NUS National University of Singapore | School of Computing

CS5340
Uncertainty Modeling in AI

Lecture 11:
Variational Inference

Asst. Prof. Lee Gim Hee

AY 2018/19

Semester 1

Course Schedule

Week	Date	Topic	Remarks
1	15 Aug	Introduction to probabilities and probability distributions	
2	22 Aug	Fitting probability models	Hari Raya Haji*
3	29 Aug	Bayesian networks (Directed graphical models)	
4	05 Sep	Markov random Fields (Undirected graphical models)	
5	12 Sep	I will be traveling	No Lecture
6	19 Sep	Variable elimination and belief propagation	
-	26 Sep	Recess week	No lecture
7	03 Oct	Factor graph and the junction tree algorithm	
8	10 Oct	Parameter learning with complete data	
9	17 Oct	Mixture models and the EM algorithm	
10	24 Oct	Hidden Markov Models (HMM)	
11	31 Oct	Monte Carlo inference (Sampling)	
12	07 Nov	Variational inference	
13	14 Nov	Graph-cut and alpha expansion	

* **Make-up lecture**: 25 Aug (Sat), 9.30am-12.30pm, LT 15

Acknowledgements

- A lot of slides and content of this lecture are adopted from:

1. Christopher Bishop, “Pattern Recognition and Machine Learning”, Chapter 10.
2. Kevin Murphy, "Machine learning: a probabilistic approach“, Chapter 21 and 22.
3. David Barber, "Bayesian reasoning and machine learning“, Chapter 28.
4. Daphne Koller and NirFriedman, "Probabilistic graphical models“, Chapter 11.

Learning Outcomes

- Students should be able to:

1. Explain the concept of variational approach using Lower-Bound of maximum likelihood and KL-divergence.

2. Use variational approach to do inference on graphical models containing both hidden variables and unknown parameters.

3. Use Loopy Belief Propagation to do message passing.

Approximate Inference

- A central task in the application of probabilistic models is the evaluation of the posterior distribution $p(z|x)$.
- And the evaluation of expectations computed with respect to this distribution.
- Z is the latent variables (including the unknown parameters θ) and X is the observed variables.

Approximate Inference

- Could be infeasible to evaluate the posterior distribution or to compute expectations with respect to this distribution due to:

1. The dimensionality is too high in the latent space to work with directly.

2. The posterior distribution has a highly complex form for which expectations are not analytically tractable.

Approximate Inference

- In such situations, we need to resort to approximation schemes, and these fall broadly into two classes:

1. Stochastic approximation: Markov Chain Monte-Carlo (MCMC).

2. Deterministic approximation: Variational approach.

Variational Approach

- Given a joint distribution $p(x, z)$, our goal is to find an approximation $q(z)$ for the posterior distribution $p(z|x)$ which is intractable.

- **Key idea**: We choose the approximation $q(z)$ such that it minimizes the KL-divergence

$$\mathrm{KL}(q\|p) = -\int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} \right\} \mathrm{d}\mathbf{Z} \geq 0.$$

- i.e. $q(z)$ that is as close as possible to $p(z|x)$.

Variational Approach

$$\mathrm{KL}(q\|p) = -\int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} \right\} \mathrm{d}\mathbf{Z} \geq 0$$

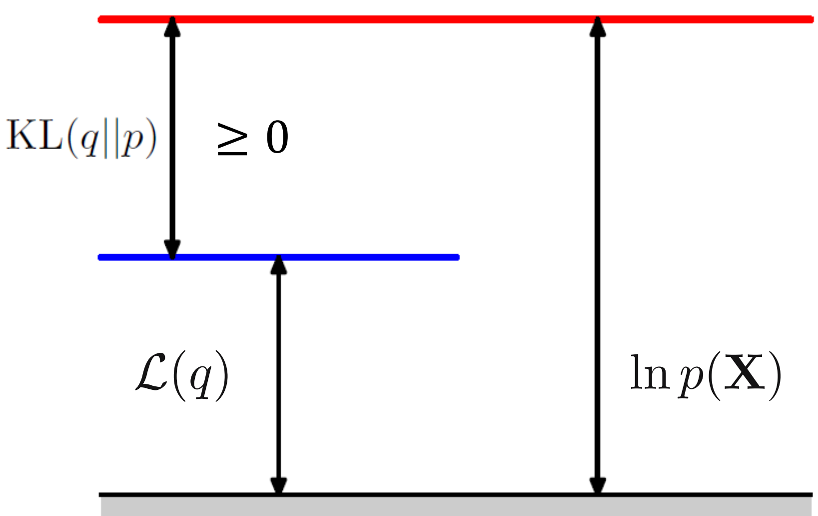
- Unfortunately, minimizing the KL-divergence is hard since $p(z|x)$ is intractable.

- **Solution:** Maximize the lower-bound of log-likelihood instead!

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

Variational Approach

- Recall in our discussion of EM, we can decompose the log marginal probability using:



$$\ln p(\mathbf{X}) = \underbrace{\mathcal{L}(q)}_{\text{Lower bound}} + \underbrace{\mathrm{KL}(q\|p)}_{\text{KL-divergence}}$$

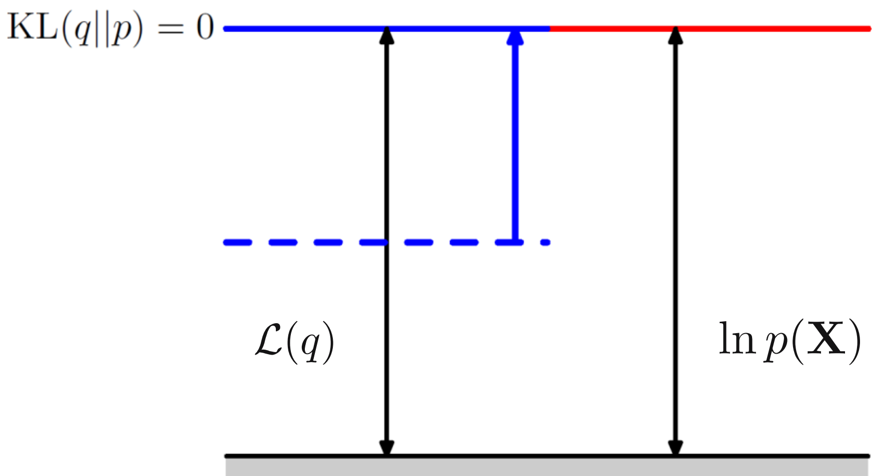
where

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

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

Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Variational Approach



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

where

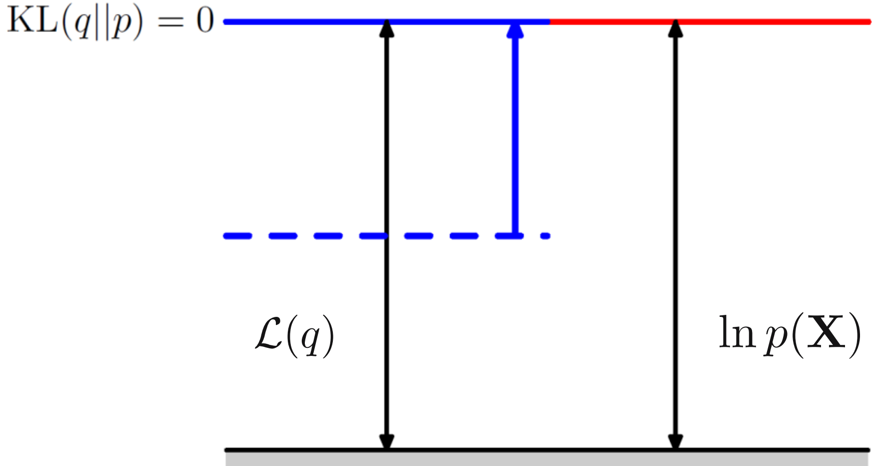
$$\mathcal{L}(q) = \int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} \right\} \mathrm{d}\mathbf{Z}$$

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

- Maximizing the lower bound $\mathcal{L}(q)$ by optimization with respect to the distribution $q(Z)$ is equivalent to minimizing the KL divergence.

Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Variational Approach



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

where

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

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

- What is a good approximation distribution $q(z)$ for the maximization of the lower-bound $\mathcal{L}(q)$?

Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Mean-Field Approximation

- Mean-field theory: an approximation framework developed in physics.

- Suppose we partition the elements of Z into disjoint groups that we denote by Z_i where $i = 1, \ldots, M$.

- We then assume that $q(z)$ factorizes with respect to these groups, so that:

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

Mean-Field Approximation

- We now seek that distribution for which the lower bound $\mathcal{L}(q)$ is largest amongst all distributions $q(z)$ having the form:

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

- Make a free form (variational) optimization of $\mathcal{L}(q)$ with respect to all of the distributions $q_i(z_i)$, which we do by optimizing w.r.t. each of the factors in turn.

Mean-Field Approximation

- Putting the factorized distribution of $q(z)$ into the lower-bound $\mathcal{L}(q)$, and dissect out the dependence on one of the factors $q_j(z_j)$, we get:

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

We want to maximize w.r.t. each of the $q_j(z_j)$!

Mean-Field Approximation

- We have defined a new distribution $\tilde{p}(x, z_j)$ by the relation:

$$\ln \widetilde{p}(\mathbf{X}, \mathbf{Z}_j) = \mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})] \,;$$

where

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

- The notation $\mathbb{E}_{i \neq j}[\cdots]$ denotes an expectation w.r.t. the q distributions over all variables Z_i for $i \neq j$.

Mean-Field Approximation

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

$$= \int q_j \ln \frac{\tilde{p}(\mathbf{x}, \mathbf{z_j})}{q_j} d\mathbf{Z_j} + \text{const}$$

$$= -KL\big(q_j \parallel \tilde{p}(\mathbf{x}, \mathbf{z_j})\big) + \text{const}$$

- The lower-bound is a negative KL-divergence that can be maximized by choosing

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

Mean-Field Approximation

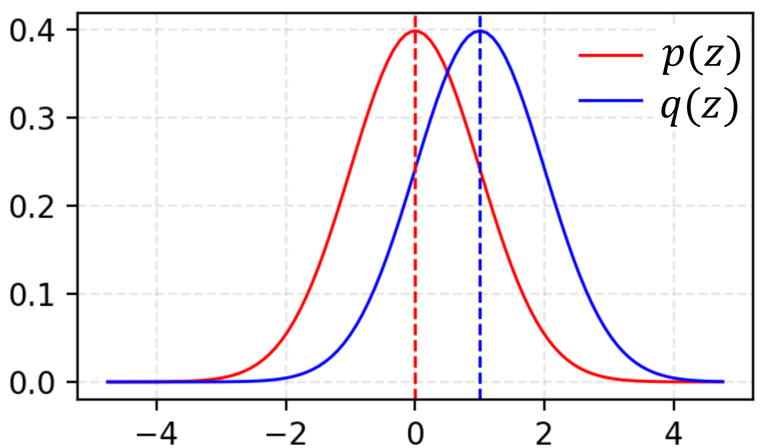
$$\ln q_j^\star(\mathbf{Z}_j) = \mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})] + \text{const}$$

- The additive constant is set by normalizing the distribution $q_j^*(z_j)$, taking the exponential of both sides and normalize, we have

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

Forward vs Backward KL-Divergence

- KL-divergence is not symmetrical, minimizing $KL(q \parallel p)$ and $KL(p \parallel q)$ will give different results.



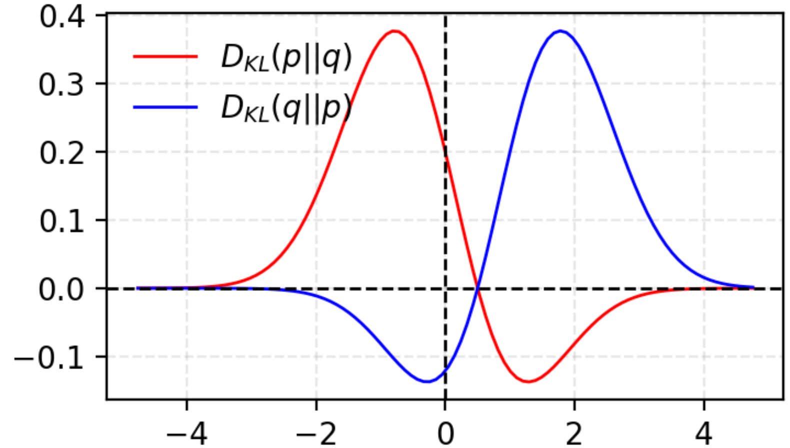


Image source: https://lilianweng.github.io/lil-log/2017/08/20/from-GAN-to-WGAN.html

Forward vs Backward KL-Divergence

- First, consider the reverse KL, $KL(q \parallel p)$, also known as an **I-projection** or **information projection**:

$$KL(q \parallel p) = \sum_{\mathrm{z}} q(\mathrm{z}) \ln \frac{q(\mathrm{z})}{p(\mathrm{z})}$$

- This is infinite if $p(z) = 0$ and $q(z) > 0$; thus if $p(z) = 0$ we must ensure $q(z) = 0$.

- We say that reverse KL is zero forcing for q, hence q will typically under-estimate the support of p.

Forward vs Backward KL-Divergence

- Next, consider the forward KL, also known as an **M-projection** or **moment projection**:

$$KL(p \parallel q) = \sum_{\mathrm{z}} p(\mathrm{z}) \ln \frac{p(\mathrm{z})}{q(\mathrm{z})}$$

- This is infinite if $q(x) = 0$ and $p(z) > 0$, thus if $p(z) > 0$, we must ensure $q(z) > 0$.

- We say that forward KL is zero avoiding for q, hence q will typically over-estimate the support of p.

Forward vs Backward KL-Divergence

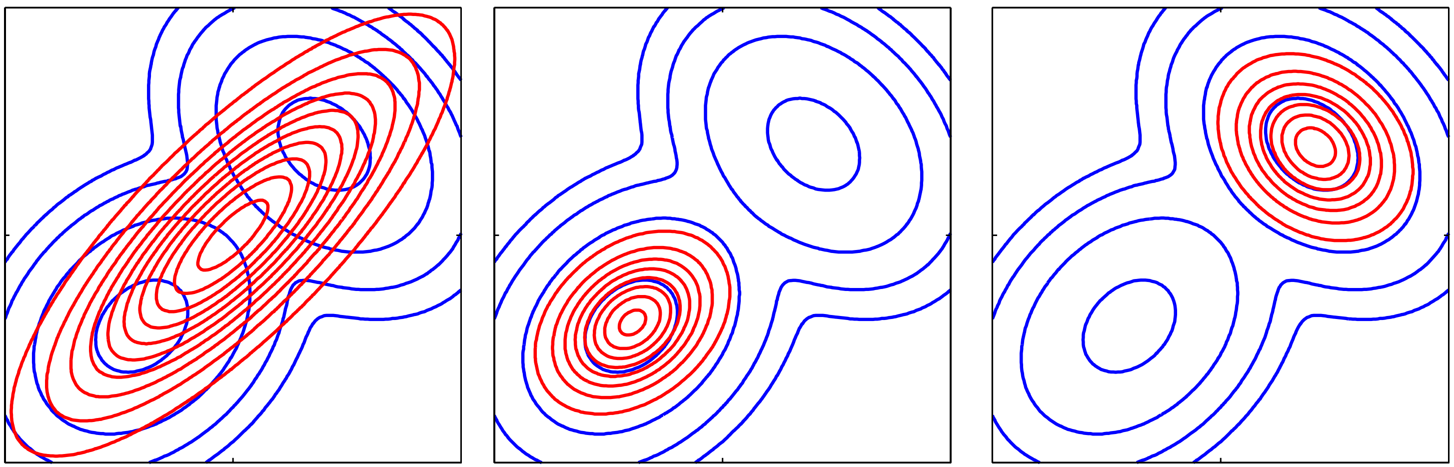
Blue contours: Bimodal distribution $p(Z)$
Red contours: $q(Z)$ that best approximates $p(Z)$

Minimizing $\boldsymbol{KL(p \parallel q)}$

Minimizing $\boldsymbol{KL(q \parallel p)}$

Local minima 1

Local minima 2



(a) (b) (c)

$q(Z)$ is nonzero in regions where $p(Z)$ is nonzero, i.e. zero avoiding

$q(Z)$ is small when $p(Z)$ is small, i.e. zero forcing

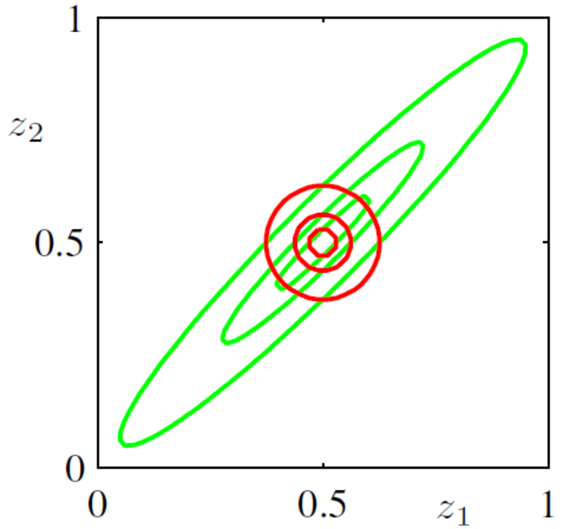
Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Forward vs Backward KL-Divergence

Red contours: approximating distribution $q(z)$

Green contours: Gaussian distribution $p(z)$

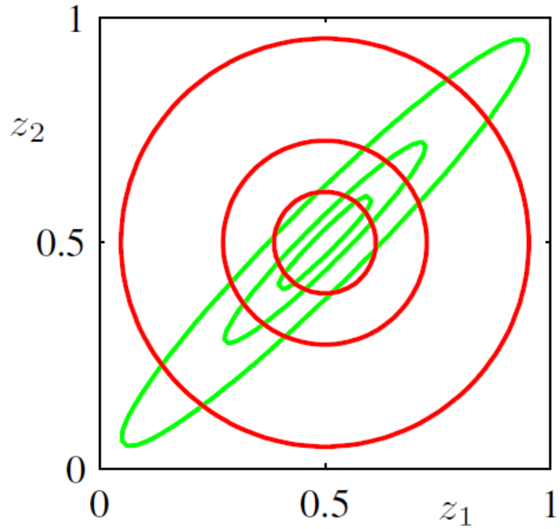
Minimizing $\boldsymbol{KL(q \parallel p)}$



(a)

Under-estimation

Minimizing $\boldsymbol{KL(p \parallel q)}$



(b)

Over-estimation

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Forward or Backward KL-Divergence?

- We use Backward KL-divergence $KL(q \parallel p)$ because it leads to a tractable lower-bound:

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

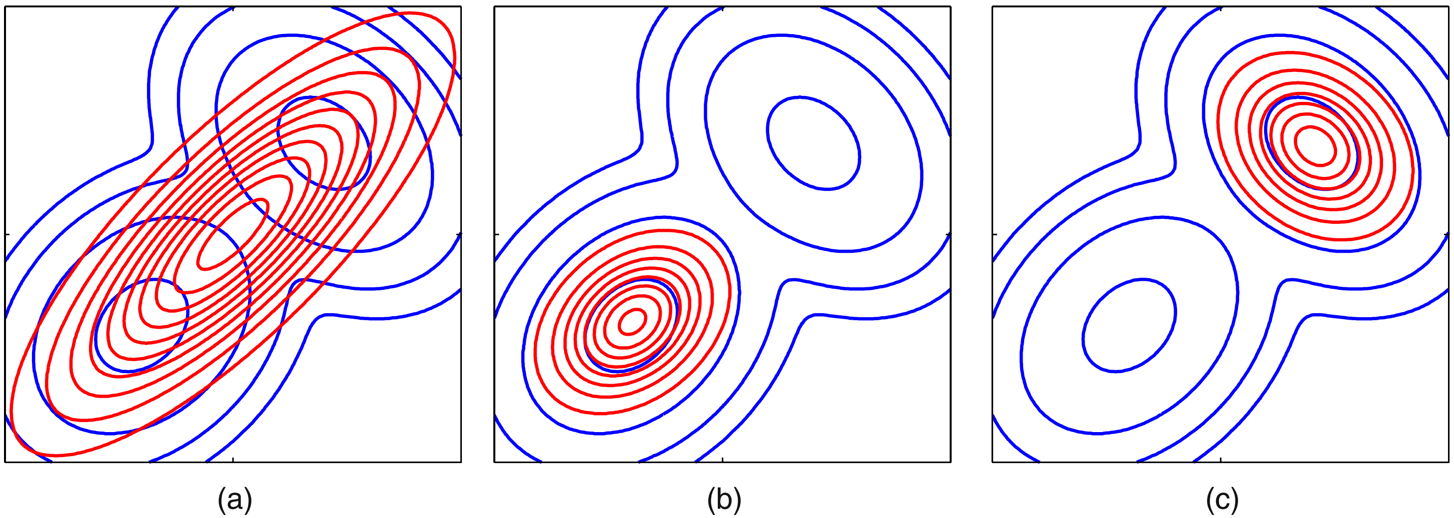
- Compared to forward KL-divergence $KL(p \parallel q)$ which leads to a intractable lower-bound:

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

Intractable to compute $p(\mathbf{Z}|\mathbf{X})$

Forward or Backward KL-Divergence?

Minimizing $KL(p \parallel q)$ **Minimizing $KL(q \parallel p)$**



- Backward KL-divergence is statistically more sensible because we saw that forward KL-divergence wrongly chose a mean in a region of low density.

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Example 1: The Univariate Gaussian

- **Given**: a data set $\mathcal{D} = \{x_1, \dots, x_N\}$ of observed values of X, which are assumed to be drawn independently from the Gaussian.

- **Goal**: infer the posterior distribution for the mean μ and precision τ (inverse of the covariance).

- The likelihood function is given by:

$$p(\mathcal{D}|\mu, \tau) = \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\left\{-\frac{\tau}{2}\sum_{n=1}^{N}(x_n - \mu)^2\right\}.$$

Example 1: The Univariate Gaussian

- The conjugate prior distributions (Gaussian-Gamma) for μ and τ given by:

$$\begin{aligned} p(\mu|\tau) &= \mathcal{N}\left(\mu|\mu_0, (\lambda_0\tau)^{-1}\right) \\ p(\tau) &= \mathrm{Gam}(\tau|a_0, b_0) \end{aligned}$$

$\longleftarrow$ (μ_0, λ_0) : hyperparameters

- Gamma distribution:

$$\mathrm{Gam}(\tau|a_0, b_0) = \frac{1}{\Gamma(a_0)} b^{a_0} \tau^{a_0 - 1} \exp(-b_0\tau)$$

where a_0 and b_0 are the hyperparameters.

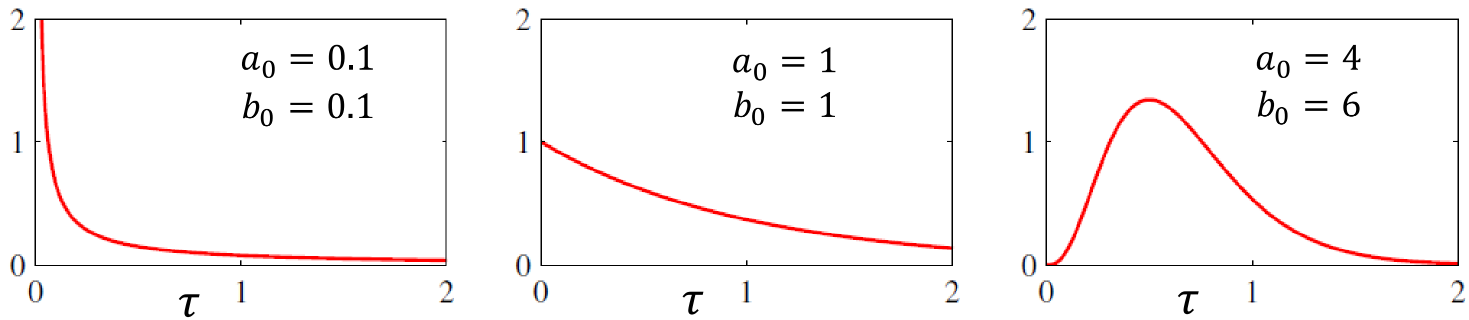


Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Example 1: The Univariate Gaussian

Note: For this simple problem the posterior distribution can be found exactly, but we will do this with variational approach for tutorial purpose.

Example 1: The Univariate Gaussian

- We consider a factorized variational approximation to the posterior distribution given by:

$$q(\mu, \tau) = q_\mu(\mu) q_\tau(\tau) \, ,$$

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

- The optimum factors $q_\mu(\mu)$ and $q_\tau(\tau)$ can be obtained from the general result:

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

Example 1: The Univariate Gaussian

- The optimal solution for $\boldsymbol{q_\mu(\mu)}$ is given by:

$$\begin{aligned}\ln q_\mu^\star(\mu) &= \mathbb{E}_\tau\left[\ln p(\mathcal{D}|\mu,\tau) + \ln p(\mu|\tau)\right] + \text{const} \\ &= -\frac{\mathbb{E}[\tau]}{2}\left\{\lambda_0(\mu-\mu_0)^2 + \sum_{n=1}^{N}(x_n-\mu)^2\right\} + \text{const.}\end{aligned}$$

- Completing the square over μ, we see that $q_\mu(\mu)$ is a Gaussian $\mathcal{N}(\mu|\mu_N, \lambda_N^{-1})$ with means and precision given by:

$$\begin{aligned}\mu_N &= \frac{\lambda_0\mu_0 + N\overline{x}}{\lambda_0 + N} \\ \lambda_N &= (\lambda_0 + N)\mathbb{E}[\tau].\end{aligned}$$

$N \to \infty \Longrightarrow \mu_N = \overline{x}$ and precision is infinite, i.e. maximum likelihood

Example 1: The Univariate Gaussian

- Similarly, the optimal solution for the factor $\boldsymbol{q_\tau(\tau)}$ is given by:

$$\begin{aligned}
\ln q_\tau^\star(\tau) &= \mathbb{E}_\mu \left[\ln p(\mathcal{D}|\mu,\tau) + \ln p(\mu|\tau)\right] + \ln p(\tau) + \text{const} \\
&= (a_0 - 1)\ln\tau - b_0\tau + \frac{N}{2}\ln\tau \\
&\quad -\frac{\tau}{2}\mathbb{E}_\mu\left[\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right] + \text{const}
\end{aligned}$$

- Hence, $q_\tau(\tau)$ is a gamma distribution $\text{Gam}(\tau\,|a_N, b_N)$ with parameters:

$$a_N = a_0 + \frac{N+1}{2}$$

$$b_N = b_0 + \frac{1}{2}\mathbb{E}_\mu\left[\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right].$$

Example 1: The Univariate Gaussian

- It should be emphasized that we did not assume any specific functional forms for the optimal distributions $q_\mu(\mu)$ and $q_\tau(\tau)$.

- They arose naturally from the structure of the likelihood function and the corresponding conjugate priors!

Example 1: The Univariate Gaussian

Problem: solutions are coupled!

$q_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \lambda_N^{-1})$, where

$$\begin{cases} \mu_N = \dfrac{\lambda_0\mu_0 + N\overline{x}}{\lambda_0 + N} \\ \lambda_N = (\lambda_0 + N)\boxed{\mathbb{E}[\tau].} \end{cases}$$

Depends on $q_\tau(\tau)$!

$q_\tau(\tau) = \mathrm{Gam}(\tau\,|a_N, b_N)$, where

Depends on $q_\mu(\mu)$!

$$\begin{cases} a_N = a_0 + \dfrac{N}{2} \\ b_N = b_0 + \dfrac{1}{2}\boxed{\mathbb{E}_\mu\left[\sum_{n=1}^{N}(x_n - \mu)^2 + \lambda_0(\mu - \mu_0)^2\right].} \end{cases}$$

Example 1: The Univariate Gaussian

Solution: an iterative approach

1. Make an initial guess for $\mathbb{E}[\tau]$ and use this to re-compute $q_\mu(\mu)$.

2. Use the revised $q_\mu(\mu)$ to extracted the moments $\mathbb{E}[\mu]$ and $\mathbb{E}[\mu^2]$, and use these to re-compute $q_\tau(\tau)$.

3. Use the revised $q_\tau(\tau)$ to extract the moment $\mathbb{E}[\tau]$ and use this to re-compute $q_\mu(\mu)$.

4. Repeat until convergence.

Example 1: The Univariate Gaussian

Contours of the true posterior distribution $p(\mu, \tau \,|\mathcal{D})$ are shown in green

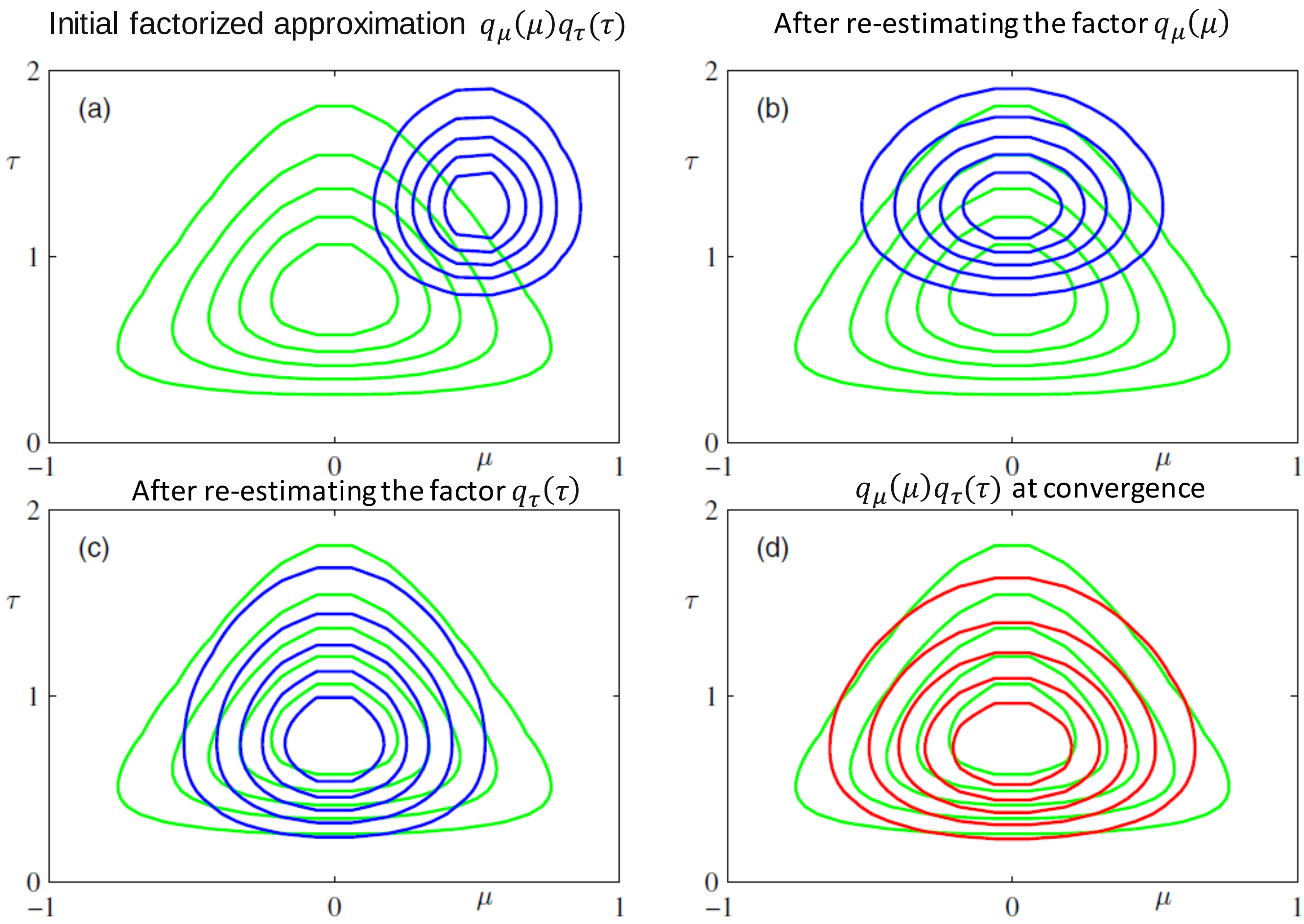


Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Example 2: Mixture of Gaussian

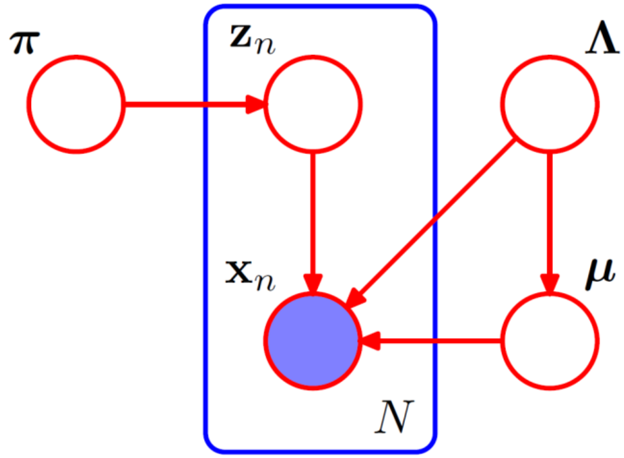


Plate denotes a set of N i.i.d. observations
$\boldsymbol{\mu}$ denotes $\{\boldsymbol{\mu}_k\}$ and $\boldsymbol{\Lambda}$ denotes $\{\boldsymbol{\Lambda}_k\}$.

- Let's look at a slightly more complicated example of applying variational inference on mixture of Gaussian.

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Example 2: Mixture of Gaussian

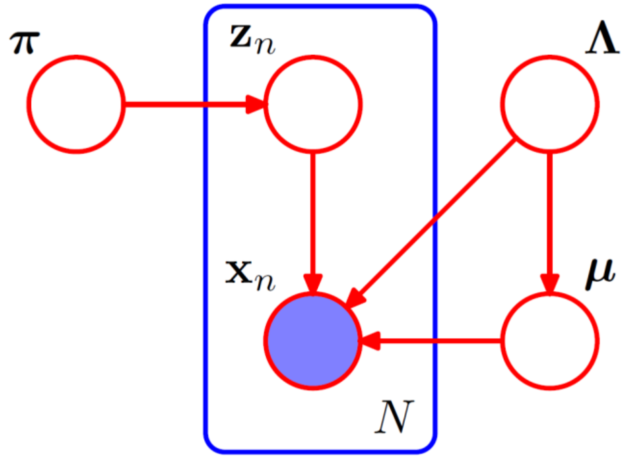


Plate denotes a set of N i.i.d. observations
$\boldsymbol{\mu}$ denotes $\{\boldsymbol{\mu}_k\}$ and $\boldsymbol{\Lambda}$ denotes $\{\boldsymbol{\Lambda}_k\}$.

- For each observation X_n, we have a corresponding latent variable Z_n comprising a 1-of-K binary vector with elements Z_{nk} for $k = 1, \ldots, K$.
- We denote the observed data set by $X = \{X_1, \ldots, X_N\}$, and similarly we denote the latent variables set by $Z = \{Z_1, \ldots, Z_N\}$.

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Example 2: Mixture of Gaussian

- Conditional distribution of Z, given the mixing coefficients π:

$$p(\mathbf{Z}|\boldsymbol{\pi}) = \prod_{n=1}^{N}\prod_{k=1}^{K}\pi_k^{z_{nk}}.$$

(Categorial distribution)

- Dirichlet distribution conjugate prior over the mixing coefficients π:

Normalizing constant (see Lecture 1)

$$p(\boldsymbol{\pi}) = \mathrm{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_0) = C(\boldsymbol{\alpha}_0)\prod_{k=1}^{K}\pi_k^{\alpha_0 - 1}$$

- Where we chose the same hyperparameter α_0 for each component.

Example 2: Mixture of Gaussian

- Conditional distribution of observed data vectors, given latent variables and component parameters:

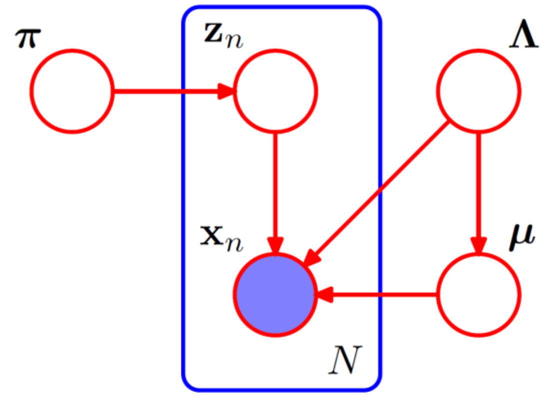
$$p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right)^{z_{nk}}$$

- Independent Gaussian-Wishart prior governing the mean and precision of each Gaussian component:

$$\begin{aligned} p(\boldsymbol{\mu}, \boldsymbol{\Lambda}) &= p(\boldsymbol{\mu}|\boldsymbol{\Lambda})p(\boldsymbol{\Lambda}) \\ &= \prod_{k=1}^{K} \mathcal{N}\left(\boldsymbol{\mu}_k | \mathbf{m}_0, (\beta_0 \boldsymbol{\Lambda}_k)^{-1}\right) \mathcal{W}(\boldsymbol{\Lambda}_k | \mathbf{W}_0, \nu_0) \end{aligned}$$

- Where $\mathrm{m}_0, \mathrm{W}_0, \nu_0$ are the hyperparameters.

Example 2: Mixture of Gaussian



- Joint distribution:

$$p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\mu}, \boldsymbol{\Lambda})p(\mathbf{Z}|\boldsymbol{\pi})p(\boldsymbol{\pi})p(\boldsymbol{\mu}|\boldsymbol{\Lambda})p(\boldsymbol{\Lambda})$$

- Consider a variational distribution which factorizes between the latent variables and parameters:

$$q(\mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = q(\mathbf{Z})q(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}).$$

Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Example 2: Mixture of Gaussian

- The log of the optimized factor for $\boldsymbol{q}(\boldsymbol{z})$ is given by:

$$\ln q^\star(\mathbf{Z}) = \mathbb{E}_{\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Lambda}}[\ln p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})] + \text{const.}$$

- Substituting the joint distribution and absorbing all terms that do not depend on Z into the additive constant, we get:

$$\ln q^\star(\mathbf{Z}) = \mathbb{E}_{\boldsymbol{\pi}}[\ln p(\mathbf{Z}|\boldsymbol{\pi})] + \mathbb{E}_{\boldsymbol{\mu},\boldsymbol{\Lambda}}[\ln p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\mu}, \boldsymbol{\Lambda})] + \text{const.}$$

Example 2: Mixture of Gaussian

- Substituting the two conditional distributions, and again absorbing all terms independent of Z into the additive constant, we have:

$$\ln q^\star(\mathbf{Z}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \ln \rho_{nk} + \text{const}$$

where we have defined

Dimensionality of data variable x

$$\begin{aligned}\ln \rho_{nk} \quad = \quad & \mathbb{E}[\ln \pi_k] + \frac{1}{2}\mathbb{E}\left[\ln |\boldsymbol{\Lambda}_k|\right] - \frac{D}{2}\ln(2\pi) \\ & -\frac{1}{2}\mathbb{E}_{\boldsymbol{\mu}_k,\boldsymbol{\Lambda}_k}\left[(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}\boldsymbol{\Lambda}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)\right]\end{aligned}$$

Example 2: Mixture of Gaussian

- Taking the exponential of both sides, we obtain:

$$q^\star(\mathbf{Z}) \propto \prod_{n=1}^{N} \prod_{k=1}^{K} \rho_{nk}^{z_{nk}}.$$

- Normalizing this distribution, and noting that $z_{nk} = \{0,1\}$ and sum to 1 over all values of k, we obtain:

$$q^\star(\mathbf{Z}) = \prod_{n=1}^{N} \prod_{k=1}^{K} r_{nk}^{z_{nk}}$$

Same functional form as $p(\mathrm{z}|\pi)$!

where

$$r_{nk} = \frac{\rho_{nk}}{\sum_{j=1}^{K} \rho_{nj}}.$$

Note that quantities r_{nk} are playing the role of responsibilities (i.e. this is similar to the E-Step in EM)!

Example 2: Mixture of Gaussian

- Let us define three statistics of the observed data set evaluated with respect to the responsibilities:

$$
\begin{aligned}
N_k &= \sum_{n=1}^{N} r_{nk} \\
\overline{\mathbf{x}}_k &= \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} \mathbf{x}_n \\
\mathbf{S}_k &= \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} (\mathbf{x}_n - \overline{\mathbf{x}}_k)(\mathbf{x}_n - \overline{\mathbf{x}}_k)^{\mathrm{T}}.
\end{aligned}
$$

- These are analogous to quantities evaluated in the maximum likelihood EM algorithm for the Gaussian mixture model.

Example 2: Mixture of Gaussian

- The log of the optimized factor for $\boldsymbol{q(\pi, \mu, \Lambda)}$ is given by:

Depends only on π

$$\ln q^{\star}(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = \boxed{\ln p(\boldsymbol{\pi})} + \boxed{\sum_{k=1}^{K} \ln p(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k)} + \boxed{\mathbb{E}_{\mathbf{Z}}\left[\ln p(\mathbf{Z}|\boldsymbol{\pi})\right]}$$
$$+ \boxed{\sum_{k=1}^{K}\sum_{n=1}^{N} \mathbb{E}[z_{nk}] \ln \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right)} + \text{const.}$$

Depends only on (μ, Λ)

Further factorizes into

$$q(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = q(\boldsymbol{\pi}) \prod_{k=1}^{K} q(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k)$$

Example 2: Mixture of Gaussian

$\ln q^*(\pi)$ is given by:

$$\ln q^\star(\boldsymbol{\pi}) = (\alpha_0 - 1)\sum_{k=1}^{K} \ln \pi_k + \sum_{k=1}^{K}\sum_{n=1}^{N} r_{nk} \ln \pi_k + \text{const}$$

Taking exponential of both sides, we get:

$$q^\star(\boldsymbol{\pi}) = \text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha})$$

Dirichlet distribution!

where $\boldsymbol{\alpha}$ has components α_k given by:

$$\alpha_k = \alpha_0 + N_k.$$

Example 2: Mixture of Gaussian

And $\ln q^*(\mu, \Lambda)$ is given by:

r_{nk}: responsibility defined earlier

$$\ln q^\star(\boldsymbol{\mu}, \boldsymbol{\Lambda}) = \sum_{k=1}^{K} \ln \underbrace{p(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k)}_{\mathcal{N}\left(\boldsymbol{\mu}_k|\mathbf{m}_0, (\beta_0\boldsymbol{\Lambda}_k)^{-1}\right)\,\mathcal{W}(\boldsymbol{\Lambda}_k|\mathbf{W}_0, \nu_0)} + \sum_{k=1}^{K}\sum_{n=1}^{N} \boxed{\mathbb{E}[z_{nk}]} \ln \mathcal{N}\left(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right) + \text{const.}$$

Proof:

$$\mathbb{E}[z_{nk}] = \sum_z q(z) z_{nk} \qquad \text{where} \quad q^\star(\mathbf{Z}) = \prod_{n=1}^{N}\prod_{k=1}^{K} r_{nk}^{z_{nk}}$$

$$= \sum_z \prod_n \prod_k r_{nk}^{z_{nk}} \, z_{nk}$$

$$= r_{nk}$$

Example 2: Mixture of Gaussian

Taking exponent on both sides, we get $q^*(\mu_k, \Lambda_k) = q^*(\mu_k|\Lambda_k)q^*(\Lambda_k)$, where:

$$q^\star(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) = \underbrace{\mathcal{N}\left(\boldsymbol{\mu}_k|\mathbf{m}_k, (\beta_k\boldsymbol{\Lambda}_k)^{-1}\right)}_{q^*(\mu_k|\Lambda_k)} \underbrace{\mathcal{W}(\boldsymbol{\Lambda}_k|\mathbf{W}_k, \nu_k)}_{q^*(\Lambda_k)}$$

Gaussian-Wishart distribution!

with:

$$\begin{aligned}
\beta_k &= \beta_0 + N_k \\
\mathbf{m}_k &= \frac{1}{\beta_k}(\beta_0\mathbf{m}_0 + N_k\overline{\mathbf{x}}_k) \\
\mathbf{W}_k^{-1} &= \mathbf{W}_0^{-1} + N_k\boxed{\mathbf{S}_k} + \frac{\beta_0 N_k}{\beta_0 + N_k}(\overline{\mathbf{x}}_k - \mathbf{m}_0)(\overline{\mathbf{x}}_k - \mathbf{m}_0)^{\mathrm{T}} \\
\nu_k &= \nu_0 + N_k.
\end{aligned}$$

Similar to M-step of the EM algorithm for mixture of Gaussians!

Dependent on responsibility $\mathbb{E}[z_{nk}]$

Example 2: Mixture of Gaussian

- As before, the solutions are coupled; we will use the iterative approach (similar to EM iterations).

$$\ln q^\star(\mathbf{Z}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} \ln \rho_{nk} + \text{const}$$

Depends on $q(\pi, \mu, \Lambda)$

where

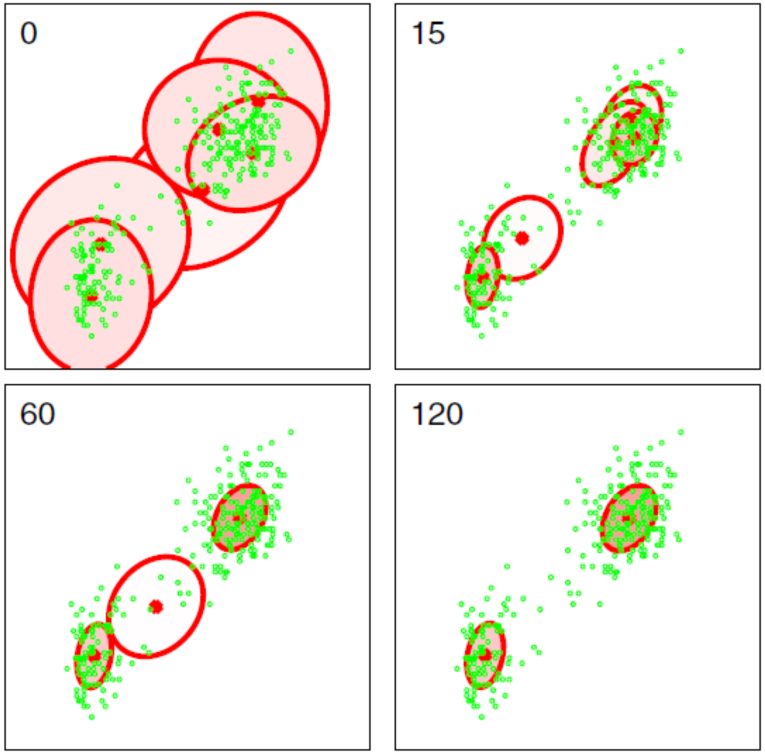
$$\ln \rho_{nk} = \boxed{\mathbb{E}[\ln \pi_k]} + \frac{1}{2}\boxed{\mathbb{E}\left[\ln |\boldsymbol{\Lambda}_k|\right]} - \frac{D}{2}\ln(2\pi) - \frac{1}{2}\boxed{\mathbb{E}_{\boldsymbol{\mu}_k,\boldsymbol{\Lambda}_k}\left[(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}\boldsymbol{\Lambda}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)\right]}$$

$$\ln q^\star(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = \ln p(\boldsymbol{\pi}) + \sum_{k=1}^{K} \ln p(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) + \boxed{\mathbb{E}_{\mathbf{Z}}\left[\ln p(\mathbf{Z}|\boldsymbol{\pi})\right]} + \sum_{k=1}^{K}\sum_{n=1}^{N} \boxed{\mathbb{E}[z_{nk}]} \ln \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right) + \text{const.}$$

Depends on $q(Z)$

Example 2: Mixture of Gaussian

- Initialized with $K = 6$, but eventually converged to two unique clusters.
- All other unused components have the respective $r_{nk} \approx 0$.

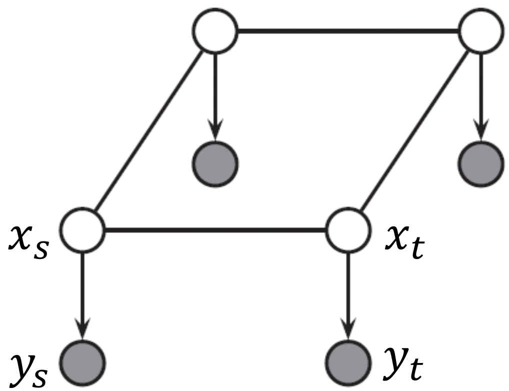


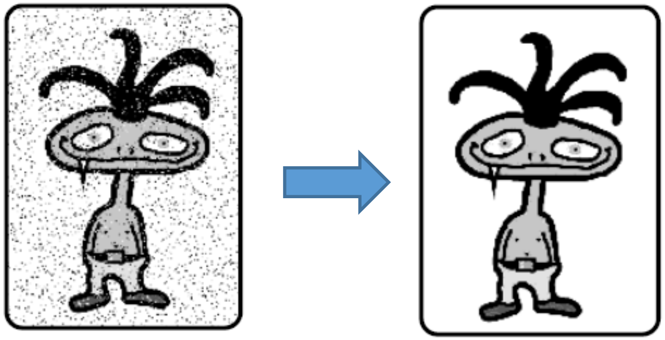
Model selection!

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Example 3: Ising Model

Image denoising problem: Get the “clean” image!





Observed Variables
$y \in \{-1, +1\}$

Latent Variables
$x \in \{-1, +1\}$

The joint distribution is given by:

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y}|\mathbf{x})$$

Image Source: “Computer Vision: Models, Learning, and Inference”, Simon Prince

Example 3: Ising Model

- The prior has the form:

$$p(\mathbf{x}) = \frac{1}{Z_0}\exp(-E_0(\mathbf{x}))$$

$$E_0(\mathbf{x}) = -\sum_{i=1}^{D}\sum_{j\in\text{nbr}_i} W_{ij}\boxed{x_i x_j}$$

Ising prior normally set to 1

"Pairwise smoothness" term, i.e. we want all neighbors to take same value

- The likelihood has the form:

$$p(\mathbf{y}|\mathbf{x}) = \prod_i p(\mathbf{y}_i|x_i) = \exp\left(\sum_i -L_i(x_i)\right)$$

High energy $L(x_i)$ when $x_i \neq y_i$, and vice-versa.

"Unary potential" term, i.e. we want latent variable to agree with the observation.

Example 3: Ising Model

- Therefore, the joint probability has the form:

$$p(x, y) = p(x)p(x|y) = \frac{1}{Z_0} \exp(-E_0(x) - \sum_i L_i(x_i))$$

$$= \frac{1}{Z_0} \exp\big(-E(x)\big) ,$$

where

$$-E(x) = x_i \sum_{j \in nbr_i} W_{ij} x_j + L_i(x_i)$$

$$\Rightarrow \ln p(x, y) = x_i \sum_{j \in nbr_i} W_{ij} x_j + L_i(x_i) + \ln Z_0$$

Example 3: Ising Model

- We will now approximate this by a fully factored approximation:

$$q(\mathrm{x}) = \prod_i q(x_i)$$

- The log of the optimized factor $q_i(x_i)$ is given by:

$$\log q_i(x_i) = \mathbb{E}_{x_{\setminus i}}[\log p(x, y)] + \text{const}$$

$$= \mathbb{E}_{x_{\setminus i}}\left[x_i \sum_{j \in nbr_i} W_{ij} x_j + L_i(x_i)\right] + \underbrace{\text{const}}_{}$$

All terms that do not include x_i go to const (including Z_0)

Example 3: Ising Model

- We get:

$$q_i(x_i) \propto \exp\left(x_i \sum_{j \in \text{nbr}_i} W_{ij}\mu_j + L_i(x_i) \right)$$

where $\mu_j = \sum_j x_j q(x_j)$ is the mean value of node j.

The results are coupled as before, do iterative update with an initialization of all μ_j!

Example 3: Ising Model

- We define m_i as the mean field influence on node i:

$$m_i = \sum_{j \in \text{nbr}_i} W_{ij} \mu_j$$

- And let:

$$L_i^+ \triangleq L_i(+1) \quad \text{and} \quad L_i^- \triangleq L_i(-1).$$

- The approximate marginal posterior is given by

$$q_i(x_i = 1) = \frac{e^{m_i + L_i^+}}{e^{m_i + L_i^+} + e^{-m_i + L_i^-}} = \frac{1}{1 + e^{-2m_i + L_i^- - L_i^+}} = \text{sigm}(2a_i)$$

$$a_i \triangleq m_i + 0.5(L_i^+ - L_i^-)$$

$$q_i(x_i = -1) = \text{sigm}(-2a_i)$$

Example 3: Ising Model

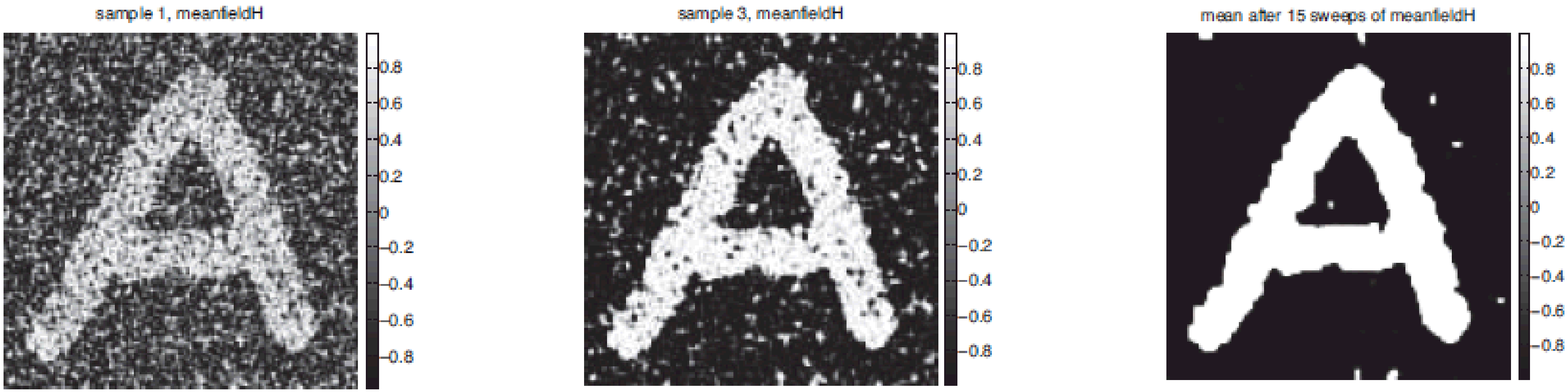
- we can compute the new mean for site i:

$$\begin{aligned}\mu_i &= \mathbb{E}_{q_i}[x_i] = q_i(x_i = +1)\cdot(+1) + q_i(x_i = -1)\cdot(-1) \\ &= \frac{1}{1+e^{-2a_i}} - \frac{1}{1+e^{2a_i}} = \frac{e^{a_i}}{e^{a_i}+e^{-a_i}} - \frac{e^{-a_i}}{e^{-a_i}+e^{a_i}} = \tanh(a_i)\end{aligned}$$

$$= \tanh\left(\sum_{j\in \mathrm{nbr}_i} W_{ij}\mu_j + 0.5(L_i^+ - L_i^-)\right)$$

Iterate until convergence!

Example 3: Ising Model



(a) (b) (c)

Image source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

Loopy Belief Propagation

- Loopy Belief Propagation is a simple algorithm for belief propagation in graphs with cycles.
- We will just look at the algorithm without proof of a variational point of view.
- Proof of the Loopy Belief Propagation algorithm from a variational point of view can be found in a 300 pages paper (Wainwright and Jordan 2008).

Loopy Belief Propagation

The **basic idea** is extremely simple: we apply the belief propagation algorithm to the graph, even if it has loops, i.e. even if it is not a tree.

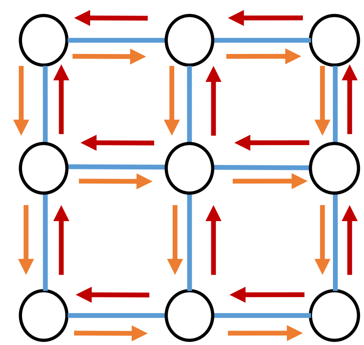
Convergence is however NOT Guaranteed!

Loopy Belief Propagation

All messages and beliefs initialized to 1: $\begin{cases} m_{s\to t}(x_t) = 1 \\ bel_s(x_s) = 1 \end{cases}$

Algorithm: Loopy belief propagation for a pairwise MRF

```
Input: node potentials ψ_s(x_s), edge potentials ψ_st(x_s, x_t);
Initialize messages m_{s→t}(x_t) = 1 for all edges s − t;
Initialize beliefs bel_s(x_s) = 1 for all nodes s;
repeat
    Send message on each edge
    m_{s→t}(x_t) = Σ_{x_s} ( ψ_s(x_s) ψ_st(x_s, x_t) Π_{u∈nbr_s \ t} m_{u→s}(x_s) );
    Update belief of each node bel_s(x_s) ∝ ψ_s(x_s) Π_{t∈nbr_s} m_{t→s}(x_s);
until beliefs don't change significantly;
Return marginal beliefs bel_s(x_s);
```



Source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

Loopy Belief Propagation

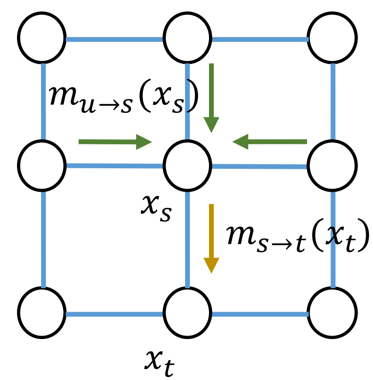
Algorithm: Loopy belief propagation for a pairwise MRF

Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
Initialize messages $m_{s\to t}(x_t) = 1$ for all edges $s - t$;
Initialize beliefs $\mathrm{bel}_s(x_s) = 1$ for all nodes s;
repeat
    Send message on each edge

Message passing

$$\boxed{m_{s\to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s)\psi_{st}(x_s, x_t) \prod_{u \in \mathrm{nbr}_s \backslash t} m_{u\to s}(x_s) \right);}$$

    Update belief of each node $\mathrm{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \mathrm{nbr}_s} m_{t\to s}(x_s)$;
until *beliefs don't change significantly*;
Return marginal beliefs $\mathrm{bel}_s(x_s)$;



$u \in nbr_s \backslash t$

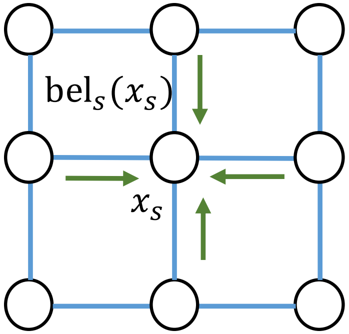
Source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

Loopy Belief Propagation

Algorithm: Loopy belief propagation for a pairwise MRF

Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
Initialize messages $m_{s\to t}(x_t) = 1$ for all edges $s - t$;
Initialize beliefs $\mathrm{bel}_s(x_s) = 1$ for all nodes s;
repeat
  Send message on each edge
  $m_{s\to t}(x_t) = \sum_{x_s}\left(\psi_s(x_s)\psi_{st}(x_s, x_t)\prod_{u\in \mathrm{nbr}_s\setminus t} m_{u\to s}(x_s)\right)$;
  Update belief of each node $\mathrm{bel}_s(x_s) \propto \psi_s(x_s)\prod_{t\in \mathrm{nbr}_s} m_{t\to s}(x_s)$;
until *beliefs don't change significantly*;
Return marginal beliefs $\mathrm{bel}_s(x_s)$;

Belief is updated at every iteration!



Source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

Loopy Belief Propagation

Algorithm: Loopy belief propagation for a pairwise MRF

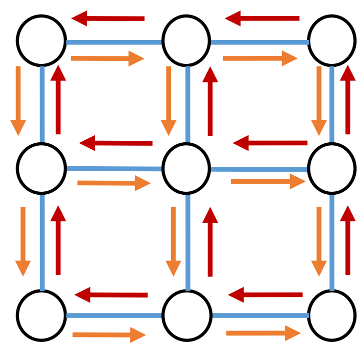
Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
Initialize messages $m_{s \to t}(x_t) = 1$ for all edges $s - t$;
Initialize beliefs $\text{bel}_s(x_s) = 1$ for all nodes s;
repeat
    Send message on each edge
    $$m_{s \to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s) \right);$$
    Update belief of each node $\text{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \text{nbr}_s} m_{t \to s}(x_s)$;
until *beliefs don't change significantly*;
Return marginal beliefs $\text{bel}_s(x_s)$;

Can be asynchronous or synchronous!

Source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

Loopy Belief Propagation: Synchronous

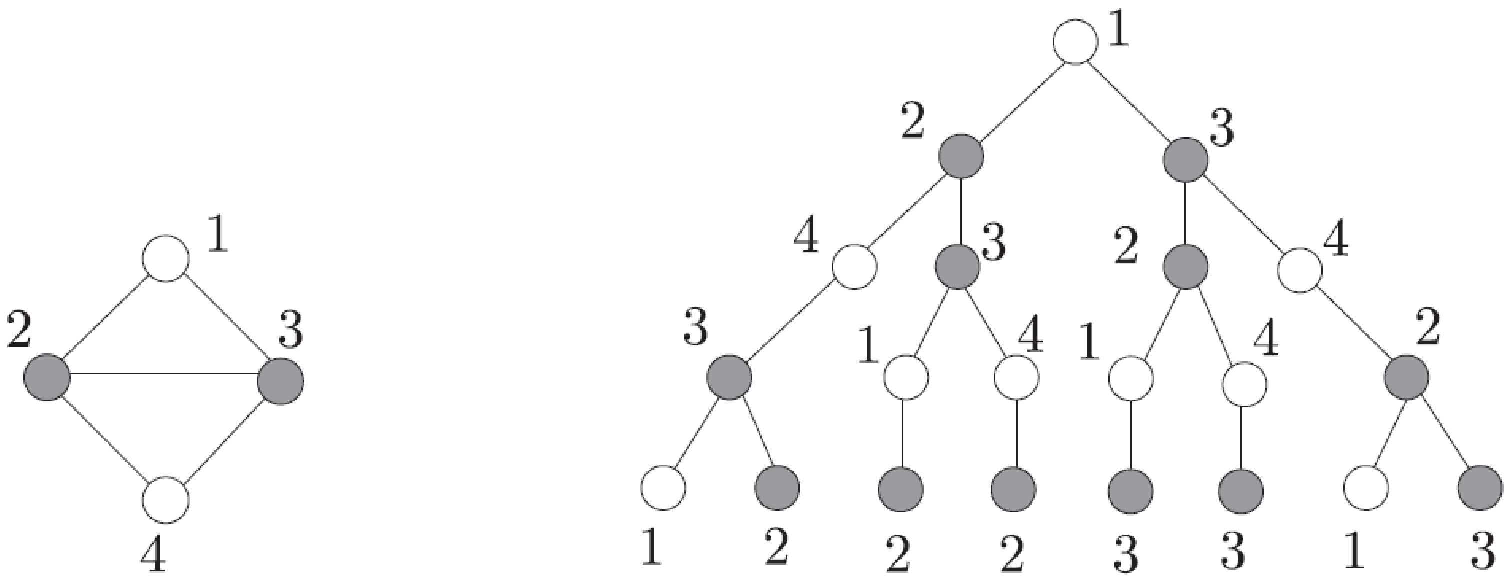
All messages are passed concurrently!



$$m_{s\to t}^{(k)}(x_t) = \sum_{x_s}\Big(\psi_s(x_s)\psi_{st}(x_s, x_t)\prod_{u\in \text{nbr}_s\backslash t} m_{u\to s}^{(k-1)}(x_s)\Big);$$

- All current messages $m_{s\to t}^{(k)}$ are updated with messages from the previous time step $m_{u\to s}^{(k-1)}$

Loopy Belief Propagation: Asynchronous



(a) (b)

- Messages are passed asynchronously according to the herachical order given by the tree.
- Notice that a node would never pass a message to its parent in the tree.

Image Source: “Machine Learning: A probabilistic Perspective”, Kevin Murphy

Summary

- We have looked at how to:

1. Explain the concept of variational approach using Lower-Bound of maximum likelihood and KL-divergence.

2. Use variational approach to do inference on graphical models containing both hidden variables and unknown parameters.

3. Use Loopy Belief Propagation to do message passing.