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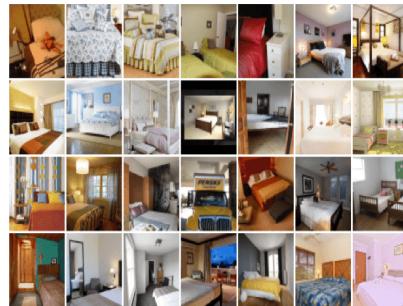
Deep Learning

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Variational Inference

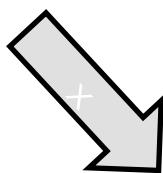
Statistical Generative Models



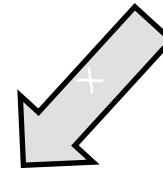
+

Model family, loss function,
optimization algorithm, etc.

Data



Learning



Prior Knowledge

Image x 

A probability
distribution
 $p(x)$

probability $p(x)$

Sampling from $p(x)$ **generates**
new images:



Statistical Generative Models



Training
Data(CelebA)

Model Samples (Karras et.al.,
2018)

4 years of progression on Faces



Brundage et al.,
2017

Conditional Generation

- ▶ Conditional generative model $P(\text{zebra images} | \text{horse images})$



- ▶ Style Transfer



Input Image



Monet



Van Gogh

Zhou et al., Cycle GAN 2017

Conditional Generation

- ▶ Conditional generative model $P(\text{zebra images} | \text{horse images})$

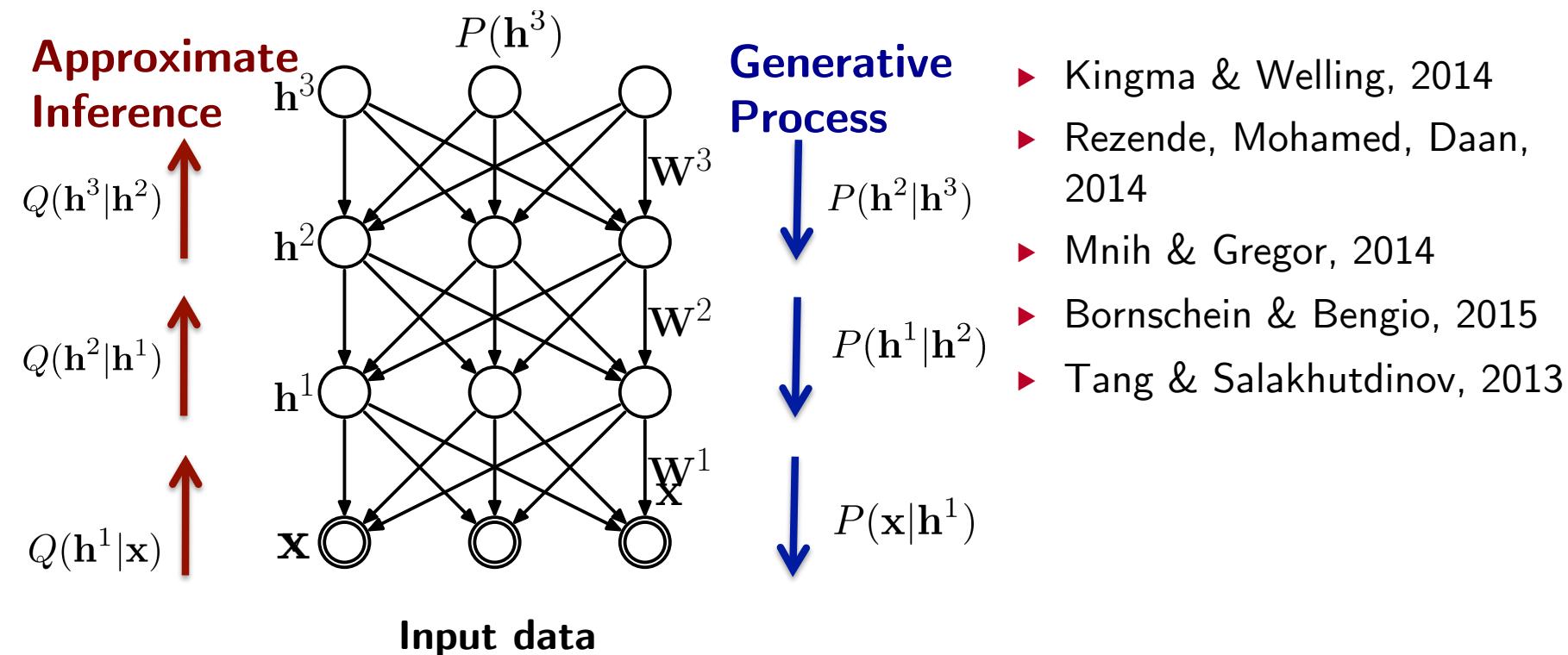


- ▶ Failure Case



Helmholtz Machines

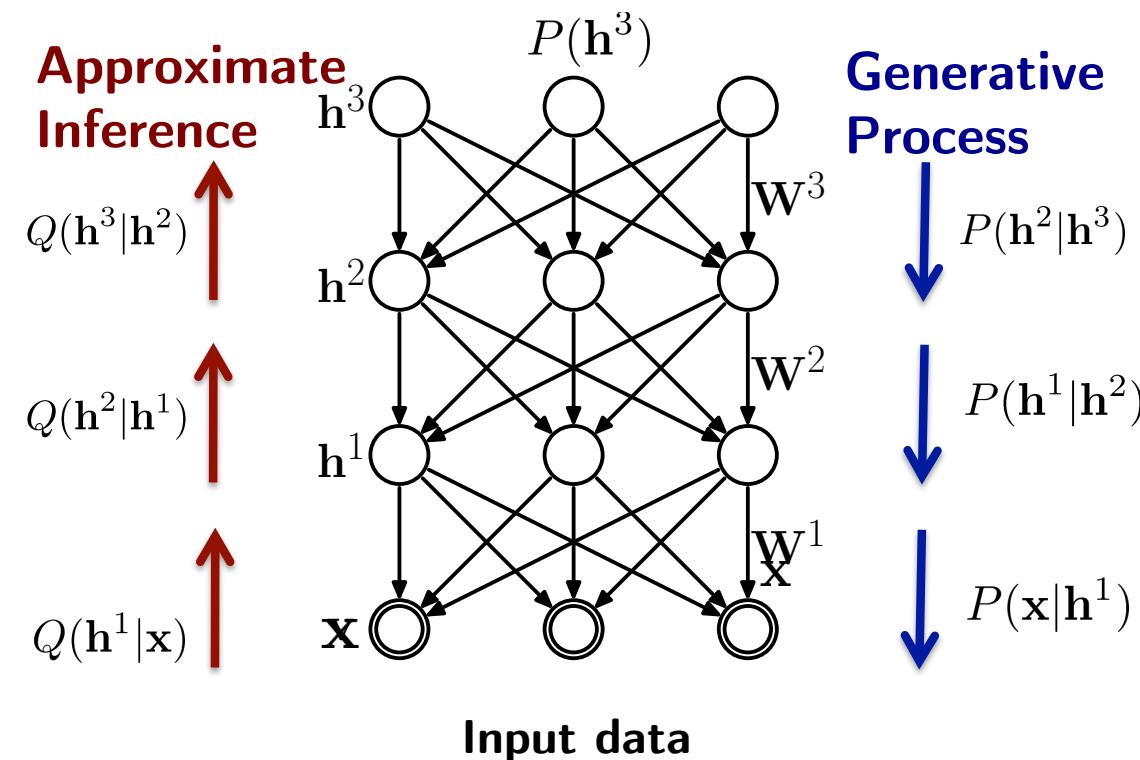
- ▶ Hinton, G. E., Dayan, P., Frey, B. J. and Neal, R., Science 1995



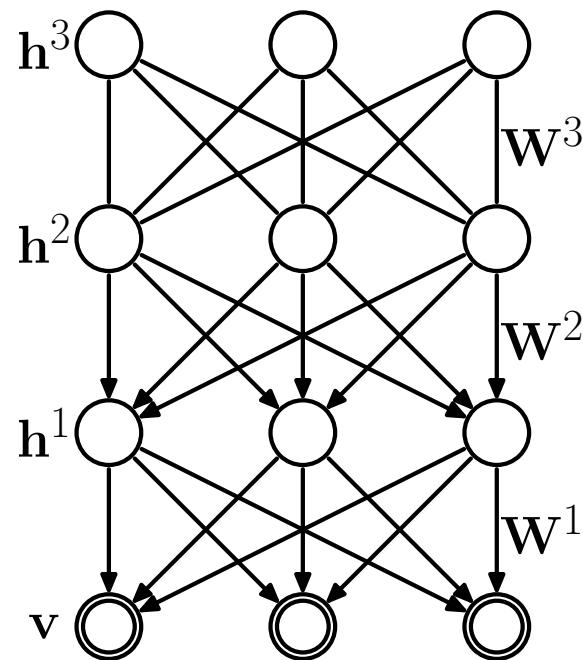
- ▶ Kingma & Welling, 2014
- ▶ Rezende, Mohamed, Daan, 2014
- ▶ Mnih & Gregor, 2014
- ▶ Bornschein & Bengio, 2015
- ▶ Tang & Salakhutdinov, 2013

Helmholtz Machines

Helmholtz Machine

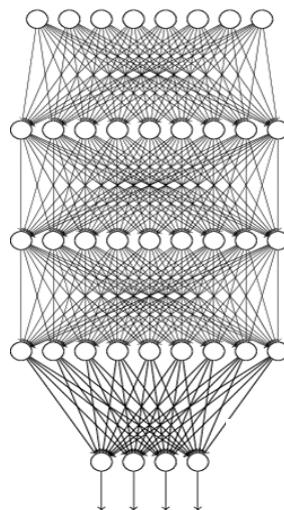


Deep Belief Network

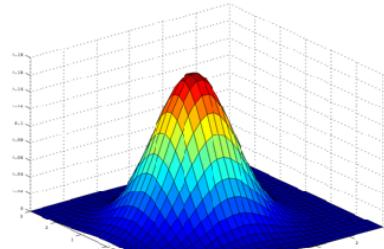


Deep Directed Generative Models

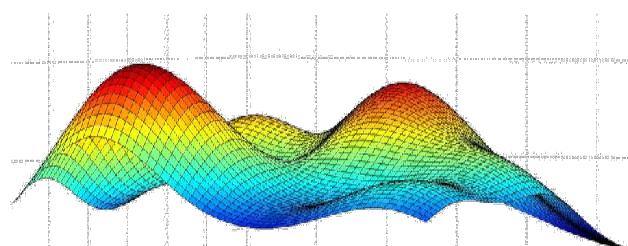
White
Noise



Code Z

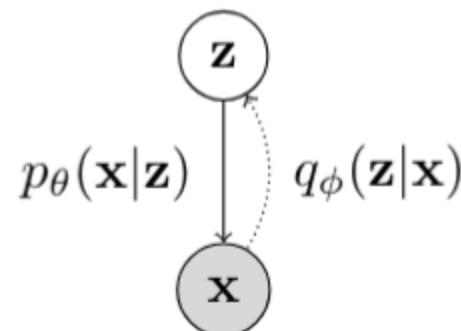


- ▶ Recognition
- ▶ Bottom-up
- ▶ $Q(z|x)$
- ▶ Generative
- ▶ Top-Down
- ▶ $P(x|z)$



D_{real}

▶ Latent Variable Models

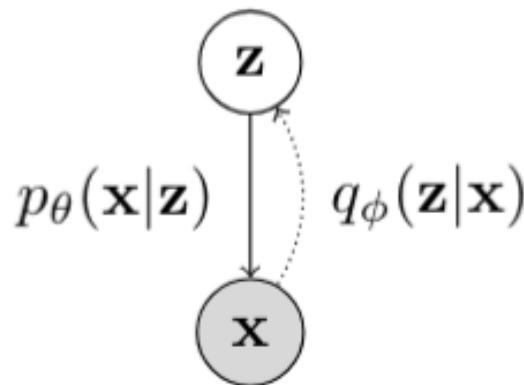


$$\log p_\theta(\mathbf{x}) = \log \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

- ▶ Conditional distributions are parameterized by deep neural networks

Directed Deep Generative Models

- Directed Latent Variable Models with Inference Network



- Maximum log-likelihood objective

$$\max_{\theta} \sum_{\mathbf{x} \in \mathcal{D}} \log p_{\theta}(\mathbf{x})$$

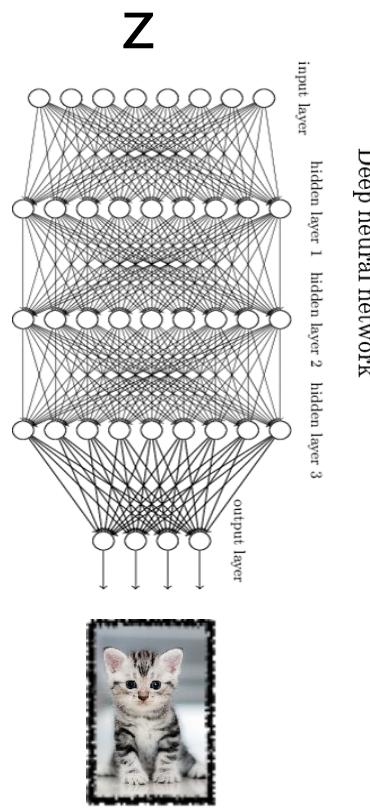
- Marginal log-likelihood is **intractable**:

$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

- **Key idea:** Approximate true posterior $p(z|x)$ with a simple, tractable distribution $q(z|x)$ (inference/recognition network).

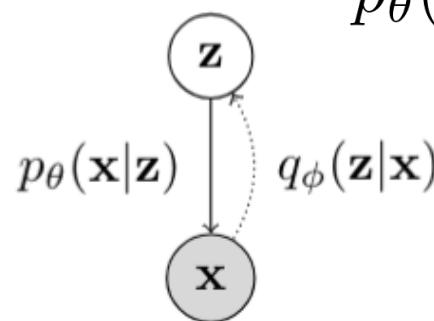
Variational Autoencoders (VAEs)

- Single stochastic (Gaussian) layer, followed by many deterministic layers



$$p(\mathbf{z}) = \mathcal{N}(0, I)$$

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



Deep neural network
parameterized by θ .
(Can use different noise models)

$$q_{\phi}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu(\mathbf{x}, \phi), \Sigma(\mathbf{x}, \phi))$$

Deep neural network
parameterized by ϕ .

Approximate Inference

- When using probabilistic graphical models, we will be interested in evaluating the **posterior distribution** $p(\mathbf{Z}|\mathbf{X})$ of the latent variables \mathbf{Z} given the observed data \mathbf{X} .
- For example, in the EM algorithm, we need to evaluate the expectation of the **complete-data log-likelihood** with respect to the **posterior distribution** over the latent variables.
- For more complex models, it may be **infeasible to evaluate the posterior distribution**, or compute expectations with respect to this distribution.
- This typically occurs when working with high-dimensional latent spaces, or when the **posterior distribution has a complex form**, for which expectations are not analytically tractable (e.g. Boltzmann machines).

Probabilistic Model

- The model may have **latent variables and parameters**, and we will denote the set of all latent variables and parameters by \mathbf{Z} .
- We will also denote the set of all **observed variables** by \mathbf{X} .
- For example, we may be given **a set of N i.i.d data points**, so that $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ and $\mathbf{Z} = \{\mathbf{z}_1, \dots, \mathbf{z}_N\}$ (as we saw in our previous class).
- Our probabilistic model specifies **the joint distribution** $P(\mathbf{X}, \mathbf{Z})$.
- Our goal is to **find approximate posterior distribution** $P(\mathbf{Z}|\mathbf{X})$ and the **model evidence** $p(\mathbf{X})$.

Variational Bound

- Given a joint distribution $p(\mathbf{Z}, \mathbf{X}|\theta)$ over observed and latent variables governed by parameters θ , the goal is to **maximize the likelihood function** $p(\mathbf{X}|\theta)$ with respect to θ :

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta).$$

- We will assume that \mathbf{Z} is **discrete**, although derivations are identical if \mathbf{Z} contains continuous, or a combination of discrete and continuous variables.
- For any distribution $q(\mathbf{Z})$ over latent variables we can derive the following **variational lower bound**:

$$\ln p(\mathbf{X}|\theta) = \ln \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})}$$

Jensen's
inequality

$$\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} = \mathcal{L}(q, \theta).$$

Variational Bound

- Variational lower-bound:

$$\begin{aligned}\ln p(\mathbf{X}|\theta) &= \ln \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \\ &\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} \\ &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln p(\mathbf{X}, \mathbf{Z}|\theta) + \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{1}{q(\mathbf{Z})} \\ &= \mathbb{E}_{q(\mathbf{Z})} [\ln p(\mathbf{X}, \mathbf{Z}|\theta)] + \mathcal{H}(q(\mathbf{Z})) = \mathcal{L}(q, \theta).\end{aligned}$$



Expected complete
log-likelihood



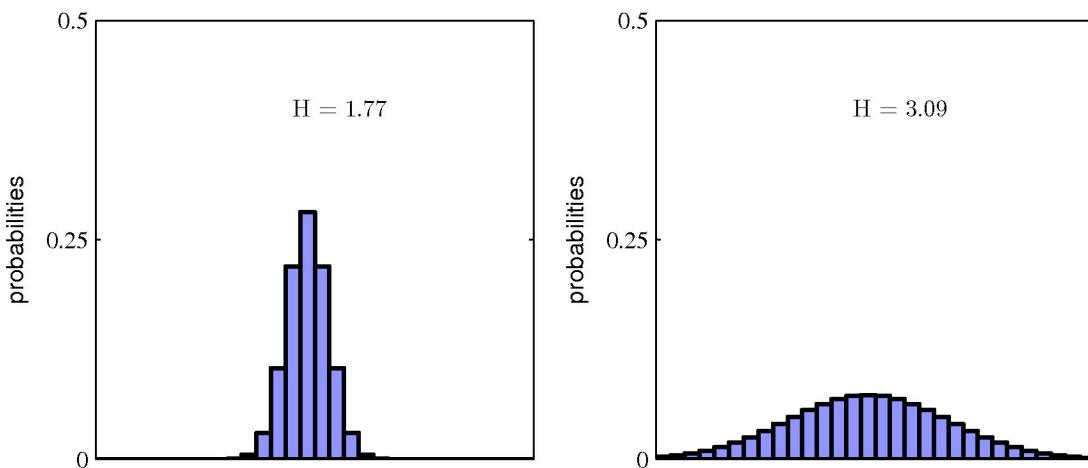
Entropy functional. Variational lower-
bound

Entropy

- For a discrete random variable X , where $P(X=x_i) = p(x_i)$, the entropy of a random variable is:

$$\mathcal{H}(p) = - \sum_i p(x_i) \log p(x_i).$$

- Distributions that are **sharply peaked** around a few values will have a relatively **low entropy**, whereas those that are **spread more evenly** across many values will have **higher entropy**



- Histograms of two probability distributions over 30 bins.
- The largest entropy will arise from a uniform distribution $H = -\ln(1/30) = 3.40$.

- For a density defined over continuous random variable, the **differential entropy** is given by:
$$\mathcal{H}(p) = - \int p(x) \log p(x) dx.$$

Variational Bound

- We saw:

$$\ln p(\mathbf{X}|\theta) \geq \mathbb{E}_{q(\mathbf{Z})} [\ln p(\mathbf{X}, \mathbf{Z}|\theta)] + \mathcal{H}(q(\mathbf{Z})) = \mathcal{L}(q, \theta).$$

- We also note that the following decomposition holds:

$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + \text{KL}(q||p),$$

where

$$\mathcal{L}(q, \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})},$$

Variational lower-bound

$$\text{KL}(q||p) = - \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{Z}|\mathbf{X}, \theta)}{q(\mathbf{Z})}.$$

Kullback-Leibler (KL) divergence.
Also known as
Relative Entropy.

- KL divergence is **not symmetric**.
- $\text{KL}(q||p) \geq 0$ with equality iff $p(\mathbf{x}) = q(\mathbf{x})$.
- Intuitively, it measures the “**distance**” between the two distributions.¹⁶

Variational Bound

- Let us derive that:

$$\log p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + \text{KL}(q||p),$$

- We can write:

$$\ln p(\mathbf{X}, \mathbf{Z}|\theta) = \ln p(\mathbf{Z}|\mathbf{X}, \theta) + \ln p(\mathbf{X}|\theta),$$

and plugging into the definition of $\mathcal{L}(q, \theta)$, gives the desired result.

- Note that **variational bound becomes tight iff $q(\mathbf{Z}) = p(\mathbf{Z} | \mathbf{X}, \theta)$** .
- In other words the distribution $q(\mathbf{Z})$ is **equal to the true posterior** distribution over the latent variables, so that $\text{KL}(q||p) = 0$.
- As $\text{KL}(q||p) \geq 0$, it immediately follows that:

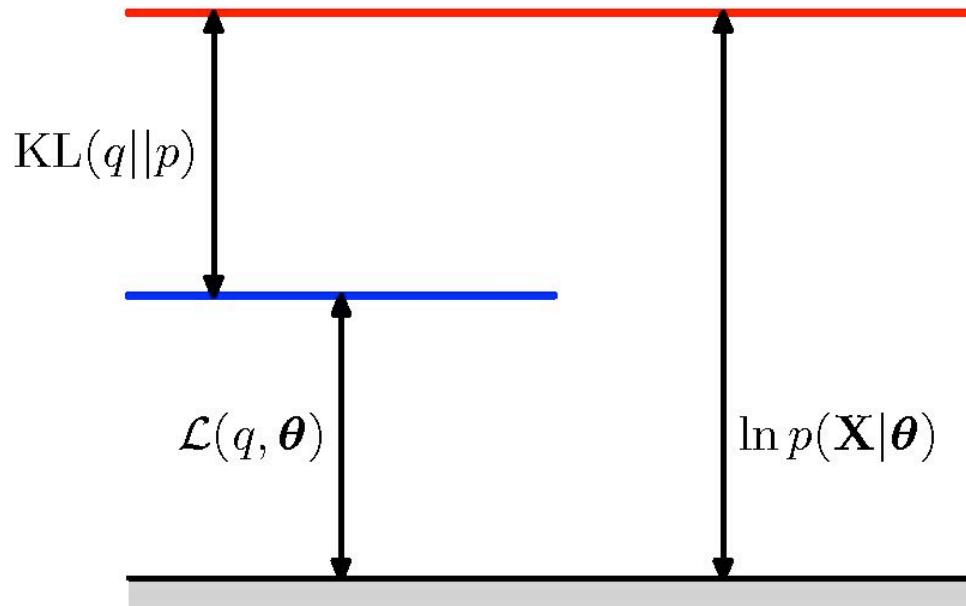
$$\ln p(\mathbf{X}|\theta) \geq \mathcal{L}(q, \theta),$$

which also showed using **Jensen's inequality**.

Decomposition

- Illustration of the decomposition which holds for any distribution $q(\mathbf{Z})$.

$$\ln p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + \text{KL}(q||p),$$



Variational Bound

- We can decompose the marginal log-probability as:

$$\log p(\mathbf{X}) = \mathcal{L}(q) + \text{KL}(q||p),$$

where

$$\mathcal{L}(q) = \int q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z}$$

$$\text{KL}(q||p) = - \int q(\mathbf{Z}) \ln \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} d\mathbf{Z}.$$

- We can maximize the variational lower bound $\mathcal{L}(q)$ with respect to the distribution $q(\mathbf{Z})$, which is equivalent to minimizing the KL divergence.
- If we allow any possible choice of $q(\mathbf{Z})$, then the maximum of the lower bound occurs when:

$$q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}).$$

In this case KL divergence becomes zero.

Variational Bound

- As in our previous lecture, we can **decompose** the marginal log-probability as:

$$\log p(\mathbf{X}) = \mathcal{L}(q) + \text{KL}(q||p),$$

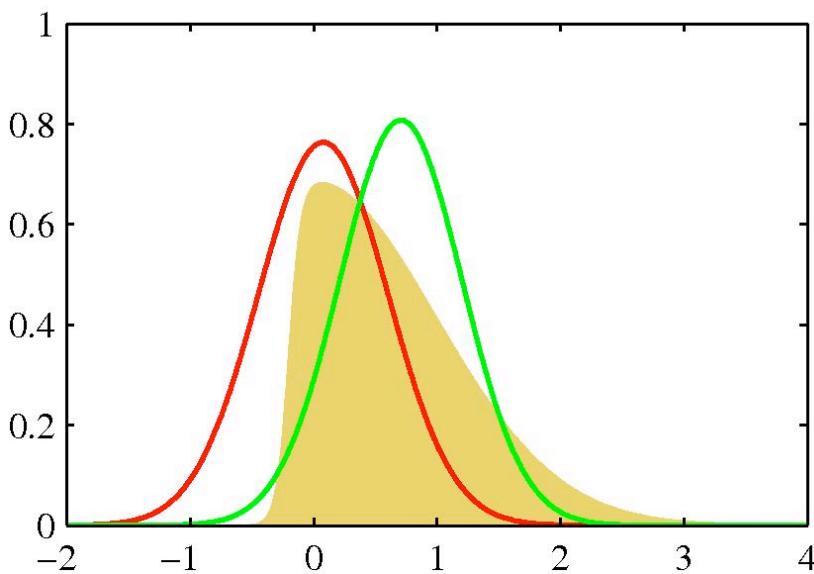
- We will assume that the **true posterior distribution** is intractable.
- We can consider a **restricted family of distributions** $q(\mathbf{Z})$ and then find the member of this family for which KL is minimized.
- Our goal is to restrict the family of distributions so that it contains **only tractable distributions**.
- At the same time, we want to allow the family to be sufficiently rich and flexible, so that it can provide a good approximation to the posterior.
- One option is to use **parametric distributions** $q(\mathbf{Z}|\omega)$, governed by parameters ω .
- The lower bound then becomes a function of ω , and we can **optimize the lower-bound** to determine the optimal values for the parameters.

Example

- One option is to use parametric distributions $q(\mathbf{Z}|\omega)$, governed by parameters ω .

$$\log p(\mathbf{X}) = \mathcal{L}(q) + \text{KL}(q||p),$$

- Here is an example, in which the variational distribution is Gaussian. We can optimize with respect to its **mean and variance**.



The original distribution (yellow), along with Laplace (red), and variational (green) approximations.

Mean-Field

- We now consider restricting the family of distributions.
- Partition the elements of \mathbf{Z} into **M disjoint groups**, denoted by \mathbf{Z}_i , $i=1,\dots,M$.
- We assume that the q distribution factorizes with respect to these groups:

$$q(\mathbf{Z}) = \prod_{i=1}^M q_i(\mathbf{Z}_i).$$

- Note that we place no restrictions on the functional form of the individual factors q_i (we will often denote $q_i(\mathbf{Z}_i)$ as simply q_i).
- This approximation framework, developed in physics, is called **mean-field theory**.

Factorized Distributions

- Among all factorized distributions, we look for a distribution for which the **variational lower bound is maximized**.
- Denoting $q_i(\mathbf{Z}_i)$ as simply q_i , we have:

$$q(\mathbf{Z}) = \prod_{i=1}^M q_i(\mathbf{Z}_i).$$

$$\begin{aligned}\mathcal{L}(q) &= \int q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z} \\ &= \int \prod_i q_i \left[\ln p(\mathbf{X}, \mathbf{Z}) - \sum_i \ln q_i \right] d\mathbf{Z} \\ &= \int q_j \left[\int \ln p(\mathbf{X}, \mathbf{Z}) \prod_{i \neq j} q_i d\mathbf{Z}_i \right] d\mathbf{Z}_j - \int q_j \ln q_j d\mathbf{Z}_j + \text{const} \\ &= \int q_j \ln \tilde{p}(\mathbf{X}, \mathbf{Z}_j) d\mathbf{Z}_j - \int q_j \ln q_j d\mathbf{Z}_j + \text{const}\end{aligned}$$

where we denote **a new distribution**:

$$\tilde{p}(\mathbf{X}, \mathbf{Z}_j) = \mathbb{E}_{i \neq j} [\ln p(\mathbf{X}, \mathbf{Z})] + \text{const.}$$

Factorized Distributions

- Among all factorized distributions, we look for a distribution for which the **variational lower bound is maximized**.
- Denoting $q_i(\mathbf{Z}_i)$ as simply q_i , we have:

$$\begin{aligned}\mathcal{L}(q) &= \int q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z} \\ &= \int q_j \ln \tilde{p}(\mathbf{X}, \mathbf{Z}_j) d\mathbf{Z}_j - \int q_j \ln q_j d\mathbf{Z}_j + \text{const}\end{aligned}$$

where

$$\ln \tilde{p}(\mathbf{X}, \mathbf{Z}_j) = \mathbb{E}_{i \neq j} [\ln p(\mathbf{X}, \mathbf{Z})] + \text{const.}$$

- Here we take an **expectation with respect to the q distribution** over all variables \mathbf{Z}_i for $i \neq j$, so that:

$$\mathbb{E}_{i \neq j} [\ln p(\mathbf{X}, \mathbf{Z})] = \int \ln p(\mathbf{X}, \mathbf{Z}) \prod_{i \neq j} q_i d\mathbf{Z}_i.$$

Maximizing Lower Bound

- Now suppose that we keep $\{q_{i \neq j}\}$ fixed, and optimize the lower bound with respect to **all possible forms of the distribution** $q_j(\mathbf{Z}_j)$.
- This optimization is easily done by recognizing that:

$$\begin{aligned}\mathcal{L}(q) &= \int q_j \ln \tilde{p}(\mathbf{X}, \mathbf{Z}_j) d\mathbf{Z}_j - \int q_j \ln q_j d\mathbf{Z}_j + \text{const} \\ &= -\text{KL}(q_j(\mathbf{Z}_j) || \tilde{p}(\mathbf{X}, \mathbf{Z}_j)) + \text{const},\end{aligned}$$

constant: does not depend on q .

$\mathcal{L}(q) = \log p(\mathbf{X}) - \text{KL}(q || p)$

so the minimum occurs when

$$q_j^*(\mathbf{Z}_j) = \tilde{p}(\mathbf{X}, \mathbf{Z}), \text{ or } \ln q_j^*(\mathbf{Z}_j) = \mathbb{E}_{i \neq j} [\ln p(\mathbf{X}, \mathbf{Z})] + \text{const.}$$

- Observe: the **log of the optimum solution for factor q_j** is given by:
 - Considering **the log of the joint distribution over all hidden and visible variables**
 - Taking the expectation with respect to all other factors $\{q_i\}$ for $i \neq j$.

Maximizing Lower Bound

- Exponentiating and normalizing, we obtain:

$$q_j^*(\mathbf{Z}_j) = \frac{\exp(\mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})])}{\int \exp(\mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})]) d\mathbf{Z}_j}.$$

- The set of these equations for $j=1, \dots, M$ represent **the set of consistency conditions for the maximum of the lower bound** subject to factorization constraint.
- To obtain a solution, we initialize all of the factors and then cycle through factors, replacing each in turn with a revised estimate.
- **Convergence is guaranteed** because the bound is convex with respect to each of the individual factors.

Factroized Gaussian

- Consider a problem of approximating a general distribution by a factorized distribution.
- To get some insight, let us look at the problem of **approximating a Gaussian distribution using a factorized Gaussian distribution**.
- Consider a Gaussian distribution over two correlated variables $\mathbf{z} = (z_1, z_2)$.

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z} | \boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}),$$
$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \boldsymbol{\Lambda} = \begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}$$

- Let us approximate this distribution using a **factorized Gaussian** of the form:

$$q(\mathbf{z}) = q_1(z_1)q_2(z_2).$$

Factroized Gaussian

- Remember:

$$\ln q_j^*(\mathbf{Z}_j) = \mathbb{E}_{i \neq j} [\ln p(\mathbf{X}, \mathbf{Z})] + \text{const.}$$

- Consider an expression for the optimal factor q_1 :

$$\begin{aligned}\ln q_1^*(z_1) &= \mathbb{E}_{q_2(z_2)} [\ln p(\mathbf{z})] + \text{const} \\ &= \mathbb{E}_{q_2(z_2)} \left[-\frac{\beta_{11}}{2}(z_1 - \mu_1)^2 - \beta_{12}(z_1 - \mu_1)(z_2 - \mu_2) \right] + \text{const} \\ &= -\frac{\beta_{11}}{2}z_1^2 + \beta_{11}z_1\mu_1 - \beta_{12}z_1(\mathbb{E}[z_2] - \mu_2) + \text{const.}\end{aligned}$$

- Note that we have a quadratic function of z_1 , and so we can identify $q_1(z_1)$ as a **Gaussian distribution**:

$$q_1^*(z_1) = \mathcal{N}(z_1 | m_1, \beta_{11}^{-1}), \quad m_1 = \mu_1 - \frac{\beta_{12}}{\beta_{11}}(\mathbb{E}[z_2] - \mu_2).$$

Factroized Gaussian

- By symmetry, we also obtain:

$$q_1^*(z_1) = \mathcal{N}(z_1 | m_1, \beta_{11}^{-1}), \quad m_1 = \mu_1 - \frac{\beta_{12}}{\beta_{11}}(\mathbb{E}[z_2] - \mu_2).$$

$$q_2^*(z_2) = \mathcal{N}(z_2 | m_2, \beta_{22}^{-1}), \quad m_2 = \mu_2 - \frac{\beta_{12}}{\beta_{22}}(\mathbb{E}[z_1] - \mu_1).$$

- There are two observations to make:

- We **did not assume** that $q_i^*(z_i)$ is Gaussian, but rather we derived this result by **optimizing variational bound over all possible distributions**.
 - The **solutions are coupled**. The optimal $q_1^*(z_1)$ depends on expectation computed with respect to $q_2^*(z_2)$.

- One option is to **cycle through the variables in turn** and update them until convergence.

Factroized Gaussian

- By symmetry, we also obtain:

$$q_1^*(z_1) = \mathcal{N}(z_1 | m_1, \beta_{11}^{-1}), \quad m_1 = \mu_1 - \frac{\beta_{12}}{\beta_{11}}(\mathbb{E}[z_2] - \mu_2).$$

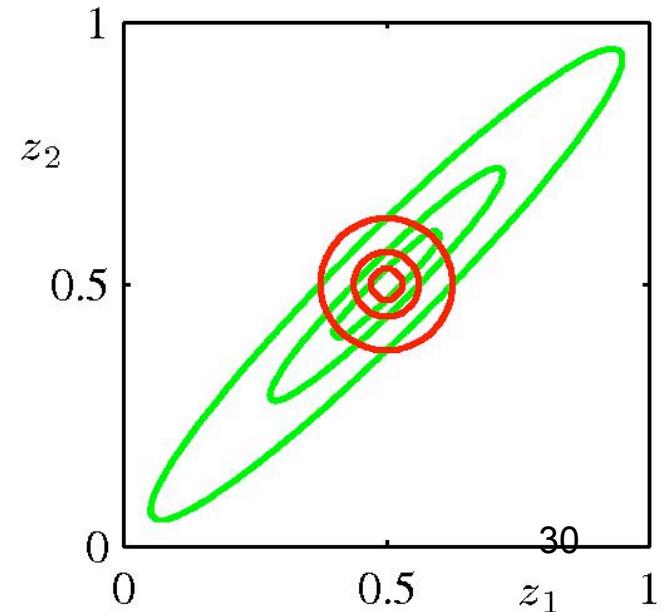
$$q_2^*(z_2) = \mathcal{N}(z_2 | m_2, \beta_{22}^{-1}), \quad m_2 = \mu_2 - \frac{\beta_{12}}{\beta_{22}}(\mathbb{E}[z_1] - \mu_1).$$

- However, in our case, $\mathbb{E}[z_1] = \mu_1$, $\mathbb{E}[z_2] = \mu_2$.

- The green contours correspond to 1,2, and 3 standard deviations of the correlated Gaussian.

- The red contours correspond to the factorial approximation $q(\mathbf{z})$ over the same two variables.

- Observe that a factorized variational approximation tends to give approximations that are too compact.



Alternative Form of KL Divergence

- We have looked at the variational approximation that minimizes $\text{KL}(q||p)$.
- For comparison, suppose that we were minimizing $\text{KL}(p||q)$.

$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} d\mathbf{Z}.$$

$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \left[\sum_{i=1}^M \ln q_i(\mathbf{Z}_i) \right] d\mathbf{Z} + \int p(\mathbf{Z}) \ln \frac{1}{p(\mathbf{Z})} d\mathbf{Z}.$$

constant: does not depend on q.

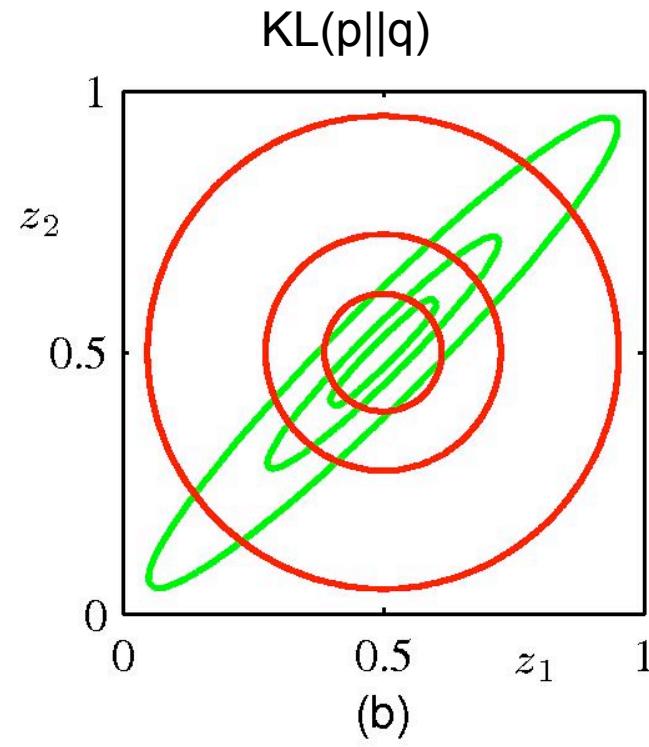
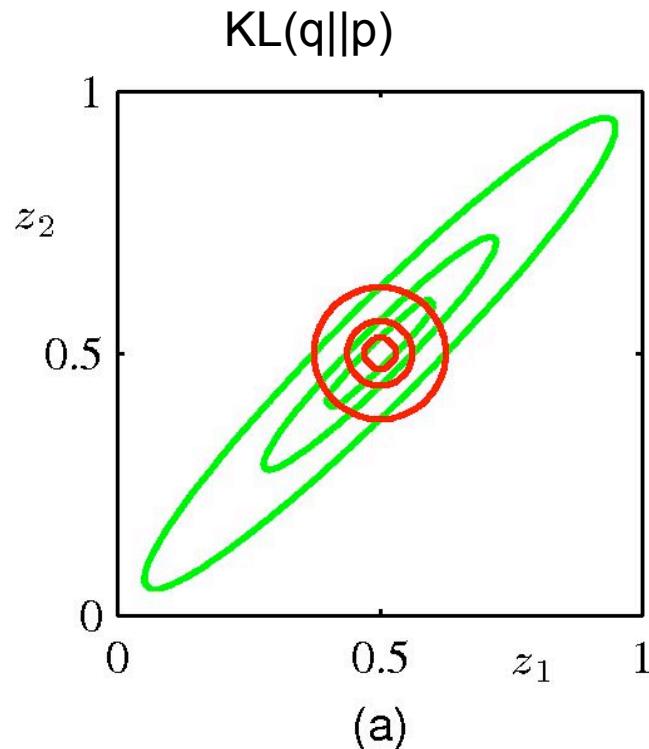
- It is easy to show that:

$$q_j^*(\mathbf{Z}_j) = \int p(\mathbf{Z}) \prod_{i \neq j} d\mathbf{Z}_i = p(\mathbf{Z}_j).$$

- The optimal factor is given by the **marginal distribution** of $p(\mathbf{Z})$.

Comparison of two KLS

- Comparison of two the alternative forms for the KL divergence.



Approximation is too compact.

Approximation is too spread.

Comparison of two KLS

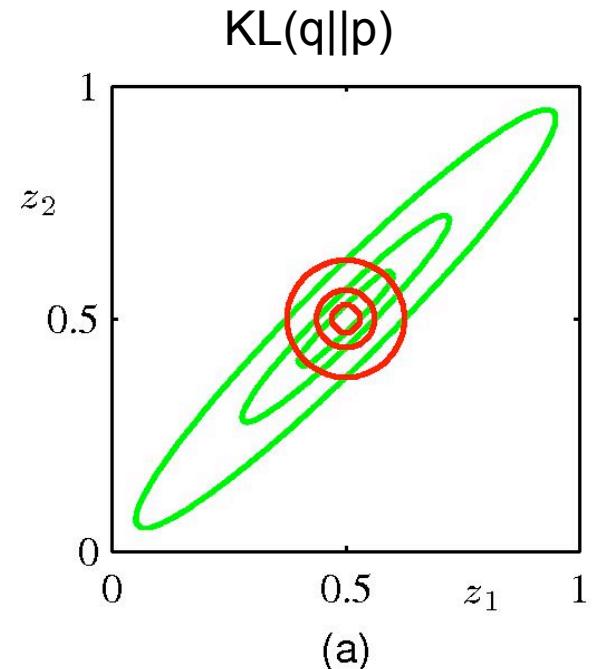
- The difference between these two approximations can be understood as follows:

$$\text{KL}(q||p) = - \int q(\mathbf{Z}) \ln \frac{p(\mathbf{Z})}{q(\mathbf{Z})} d\mathbf{Z}.$$

- There is a **large positive contribution** to the KL divergence from regions of \mathbf{Z} space in which:

- $p(\mathbf{Z})$ is **near zero**,
 - unless $q(\mathbf{Z})$ is also close to zero.

- Minimizing $\text{KL}(q||p)$ leads to distributions $q(\mathbf{Z})$ that **avoid regions in which $p(\mathbf{Z})$ is small**.

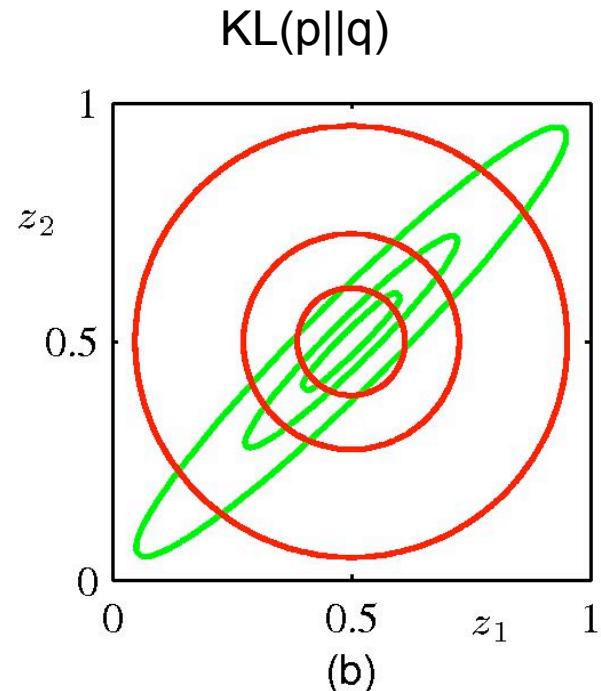


Comparison of two KLs

- Similar arguments apply for the alternative KL divergence:

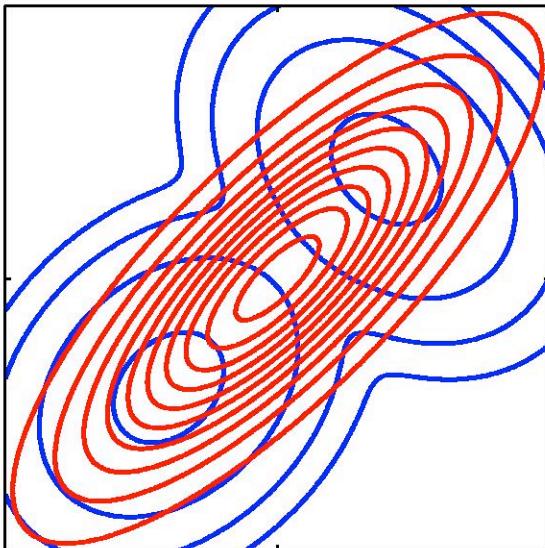
$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} d\mathbf{Z}.$$

- There is a large positive contribution to the KL divergence from regions of \mathbf{Z} space in which:
 - $q(\mathbf{Z})$ is near zero,
 - unless $p(\mathbf{Z})$ is also close to zero.
- Minimizing $KL(p||q)$ leads to distributions $q(\mathbf{Z})$ that are nonzero in regions where $p(\mathbf{Z})$ is nonzero.

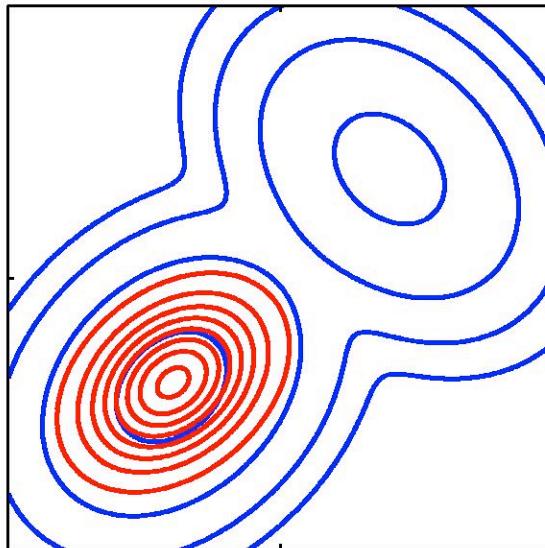


Approximating Multimodal Distribution

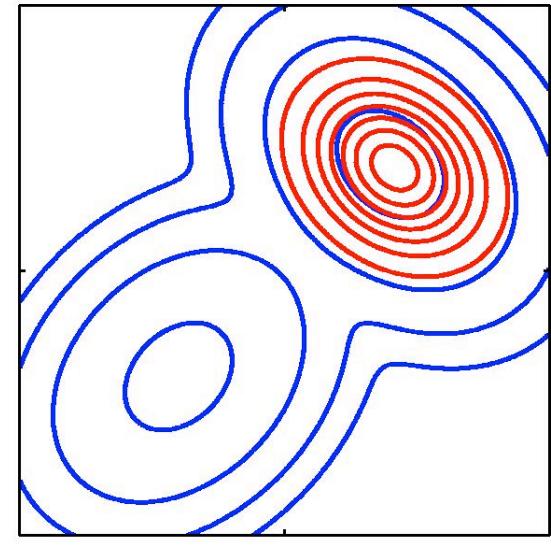
- Consider approximating **multimodal distribution** with a **unimodal one**.
- Blue contours show **bimodal distribution $p(\mathbf{Z})$** , red contours show a single Gaussian distribution that best approximates $q(\mathbf{Z})$ that best approximates $p(\mathbf{Z})$.



$\text{KL}(p||q)$



$\text{KL}(q||p)$



$\text{KL}(q||p)$

- In practice, **the true posterior will often be multimodal**.
- $\text{KL}(q||p)$ will tend to find a single mode, whereas $\text{KL}(p||q)$ will average across all of the modes.

Alpha-family of Divergences

- The two forms of KL are members of the **alpha-family divergences**:

$$D_\alpha(p||q) = \frac{4}{1-\alpha^2} \left(1 - \int p(x)^{(1+\alpha)/2} q(x)^{(1-\alpha)/2} dx \right), \quad -\infty < \alpha < \infty.$$

- Observe **three points**:

- $KL(p||q)$ corresponds to the limit $\alpha \rightarrow 1$.
- $KL(q||p)$ corresponds to the limit $\alpha \rightarrow -1$.
- $D_\alpha(p||q) \geq 0$, for all α , and $D_\alpha(p||q)=0$ iff $q(x) = p(x)$.

- Suppose $p(x)$ is fixed and we minimize $D_\alpha(p||q)$ with **respect to q** distribution.
- For $\alpha < -1$, the divergence is **zero-forcing**: $q(x)$ will underestimate the support of $p(x)$.
- For $\alpha > 1$, the divergence is **zero-avoiding**: $q(x)$ will stretch to cover all of $p(x)$.
- For $\alpha = 0$, we obtain a symmetric divergence which is related to **Hellinger Distance**:

$$D_H(p||q) = \frac{1}{2} \int \left(p(x)^{1/2} - q(x)^{1/2} \right)^2 dx.$$