\varphi(\theta)}[\log p(\theta)] - \mathbb{E}_{q_\varphi(\theta)}[\log q_\varphi(\theta)] \\
&= \mathbb{E}_{q_\varphi(\theta)}[\log p(x|\theta)] - \mathrm{KL}(q_\varphi(\theta)||\mathrm{p}(\theta)) \\
&= \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})
\end{aligned}
$$

- Maximize reconstruction accuracy $\mathbb{E}_{q_\varphi(\theta)}[\log p(x|\theta)]$
- While minimizing the KL distance between the prior $\mathrm{p}(\theta)$ and the approximate posterior $q_\varphi(\theta)$

ELBO: Formulation 2

$$
\begin{aligned}
&\geq \mathbb{E}_{q_\varphi(\theta)}\left[\log \frac{p(x,\theta)}{q_\varphi(\theta)}\right] \\
&= \mathbb{E}_{q_\varphi(\theta)}[\log p(x,\theta)] - \mathbb{E}_{q_\varphi(\theta)}\left[\log q_\varphi(\theta)\right] \\
&= \mathbb{E}_{q_\varphi(\theta)}[\log p(x,\theta)] + \mathrm{H}(\theta) \\
&= \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})
\end{aligned}
$$

- Maximize something like negative Boltzmann energy $\mathbb{E}_{q_\varphi(\theta)}[\log p(x,\theta)]$
- While maximizing the entropy the approximate posterior $q_\varphi(\theta)$
  - Avoid collapsing latents θ to a single value (like for MAP estimates)

ELBO vs. Marginal

- It is easy to see that the ELBO is directly related to the marginal

$$\log p(x) = \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) + KL(q_{\varphi}(\theta)||p(\theta|x))$$

- You can also see $\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})$ as Variational Free Energy

ELBO vs. Marginal: Derivations

- It is easy to see that the ELBO is directly related to the marginal

$$\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) =$$

ELBO vs. Marginal: Derivations

- It is easy to see that the ELBO is directly related to the marginal

$$\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) =$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(x,\theta)] - \mathbb{E}_{q_\varphi(\theta)}[\log q_\varphi(\theta)]$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(\theta|x)] + \mathbb{E}_{q_\varphi(\theta)}[\log p(x)] - \mathbb{E}_{q_\varphi(\theta)}[\log q_\varphi(\theta)]$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(x)] - KL(q_\varphi(\theta)||p(\theta|x))$$
$$= \log p(x) - KL(q_\varphi(\theta)||p(\theta|x))$$
$$\Rightarrow$$
$$\log p(x) = \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) + KL(q_\varphi(\theta)||p(\theta|x))$$

$\log p(x)$ does not depend on $q_\varphi(\theta)$

$\mathbb{E}_{q_\varphi(\theta)}[1]=1$

- You can also see $\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})$ as Variational Free Energy

ELBO interpretations

- $\log p(x) = \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) + KL(q_\varphi(\theta)||p(\theta|x))$
- The log-likelihood $\log p(x)$ constant → does not depend on any parameter
- Also, $\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) > 0$ and $KL(q_\varphi(\theta)||p(\theta|x)) > 0$

1. The higher the Variational Lower Bound $\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})$, the smaller the difference between the approximate posterior $q_\varphi(\theta)$ and the true posterior $p(\theta|x)$ → better latent representation
2. The Variational Lower Bound $\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x})$ approaches the log-likelihood → better density model

Amortized Inference

- The variational distribution $q(\theta|\varphi)$ does not depend directly on data
  - Only indirectly, via minimizing its distance to the true posterior $KL(q(\theta|\varphi)||p(\theta|x))$
- So, with $q(\theta|\varphi)$ we have a major optimization problem
- The approximate posterior must approximate the whole dataset $x = [x_1, x_2, \dots, x_N]$ jointly
- Different neural network weights for each data point x_i

Amortized Inference

- Better share weights and “amortize” optimization between individual data points

$$q(\theta|\varphi) = q_{\varphi}(\theta|x)$$

- Predict model parameters θ using a φ-parameterized model of the input x
- Use amortization for data-dependent parameters that depend on data
  - E.g., the latent activations that are the output of a neural network layer: $\mathrm{z} \sim q_{\varphi}(z|x)$

Amortized Inference (Intuitively)

- The original view on Variational Inference is that $q(\theta|\varphi)$ describes the approximate posterior of the dataset as a whole
- Imagine you don't want to make a practical model that returns latent activations for a specific input
- Instead, you want to optimally approximate the true posterior of the unknown weights with an model with latent parameters
- It doesn't matter if these parameters are "latent activations" $\boldsymbol{z}$ or "model variables" $\boldsymbol{w}$

Variational Autoencoders

- Let's rewrite the ELBO a bit more explicitly

$$\text{ELBO}_{\theta,\varphi}(x) = \mathbb{E}_{q_\varphi(\theta)}[\log p(x|\theta)] - \text{KL}(q_\varphi(\theta)||\text{p}(\theta))$$
$$= \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x)||\text{p}_\lambda(\text{z}))$$

- $p_\theta(x|z)$ instead of $p(x|\theta)$

- I.e., the likelihood model $p_\theta(x|z)$ has weights parameterized by θ
- Conditioned on latent model activations parameterized by z

Variational Autoencoders

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$$= \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x)||\text{p}_\lambda(\text{z}))$$

- $\text{p}_\lambda(\text{z})$ instead of $\text{p}(\theta)$

- I.e., a λ-parameterized prior only on the latent activations z
- Not on model weights

Variational Autoencoders

- Let's rewrite the ELBO a bit more explicitly

$$\text{ELBO}_{\theta,\varphi}(x) = \mathbb{E}_{q_\varphi(\theta)}[\log p(x|\theta)] - \text{KL}(q_\varphi(\theta)||\text{p}(\theta))$$
$$= \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x)||\text{p}_\lambda(\text{z}))$$

- $q_\varphi(z|x)$ instead of $q(\theta|\varphi)$

- The model $q_\varphi(z|x)$ approximates the posterior density of the latents z
- The model weights are parameterized by φ

Variational Autoencoders

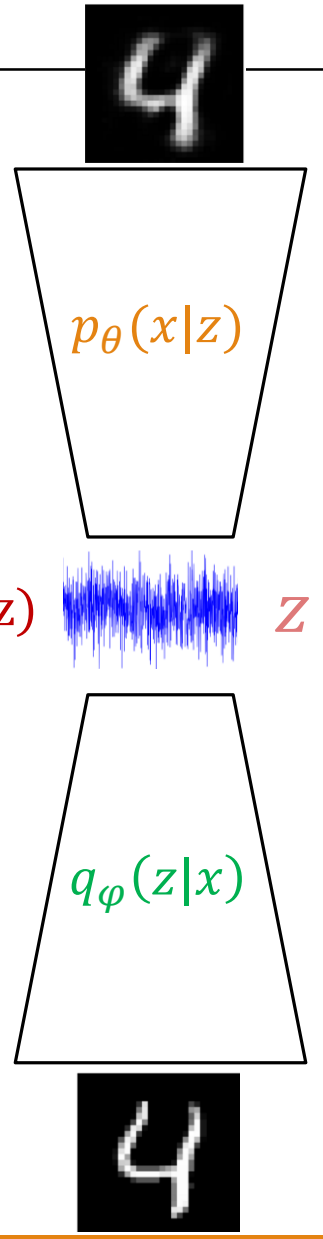
- $\text{ELBO}_{\theta,\varphi}(x) = \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x)||\text{p}_\lambda(\text{z}))$
- How to model $p_\theta(x|z)$ and $q_\varphi(z|x)$?

Variational Autoencoders

- $\text{ELBO}_{\theta,\varphi}(x) = \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x)||\text{p}_\lambda(\text{z}))$
- How to model $p_\theta(x|z)$ and $q_\varphi(z|x)$?
- What about modelling them as neural networks

Variational Autoencoders

- The approximate posterior $q_\varphi(z|x)$ is a CovnNet (or MLP)
  - Input x is an image
  - Given input the output is a feature map from a latent variable z
  - Also known as encoder or inference or recognition network, because it infers/recognizes the latent codes
- The likelihood density $p_\theta(x|z)$ is an inverted ConvNet (or MLP)
  - Given the latent z as input, it reconstructs the input $\tilde{x}$
  - Also known as decoder or generator network
- If we ignore the distribution of the latents z, $\mathrm{p}_\lambda(\mathrm{z})$, then we get the Vanilla Autoencoder



Training Variational Autoencoders

- Maximize the Evidence Lower Bound (ELBO)
  - Or minimize the negative ELBO

$$\mathcal{L}(\theta, \varphi) = \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \mathrm{KL}(q_\varphi(z|x)||\mathrm{p}_\lambda(\mathrm{z}))$$

- How to we optimize the ELBO?

Training Variational Autoencoders

- Maximize the Evidence Lower Bound (ELBO)
  - Or minimize the negative ELBO

$$\mathcal{L}(\theta, \varphi) = \mathbb{E}_{q_\varphi(Z|x)}[\log p_\theta(x|Z)] - \mathrm{KL}(q_\varphi(Z|x)||\mathrm{p}_\lambda(\mathrm{Z}))$$

$$= \int_z q_\varphi(z|x) \log p_\theta(x|z)\, dz - \int_z q_\varphi(z|x) \log \frac{q_\varphi(z|x)}{p_\lambda(z)} dz$$

- Forward propagation → compute the two terms
- The first term is an integral (expectation) that we cannot solve analytically. So, we need to sample from the pdf instead
  - When $p_\theta(x|z)$ contains even a few nonlinearities, like in a neural network, the integral is hard to compute analytically

Training Variational Autoencoders

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- So, we need to sample from the pdf instead
- VAE is a stochastic model
- The second term is the KL divergence between two distributions that we know

Training Variational Autoencoders

- $\int_z q_\varphi(z|x) \log p_\theta(x|z)\, dz$
- The first term is an integral (expectation) that we cannot solve analytically.
  - When $p_\theta(x|z)$ contains even a few nonlinearities, like in a neural network, the integral is hard to compute analytically
- As we cannot compute analytically, we sample from the pdf instead
  - Using the density $q_\varphi(z|x)$ to draw samples
  - Usually one sample is enough → stochasticity reduces overfitting
- VAE is a stochastic model
- The second term is the KL divergence between two distributions that we know

Training Variational Autoencoders

- $\int_z q_\varphi(z|x) \log \frac{q_\varphi(z|x)}{p_\lambda(z)} dz$
- The second term is the KL divergence between two distributions that we know
- E.g., compute the KL divergence between a centered $N(0,1)$ and a non-centered $N(\mu, \sigma)$ gaussian

Typical VAE

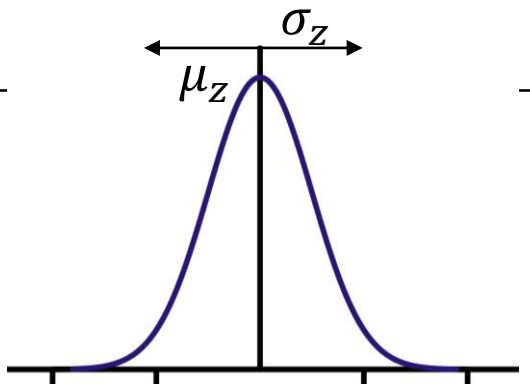
- We set the prior $\mathrm{p}_\lambda(\mathrm{z})$ to be the unit Gaussian

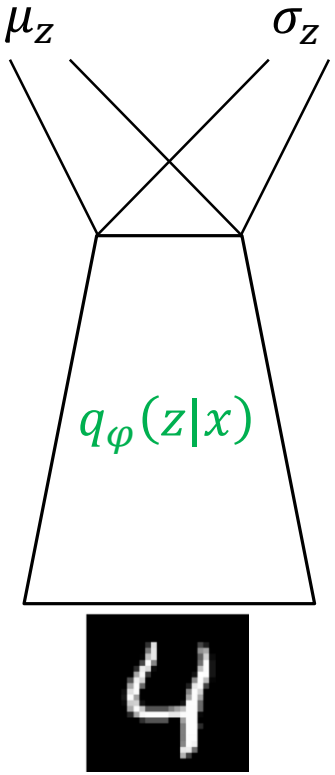
$$\mathrm{p}(z) \sim N(0,1)$$

- We set the likelihood to be a Bernoulli for binary data

$$p(x|z) \sim Bernoulli(\pi)$$

- We set $q_\varphi(\mathrm{z}|\mathrm{x})$ to be a neural network (MLP, ConvNet), which maps an input $\mathbf{x}$ to the Gaussian distribution, specifically it's mean and variance
  - $\mu_z, \sigma_z \sim q_\varphi(\mathrm{z}|\mathrm{x})$
  - The neural network has two outputs, one is the mean μ_x and the other the σ_x, which corresponds to the covariance of the Gaussian

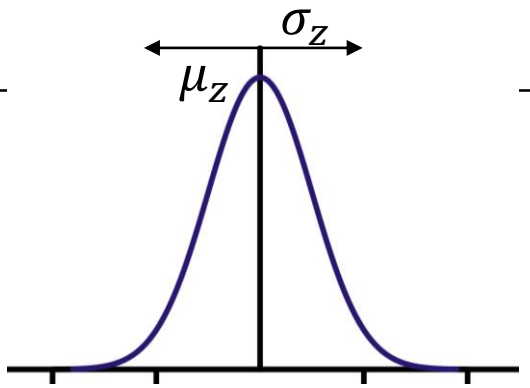


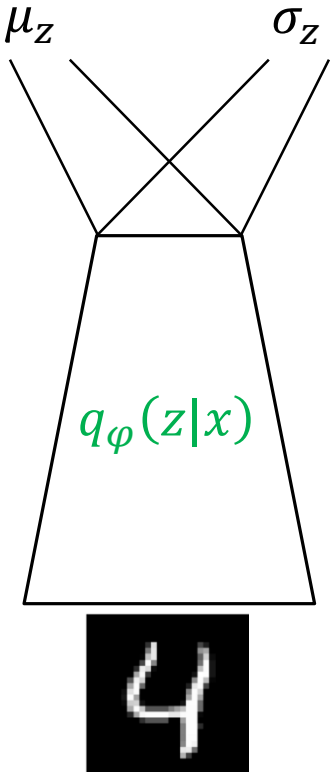


Typical VAE

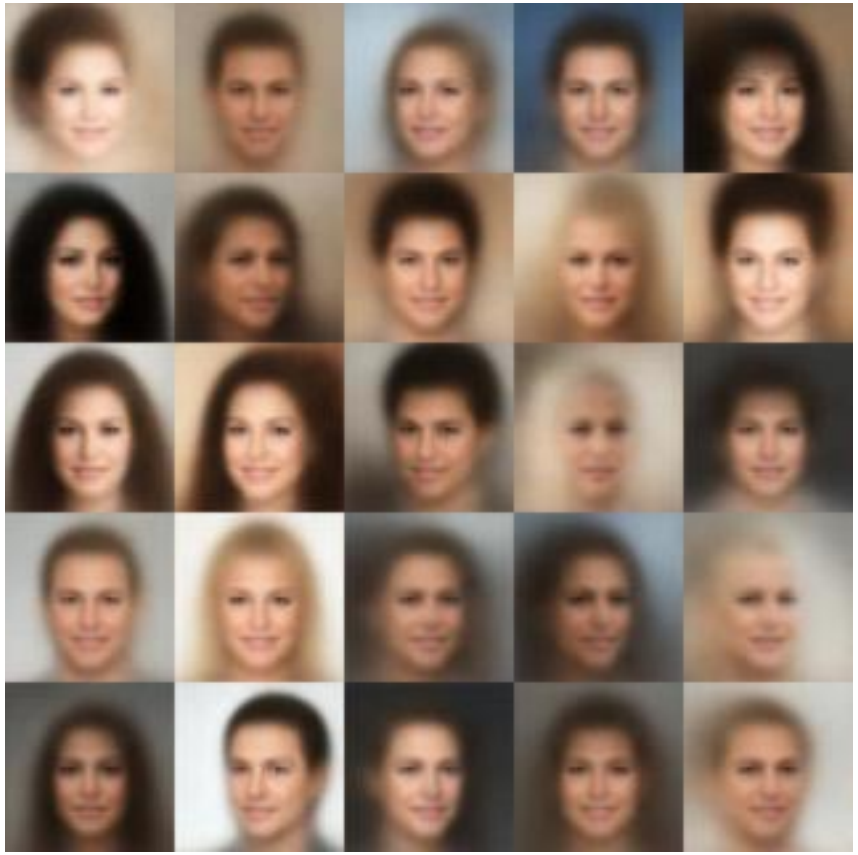
- We set $p_\theta(\mathrm{x}|\mathrm{z})$ to be an inverse neural network, which maps Z to the Bernoulli distribution if our outputs binary (e.g. Binary MNIST)

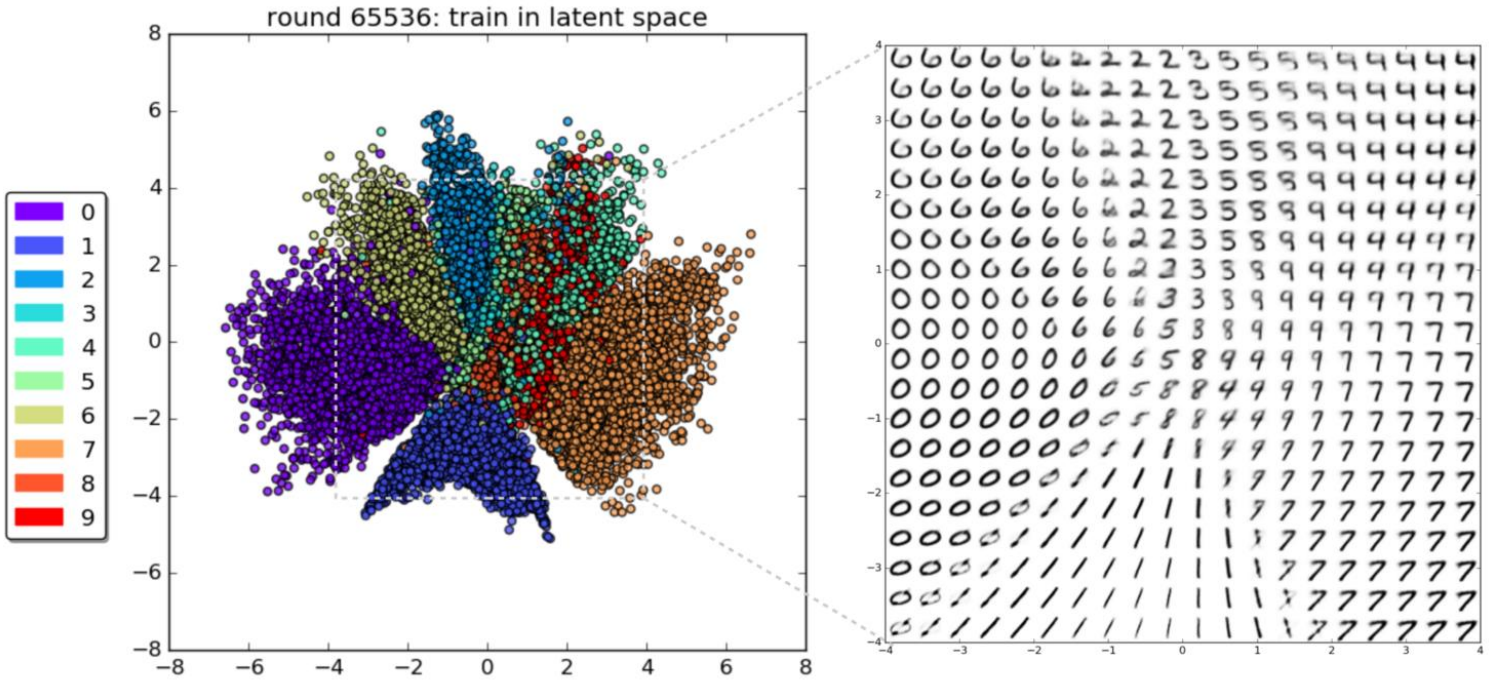
- Good exercise: Derive the ELBO for the standard VAE





VAE: Interpolation in the latent space





Summary

- Gentle intro to Bayesian Modelling and Variational Inference
- Restricted Boltzmann Machines
- Deep Boltzmann Machines
- Deep Belief Network
- Contrastive Divergence
- Variational Autoencoders
- Normalizing Flows