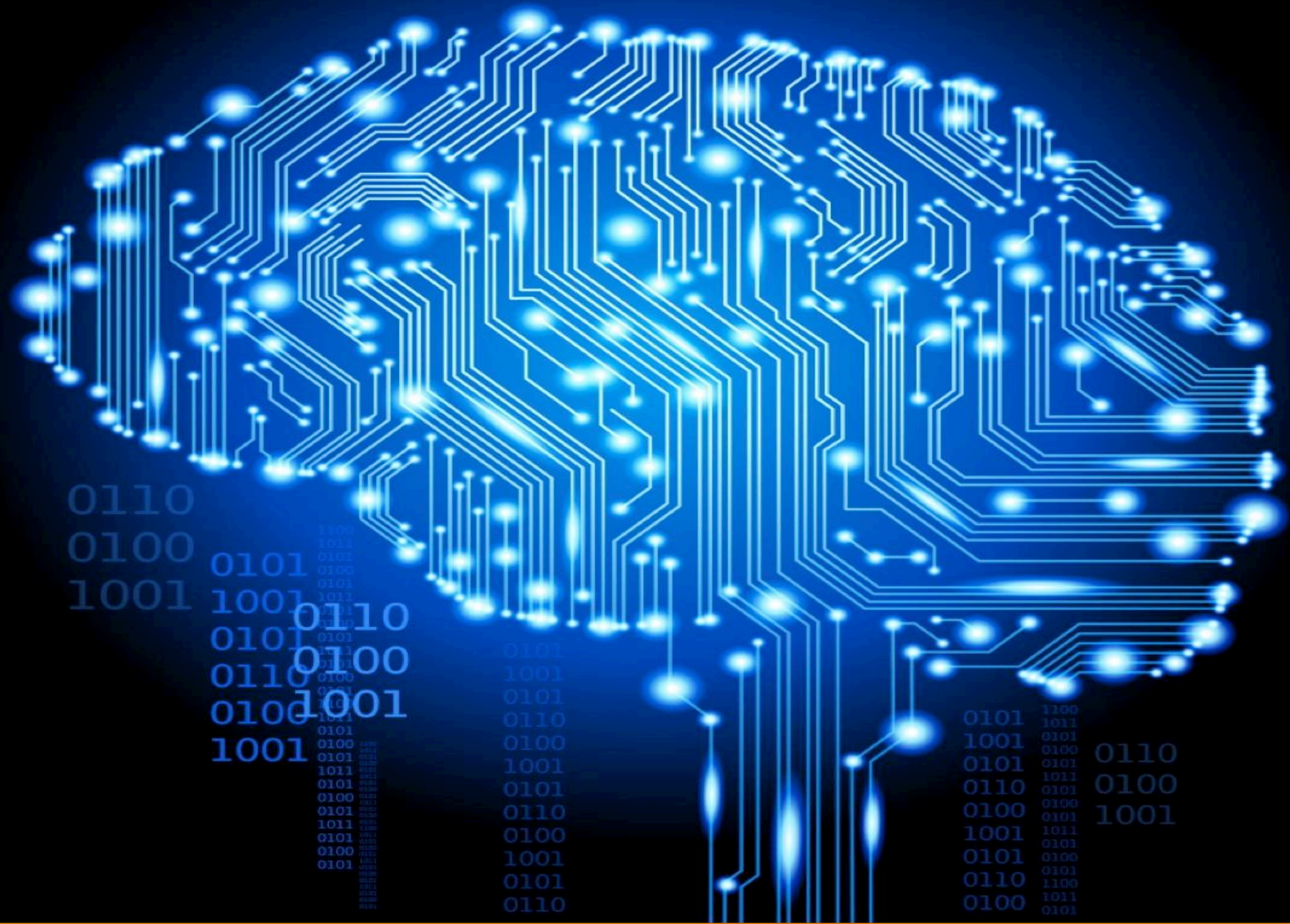

Lecture 9: Explicit Generative Models

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Lecture overview

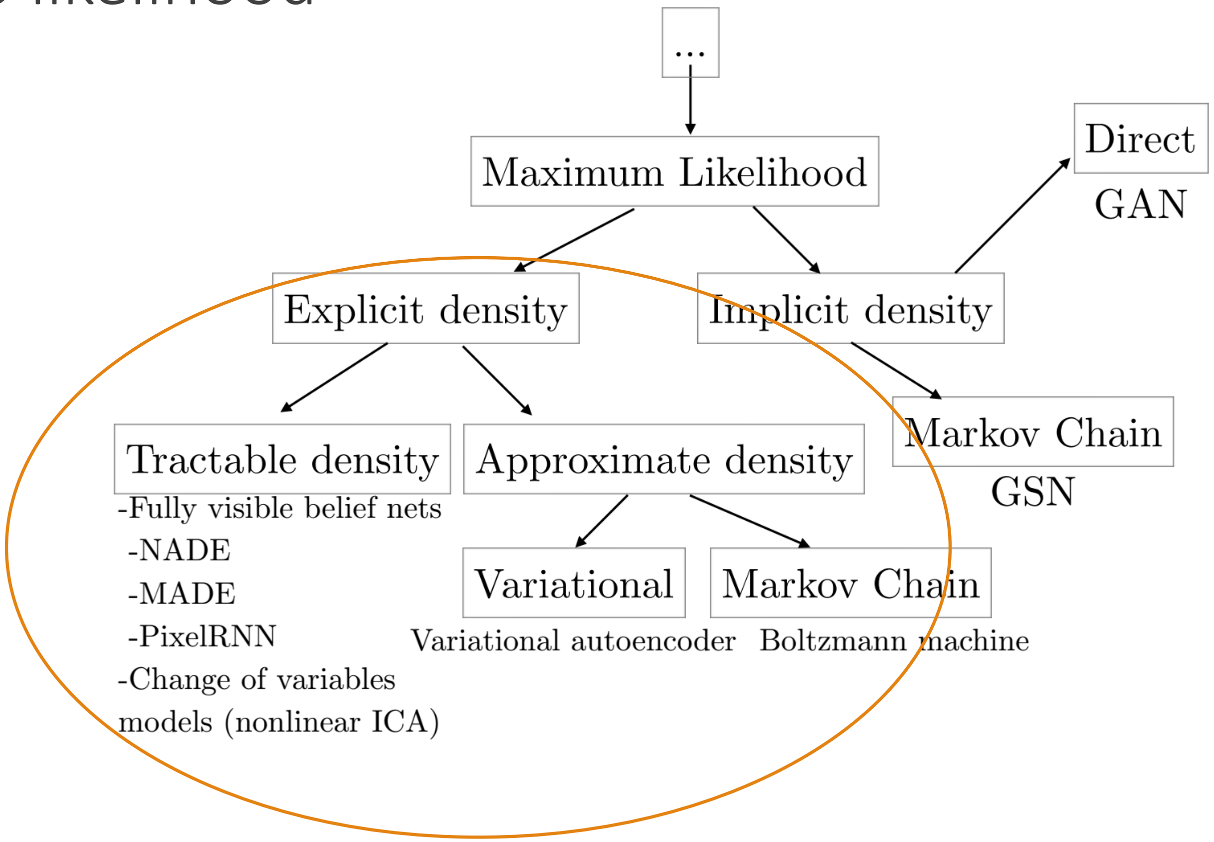
- Gentle intro to Bayesian Modelling and Variational Inference
- Restricted Boltzmann Machines
- Deep Boltzmann Machines
- Deep Belief Network
- Contrastive Divergence
- Variational Autoencoders
- Normalizing Flows

Explicit density models

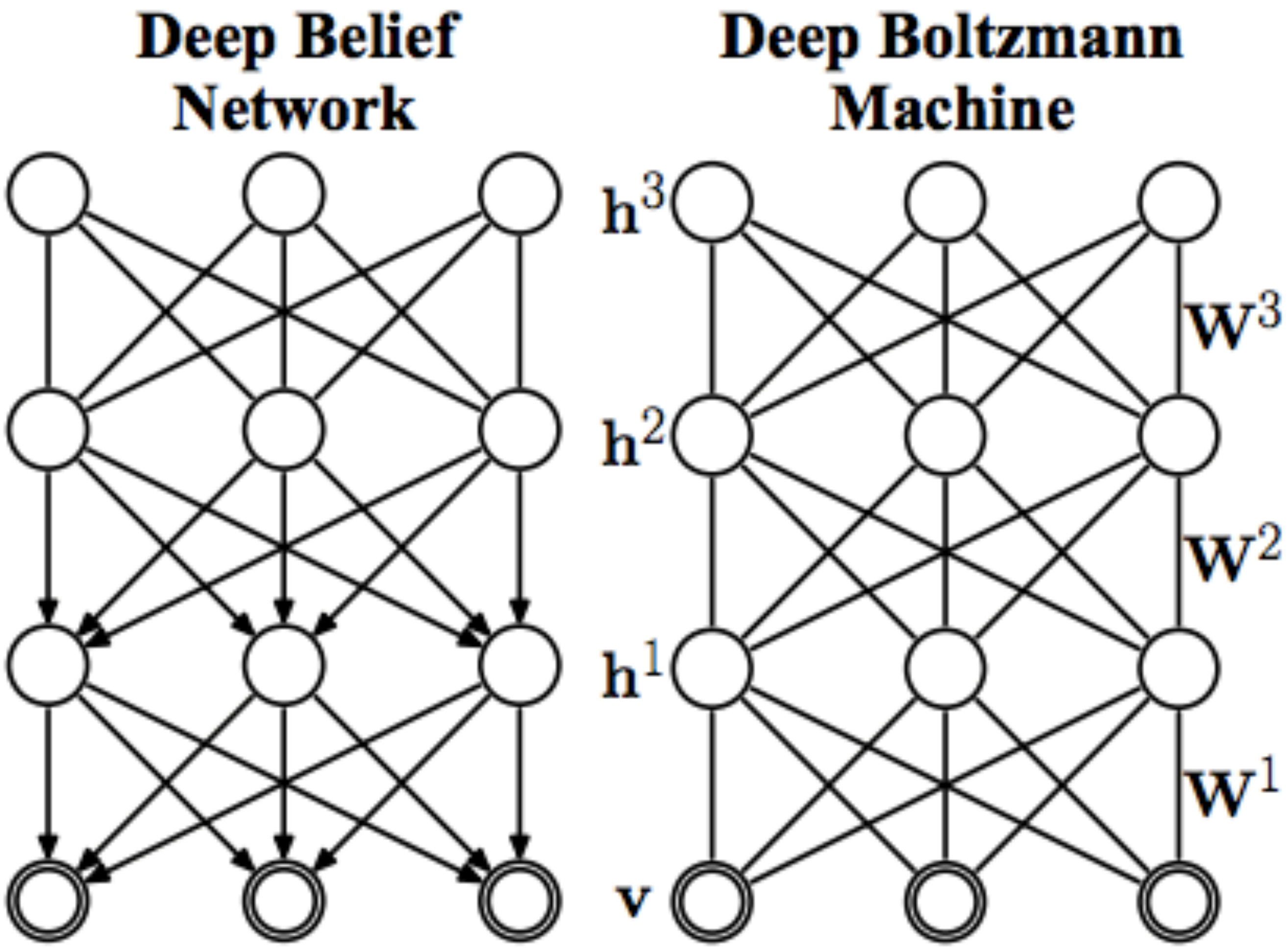
- Plug in the model density function to likelihood
- Then maximize the likelihood

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

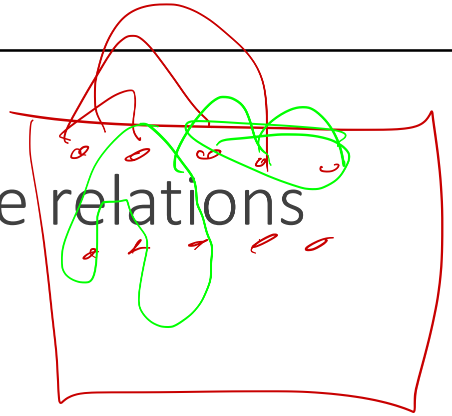


Bayesian Modelling
Variational Inference



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



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

$\psi_c(x_1, x_2) = w_1 x_1 x_2$

- Quite inefficient → think of all possible relations (not just pairwise) between $256 \times 256 = 65K$ input variables
- Solution: Define an energy function to model the relations between the inputs variables

Restricted Boltzmann Machines

0 1

- Boltzmann (or Gibbs) distribution defined over a free energy function $E(x)$

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

- Z is the normalization factor that makes sure $\int_x p(x)\,dx = 1$
  - Very expensive to compute → if $x = \{0,1\}$ computing Z requires 2^d computations
- Better restrict the model further to a bottleneck

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

pixel inputs

XWx

feature maps

Why Boltzmann?

- In statistical mechanics and mathematics, 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

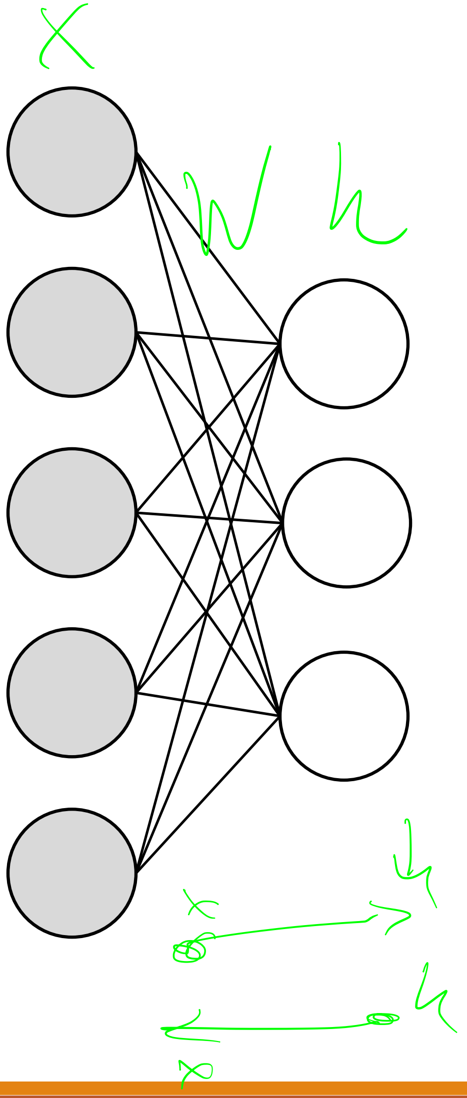
Restricted Boltzmann Machines

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

- $E(x) = -x^T W h - b^T x - c^T h, \quad \theta = \{W, b, c\}$

- The free energy function $F(x) = -\log \sum_h \exp(-E(x,h))$ defines a bipartite graph with undirected connections
  - Information flows forward and backward



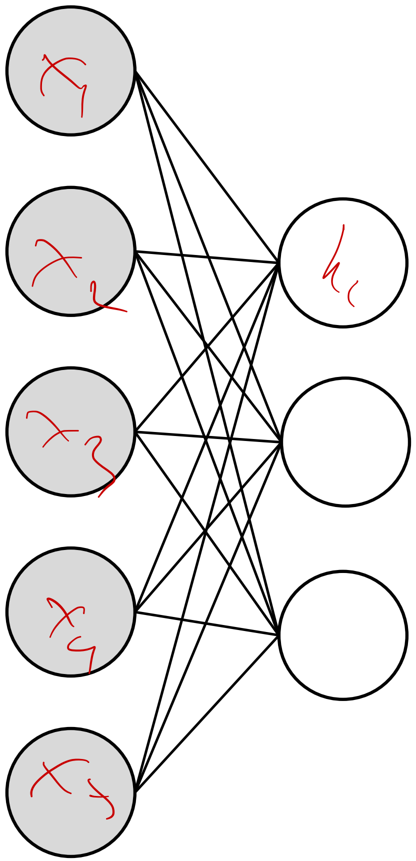
Restricted Boltzmann Machines

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

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

- 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

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

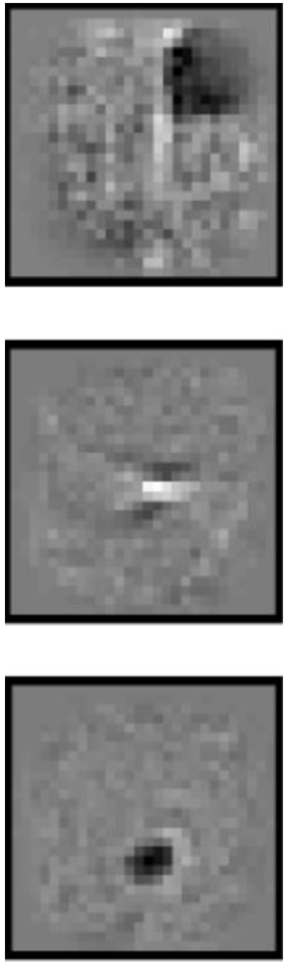
$\theta = \{w, b\}$

- Maximize log-likelihood

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

- 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

hard

- Let's take the gradients

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

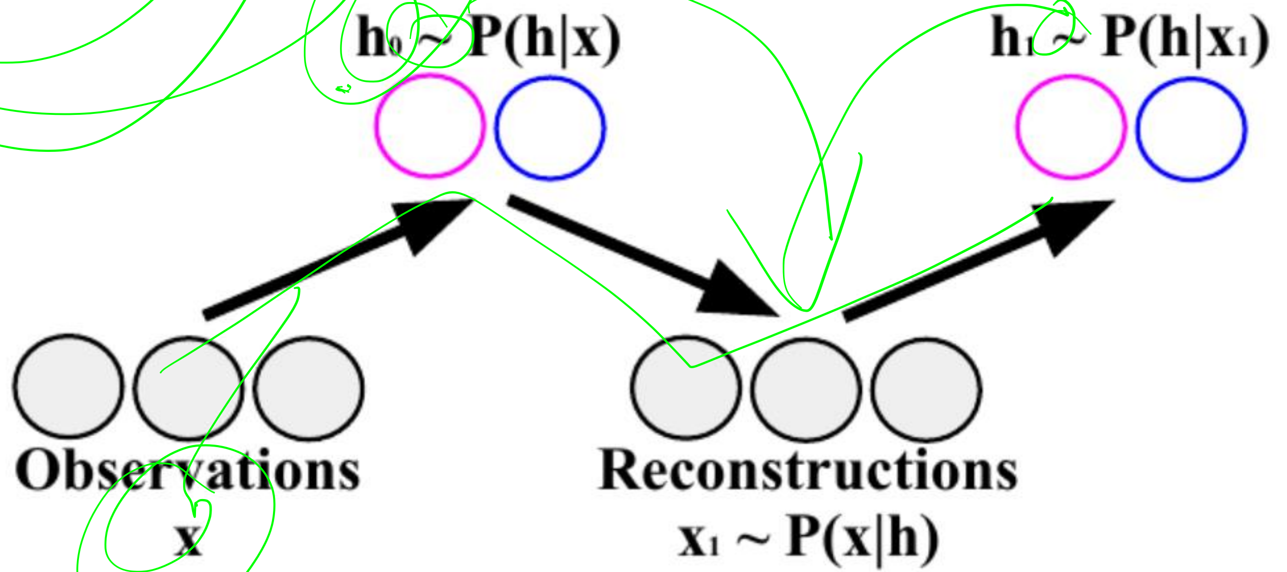
$$= -\sum_h p(h|x_n,\theta)\frac{\partial E(x_n|h,\theta)}{\partial \theta} + \sum_{\tilde{x},h} p(\tilde{x},h|\theta)\frac{\partial E(\tilde{x},h|\theta)}{\partial \theta}$$

- 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

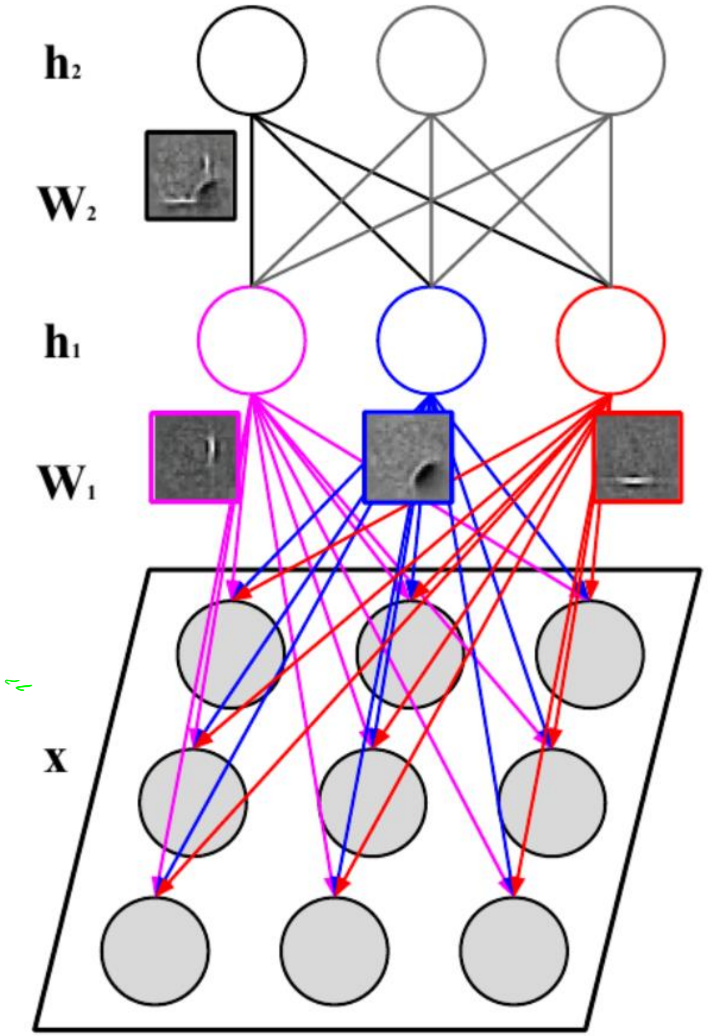
- RBMs are just one layer
- Use RBM as a building block
- Stack multiple RBMs one on top of the other

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

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

2

1

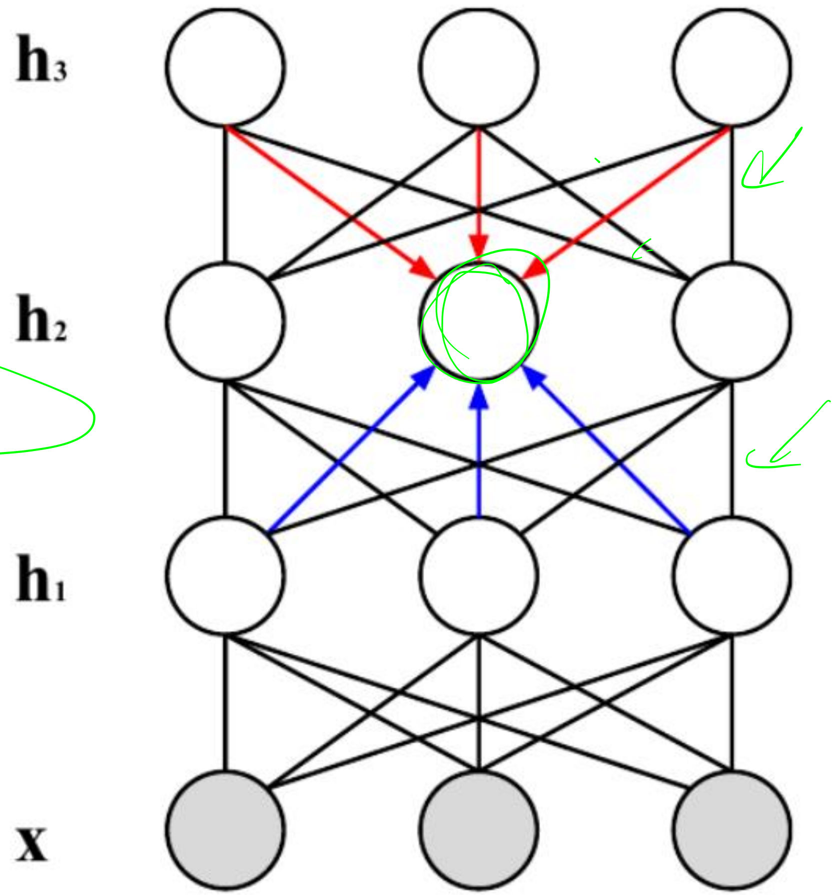


Deep Boltzmann Machines

- 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

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

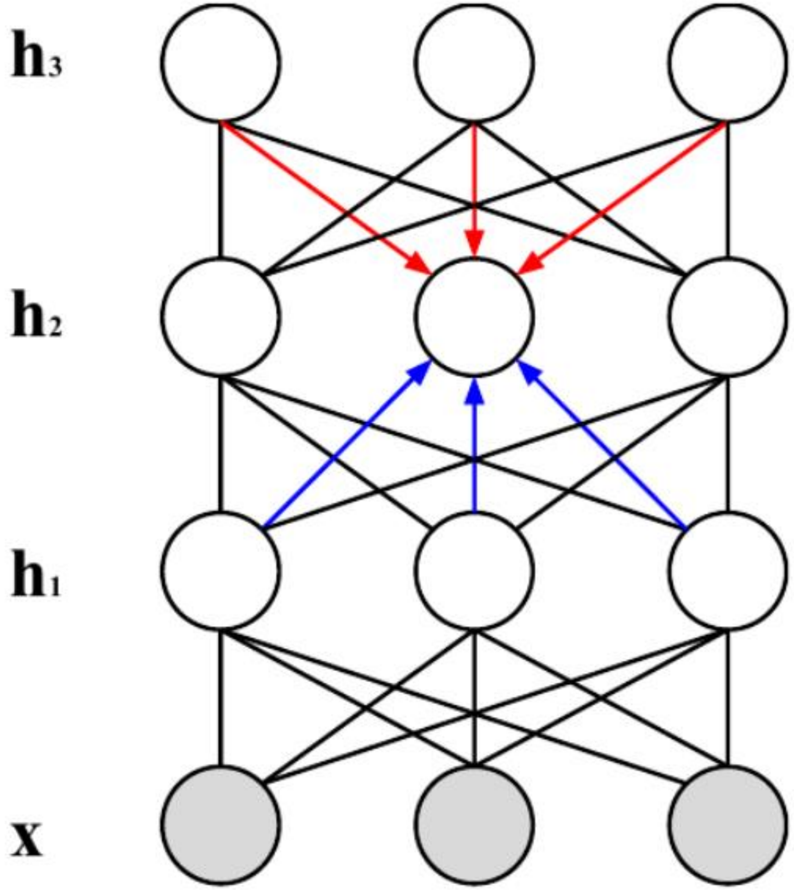
$$p(h_2^k|h_1, h_3) = \sigma(\sum_j W_1^{jk} h_1^j + \sum_l W_3^{kl} h_3^k)$$



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

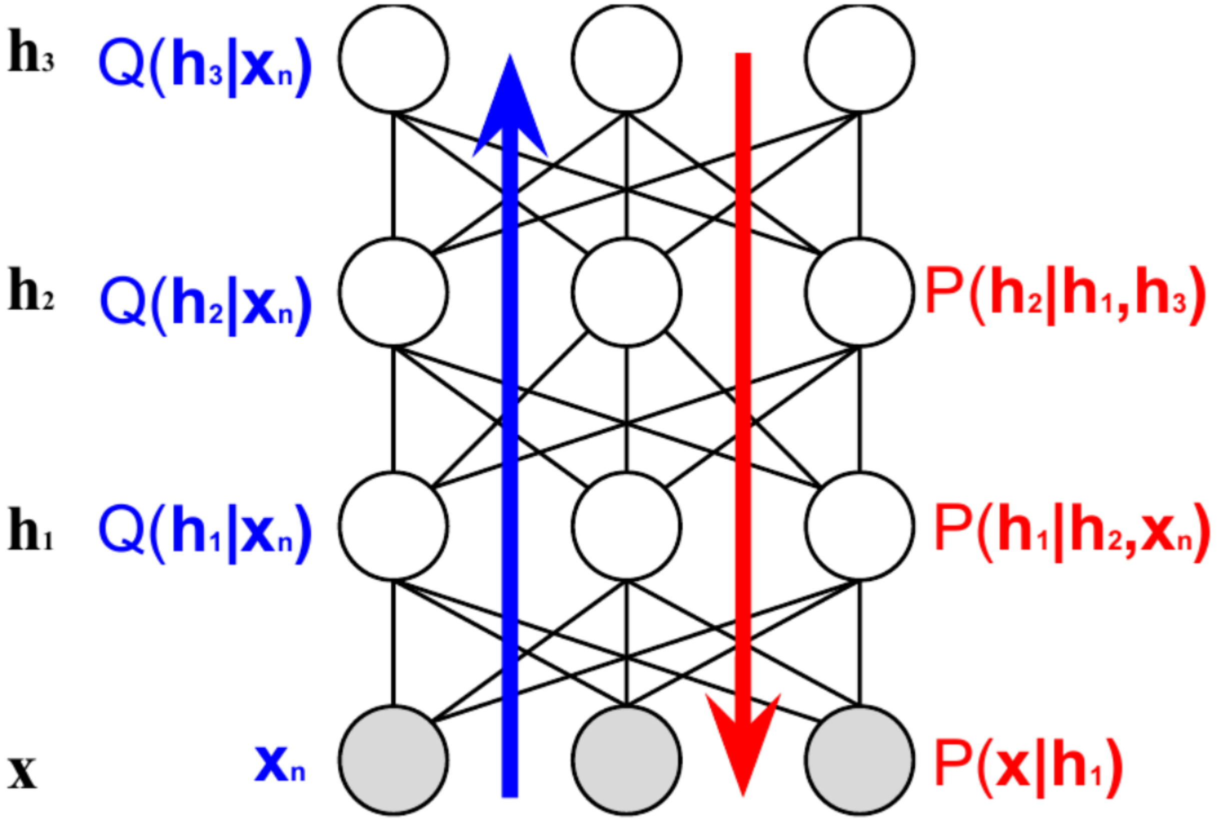
$$p(h_2^k | h_1, h_3) = \sigma(\sum_j W_1^{jk} h_1^j + \sum_l W_3^{kl} h_3^k)$$



Training Deep Boltzmann Machines

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

DBM

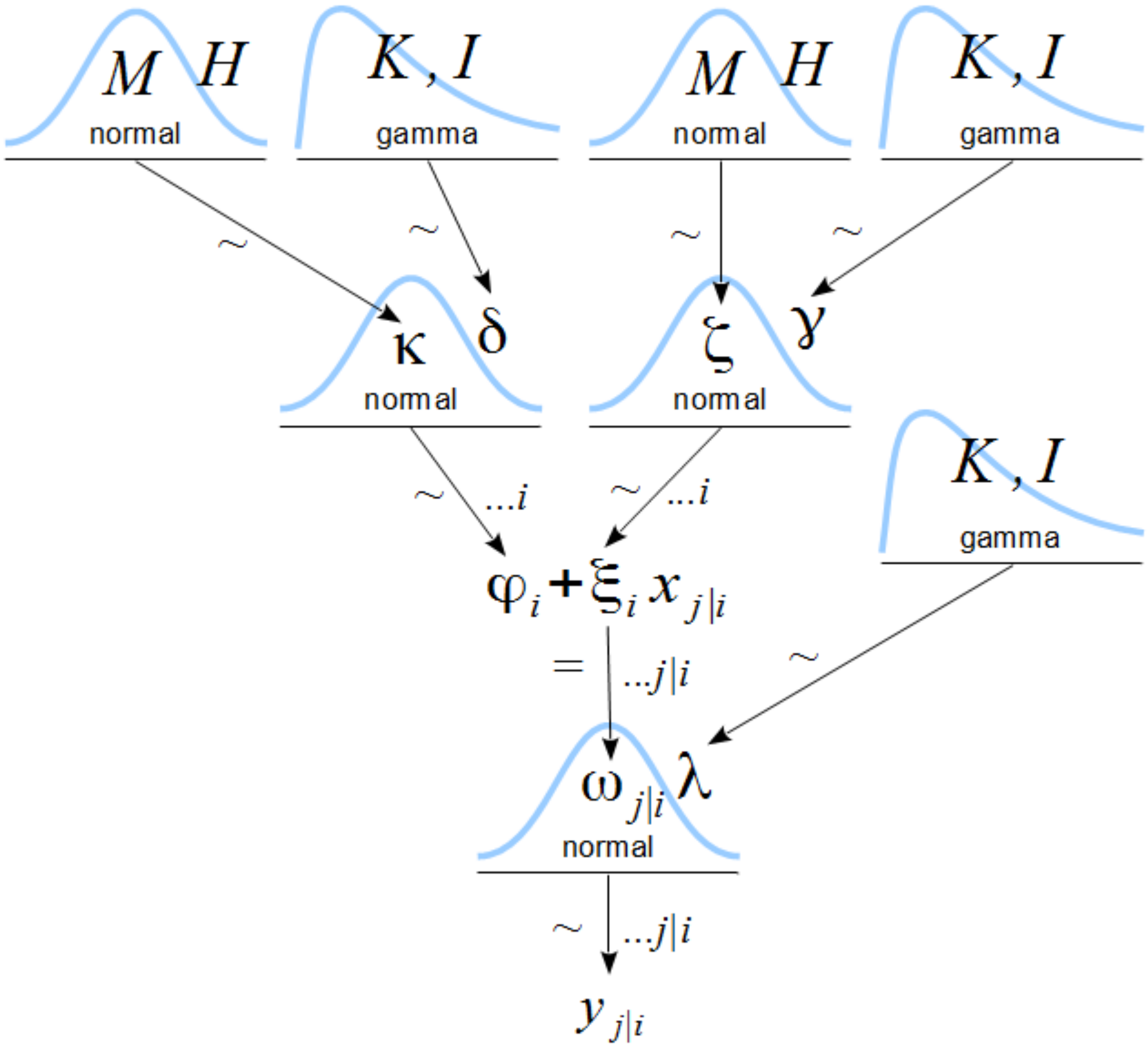


Standard NN

FP

BP

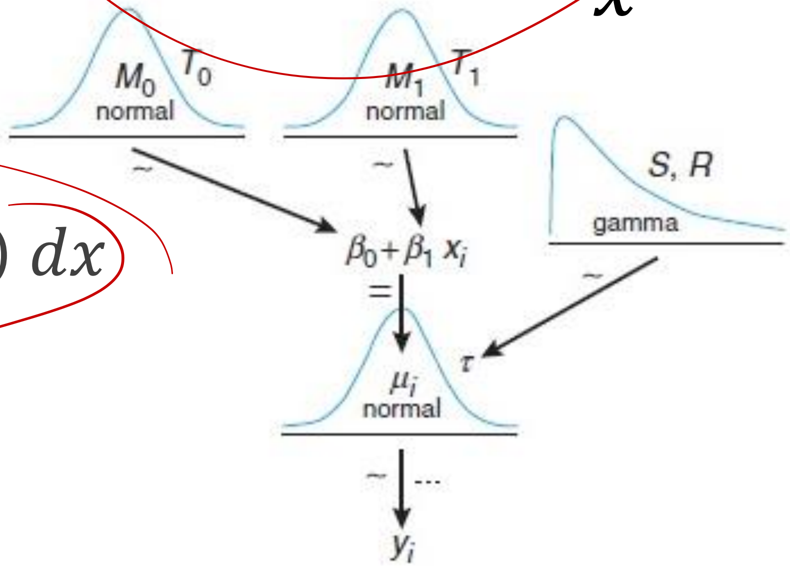
Bayesian Modelling
Variational Inference



Bayesian 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

Bayes Rule

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

$$p(\theta|x) =$$

1. $$= \frac{p(x,\theta)}{p(x)}$$ ← Conditional probability

2. $$= \frac{p(x|\theta)\, p(\theta)}{p(x)}$$ ← Bayes Rule

3. $$= \frac{p(x|\theta)\, p(\theta)}{\int_{\theta'} p(x, \theta')\; d\theta'}$$ ← Marginal probability

4. $$\boxed{\propto p(x|\theta)\, p(\theta)}$$ ← $p(x\ )$ is constant

- Posterior Predictive pdf

$$p(\cancel{x}_{new}|\cancel{x}) = \int_{\theta} p(\cancel{x}_{new}|\theta)\, p(\theta|\cancel{x})\, d\theta$$

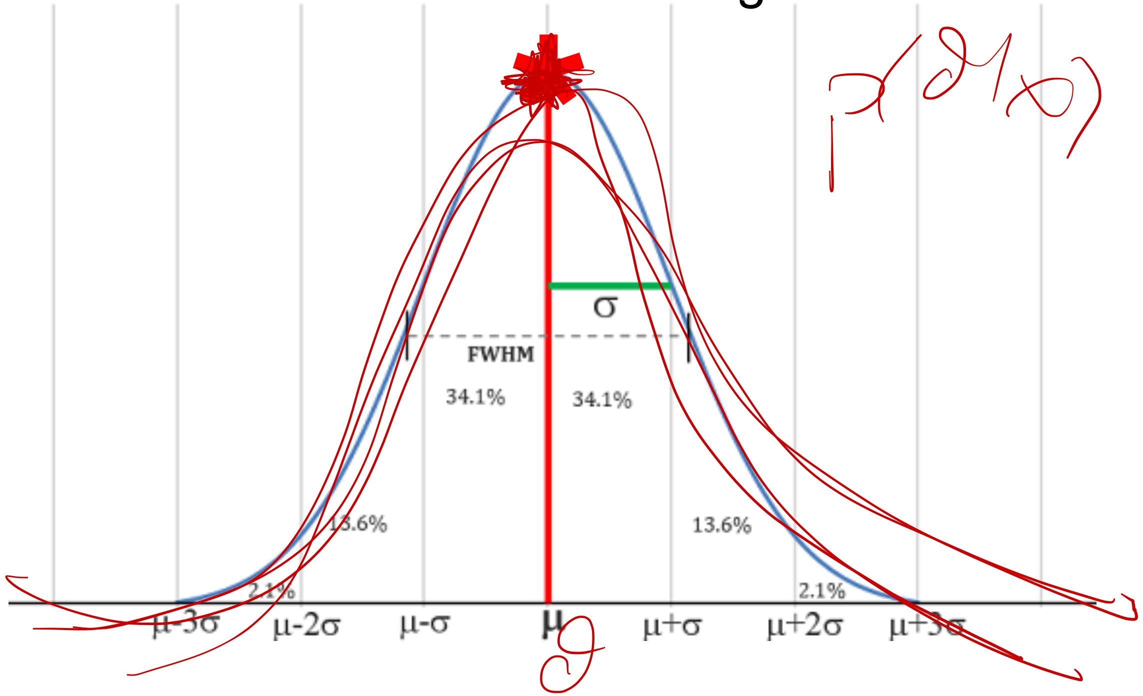
Bayesian Terminology

- 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)

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

  - 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)

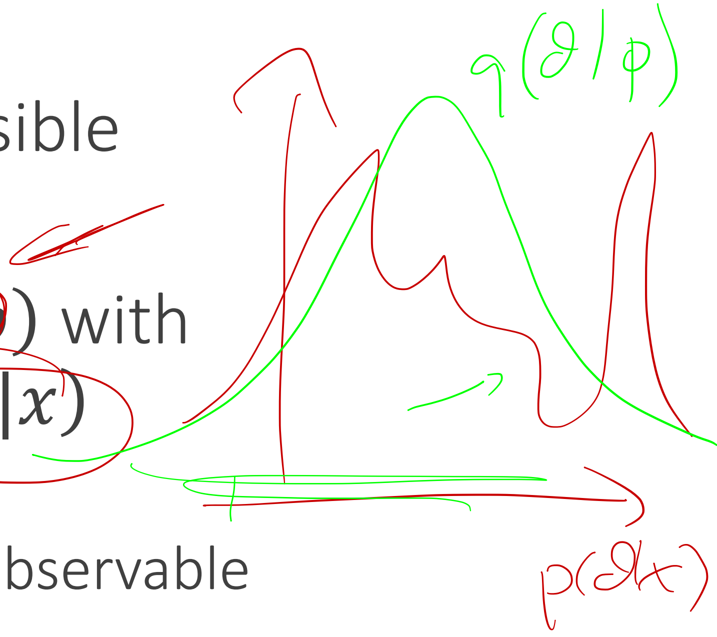
- But how to estimate the posterior density?
  - Markov Chain Monte Carlo (MCMC) → Simulation-like estimation
  - Variational Inference → Turn estimation to optimization

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

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

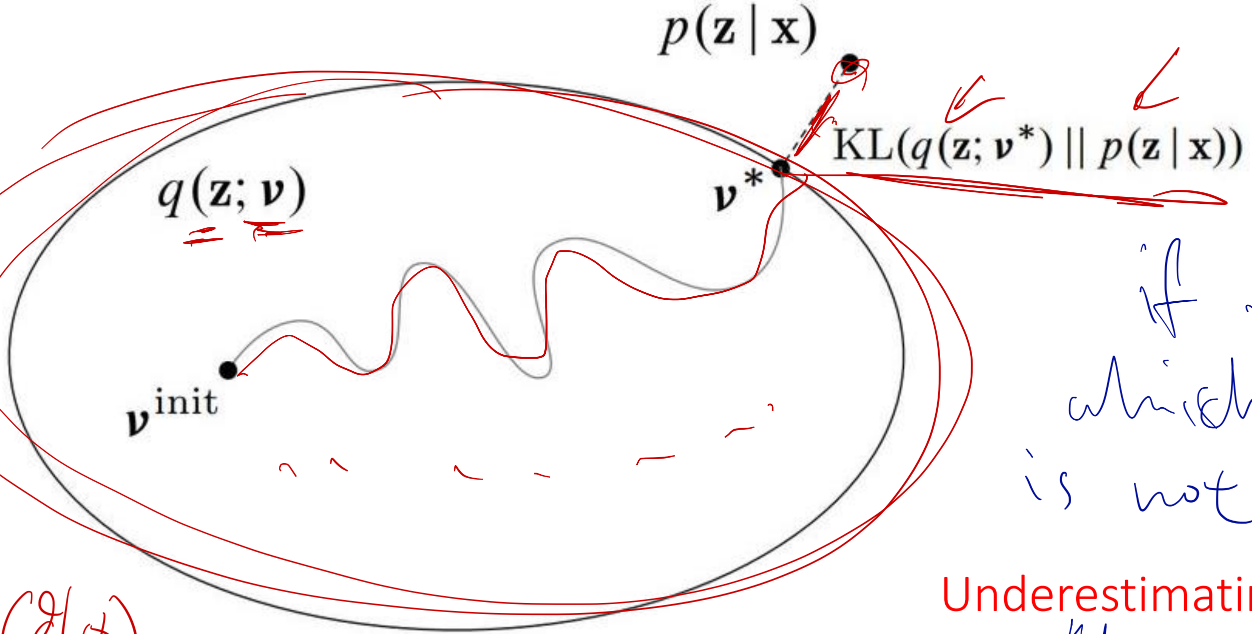
- Turn inference into optimization



Variational Inference (graphically)

Forward KL

$\sum_p \log \frac{p}{q}$



$= \sum_q \log \frac{q}{p}$

if $p=0$ and q which is an approx is not 0 $\log \frac{q}{p}$ ↗

Underestimating variance. Why?

model

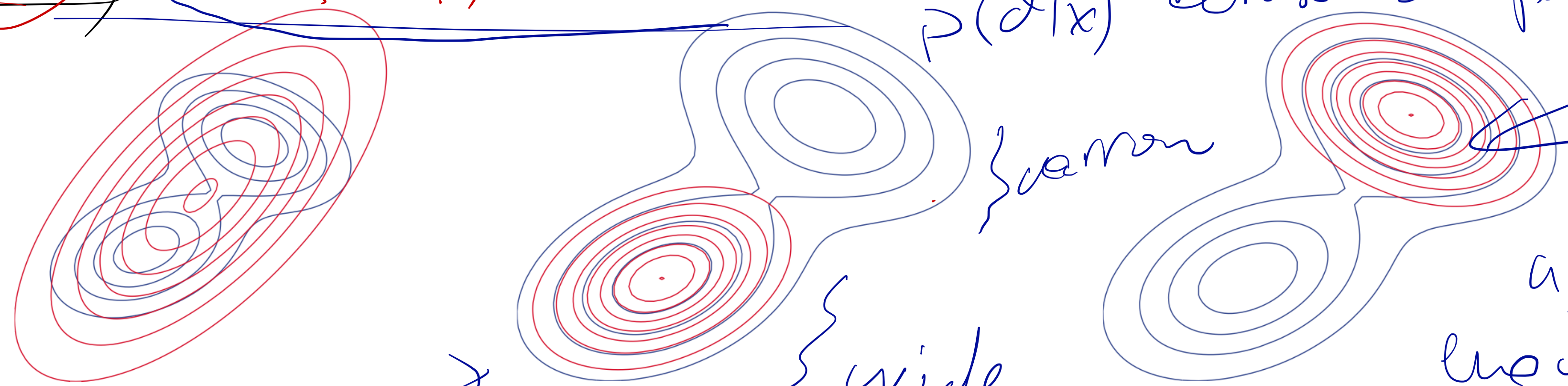
model

$q(\vartheta|\phi)$

$p(\vartheta|x)$

Reverse KL

prefer to set $q=0$ when it cannot approximate well enough p.

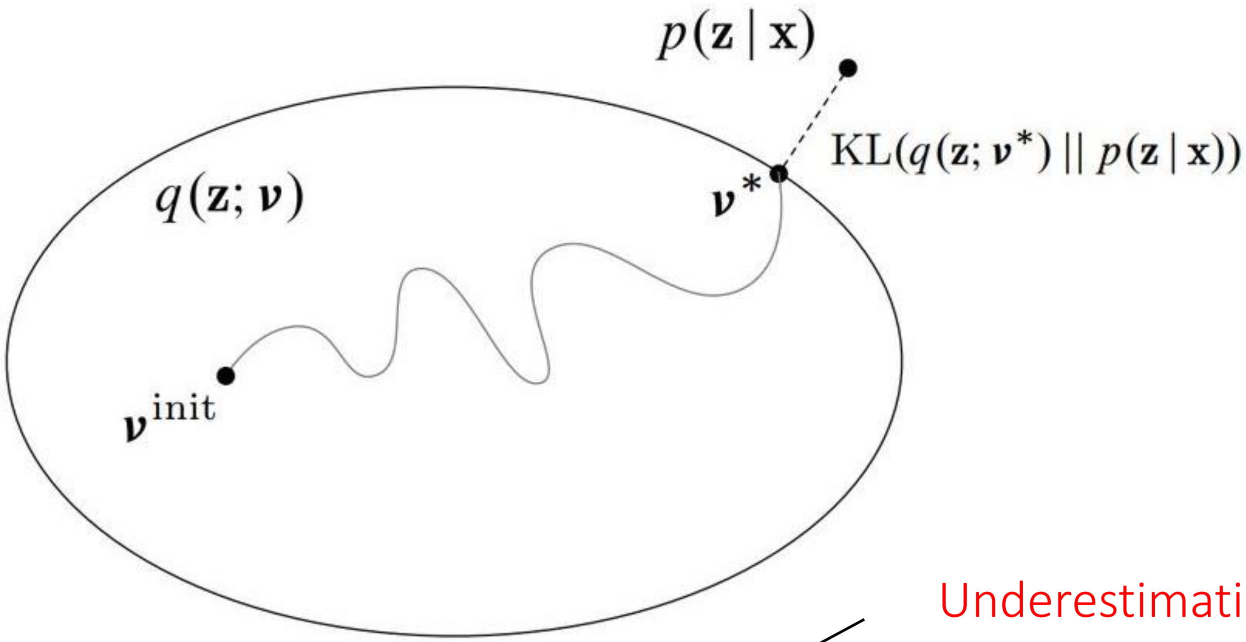


narrow

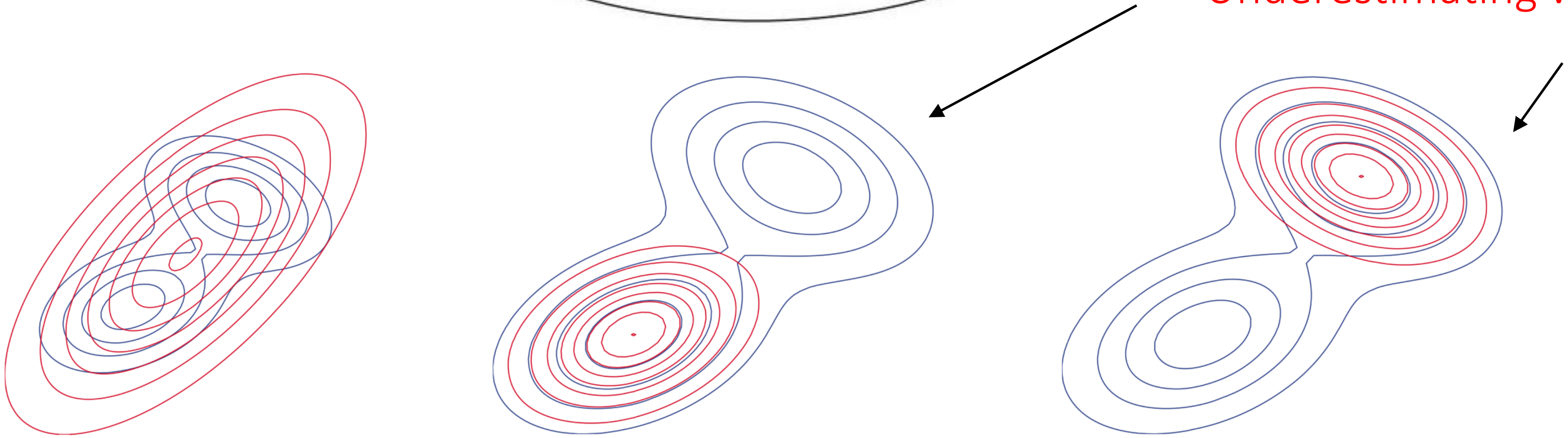
wide

overestimation

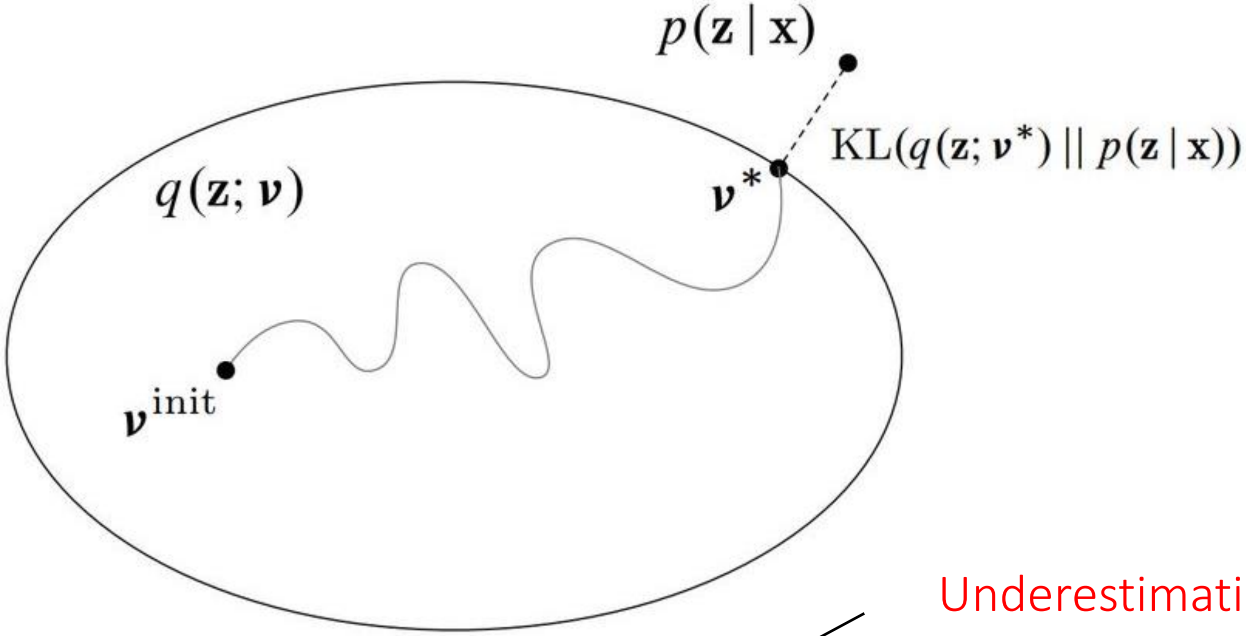
Variational Inference (graphically)



Underestimating variance. Why?

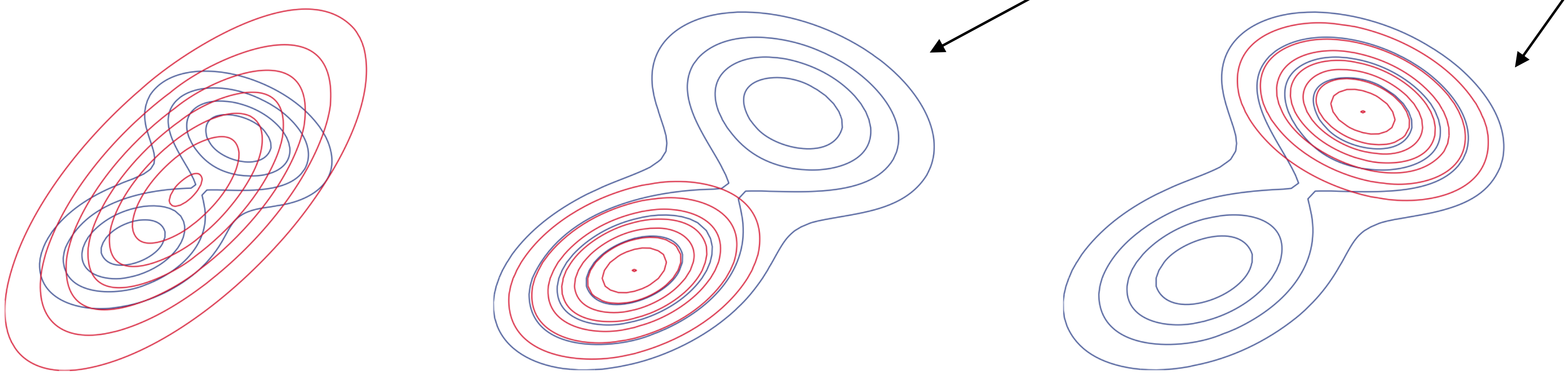


Variational Inference (graphically)

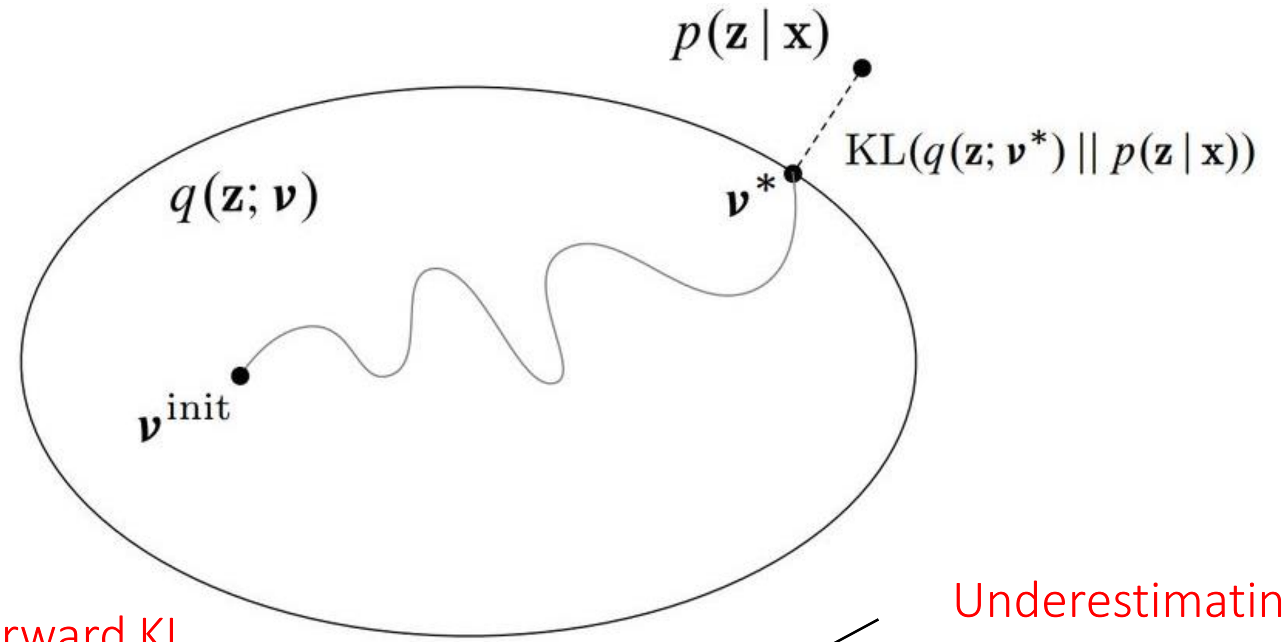


Underestimating variance. Why?

How to overestimate variance?

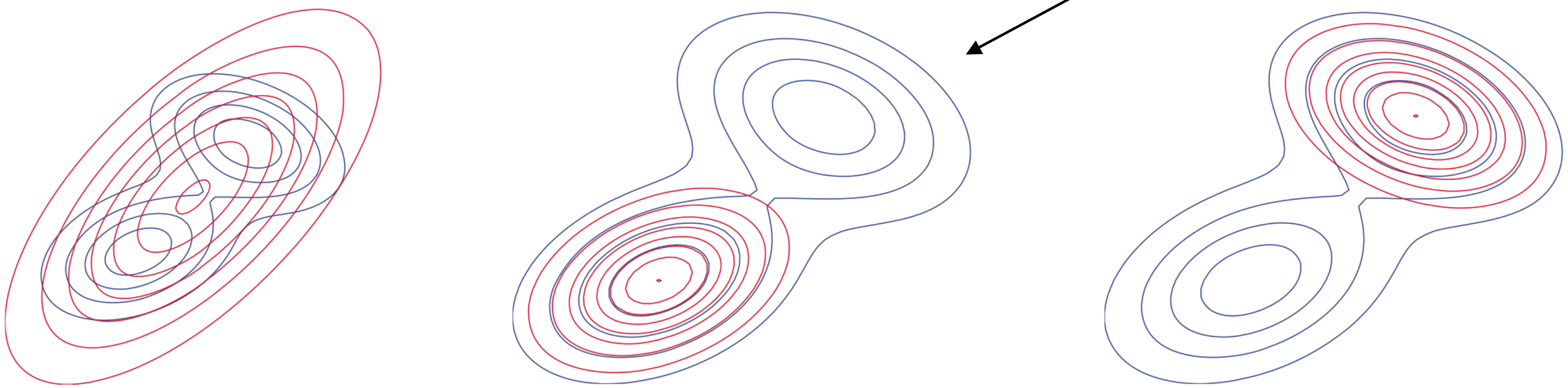


Variational Inference (graphically)



How to overestimate variance? Forward KL

Underestimating variance. Why?



Mean-Field Approximation and CAVI Optimization

- To make the optimization of the VI easier, one can assume the latent variables are independent of each other

$$q(\theta|\varphi) = \prod_j q_j(\theta_j|\varphi_j)$$

- The optimization is often done with CAVI
  - Coordinate-Ascent Variational Inference
  - Initially set φ randomly
  - For each j in turn you set $q_j(\theta_j|\varphi_j) = \mathbb{E}_{g_{-j}}[\log p(\theta|x)]$

Variational Inference - Evidence Lower Bound (ELBO)

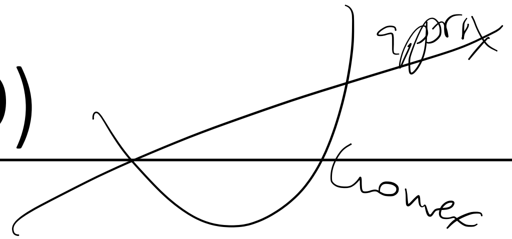
- Given latent variables θ and the approximate posterior
$$q_\varphi(\theta) = q(\theta|\varphi)$$
- The log marginal is
$$\log p(x) = \log \int_\theta p(x,\theta)\, d\theta$$
$$= \log \int_\theta p(x,\theta) \frac{q_\varphi(\theta)}{q_\varphi(\theta)}\, d\theta$$
$$= \log \mathbb{E}_{q_\varphi(\theta)}\left[\frac{p(x,\theta)}{q_\varphi(\theta)}\right]$$
$$\leq \mathbb{E}_{q_\varphi(\theta)}\left[\log \frac{p(x,\theta)}{q_\varphi(\theta)}\right]$$

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

or

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

Variational Inference - Evidence Lower Bound (ELBO)



- Given latent variables $\boldsymbol{\theta}$ and the approximate posterior
$$q_\varphi(\theta) = q(\theta|\varphi)$$
- The log marginal is

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

multiply and divide by $q(\theta|\phi)$

$$= \log \int_\theta p(x,\theta) \frac{q(\theta|\phi)}{q(\theta|\phi)}\, d\theta$$

by definition of Expect.

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

Jensen ineq.

$$\le \mathbb{E}_{q(\theta|\phi)}\left[\log \frac{p(x,\theta)}{q(\theta|\phi)}\right]$$

A

$$= \mathbb{E}_{q(\theta|\phi)}[\log p(x,\theta)] \underbrace{- \mathbb{E}_{q(\theta|\phi)}[\log q(\theta|\phi)]}_{H(q)}$$

$$= \underbrace{\mathbb{E}_{q(\theta|\phi)}[\log p(x,\theta)] - H(q)}_{\mathrm{ELBO}(\theta,\phi)}$$

B

$$= \mathbb{E}_{q(\theta|\phi)}[\log p(x|\theta)] - \mathbb{E}_{q(\theta|\phi)}[\log p(\theta)] + \mathbb{E}_{q(\theta|\phi)}[\log q_\phi(\theta)]$$

$$= \mathbb{E}_{q(\theta|\phi)}[\log p(x|\theta)] - KL(q(\theta|\phi)\,\|\,p(\theta))$$

ELBO

ELBO and the marginal

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

$$\mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) =$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(x,\theta)] - \mathbb{E}_{q_\varphi(\theta)}\left[\log q_\varphi(\theta)\right]$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(\theta|x)] + \mathbb{E}_{q_\varphi(\theta)}[\log p(x)] - \mathbb{E}_{q_\varphi(\theta)}\left[\log q_\varphi(\theta)\right]$$
$$= \mathbb{E}_{q_\varphi(\theta)}[\log p(x)] - KL(q_\varphi(\theta)||p(\theta|x))$$
$$= \log p(x) - KL(q_\varphi(\theta)||p(\theta|x)) \qquad \leftarrow \log p(x) \text{ does not depend on } q_\varphi(\theta)$$
$$\Rightarrow \qquad \leftarrow \mathbb{E}_{q_\varphi(\theta)}[1]=1$$
$$\log p(x) = \mathrm{ELBO}_{\theta,\varphi}(\mathrm{x}) + KL(q_\varphi(\theta)||p(\theta|x))$$

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

ELBO and the marginal

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

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

ELBO interpretations

- $\log p(x) = \text{ELBO}_{\theta,\varphi}(\text{x}) + KL(q_\varphi(\theta)||p(\theta|x))$
- The log-likelihood is constant, as it does not depends on any parameter
- Also, both $\text{ELBO}_{\theta,\varphi}(\text{x}) > 0$ and $KL(q_\varphi(\theta)||p(\theta|x)) > 0$

1. The higher the Variational Lower Bound $\text{ELBO}_{\theta,\varphi}(\text{x})$, 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 $\text{ELBO}_{\theta,\varphi}(\text{x})$ approaches the log-likelihood → better density model

Amortized Inference

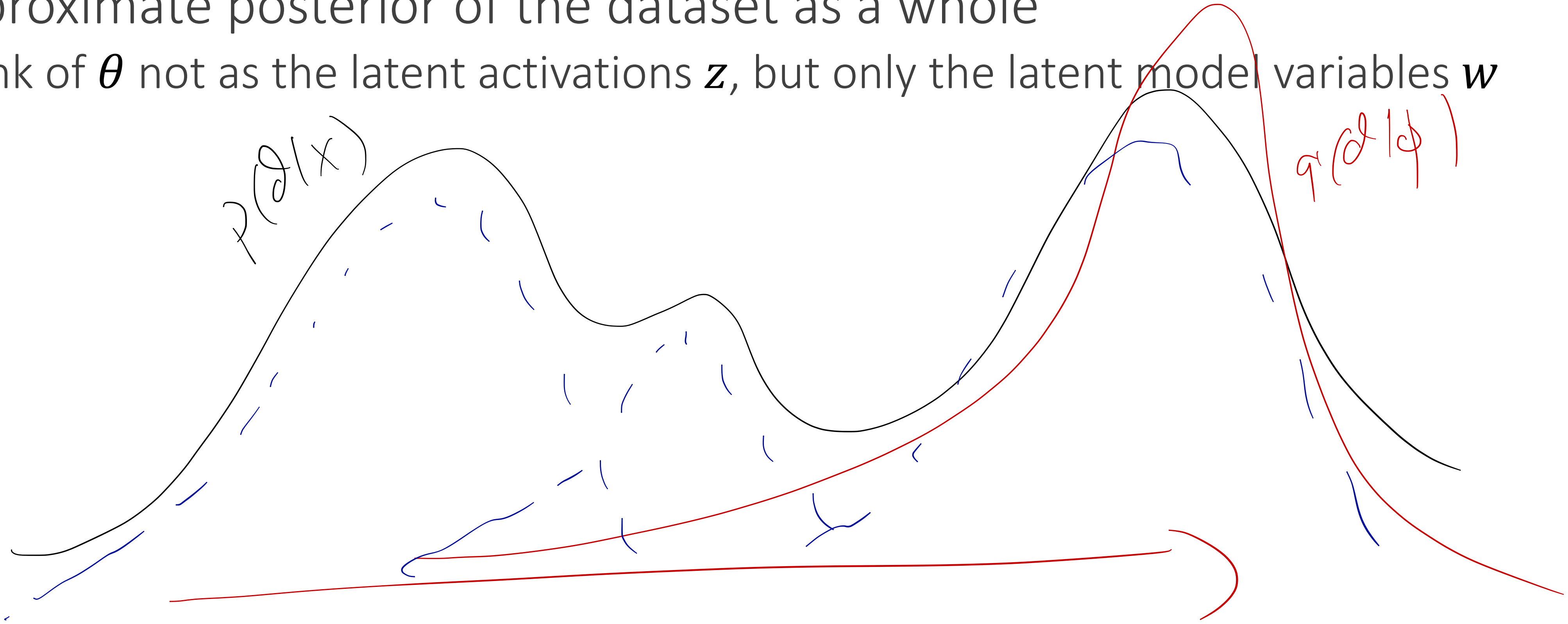
- The variational distribution $q(\theta|\varphi)$ does not depend directly on data
  - Only indirectly, via minimizing its distance to the true posterior $KL(q(\theta|\varphi)||p(\theta|x))$
- So, with $q(\theta|\varphi)$ we have a major optimization problem, as the approximate posterior must approximate the whole dataset $x = [x_1, x_2, \ldots, x_N]$ jointly
- As this is obviously quite complex, one can amortize the optimization on individual data points by setting

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

- Predict model parameters θ using a φ-parameterized model of the input x
- Use it for parameters that depend on data, such as the latent activations

Amortized Inference (Intuitively)

- Originally, Variational Inference assumed that $q(\theta|\varphi)$ describes the approximate posterior of the dataset as a whole
  - Think of θ not as the latent activations z, but only the latent model variables w



Variational Autoencoders

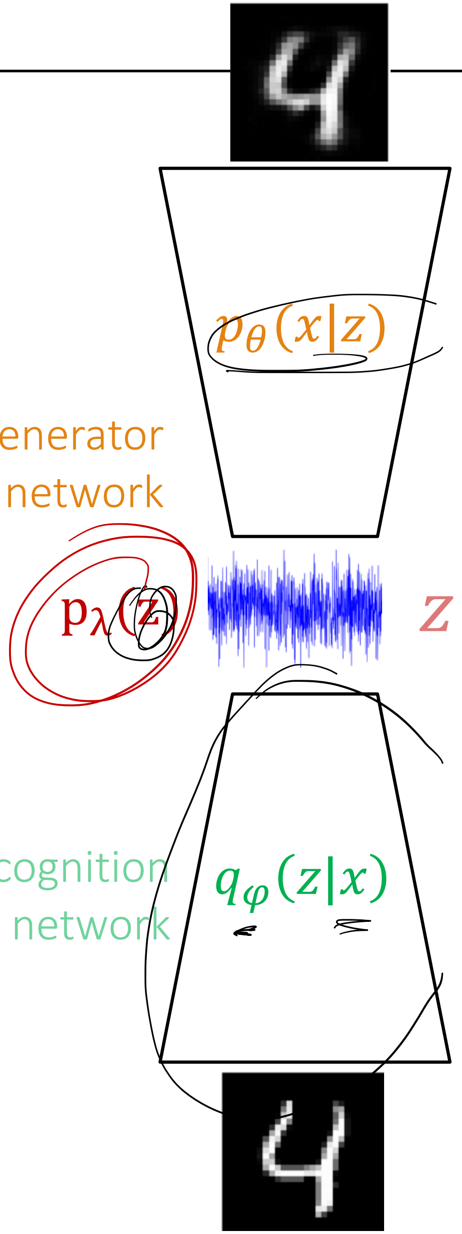
- Let's rewrite the ELBO a bit more explicitly

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

- Instead of $p(x|\theta)$ we have $p_\theta(x|z)$ to indicate that the model for the ~~posterior~~ density has weights parameterized by θ and latent model activations parameterized by z
- Instead of $\text{p}(\theta)$ we have $\text{p}_\lambda(\text{z})$, namely we put a λ-parameterized prior only on the latent activations z and not the model weights
- Instead of $q(\theta|\varphi)$ we have $q_\varphi(z|x)$ to indicate that the model approximates the posterior density of the latent activations, and the model weights are parameterized by φ

Variational Autoencoders

- So, we have $\text{ELBO}_{\theta,\varphi}(x) = \mathbb{E}_{q_\varphi(z|x)}[\log p_\theta(x|z)] - \text{KL}(q_\varphi(z|x) || \mathrm{p}_\lambda(\mathrm{z}))$
- What if we model the densities $p_\theta(x|z)$ and $q_\varphi(z|x)$ as neural networks?
- The approximate posterior looks like a standard CovnNet (or MLP), which receives an image input x and returns a feature map/latent variable z
  - Also known as encoder or inference network
- The likelihood term $p_\theta(x|z)$ looks like an inverted ConvNet (deconvolutions), which given a latent feature map z reconstructs the input x
  - Also known as decoder or generator network, because it recognizes the input given the latent variable
- A difference from a standard autoencoder is we now have an opinion of what the distribution of the latents z should look like, with $\mathrm{p}_\lambda(\mathrm{z})$



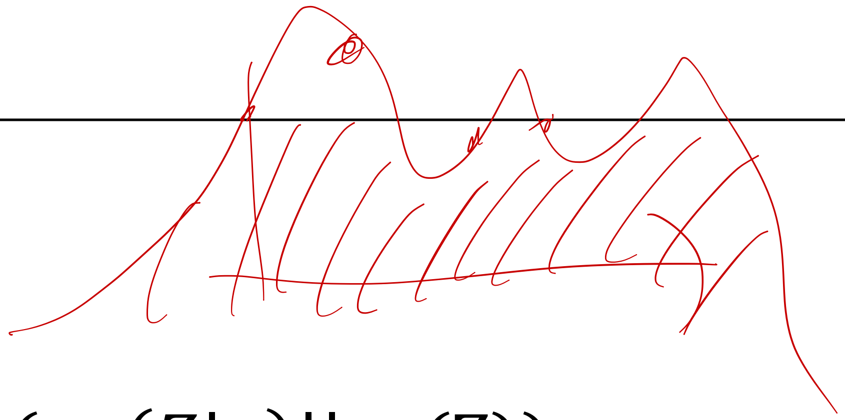
Training Variational Autoencoders

- 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

Complex integrals

Training Variational Autoencoders

$\|w\|_2^2$

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

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

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- 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
- The second term is the KL divergence between two distributions that we know

Typical VAE

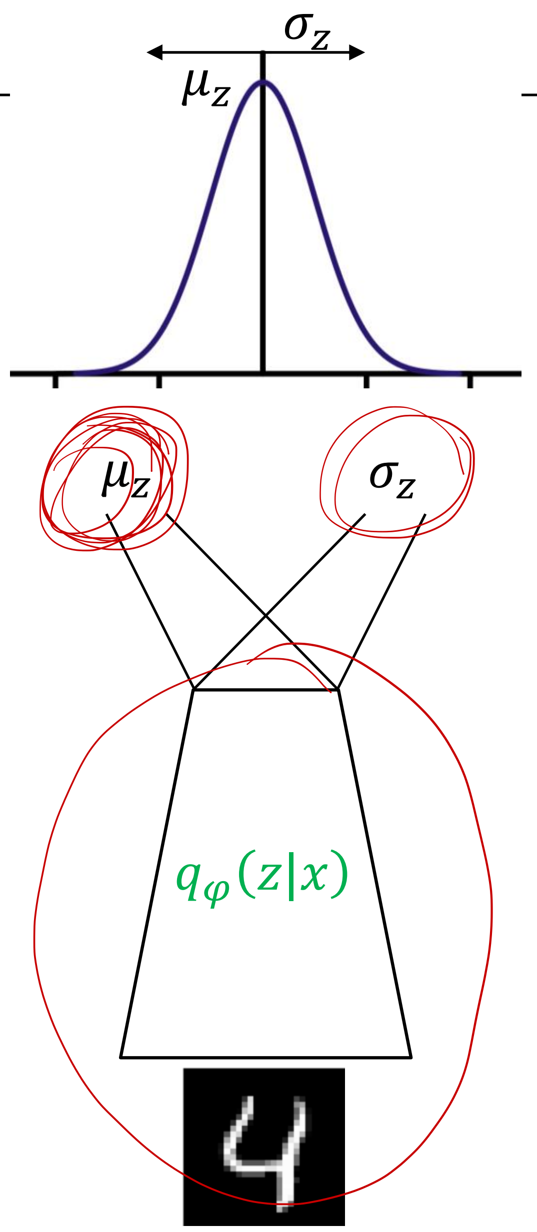
- We set the prior $p_\lambda(Z)$ to be the unit Gaussian

$$p(Z) \sim N(0,1)$$

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

$$p(X|Z) \sim Bernoulli(\pi)$$

- We set $q_\varphi(Z|x)$ to be a neural network (MLP, ConvNet), which maps an input x to the Gaussian distribution, specifically it's mean and variance
  - $\mu_z, \sigma_z \sim q_\varphi(Z|x)$
  - 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
- We set $p_\theta(X|Z)$ to be an inverse neural network, which maps Z to the Bernoulli distribution if our outputs binary (e.g. Binary MNIST)

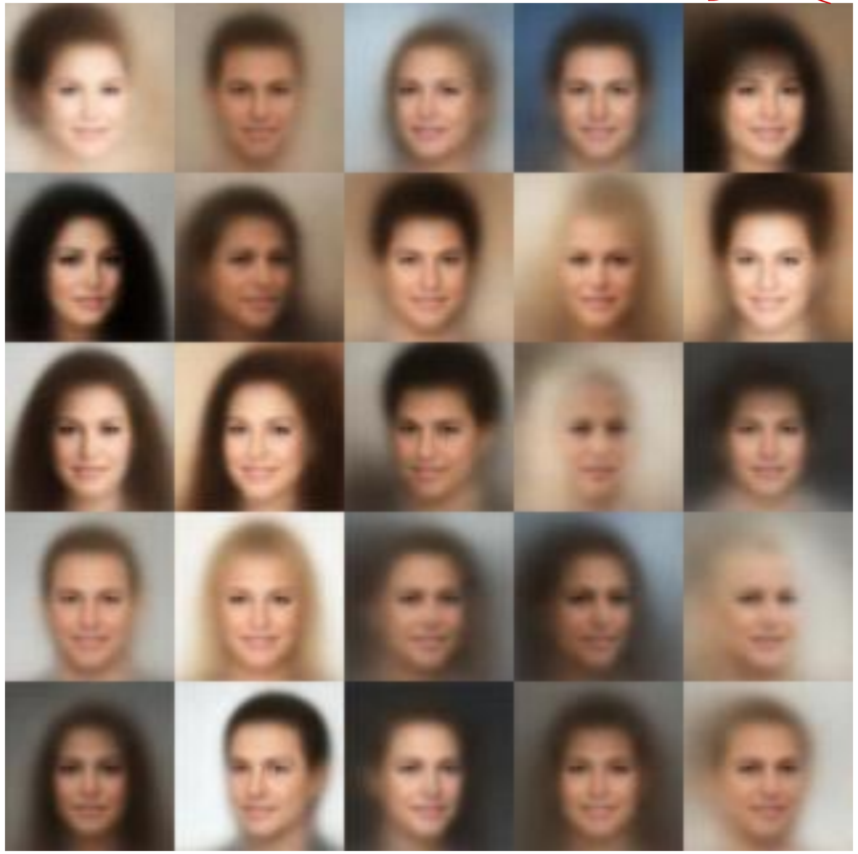


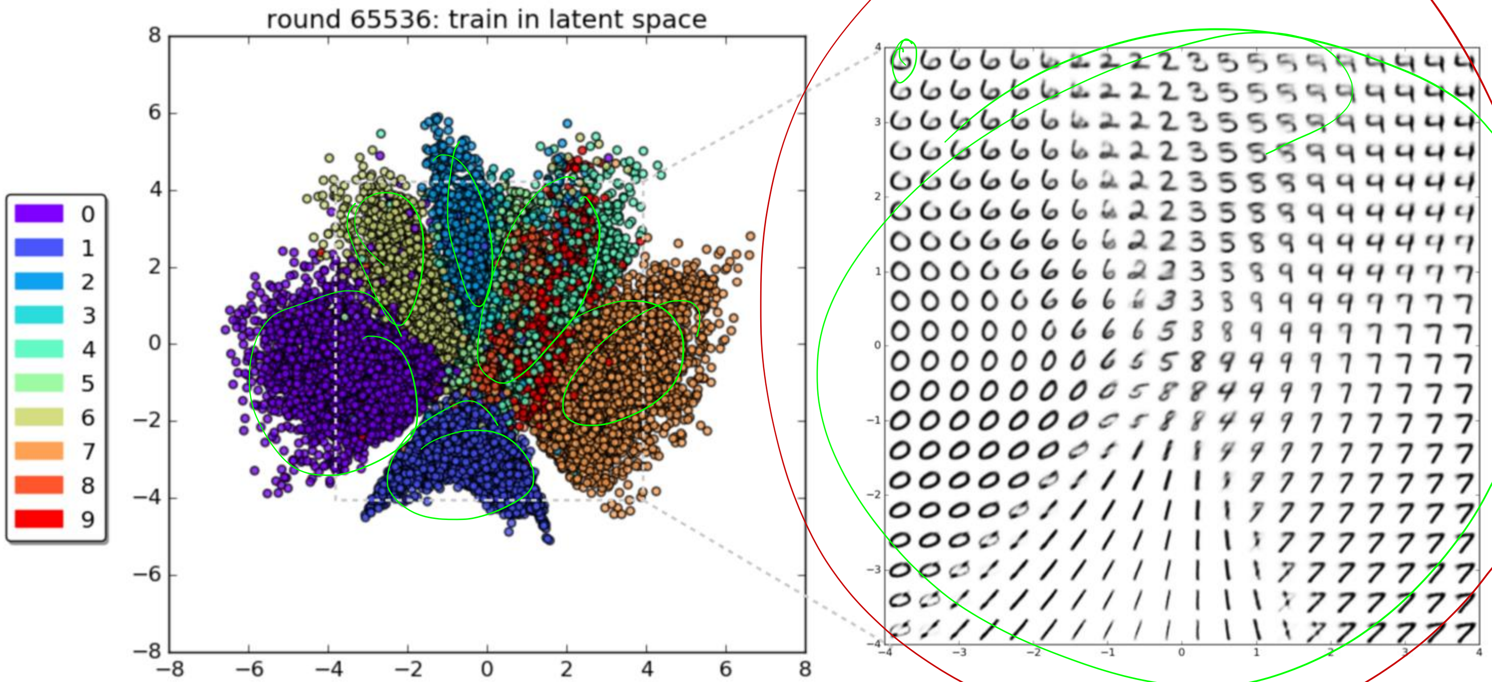
VAE: Interpolation in the latent space

$z \in \mathbb{R}^2$

#1 -1 -0.9 ... 0.9 1

#2





$h_2 \in \mathbb{R}^2$

h_2

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

Backward propagation in VAE

- Backpropagation → compute the gradients of

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

Backward propagation in VAE

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- Problem?

Backward propagation in VAE

- Backpropagation → compute the gradients of

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

- $\nabla_\theta \mathcal{L} = \mathbb{E}_{z\sim q_\varphi(Z|x)}[\nabla_\theta \log p_\theta(x|z)]$
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  - Also, the KL does not depend on θ, so no gradient from over there!
- $\nabla_\varphi \mathcal{L} = \nabla_\varphi \left[\mathbb{E}_{z\sim q_\varphi(Z|x)}[\log p_\theta(x|z)]\right] - \nabla_\varphi [\mathrm{KL}(q_\varphi(Z|x)||\mathrm{p}_\lambda(\mathrm{Z}))]$
- Problem? Sampling $z\sim q_\varphi(Z|x)$ is not differentiable → no gradients
- No gradients → No backprop → No training! → Solution?

Solution: REINFORCE?

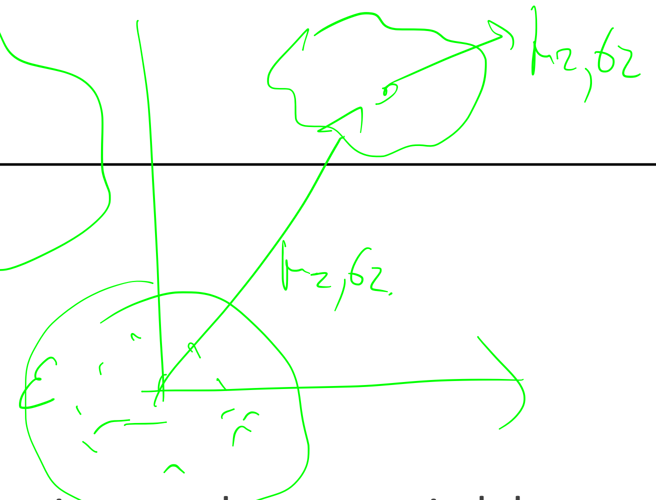
- So, our latent variable Z is a Gaussian (in the standard VAE) represented by the mean and variance μ_Z, σ_Z, which are the output of a neural net
- So, we can train by sampling randomly from that Gaussian

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

- 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

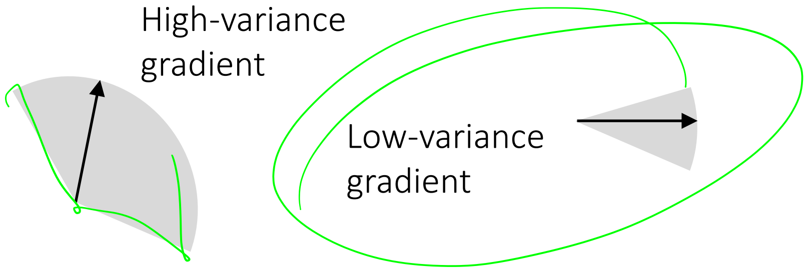
- For the Gaussian specifically, the following two formulations are equivalent

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

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

Solution: Reparameterization trick

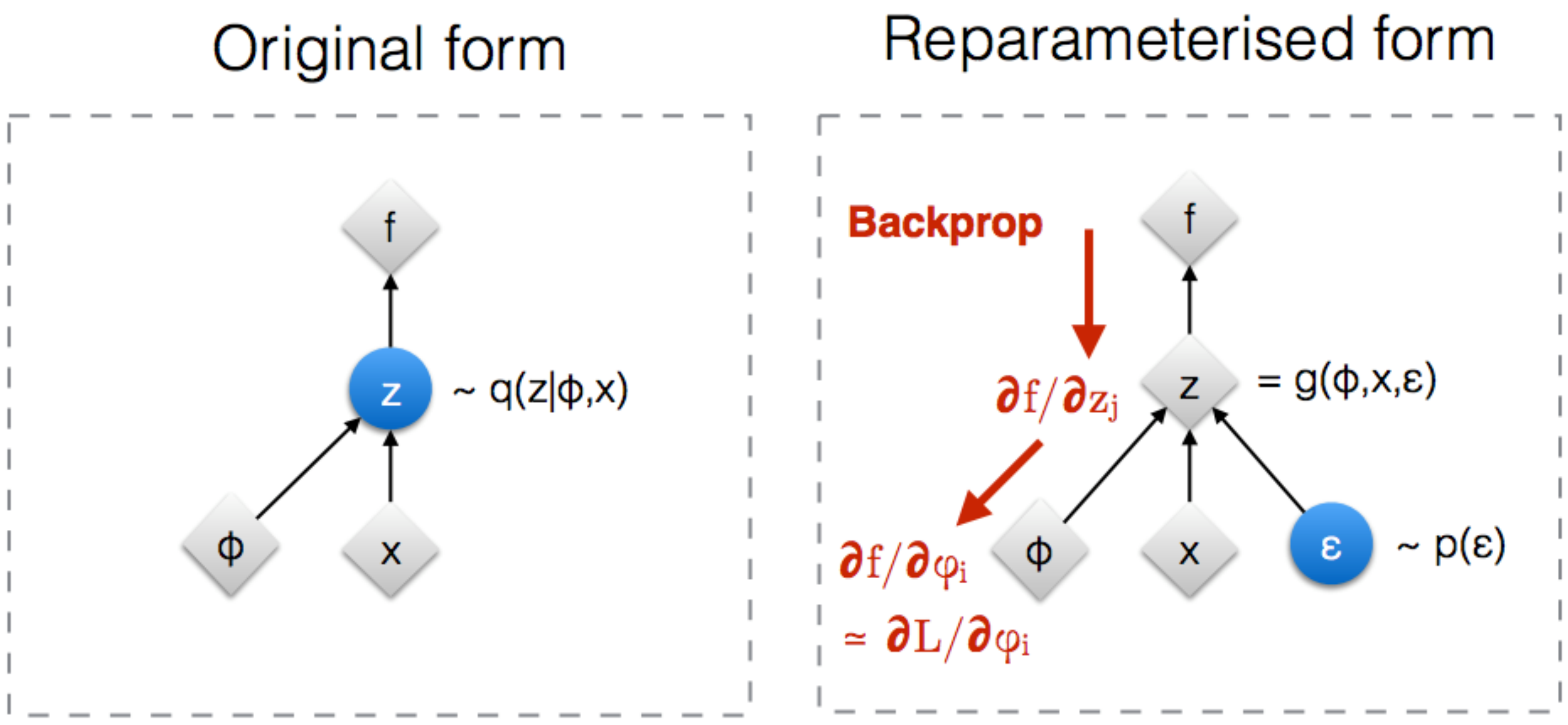
- Instead of sampling from $z \sim N(\mu_Z, \sigma_Z)$, we sample from $\varepsilon \sim N(0, 1)$ and then we compute z
- Sampling directly from $z \sim N(\mu_Z, \sigma_Z)$ leads to high-variance estimates
- Sampling directly from $\varepsilon \sim N(0,1)$ leads to low-variance estimates
  - Why low 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

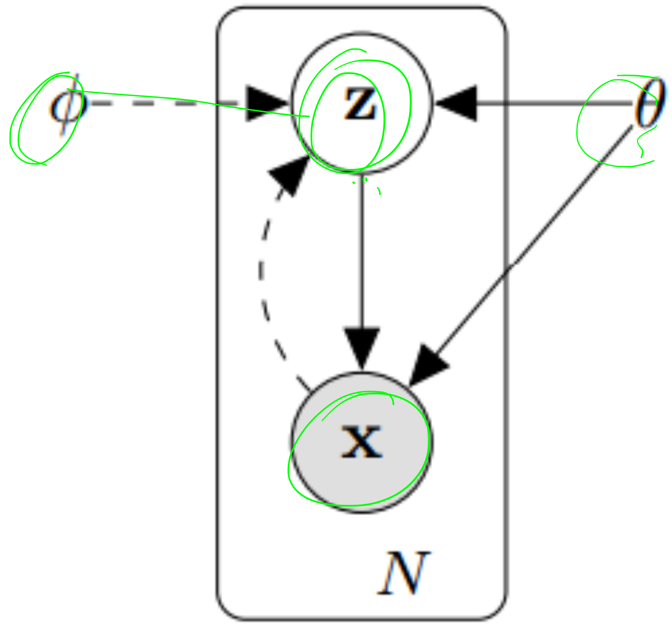


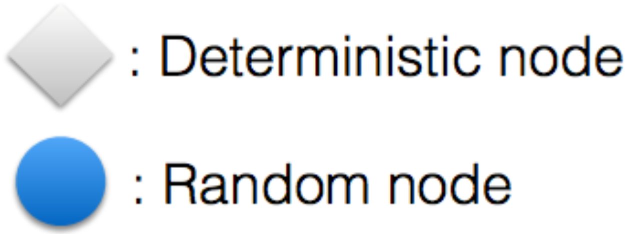
Check what is random

- 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 <u>**externally**</u>
- 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

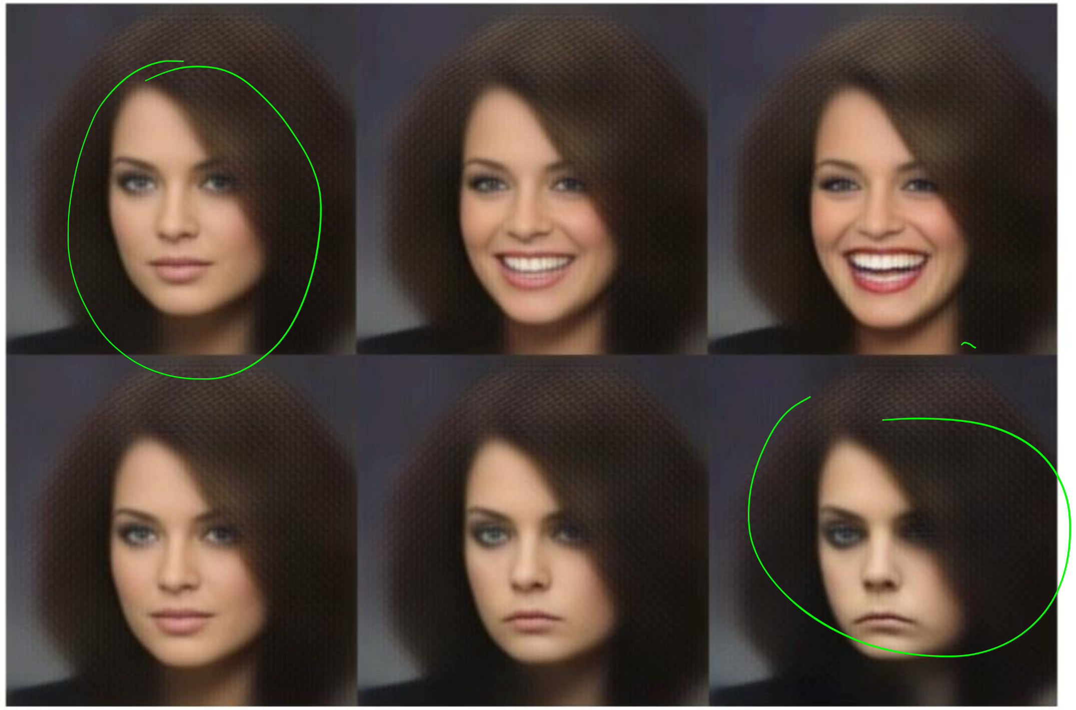
VAE for NLP

“ 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



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

Latent space arithmetic

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.

VAE for designing chemical compounds

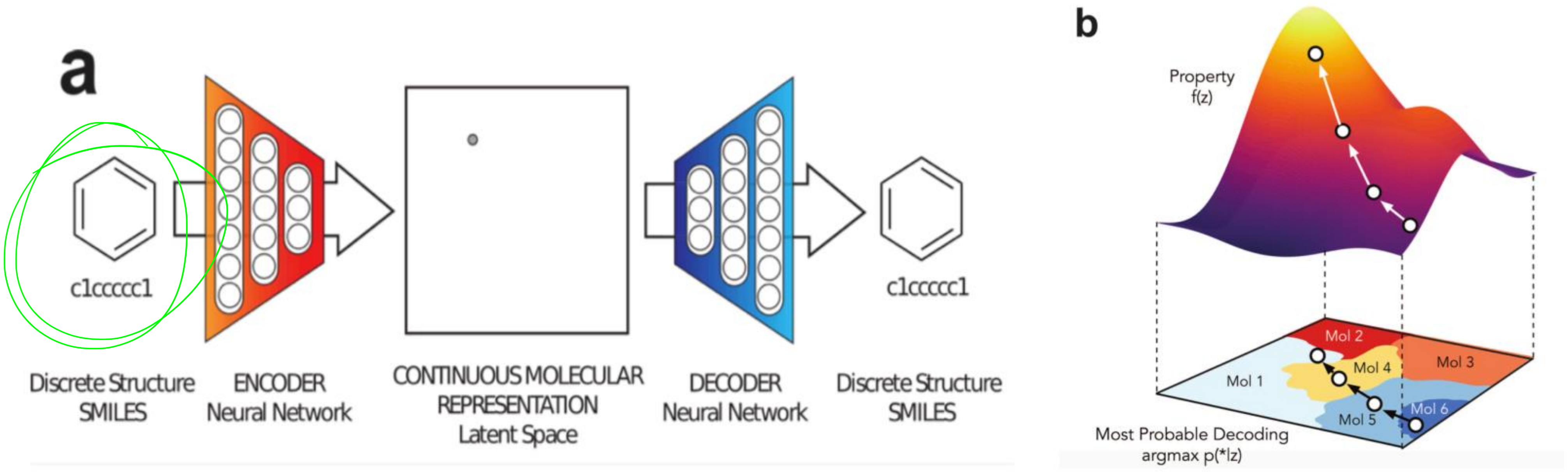
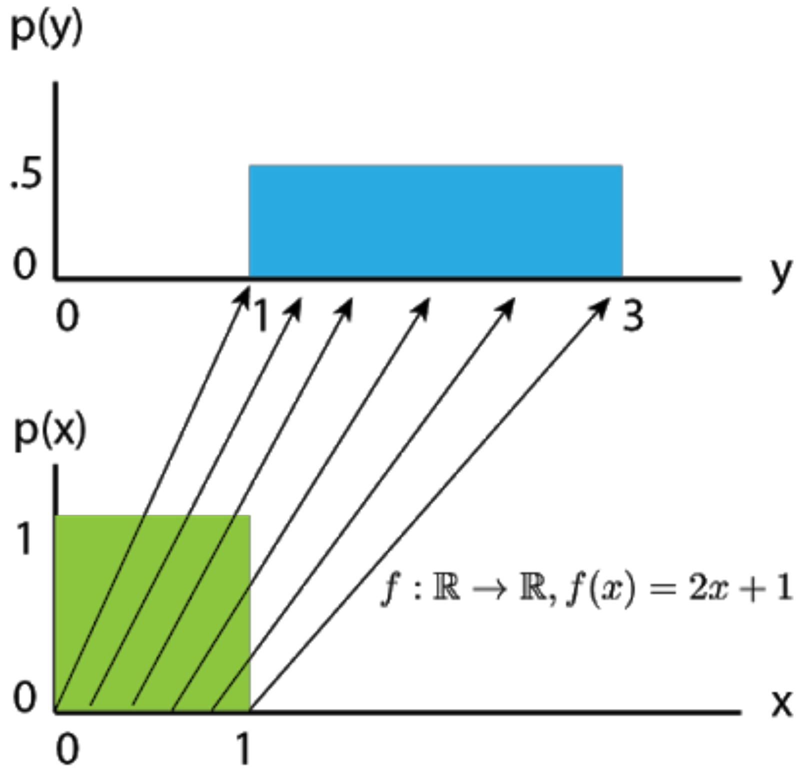


Figure 2.D.1: Example application of a VAE in [Gómez-Bombarelli et al., 2016]: design of new molecules with desired chemical properties. (a) A latent continuous representation $\mathbf{z}$ of molecules is learned on a large dataset of molecules. (b) This continuous representation enables gradient-based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

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 <u>even</u> 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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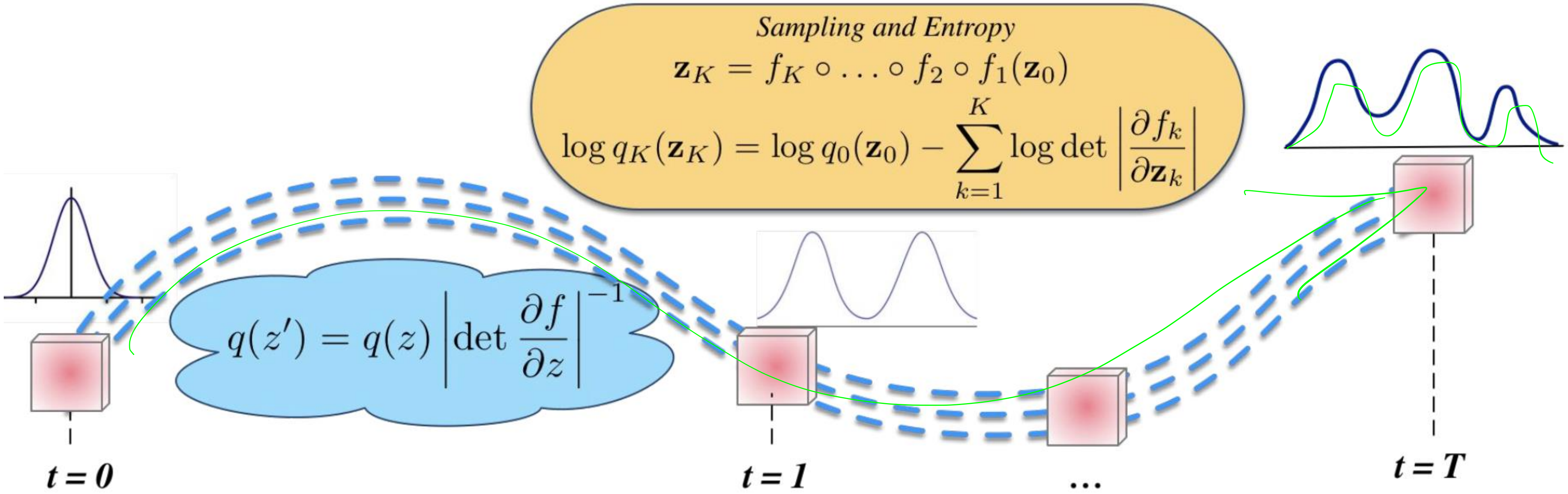
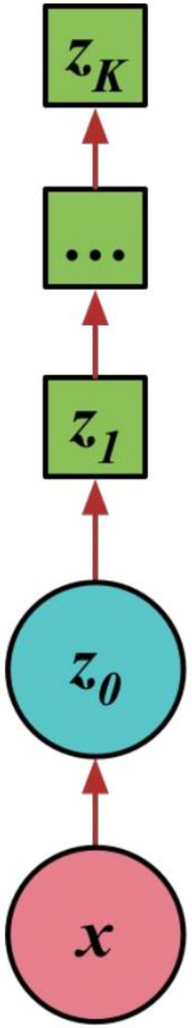
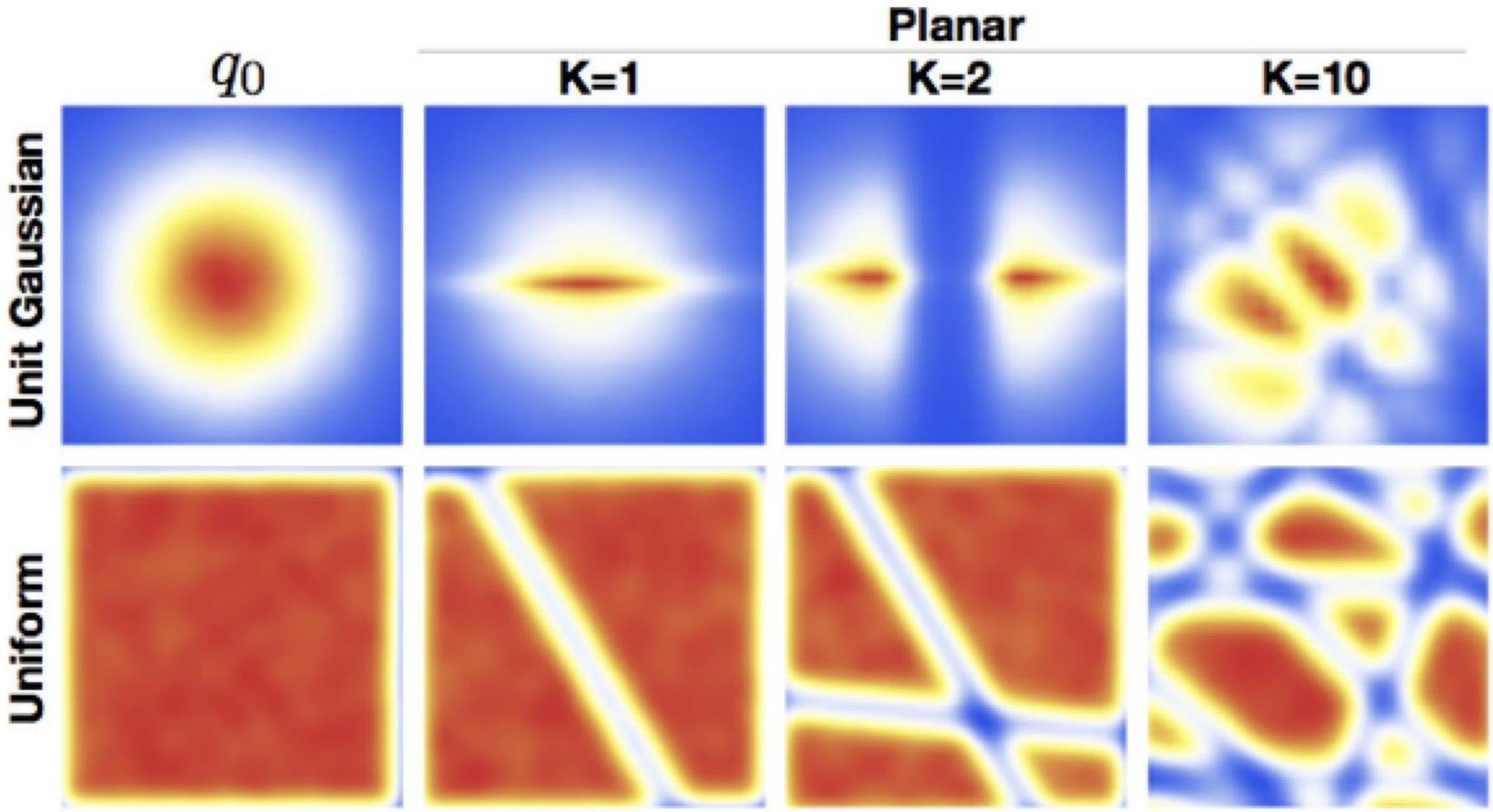




Distribution flows through a sequence of invertible transforms

Normalizing Flows



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

Normalizing Flows on Non-Euclidean Manifolds

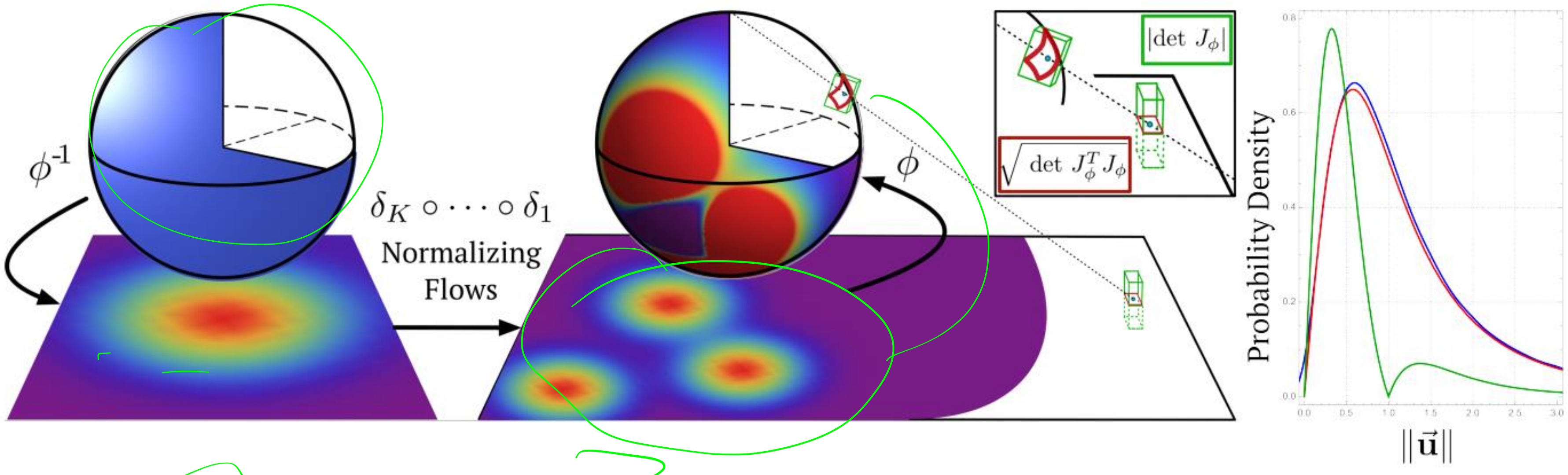


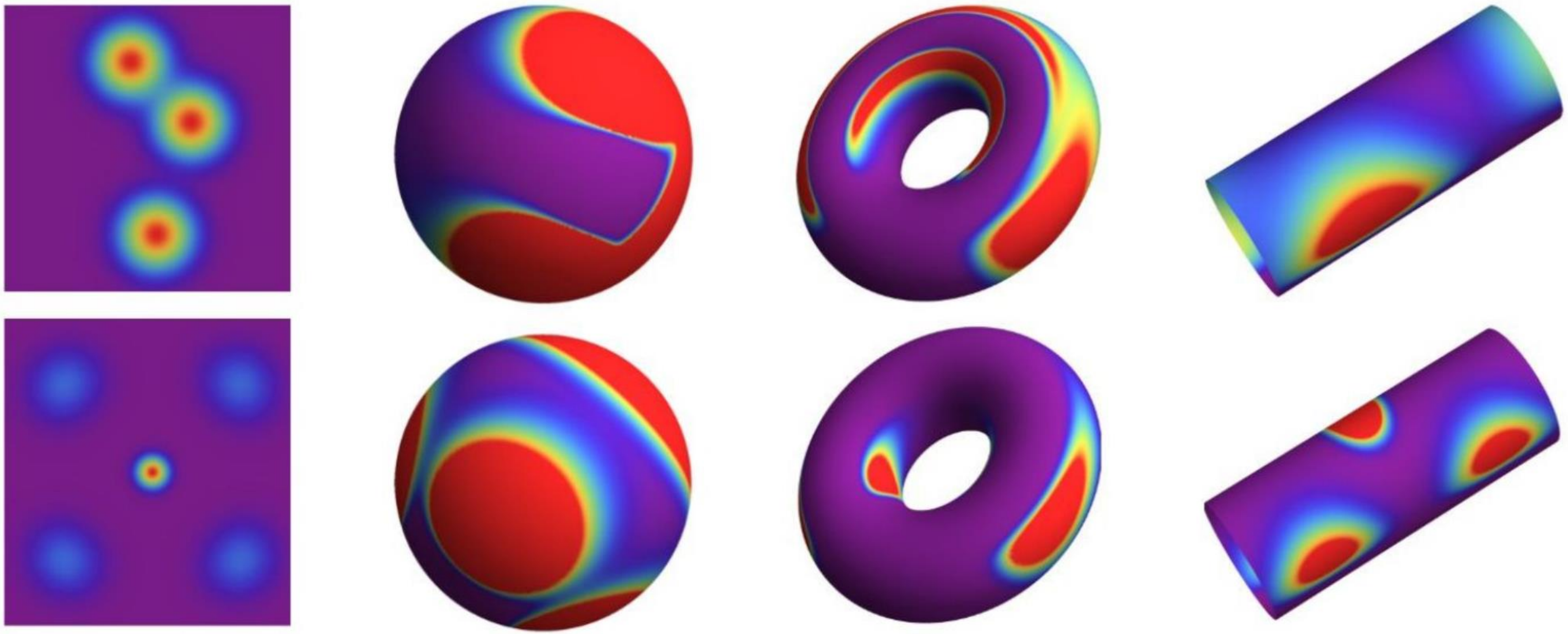
Figure 1: Left: Construction of a complex density on $\mathbf{S}^n$ by first projecting the manifold to $\mathbf{R}^n$, transforming the density and projecting it back to $\mathbf{S}^n$. Right: Illustration of transformed ($\mathbf{S}^2 \to \mathbf{R}^2$) densities corresponding to an uniform density 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



Summary

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