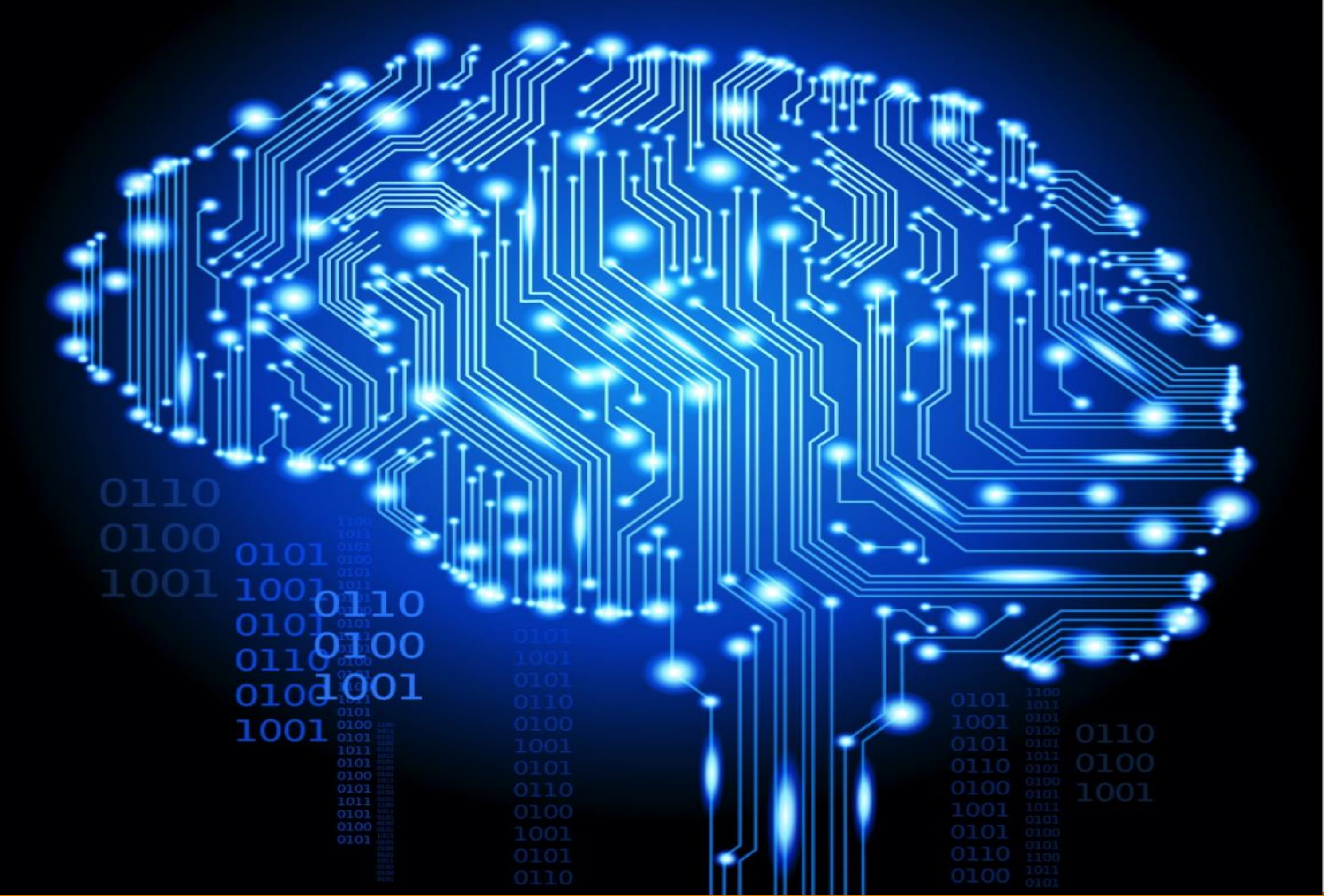


Lecture 9: Deep Generative Models

Efstratios Gavves

Lecture overview

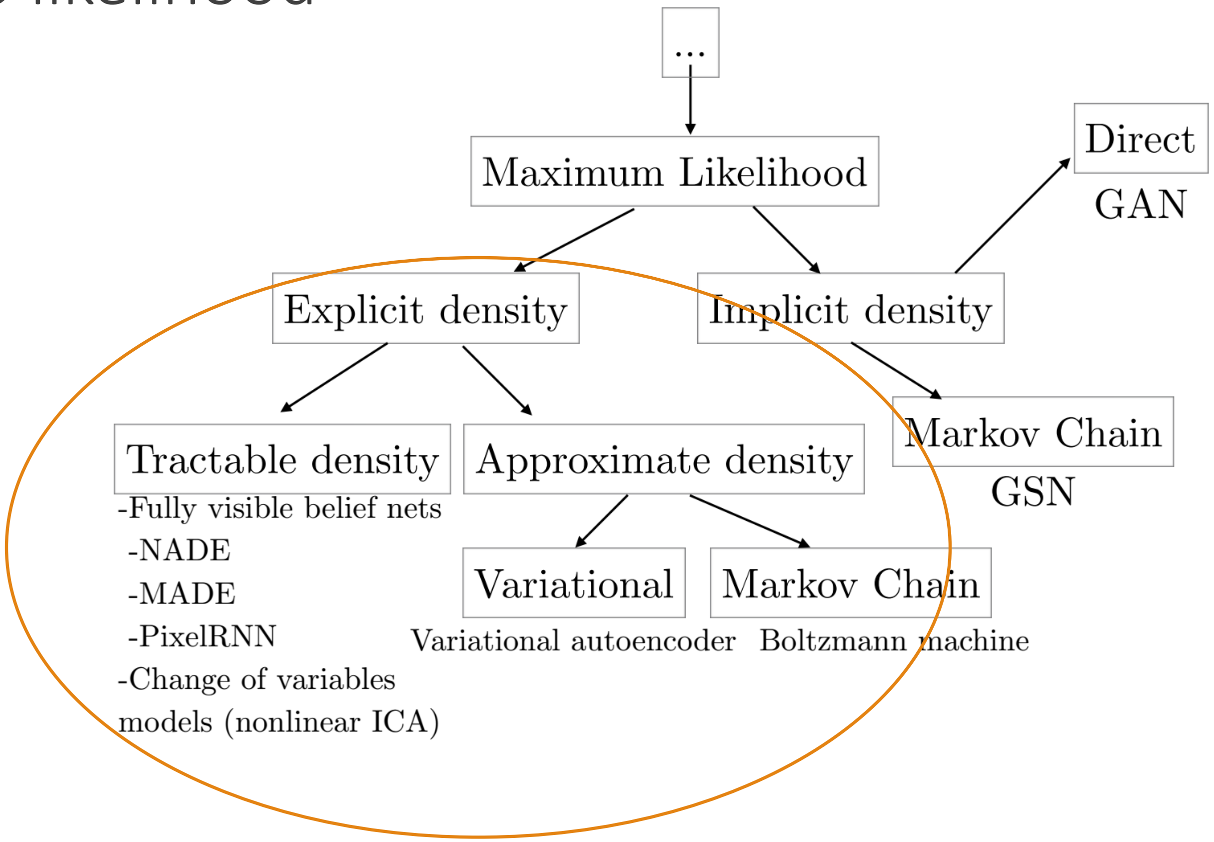
- Early Generative Models
- Restricted Boltzmann Machines
- Deep Boltzmann Machines
- Deep Belief Network
- Contrastive Divergence
- Gentle intro to Bayesian Modelling and Variational Inference
- Variational Autoencoders
- Normalizing Flows

Explicit density models

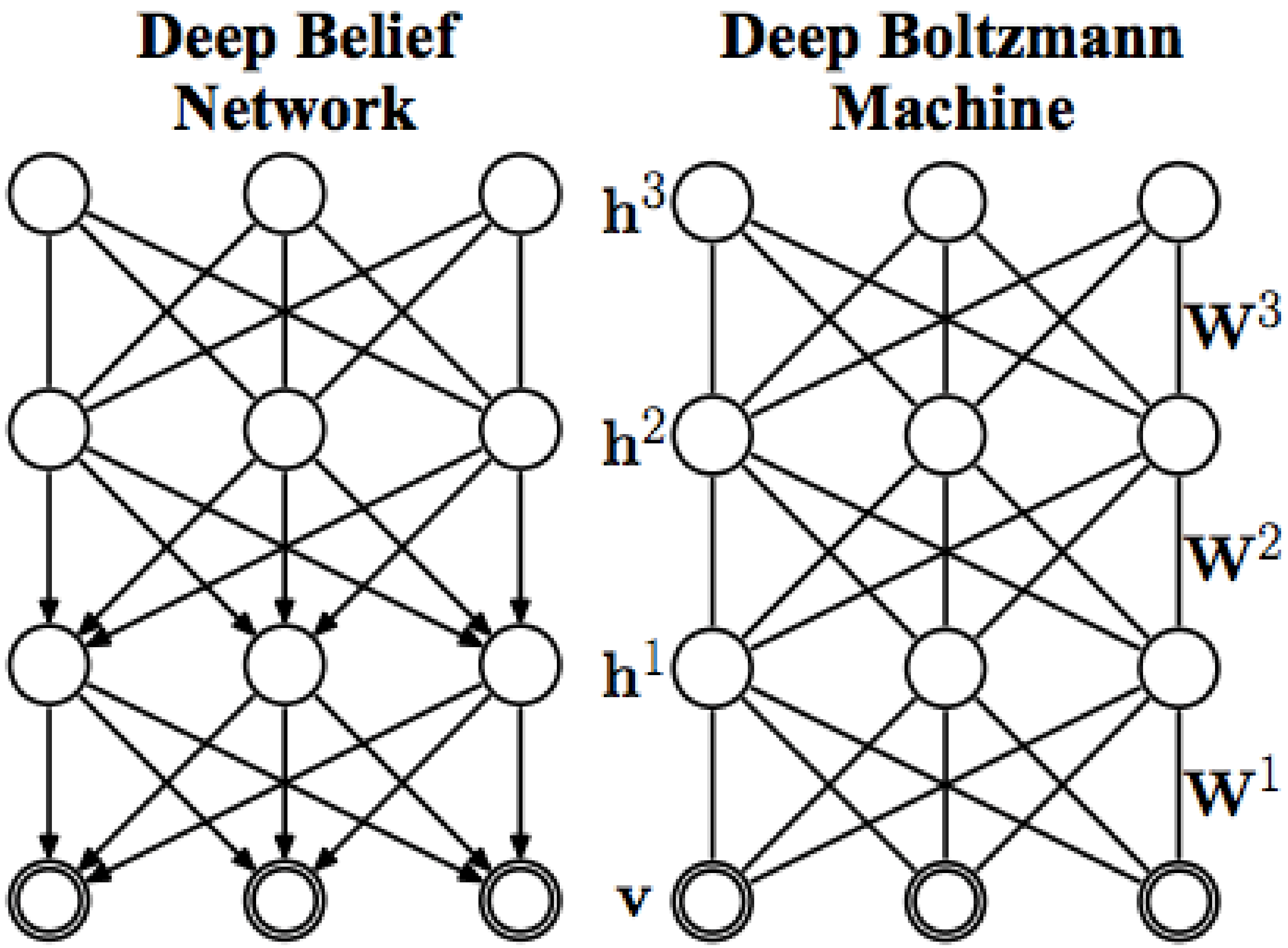
- Plug in the model density function to likelihood
- Then maximize the likelihood

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 $\psi_c$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?

- 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

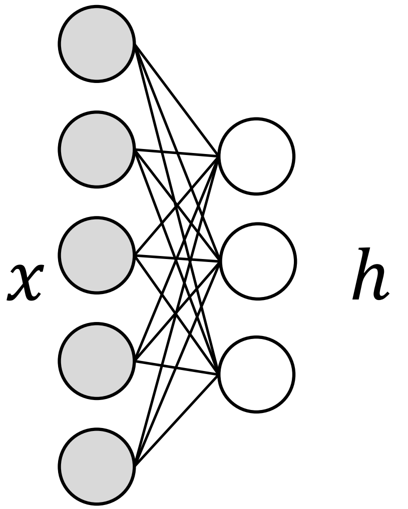
- $E(x) = -x^T W h - b^T x - c^T h$
- The $x^T W h$ models correlations between x and the latent activations via the parameter matrix W
- The $b^T x, c^T h$ model the priors
- Restricted Boltzmann Machines (RBM) assume x, h to be binary

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 $\propto \exp(\mathrm{x})/\mathrm{Z}$ because of the $\sum$



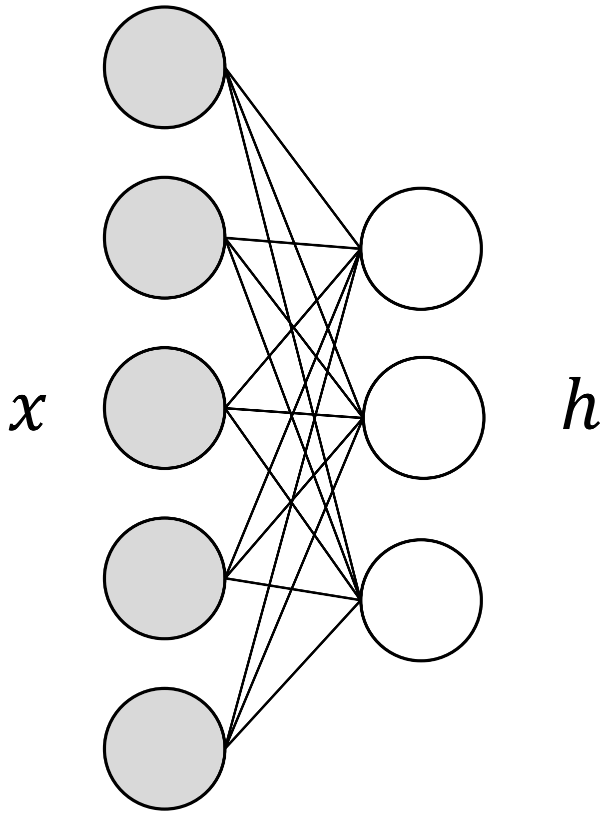
- Free energy function: $F(x) = -b^T x - \sum_i \log \sum_{h_i} \exp(h_i (c_i + W_i x))$

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

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

Restricted Boltzmann Machines

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



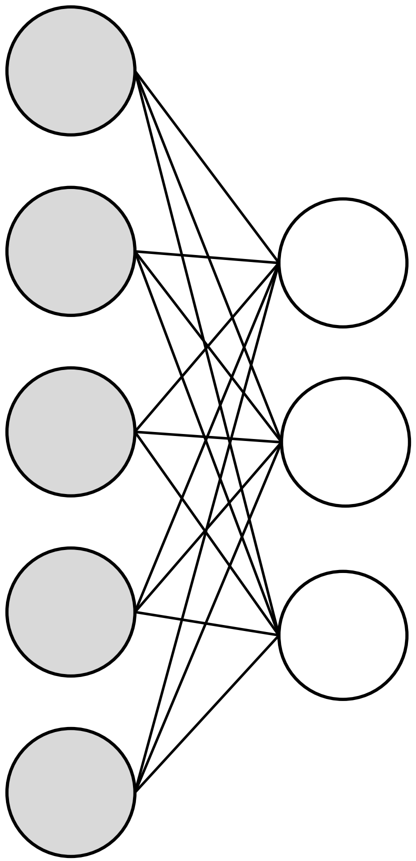
Restricted Boltzmann Machines

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

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



Training RBMs

- The conditional probabilities are defined as sigmoids

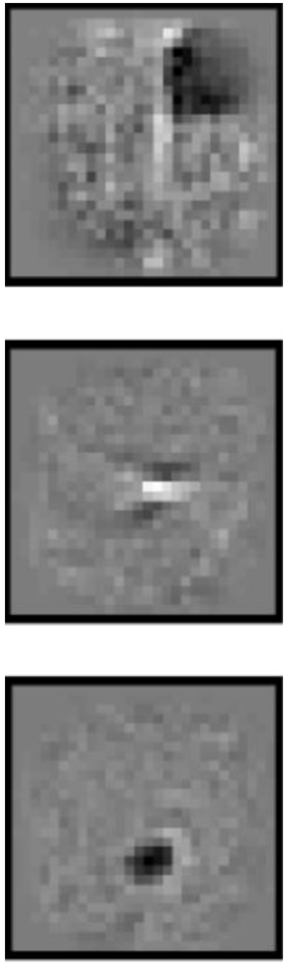
$$p\left(h_j \middle| x, \theta\right) = \sigma\left(W_{\cdot j} x + b_j\right)$$
$$p(x_i | h, \theta) = \sigma(W_{\cdot i} x + c_i)$$

- 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

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

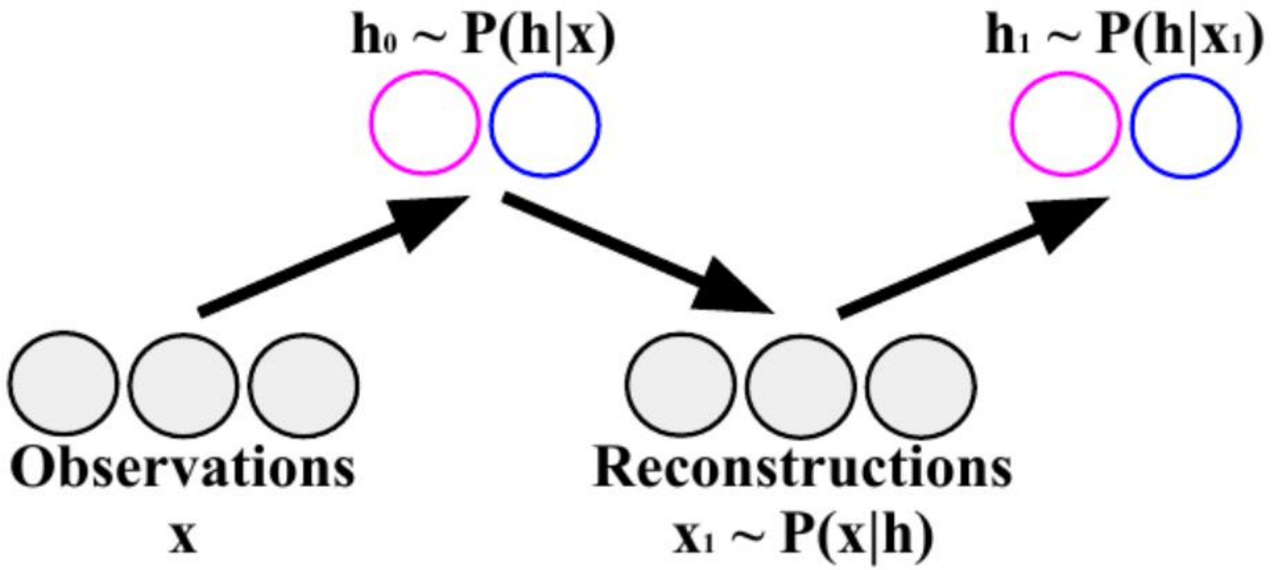
$$= -\sum_h p(h|x_n,\theta)\frac{\partial E(x_n|h,\theta)}{\partial \theta} + \sum_{\tilde{x},h} p(\tilde{x},h|\theta)\frac{\partial E(\tilde{x},h|\theta)}{\partial \theta}$$

- 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

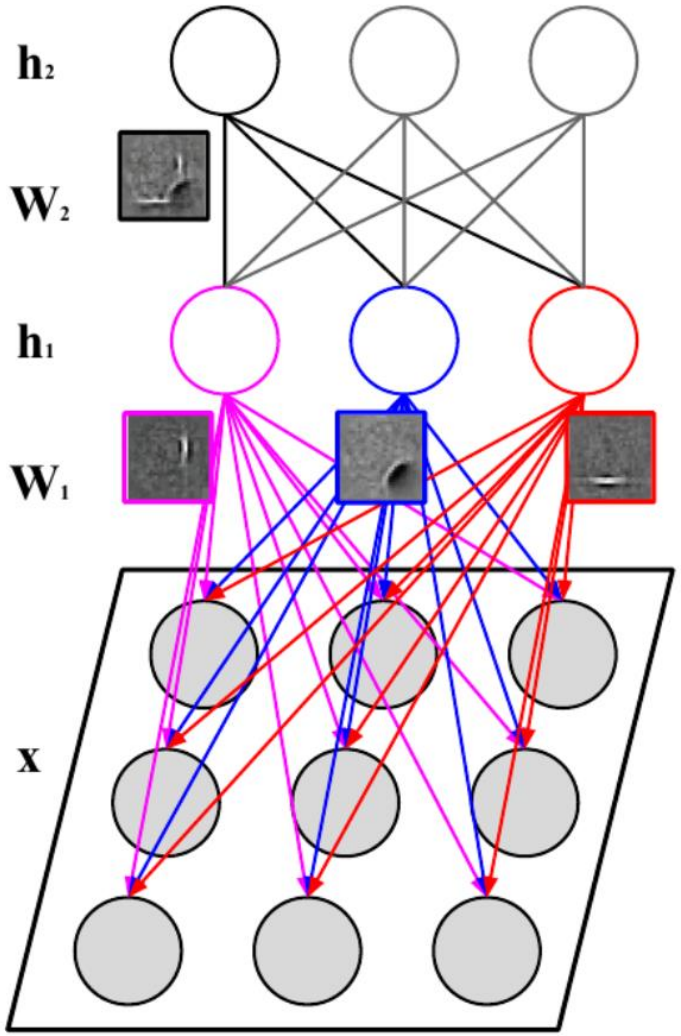
- RBMs are just one layer

- 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, $p(x_i|h, \theta) = \sigma(W_{\cdot i}x + c_i)$, namely the input argument has only variable only from below

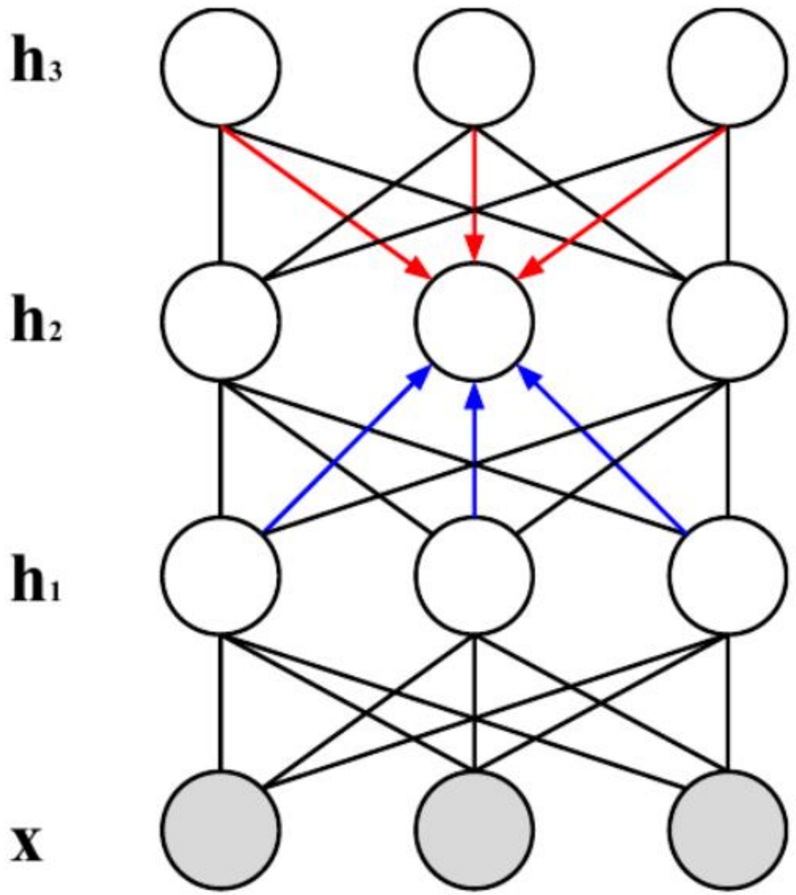


Deep Boltzmann Machines

- 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

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

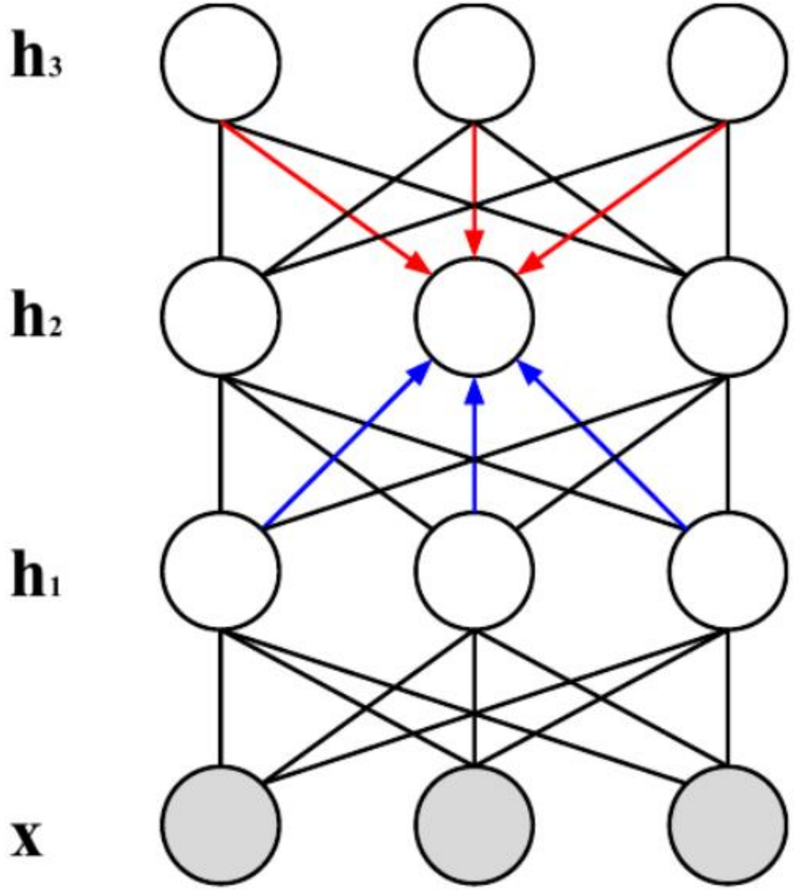
$$p(h_2^k|h_1, h_3) = \sigma(\sum_j W_1^{jk} h_1^j + \sum_l W_3^{kl} h_3^k)$$



Deep Boltzmann Machines

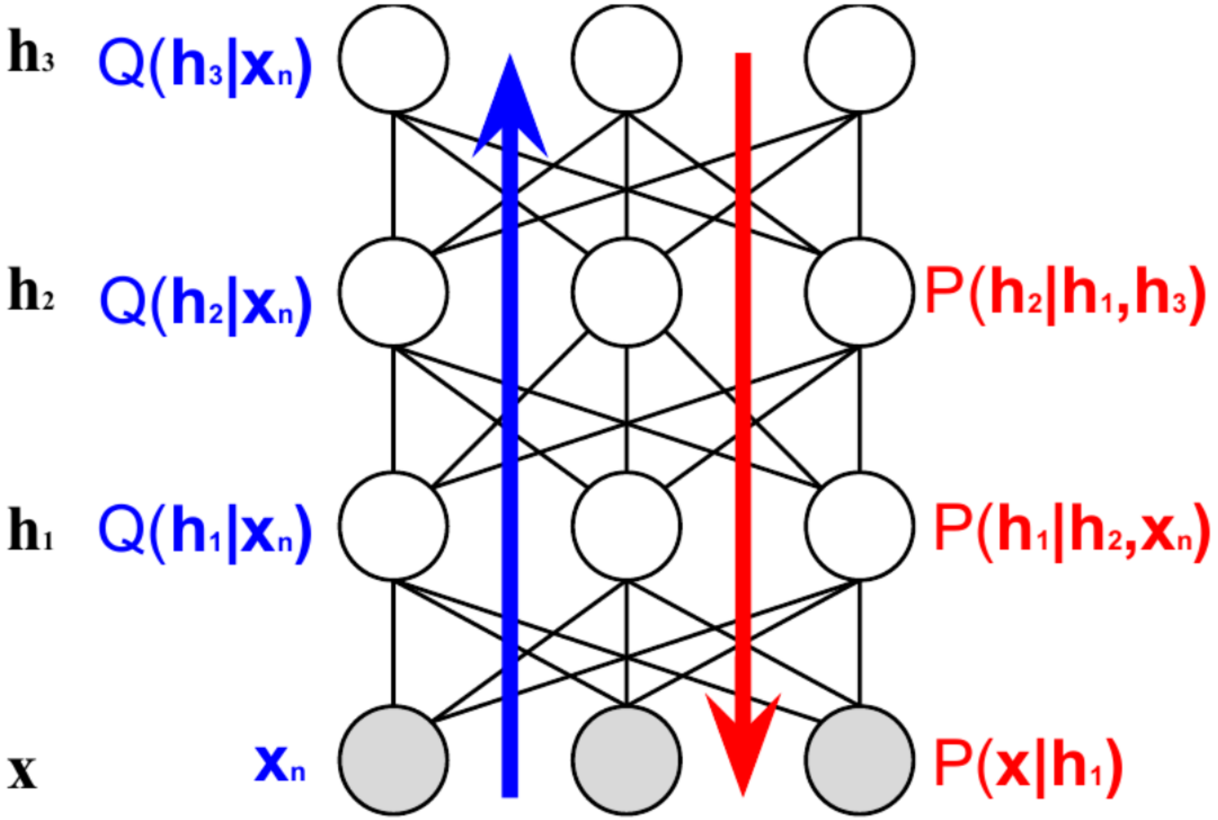
- Schematically similar to Deep Belief Networks
- But, Deep Boltzmann Machines (DBM) are undirected models
  - Belong to the Markov Random Field family
- So, two types of relationships: bottom-up and up-bottom

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

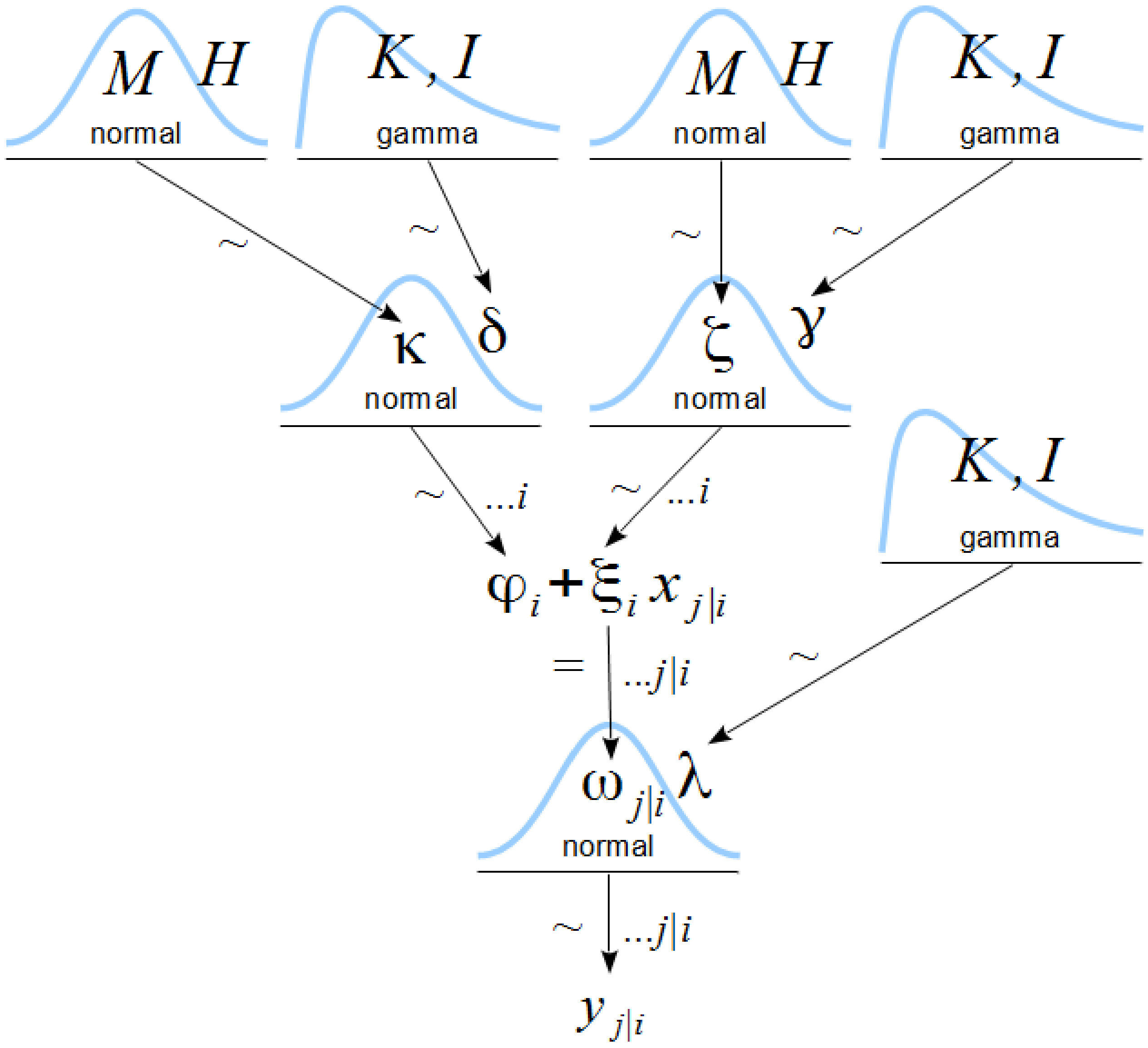


Training Deep Boltzmann Machines

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



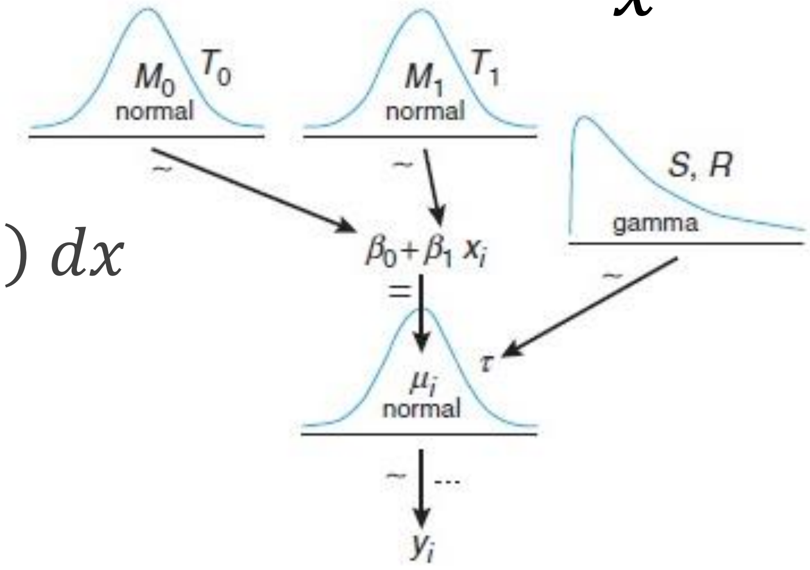
Variational Inference



Some (Bayesian) Terminology

x

- 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: $p(x|\theta)$



Bayesian Terminology

- Posterior pdf

$$
\begin{aligned}
p(\theta|x) &= \\
&= \frac{p(x,\theta)}{p(x)} \\
&= \frac{p(x|\theta)\, p(\theta)}{p(x)} \\
&= \frac{p(x|\theta)\, p(\theta)}{\int_{\theta'} p(x,\theta')\ d\theta'} \\
&\propto p(x|\theta)\, p(\theta)
\end{aligned}
$$

← Conditional probability

← Bayes Rule

← Marginal probability

← $p(x\ )$ is constant

- Posterior Predictive pdf

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

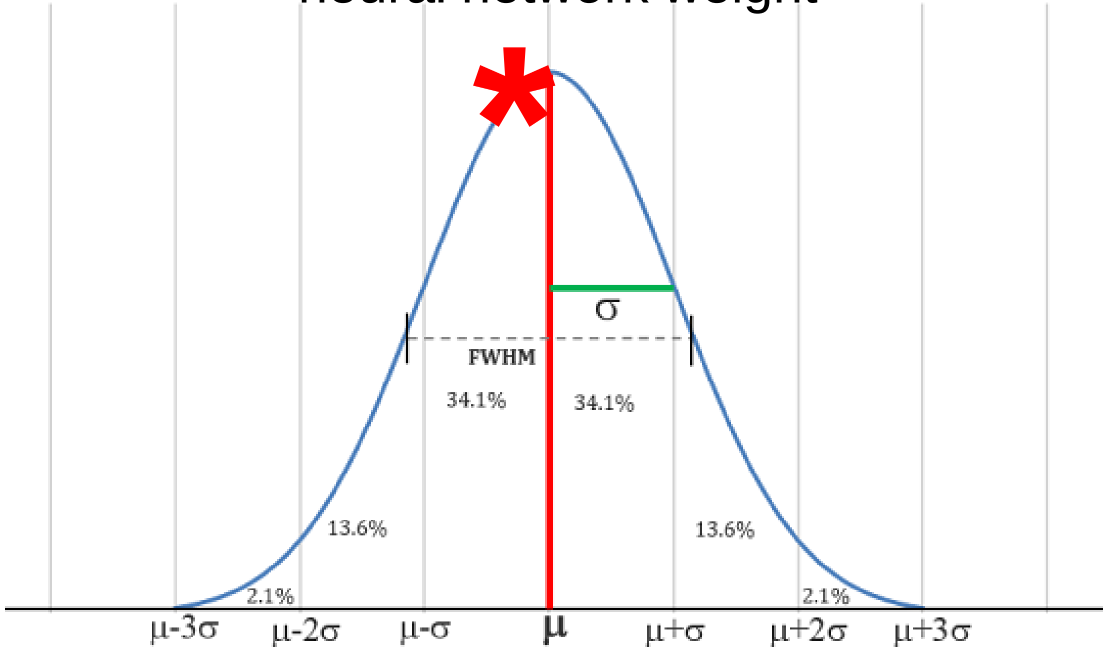
Bayesian Terminology

- 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)

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

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

Point estimate of your neural network weight



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

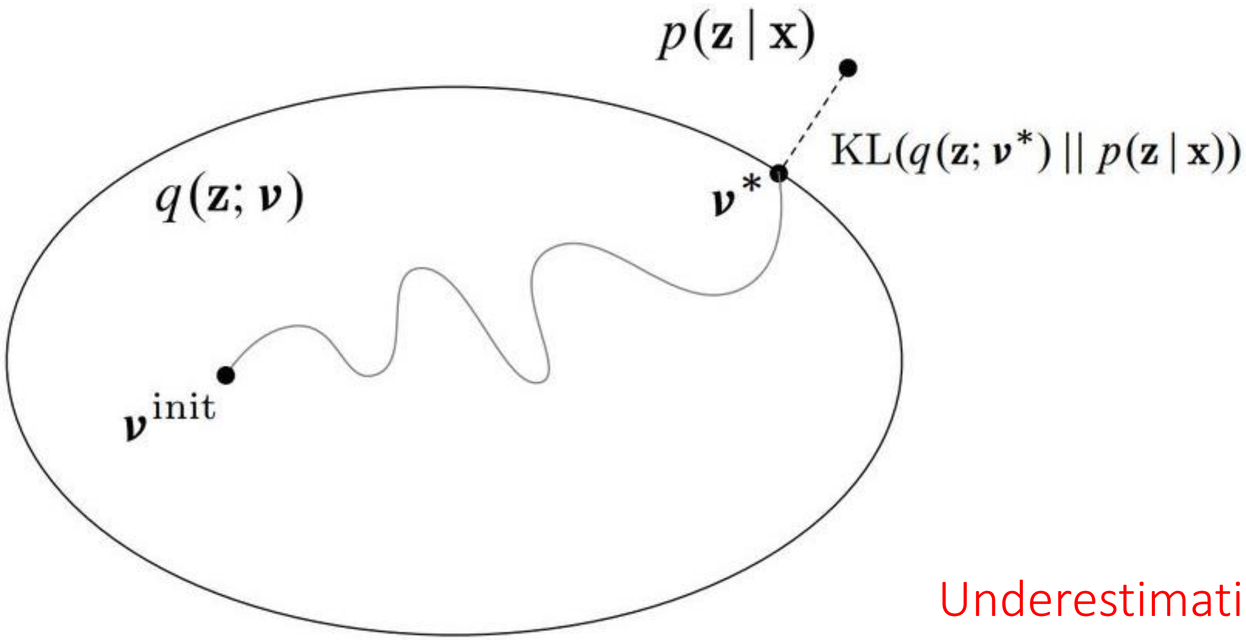
Variational Inference

- 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

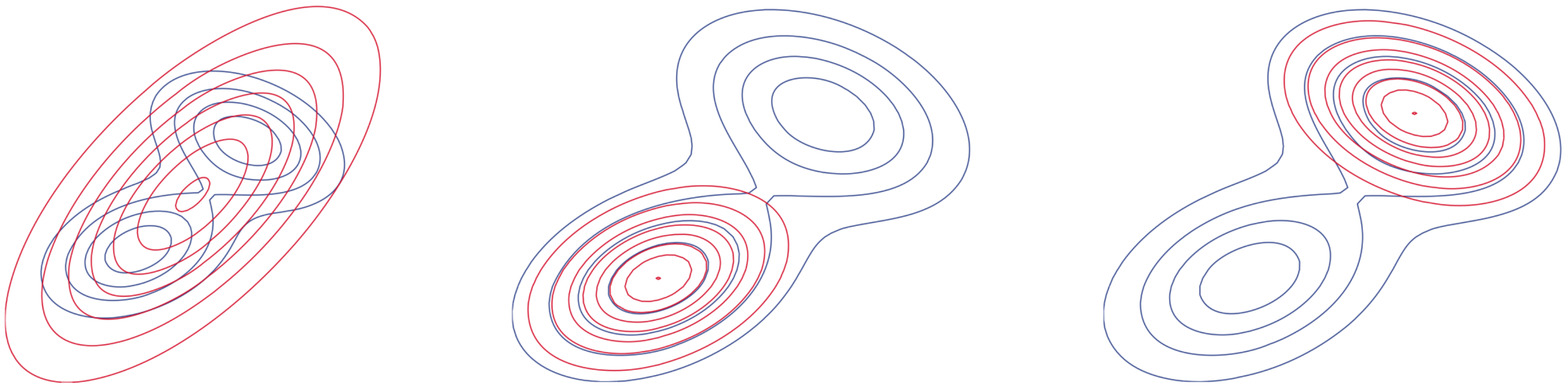
$$\varphi^* = \arg\min_{\varphi} KL(q(\theta|\varphi)||p(\theta|x))$$

- Turn inference into optimization

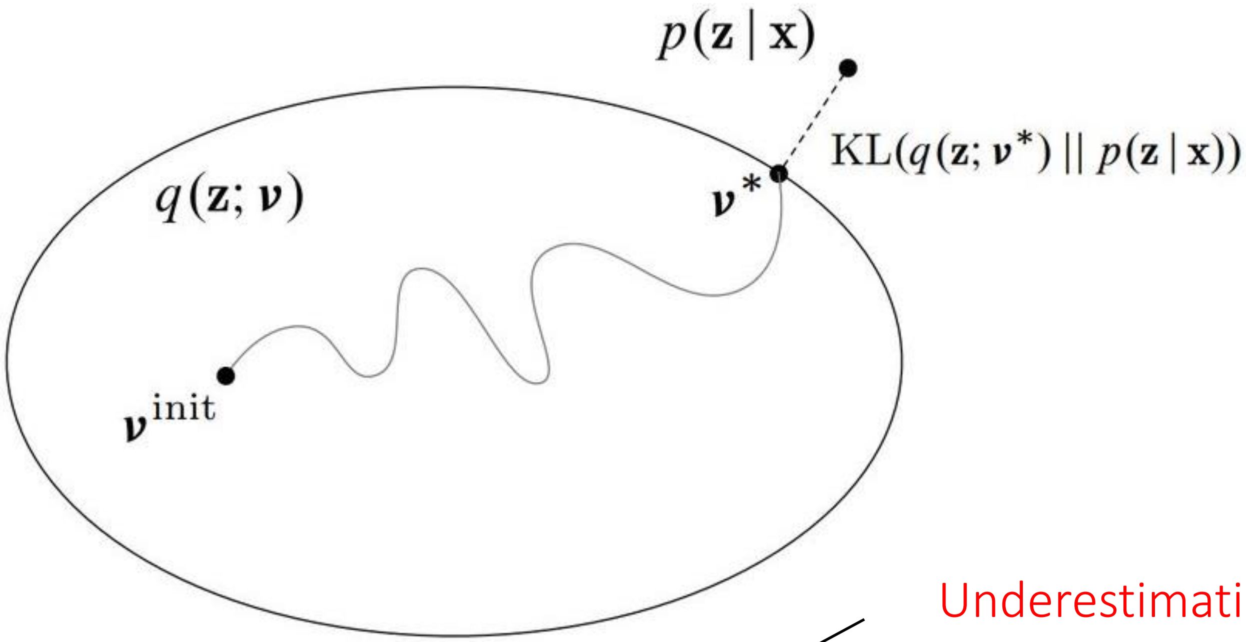
Variational Inference (graphically)



Underestimating variance. Why?



Variational Inference (graphically)



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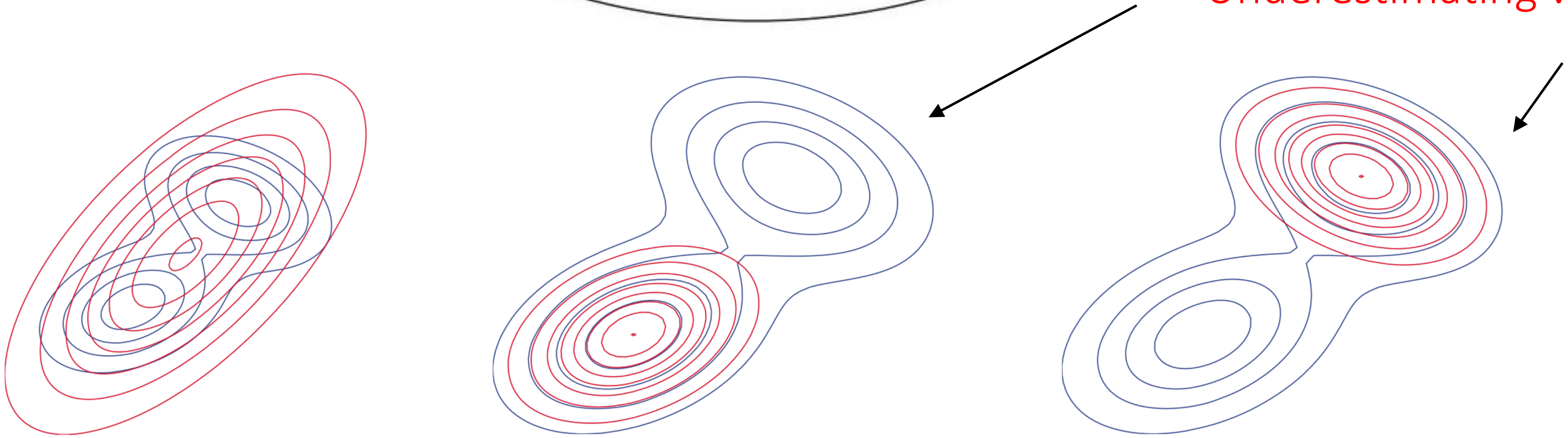
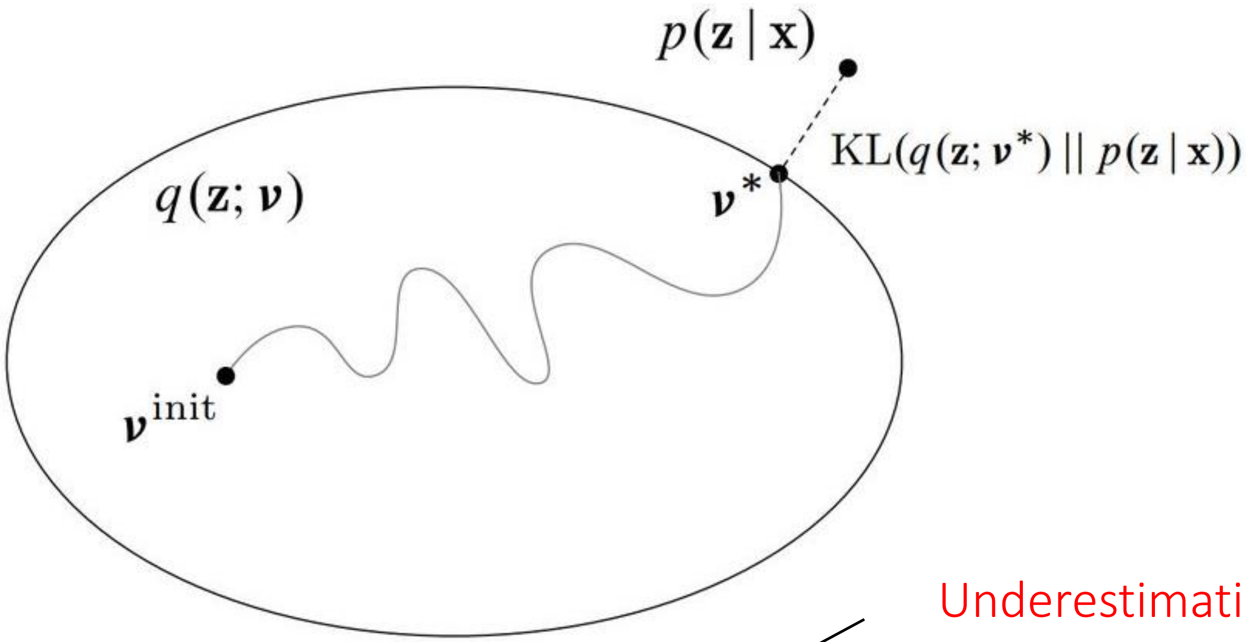
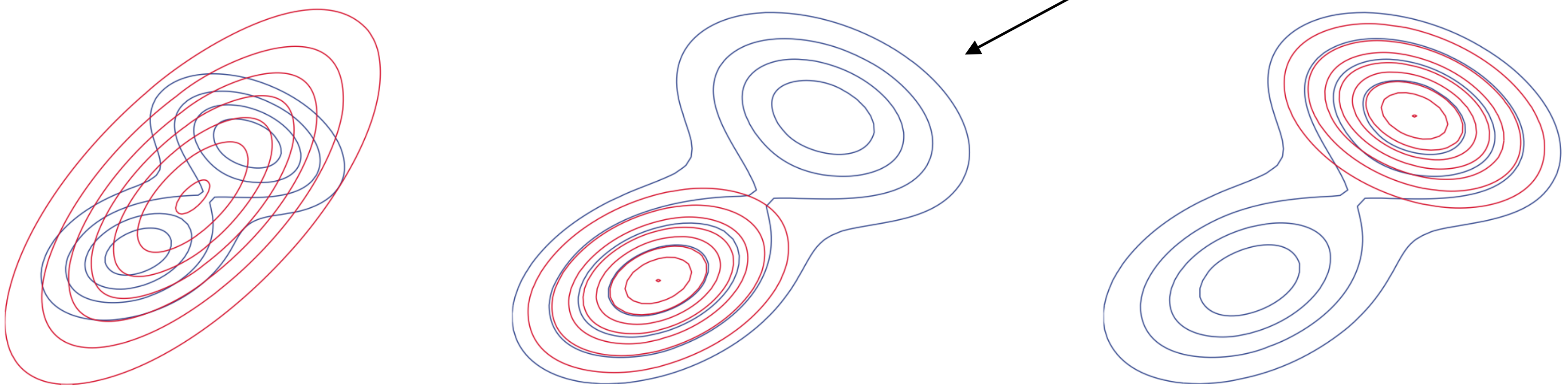


Variational Inference (graphically)

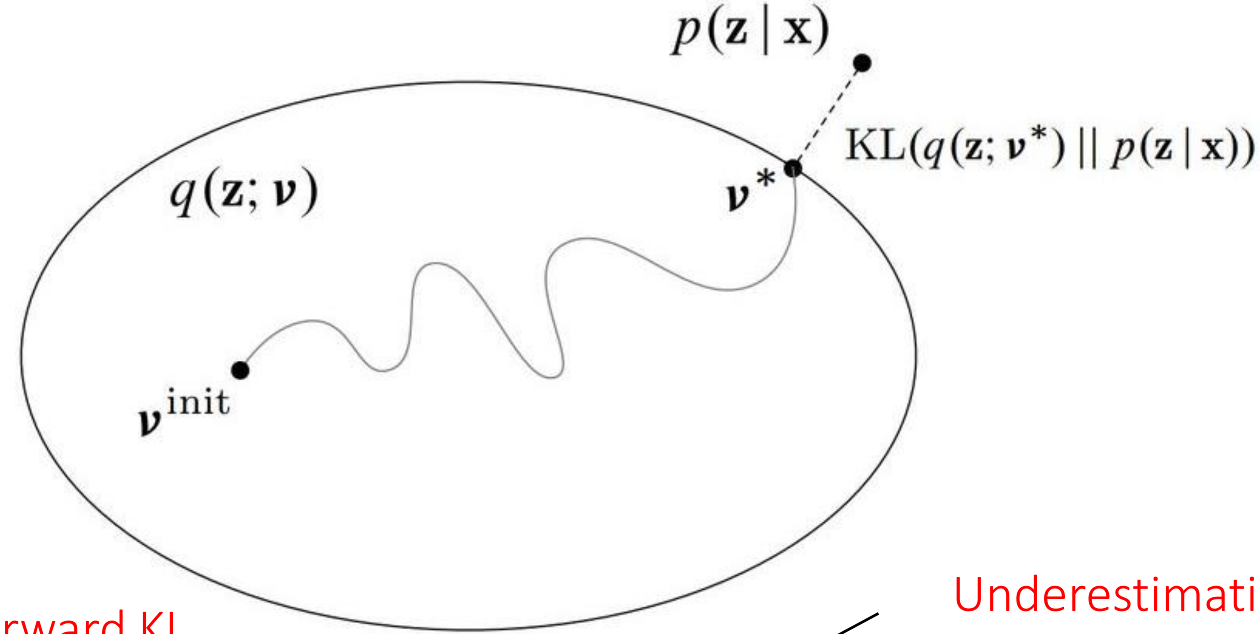


How to overestimate variance?

Underestimating variance. Why?

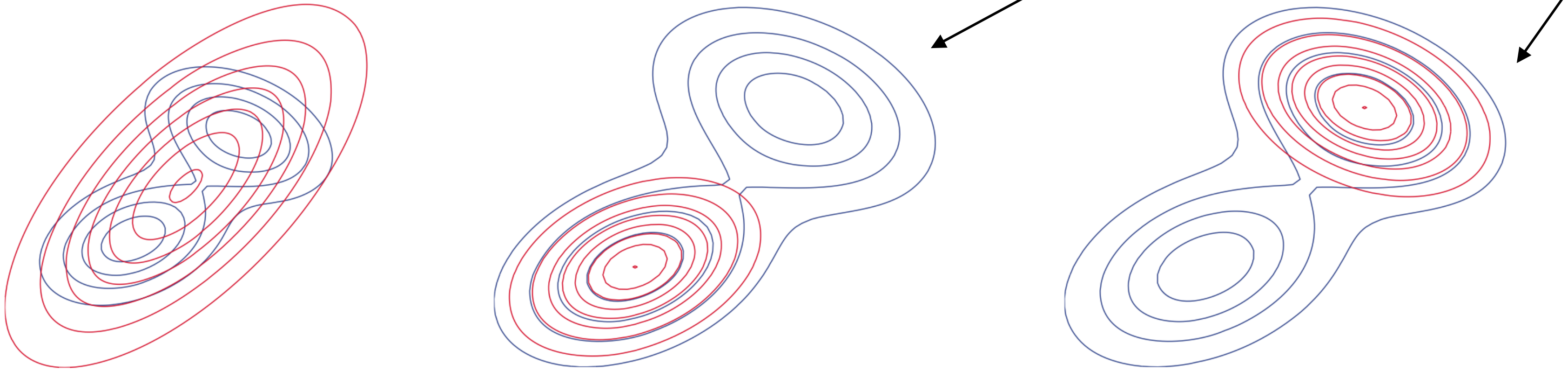


Variational Inference (graphically)



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 $\log p(x)$

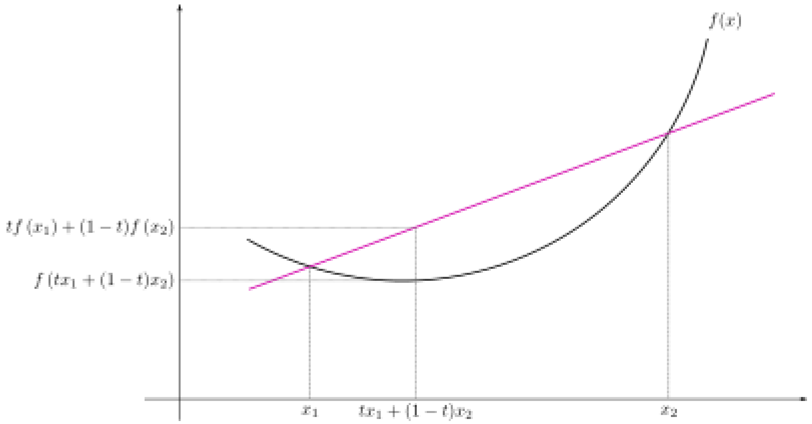
$$\log p(x) \geq \mathbb{E}_{q_\varphi(\theta)}\left[\log \frac{p(x, \theta)}{q_\varphi(\theta)}\right]$$

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

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

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

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

- 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

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

- 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" z or "model variables" w

Variational Autoencoders

- Let's rewrite the ELBO a bit more explicitly

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

- $p_\theta(x|z)$ 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

- Let's rewrite the ELBO a bit more explicitly

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

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

- I.e., a λ-parameterized prior only on the latent activations $\mathbf{z}$
- Not on model weights

Variational Autoencoders

- Let's rewrite the ELBO a bit more explicitly

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

- $q_\varphi(z|x)$ 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

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

Variational Autoencoders

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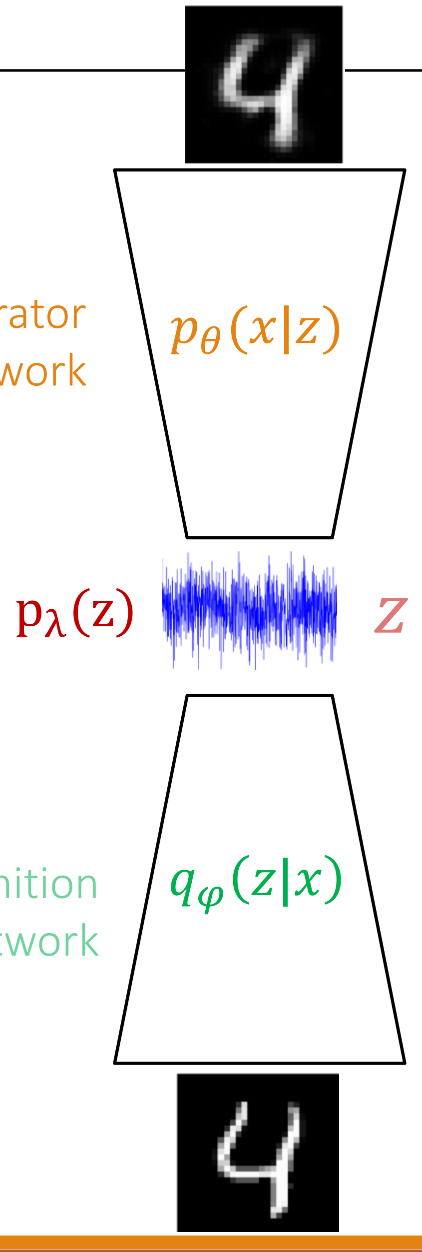
- How to model $p_\theta(x|z)$ and $q_\varphi(z|x)$?
- What about modelling them as neural networks

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 network, because it infers 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, because it recognizes the input given the latent variable
- 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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- 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

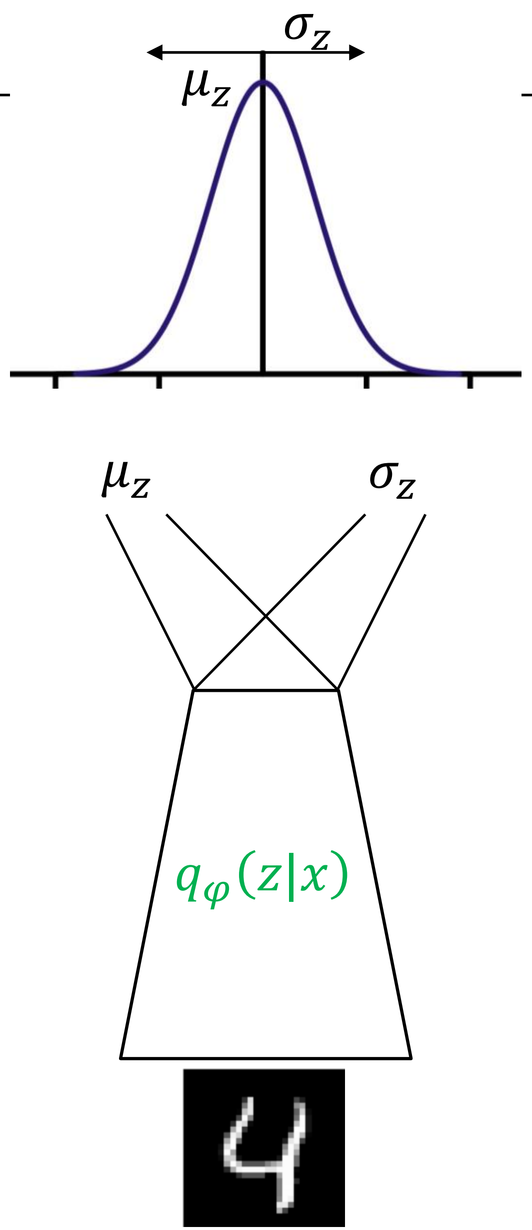
- We set the prior $\mathrm{p}_\lambda(\mathrm{z})$ to be the unit Gaussian

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

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

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

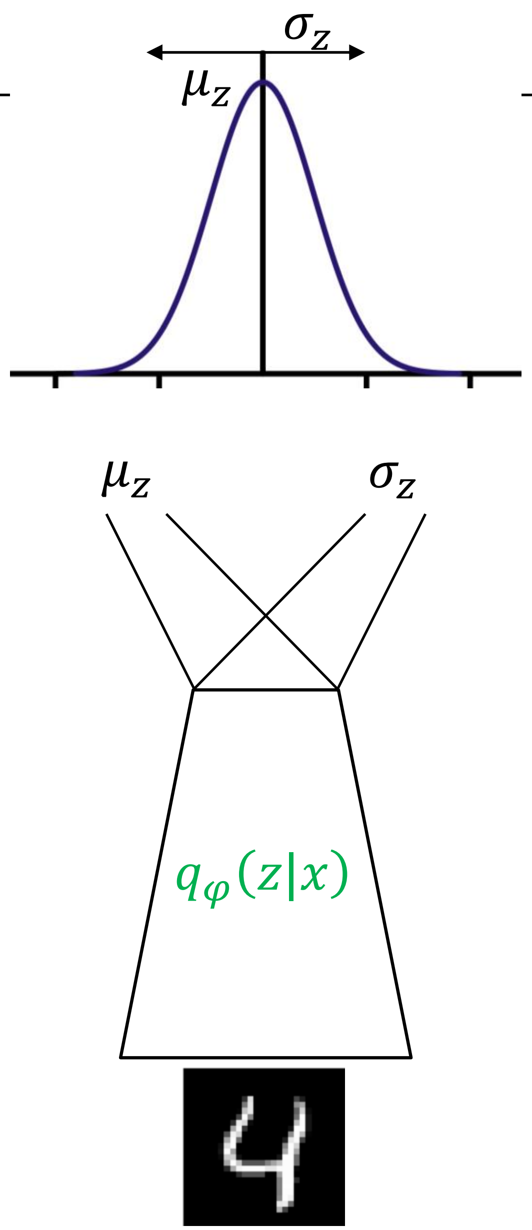
- We set $q_\varphi(\mathrm{z}|\mathrm{x})$ to be a neural network (MLP, ConvNet), which maps an input $\mathbf{x}$ to the Gaussian distribution, specifically it's mean and variance
  - $\mu_z, \sigma_z \sim q_\varphi(\mathrm{z}|\mathrm{x})$
  - The neural network has two outputs, one is the mean μ_x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



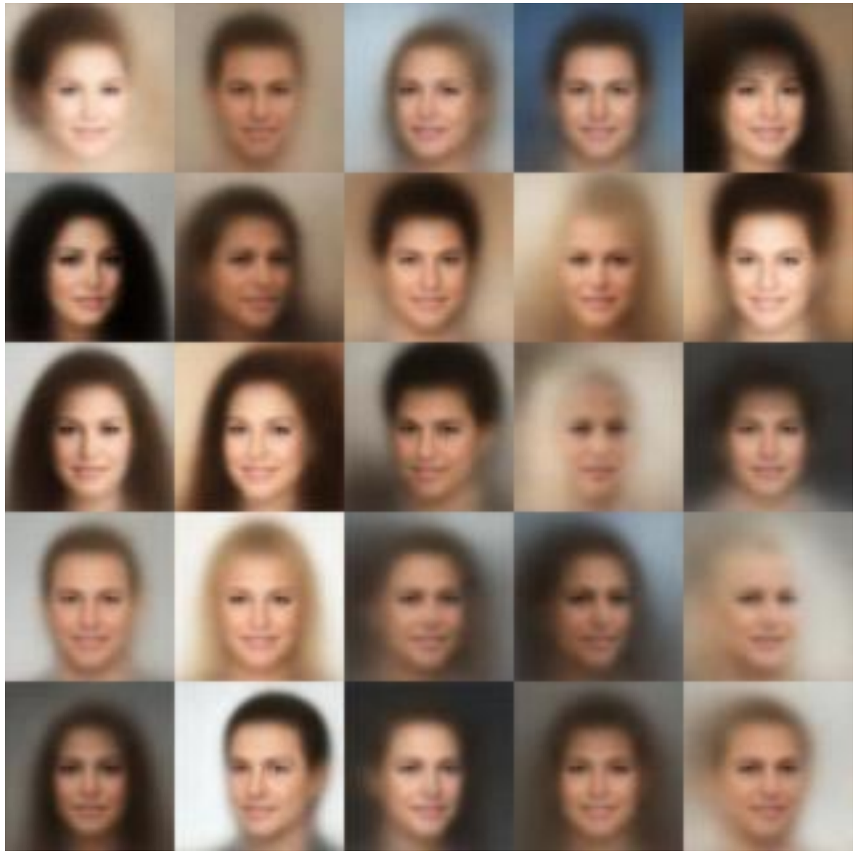
Typical VAE

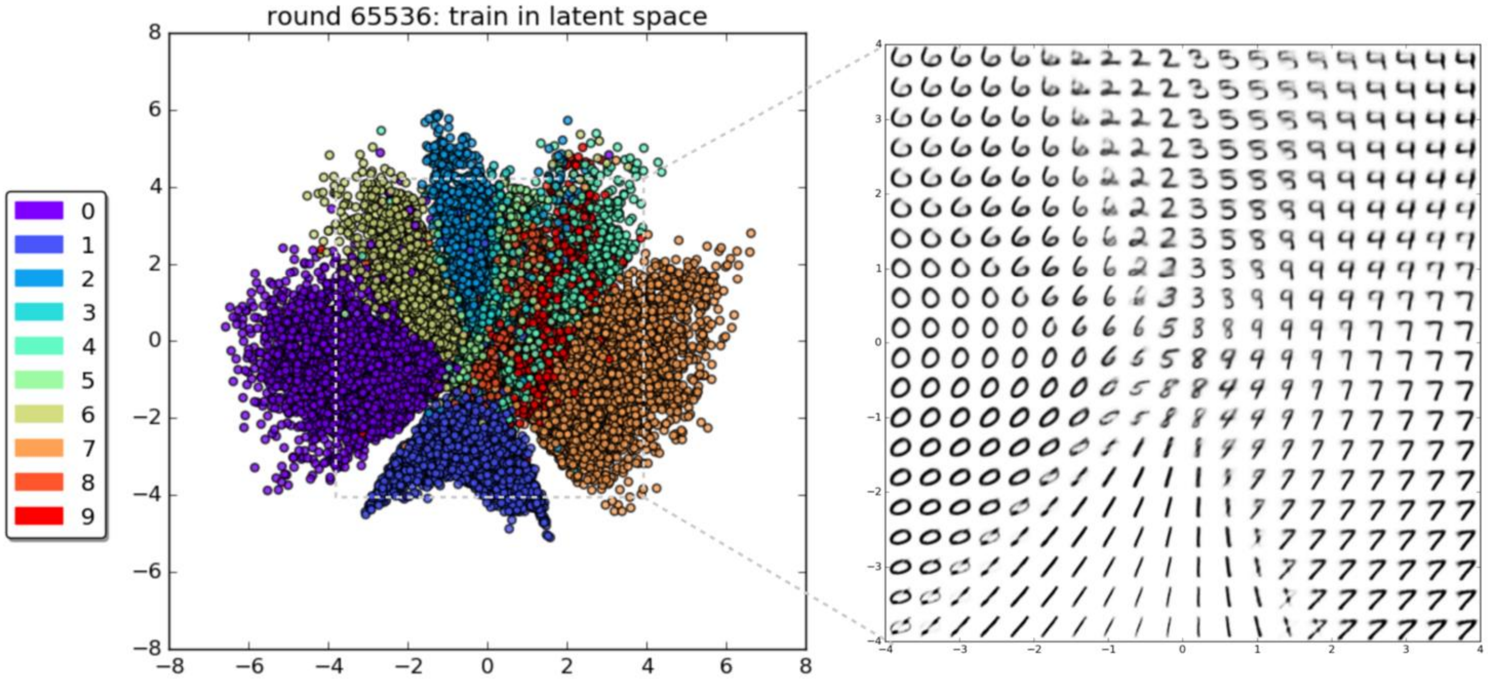
- We set $p_\theta(\mathrm{x}|\mathrm{z})$ to be an inverse neural network, which maps $\mathbf{Z}$ to the Bernoulli distribution if our outputs binary (e.g. Binary MNIST)

- Good exercise: Derive the ELBO for the standard VAE



VAE: Interpolation in the latent space





Forward propagation in VAE

- Sample z from the approximate posterior density $z \sim q_\varphi(Z|x)$
  - As q_φ is a neural network that outputs values from a specific and known parametric pdf, e.g. a Gaussian, sampling from it is rather easy
  - Often even a single draw is enough
- Second, compute the $\log p_\theta(x|Z)$
  - As p_θ is a a neural network that outputs values from a specific and known parametric pdf, e.g. a Bernoulli for white/black pixels, computing the log-prob is easy
- Computing the ELBO is rather straightforward in the standard case
- How should we optimize the ELBO?

Forward propagation in VAE

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- Computing the ELBO is rather straightforward in the standard case
- How should we optimize the ELBO? Backpropagation?

Backward propagation in VAE

- Backpropagation → compute the gradients of
$$\mathcal{L}(\theta,\varphi)=\mathbb{E}_{z\sim q_\varphi(Z|x)}[\log p_\theta(x|z)]-\mathrm{KL}(q_\varphi(Z|x)||\mathrm{p}_\lambda(\mathrm{Z}))$$
- $\nabla_\theta\mathcal{L}=\mathbb{E}_{z\sim q_\varphi(Z|x)}[\nabla_\theta \log p_\theta(x|z)]$
  - The expectation and sampling in $\mathbb{E}_{z\sim q_\varphi(Z|x)}$ does not depend on $\theta,$ so no problem!
  - Also, the KL does not depend on $\theta,$ so no gradient from over there!
- $\nabla_\varphi\mathcal{L}=\nabla_\varphi\left[\mathbb{E}_{z\sim q_\varphi(Z|x)}[\log p_\theta(x|z)]\right]-\nabla_\varphi\left[\mathrm{KL}(q_\varphi(Z|x)||\mathrm{p}_\lambda(\mathrm{Z}))\right]$

Backward propagation in VAE

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

Backward propagation in VAE

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- Problem?

Backward propagation in VAE

- Backpropagation → compute the gradients of

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

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- Problem? Sampling $z\sim q_\varphi(Z|x)$ is not differentiable → no gradients
- No gradients → No backprop → No training! → Solution?

Solution: REINFORCE?

- So, our latent variable Z is a Gaussian (in the standard VAE) represented by the mean and variance μ_Z, σ_Z, which are the output of a neural net
- So, we can train by sampling randomly from that Gaussian

$$z \sim N(\mu_Z, \sigma_Z)$$

- Once we have that z, however, it's a fixed value (not a function), so we cannot backprop
- We could use, however, the REINFORCE algorithm to compute an approximation to the gradient
  - High-variance gradients → slow and not very effective learning

Solution: Reparameterization trick

- Remember, we have a Gaussian output $z \sim N(\mu_Z, \sigma_Z)$

- For certain pdfs, including the Gaussian, we can rewrite their random variable z as deterministic transformations of a simpler random variable ε

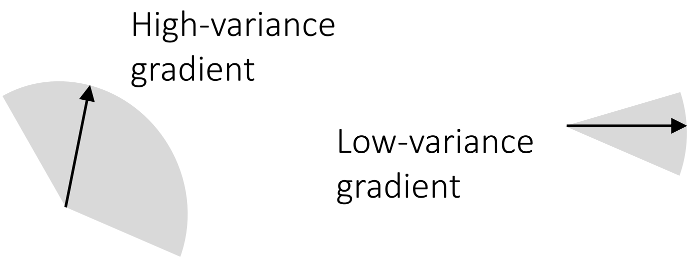
- For the Gaussian specifically, the following two formulations are equivalent

$$z \sim N(\mu_Z, \sigma_Z) \;\Leftrightarrow\; z = \mu_Z + \varepsilon \cdot \sigma_z,$$

where $\varepsilon \sim N(0, 1)$ and μ_Z, σ_Z are deterministic values from the NN function

Solution: Reparameterization trick

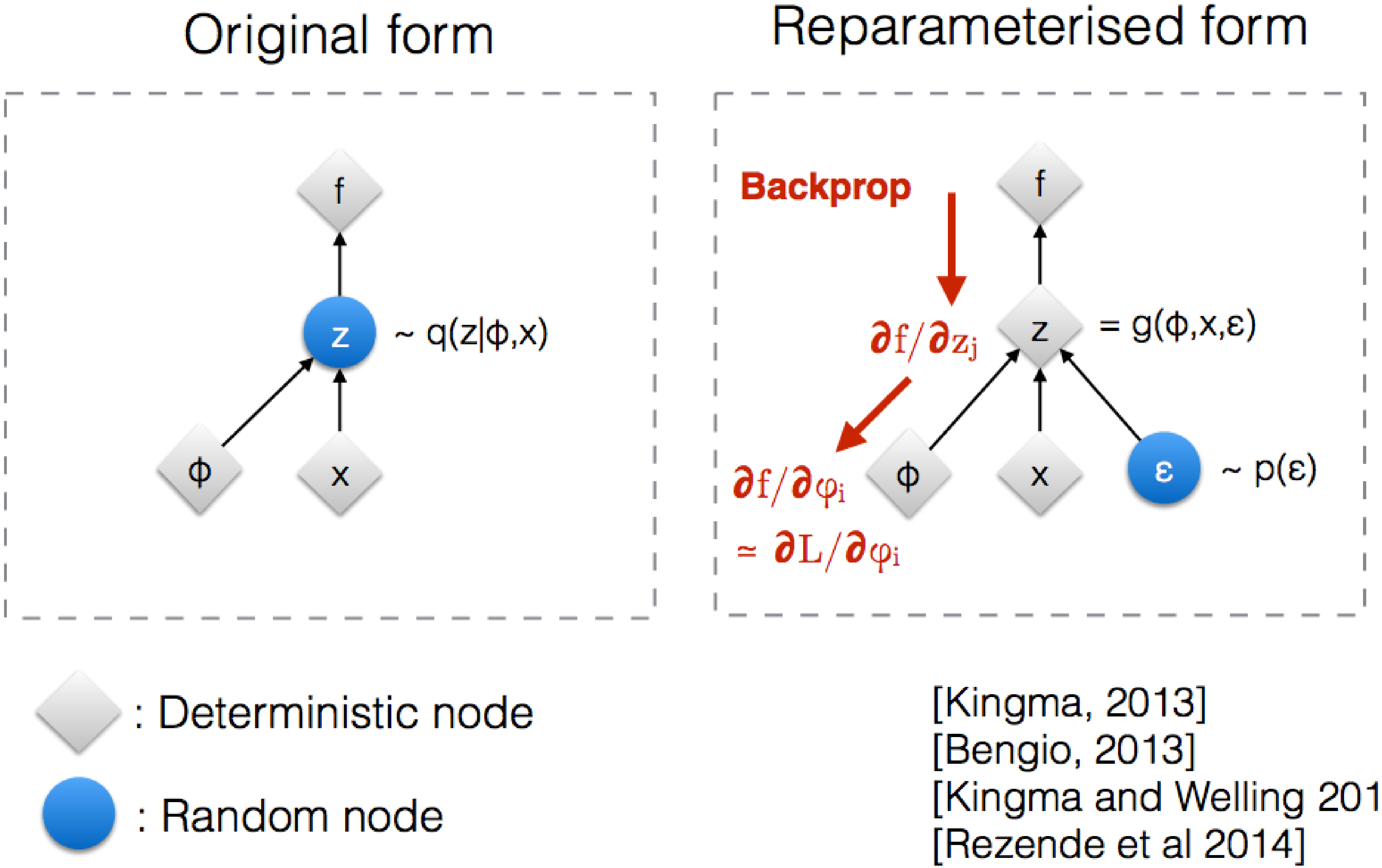
- Instead of sampling from $z \sim N(\mu_Z, \sigma_Z)$, we sample from $\varepsilon \sim N(0, 1)$ and then we compute z
- Sampling directly from $z \sim N(\mu_Z, \sigma_Z)$ leads to high-variance estimates
- Sampling directly from $\varepsilon \sim N(0,1)$ leads to low-variance estimates
  - Why low variance? Exercise for the interested reader
- Remember: since we are sampling for z, we are also sampling gradients
- More distributions beyond Gaussian possible: Laplace, Student-t, Logistic, Cauchy, Rayleight, Pareto



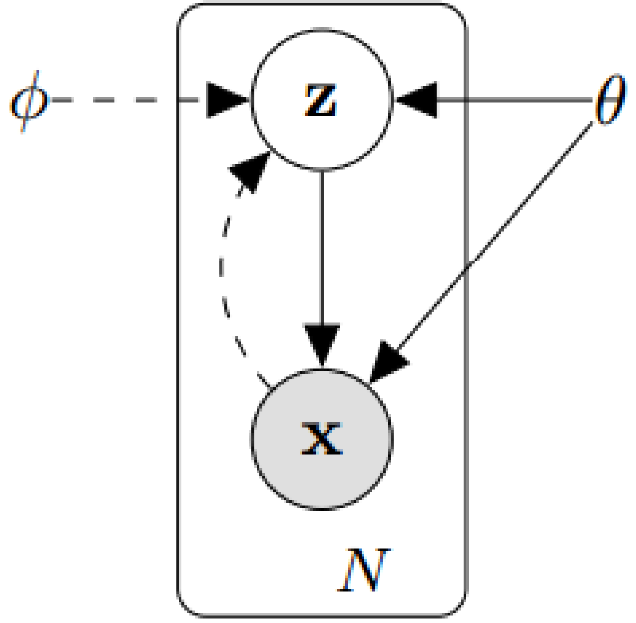
Check what is random

- Again, the latent variable is $z = \mu_Z + \varepsilon \cdot \sigma_z$
- μ_Z and σ_z are deterministic functions (via the neural network encoder)
- ε is a random variable, which comes **externally**
- The z as a result is itself a random variable, because of ε
- However, now the randomness is not associated with the neural network and its parameters that we have to learn
  - The randomness instead comes from the external ε
  - The gradients flow through μ_Z and σ_Z

Reparameterization Trick (graphically)



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



VAE Training Pseudocode

Data:

$\mathcal{D}$: Dataset

$q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$: Inference model

$p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})$: Generative model

Result:

$\boldsymbol{\theta}, \boldsymbol{\phi}$: Learned parameters

$(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow$ Initialize parameters

while *SGD not converged* **do**

$\mathcal{M} \sim \mathcal{D}$ (Random minibatch of data)

$\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$ (Random noise for every datapoint in $\mathcal{M}$)

Compute $\tilde{\mathcal{L}}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathcal{M}, \boldsymbol{\epsilon})$ and its gradients $\nabla_{\boldsymbol{\theta},\boldsymbol{\phi}} \tilde{\mathcal{L}}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathcal{M}, \boldsymbol{\epsilon})$

Update $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ using SGD optimizer

end

The ELBO's gradients

VAE for NLP

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Figure 2.D.2: An application of VAEs to interpolation between pairs of sentences, from [Bowman et al., 2015]. The intermediate sentences are grammatically correct, and the topic and syntactic structure are typically locally consistent.

VAE for Image Resynthesis

Figure 2.D.3: VAEs can be used for image re-synthesis. In this example by White [2016], an original image (left) is modified in a latent space in the direction of a *smile vector*, producing a range of versions of the original, from smiling to sadness. Notice how changing the image along a single vector in latent space, modifies the image in many subtle and less-subtle ways in pixel space.

Smile vector:
mean smiling faces –
mean no-smile faces

Latent space arithmetic

VAE for designing chemical compounds

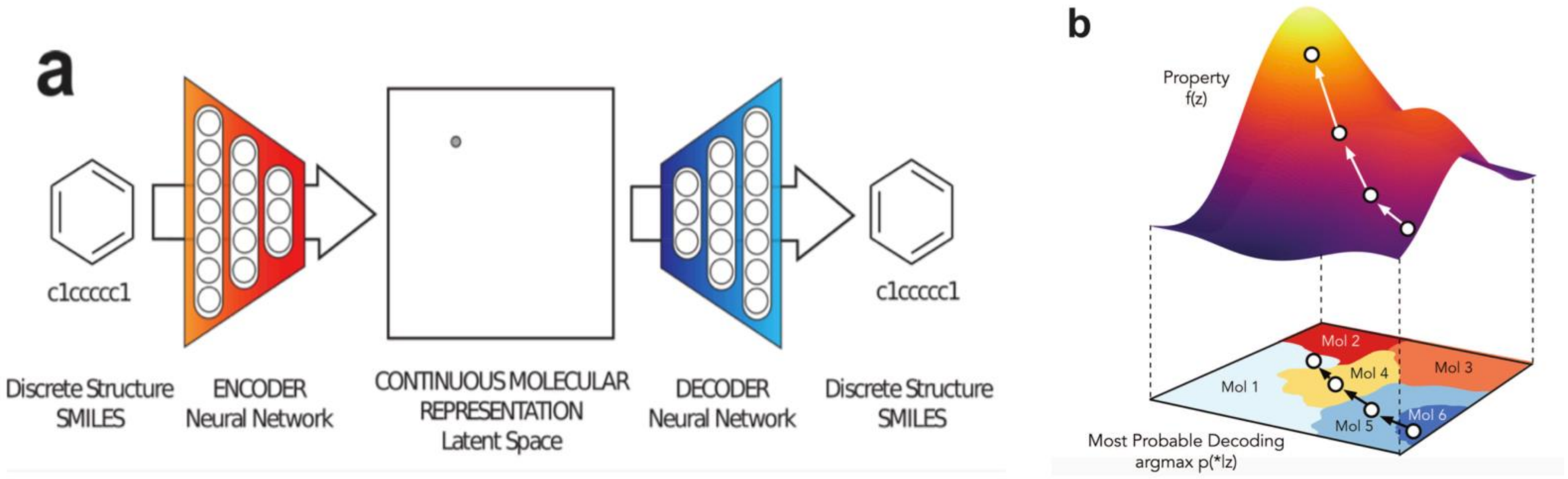


Figure 2.D.1: Example application of a VAE in [Gómez-Bombarelli et al., 2016]: design of new molecules with desired chemical properties. (a) A latent continuous representation $\mathbf{z}$ of molecules is learned on a large dataset of molecules. (b) This continuous representation enables gradient-based search of new molecules that maximizes some chosen desired chemical property given by objective function $f(\mathbf{z})$.

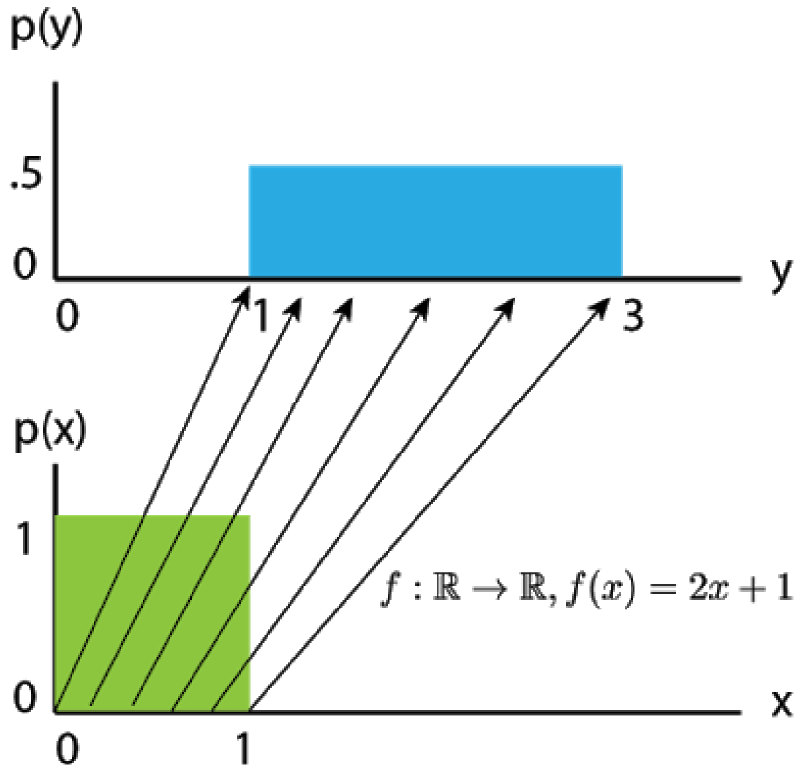
Summary

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

Normalizing Flows

https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf
https://blog.evjang.com/2018/01/nf1.html
https://arxiv.org/pdf/1505.05770.pdf

- Using simple pdfs, like a Gaussian, for the approximate posterior limits the expressivity of the model
- Better make sure the approximate posterior comes from a class of models that can even contain the true posterior
- Use a series of K invertible transformations to construct the approximate posterior
  - $z_k = f_k \circ f_{k-1} \circ \cdots f_1(z_0)$
  - Rule of change for variables



Changing from the x variable to y using the transformation $\mathrm{y} = f(x) = 2x + 1$

Normalizing Flows

https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf
https://blog.evjang.com/2018/01/nf1.html
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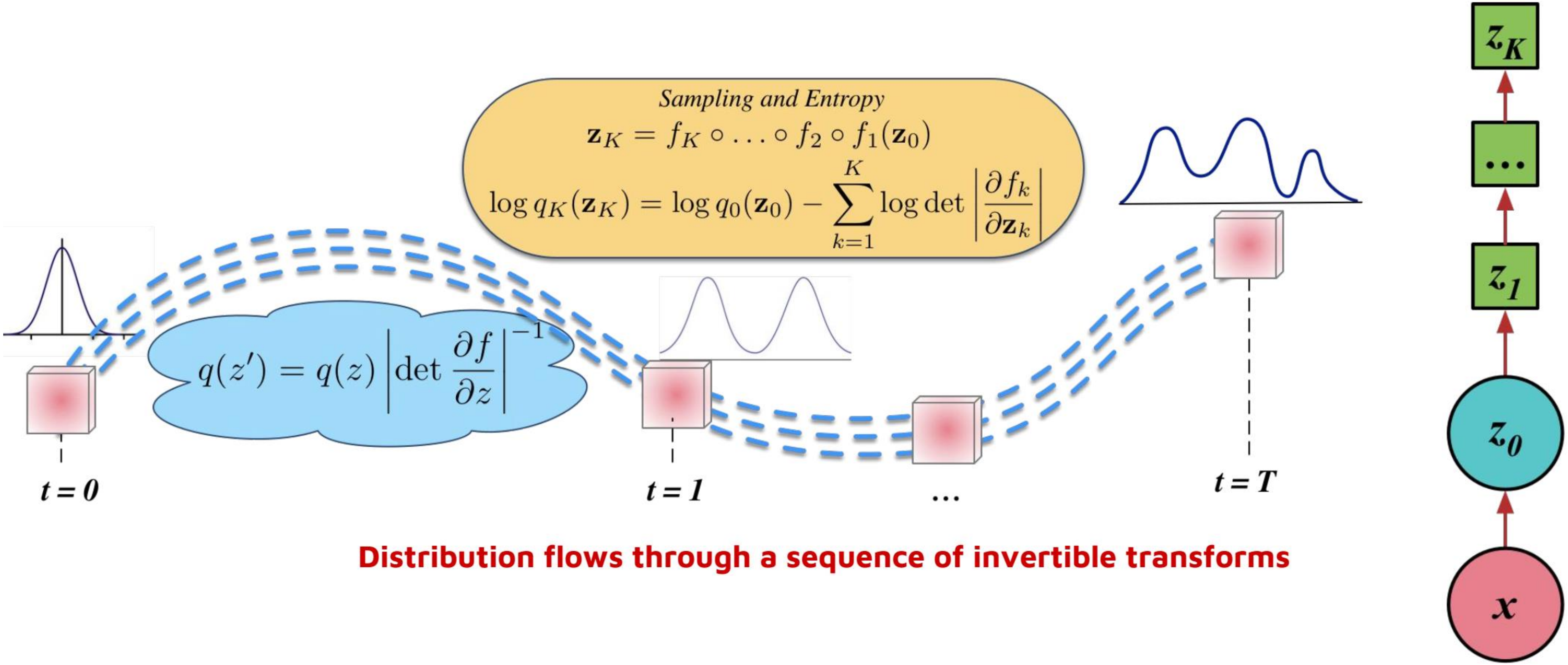
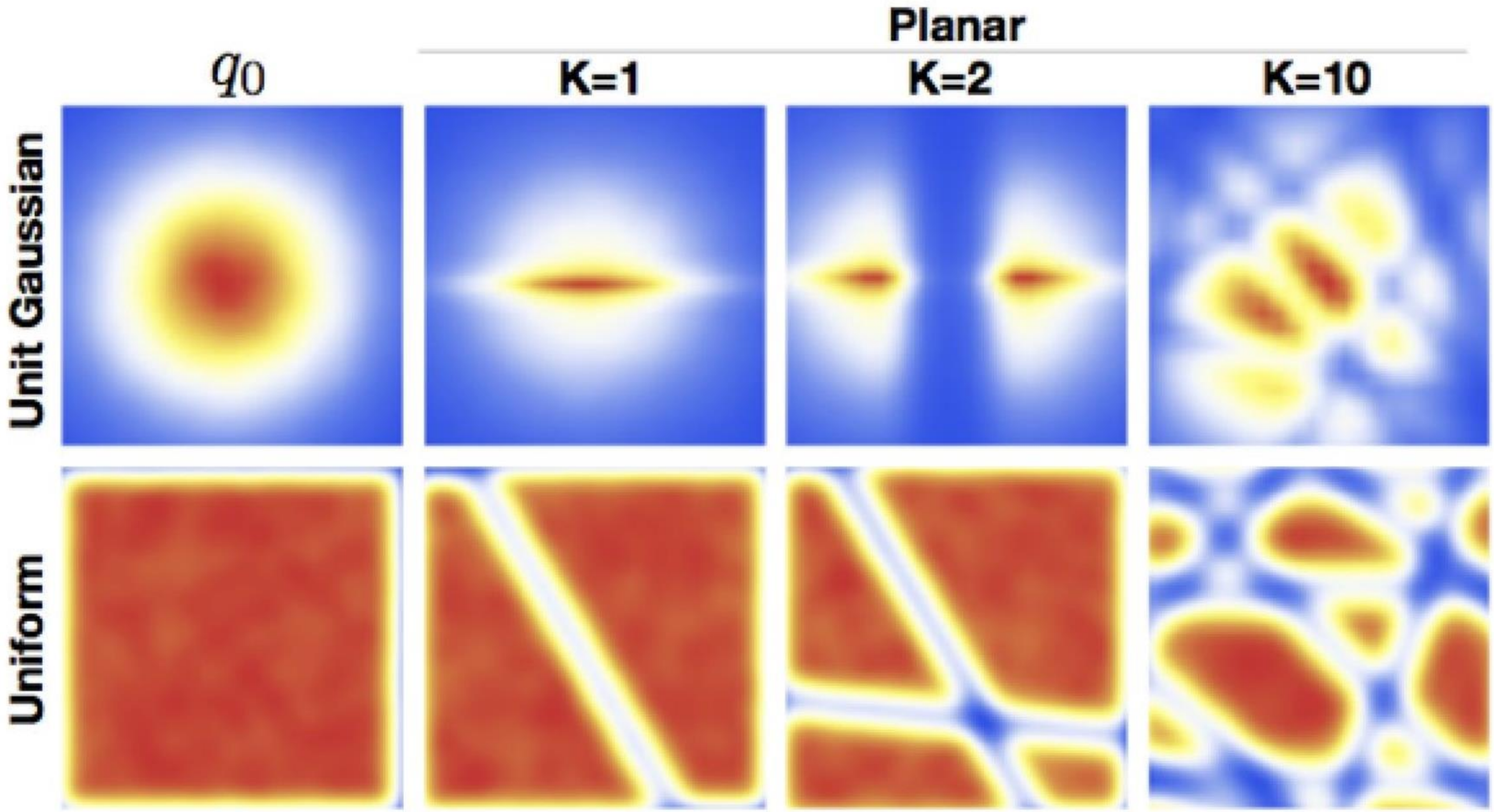


Distribution flows through a sequence of invertible transforms

Normalizing Flows



https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf

Normalizing Flows on Non-Euclidean Manifolds

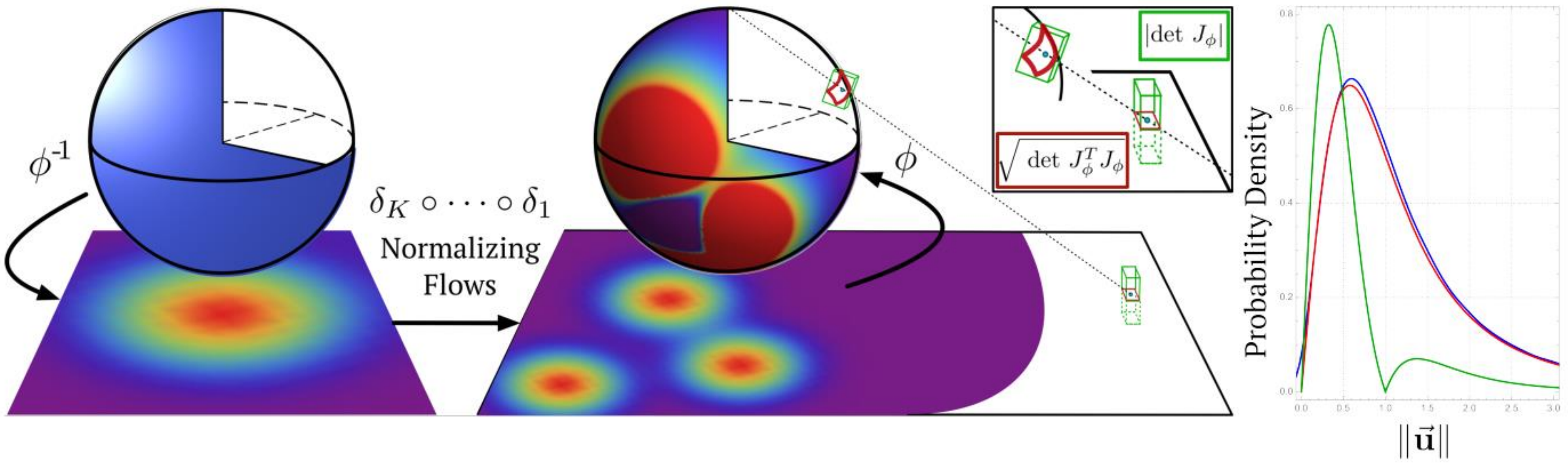


Figure 1: Left: Construction of a complex density on $\mathbf{S}^n$ by first projecting the manifold to $\mathbf{R}^n$, transforming the density and projecting it back to $\mathbf{S}^n$. Right: Illustration of transformed ($\mathbf{S}^2 \to \mathbf{R}^2$) densities corresponding to an uniform density on the sphere. Blue: empirical density (obtained by Monte Carlo); Red: Analytical density from equation (4); Green: Density computed ignoring the intrinsic dimensionality of $\mathbf{S}^n$.

$$\log q_K(\mathbf{z}_K) = \log q_0(\mathbf{z}_0) - \frac{1}{2}\sum_{k=1}^{K} \log\det\left|\mathbf{J}_\phi{}^\top \mathbf{J}_\phi\right|$$

Gemici et al., 2016

https://www.shakirm.com/slides/DeepGenModelsTutorial.pdf

Normalizing Flows on Non-Euclidean Manifolds