

**10707**

# **Deep Learning**

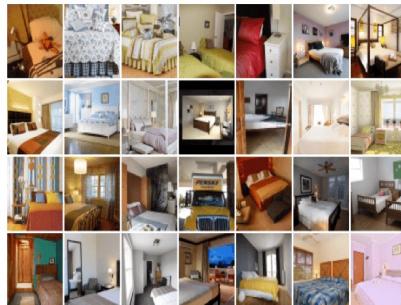
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Variational Inference

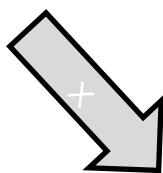
# Statistical Generative Models



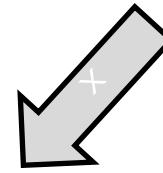
+

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



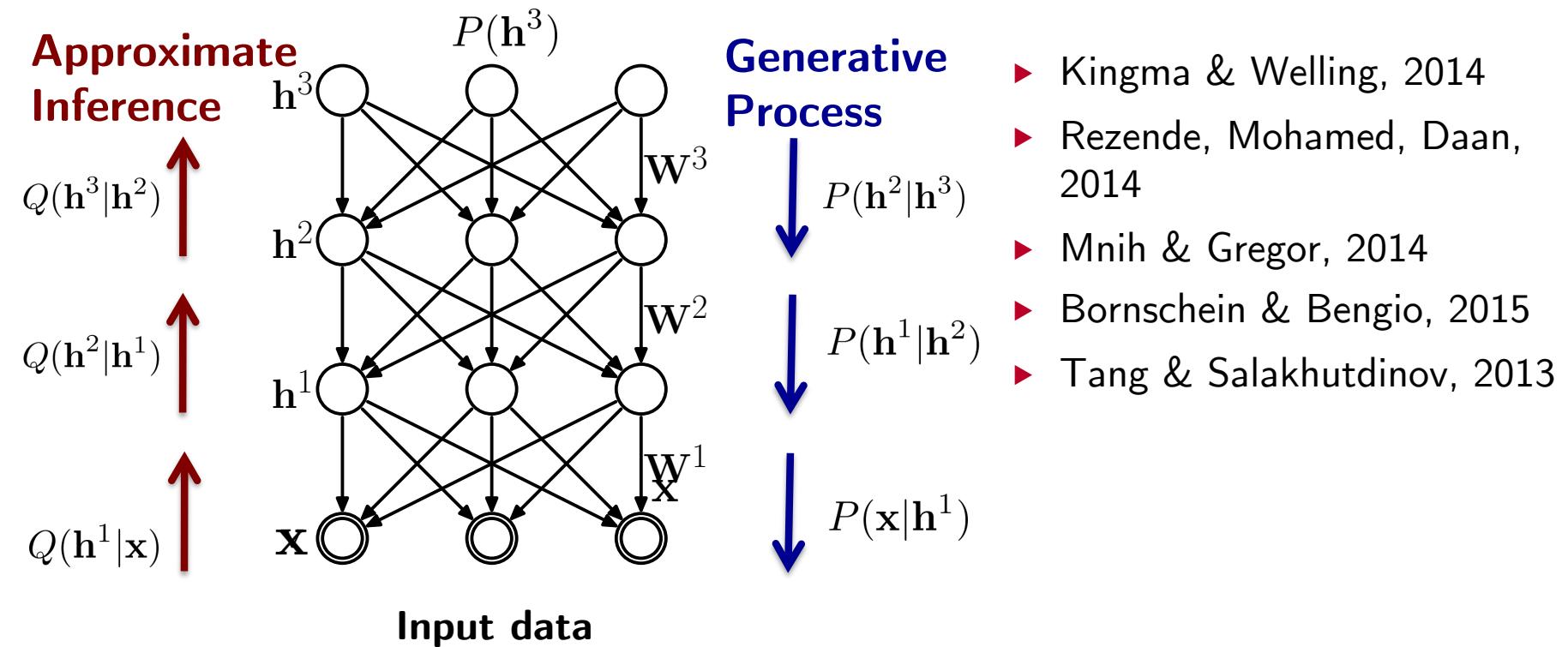
Monet



Van Gogh

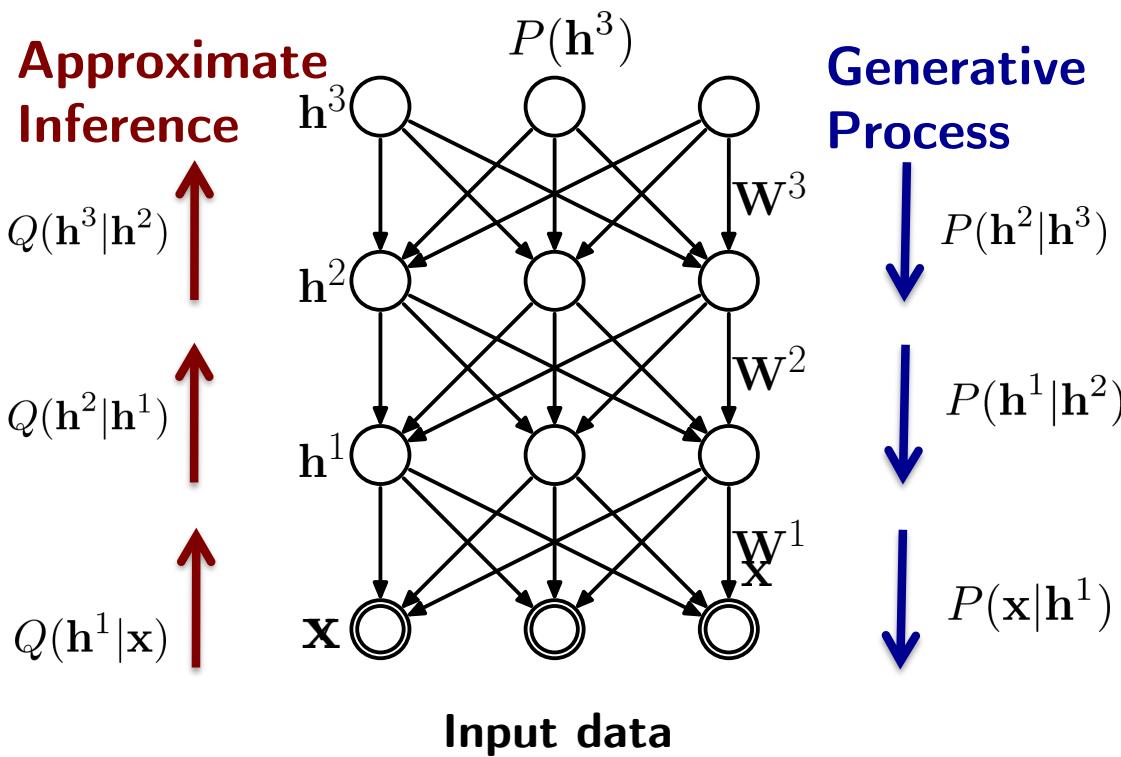
# Helmholtz Machines

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

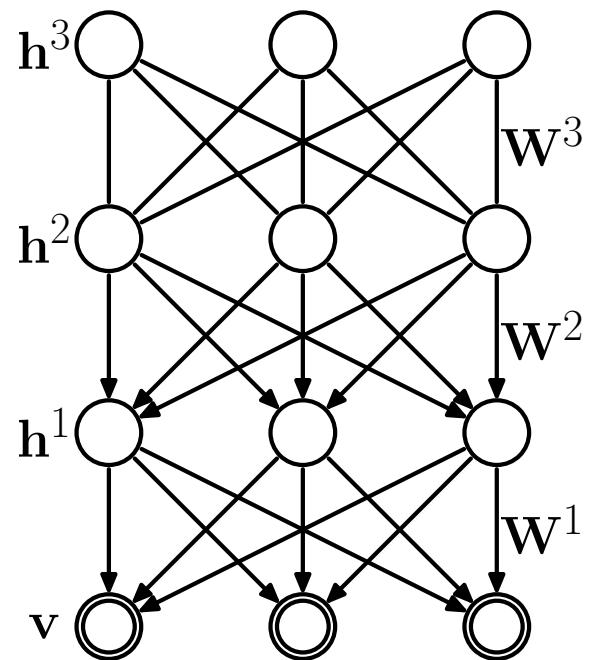


# Helmholtz Machines

Helmholtz Machine



Deep Belief Network

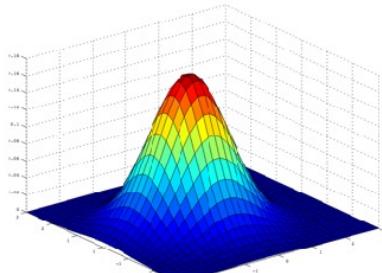
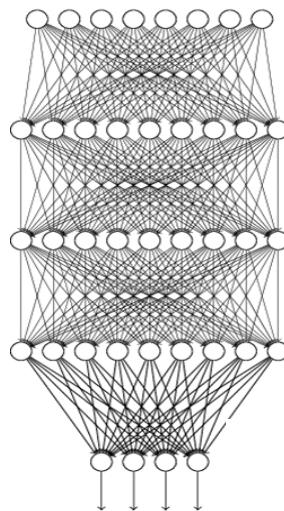


# Deep Directed Generative Models

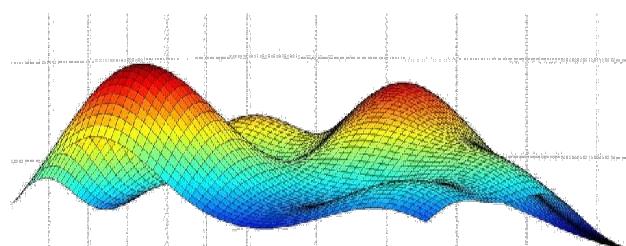
Code Z

► Latent Variable Models

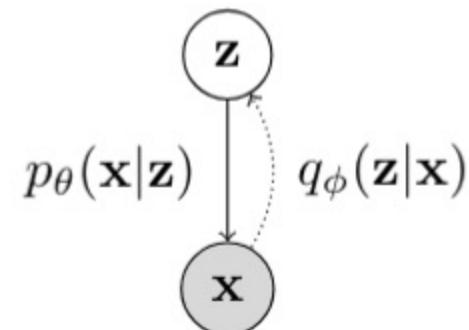
White  
Noise



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



$D_{real}$

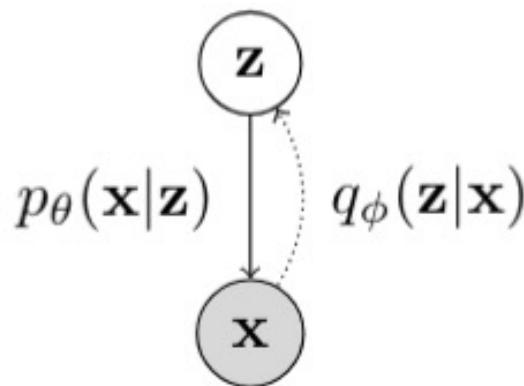


$$\log p_\theta(\mathbf{x}) = \log \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

- Conditional distributions are parameterized by deep neural networks

# Directed Deep Generative Models

- Directed Latent Variable Models with Inference Network



- Maximum log-likelihood objective

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

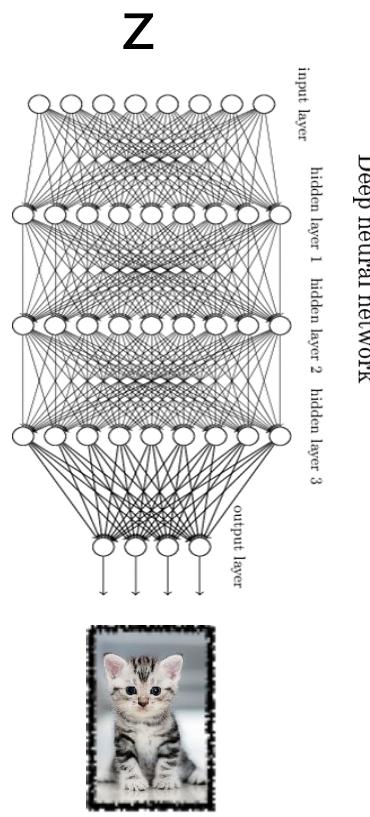
- Marginal log-likelihood is **intractable**:

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

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

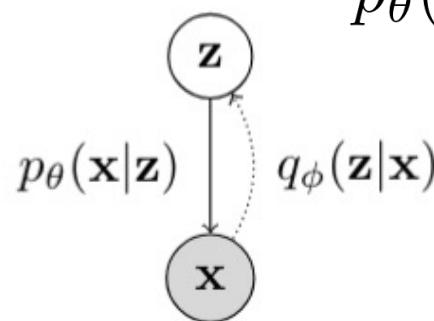
# Variational Autoencoders (VAEs)

- 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  $\theta$ .  
(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  $\phi$ .

# 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  $\theta$ , the goal is to **maximize the likelihood function**  $p(\mathbf{X}|\theta)$  with respect to  $\theta$ :

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

- 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



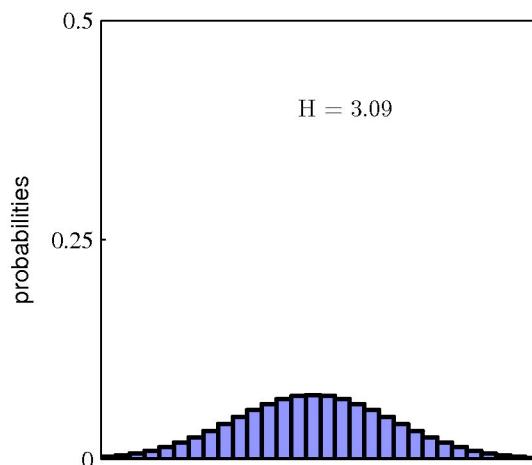
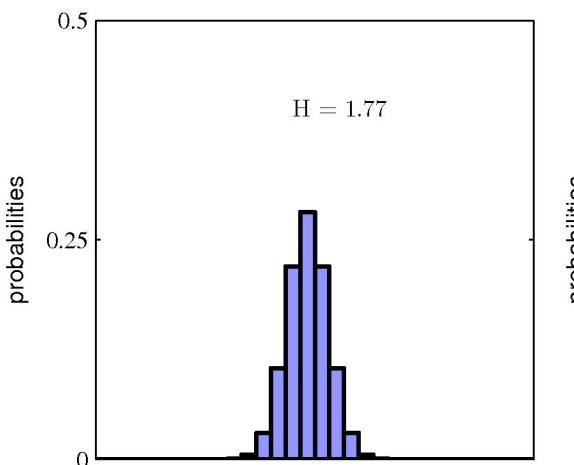
Entropy functional. Variational lower-  
bound

# 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 picked 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  $p(x) = q(x)$ .
- Intuitively, it measures the “**distance**” between the two distributions.

# 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:

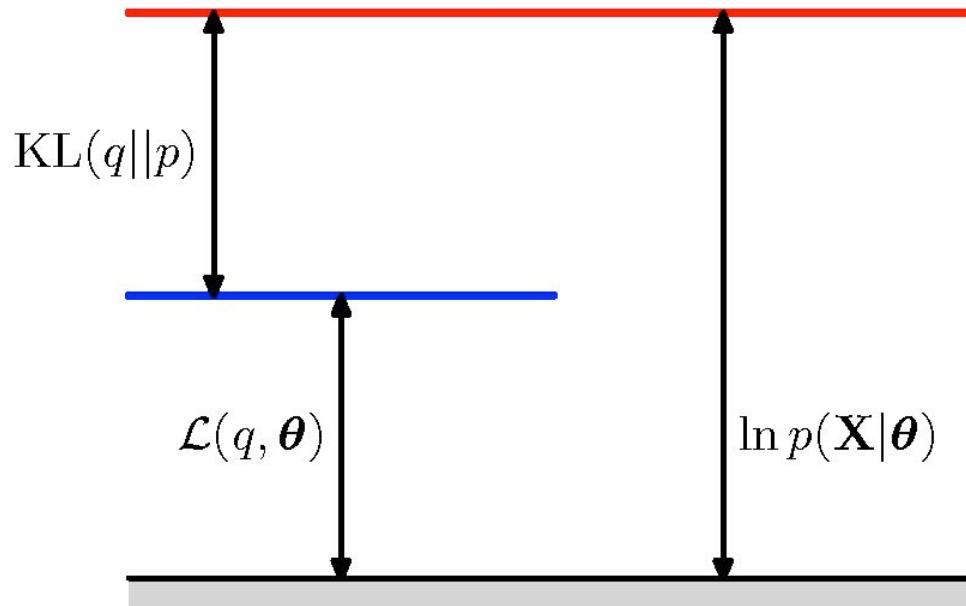
$$\ln p(\mathbf{X}|\theta) \geq \mathcal{L}(q, \theta),$$

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:

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

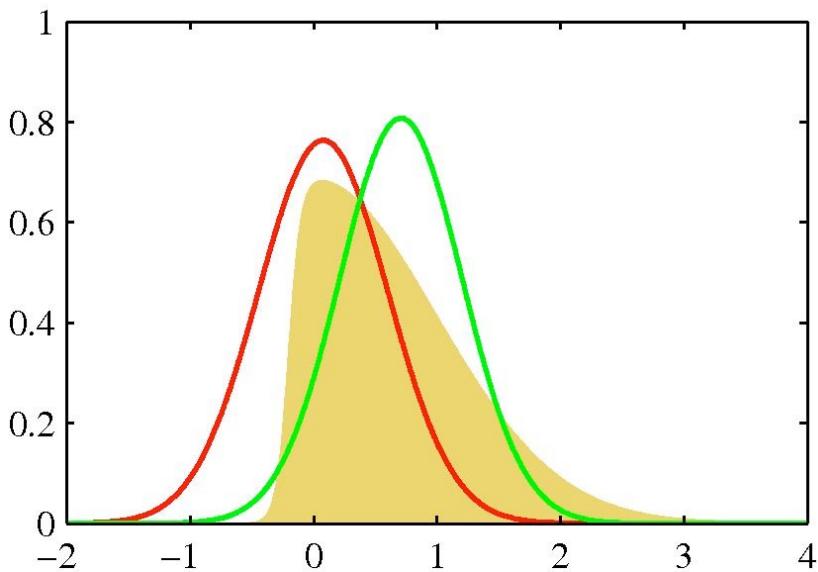
- We will assume that the **true posterior distribution is intractable**.
- We can consider a **restricted family of distributions**  $q(\mathbf{Z})$  and then find the member of this family for which KL is minimized.
- Our goal is to restrict the family of distributions so that it contains **only tractable 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  $\omega$ .
- The lower bound then becomes a function of  $\omega$ , 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  $\omega$ .

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

- 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:

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

$$= -\text{KL}(q_j(\mathbf{Z}_j) || \tilde{p}(\mathbf{X}, \mathbf{Z}_j)) + \text{const},$$

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:

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

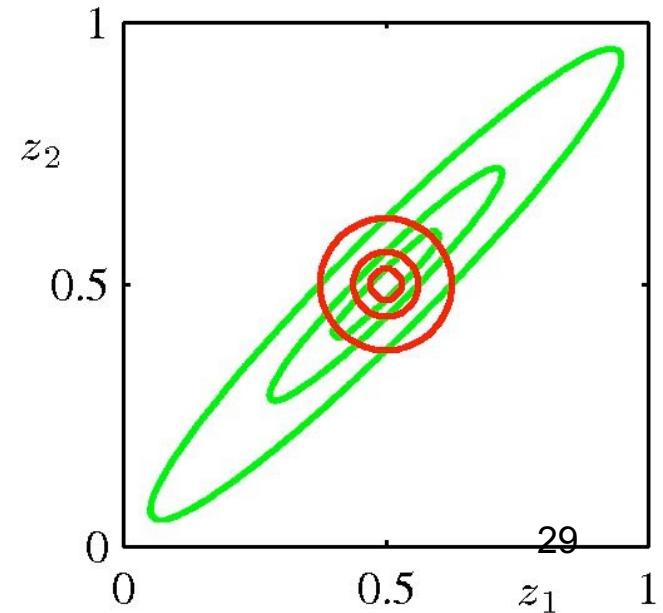
$$q_2^*(z_2) = \mathcal{N}(z_2 | m_2, \beta_{22}^{-1}), \quad m_2 = \mu_2 - \frac{\beta_{12}}{\beta_{22}}(\mathbb{E}[z_1] - \mu_1).$$

- 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.

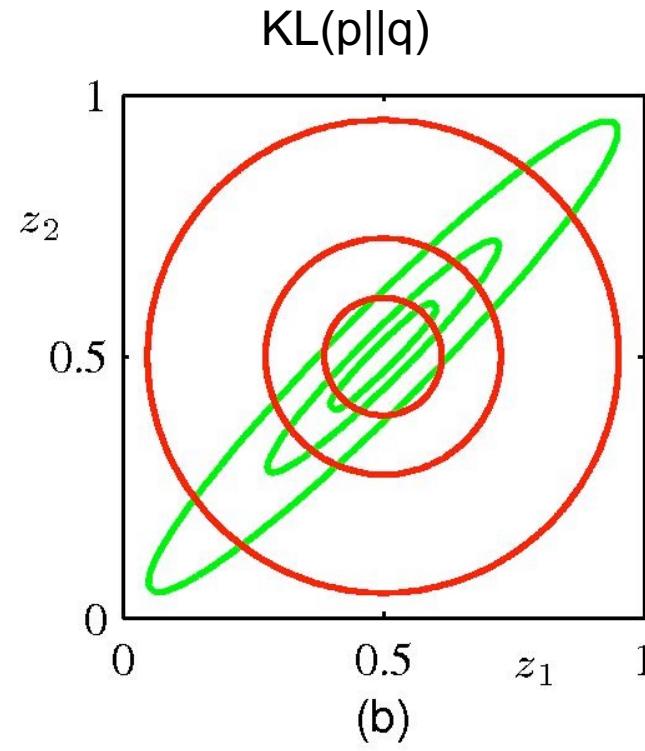
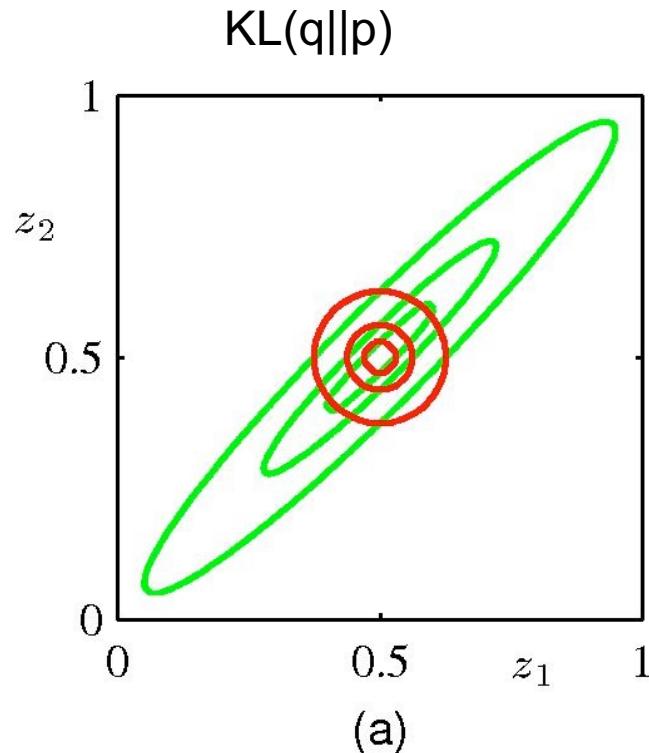
- It is easy to show that:

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

- 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

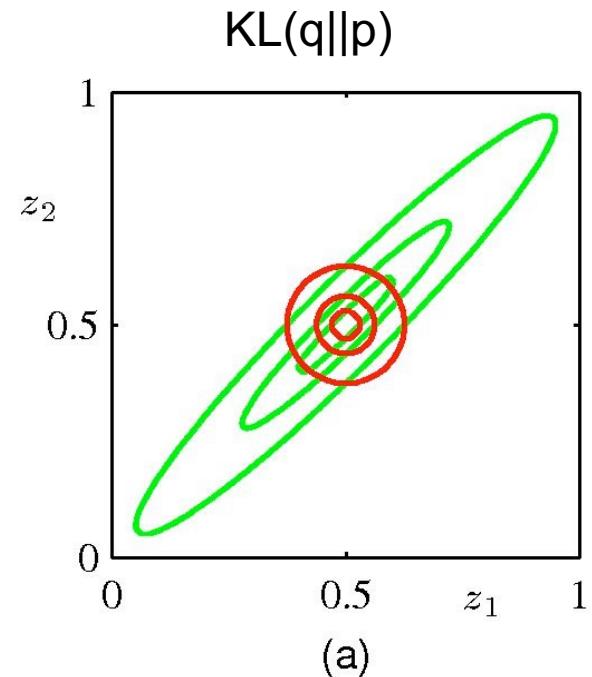
- The difference between these two approximations can be understood as follows:

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

- 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**.

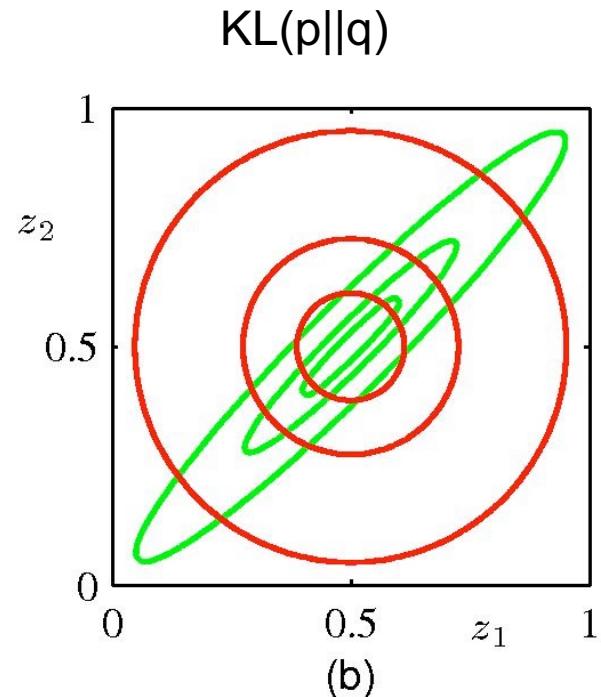


# Comparison of two KLs

- Similar arguments apply for **the alternative KL divergence**:

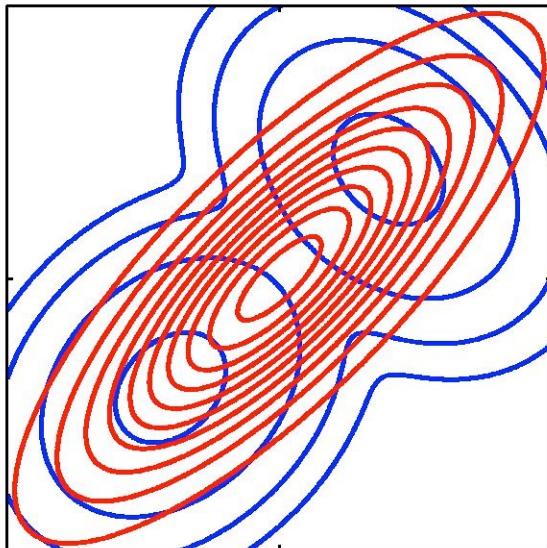
$$\text{KL}(p||q) = - \int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} d\mathbf{Z}.$$

- 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  $\text{KL}(p||q)$  leads to distributions  $q(\mathbf{Z})$  that are nonzero in regions where  $p(\mathbf{Z})$  is nonzero.

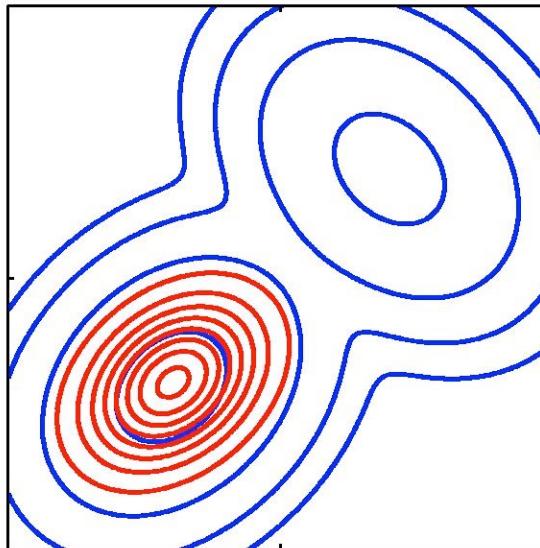


# Approximating Multimodal Distribution

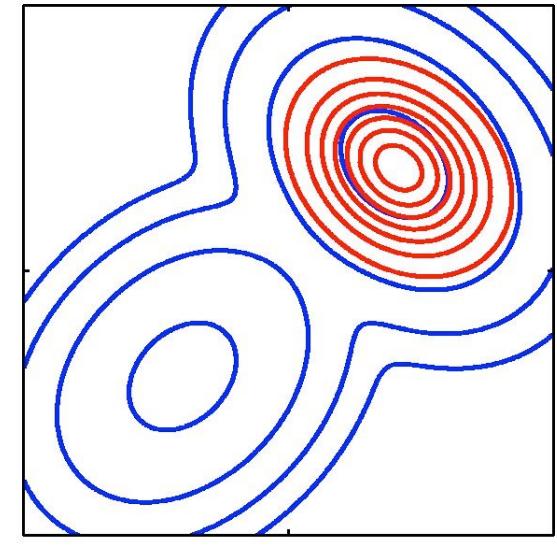
- Consider approximating multimodal distribution with a unimodal one.
- Blue contours show bimodal distribution  $p(\mathbf{Z})$ , red contours show a single Gaussian distribution that best approximates  $q(\mathbf{Z})$  that best approximates  $p(\mathbf{Z})$ .



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



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



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

- 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**:

- $\text{KL}(p||q)$  corresponds to the limit  $\alpha \rightarrow 1$ .
- $\text{KL}(q||p)$  corresponds to the limit  $\alpha \rightarrow -1$ .
- $D_\alpha(p||q) \geq 0$ , for all  $\alpha$ , 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**:

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