

CS5340 Uncertainty Modeling in Al

Lecture 10: Variational Inference

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AY 2020/21
Semester 1

Course Schedule

Week	Date	Topic	Remarks
1	12 Aug	Introduction to probabilistic reasoning	1830hrs: MS Teams (Live Introduction)
2	19 Aug	Bayesian networks (Directed graphical models)	
3	26 Aug	Markov random Fields (Undirected graphical models)	1830hrs: Zoom discussions
4	02 Sep	Variable elimination and belief propagation	Assignment 1: Belief propagation and maximal probability (15%)
5	09 Sep	Factor graph and the junction tree algorithm	
6	16 Sep	Parameter learning with complete data	Assignment 1: Due Assignment 2: Junction tree and parameter learning (15%) 1830hrs: Zoom discussions
-	23 Sep	Recess week	No lecture
7	30 Sep	Mixture models and the EM algorithm	Assignment 2: Due Online quiz 1 (20%)
8	07 Oct	Hidden Markov Models (HMM)	Assignment 3: Hidden Markov model (15%)
9	14 Oct	Monte Carlo inference (Sampling)	1830hrs: Zoom discussions
10	21 Oct	Variational inference	Assignment 3: Due Assignment 4: MCMC Sampling (15%)
11	28 Oct	Variational Auto-Encoder and Mixture Density Networks	
12	04 Nov	Graph-cut and alpha expansion	Assignment 4: Due 1830hrs: Zoom discussions
-	11 Nov		Online quiz 2 (20%)



Acknowledgements

- A lot of slides and content of this lecture are adopted from:
- 1. Christopher Bishop, "Pattern Recognition and Machine Learning", Chapter 10.
- Kevin Murphy, "Machine learning: a probabilistic approach", Chapter 21 and 22.
- 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:
- Explain the concept of variational approach using Lower-Bound of maximum likelihood and KLdivergence.
- 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.



- 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

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

• i.e. q(z) is as close as possible to p(z|x).

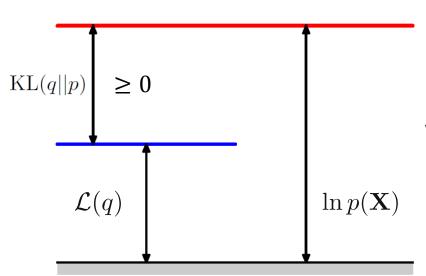
$$\mathrm{KL}(q\|p) = -\int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} \right\} d\mathbf{Z} \geq \mathbf{0}$$

- Unfortunately, minimizing the KL-divergence is hard since p(z|x) is intractable.
- **Solution:** Maximize the lower-bound of log-likelihood instead!

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



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



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

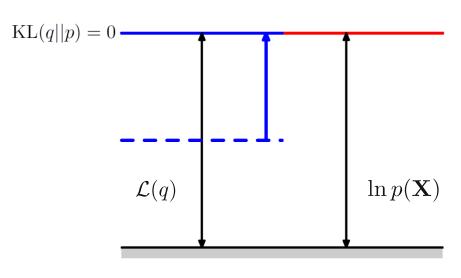
Lower bound KL-divergence

where

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

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





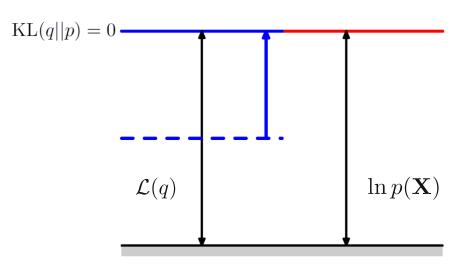
$$\ln p(\mathbf{X}) = \mathcal{L}(q) + \mathrm{KL}(q||p)$$

where

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

$$\frac{1}{2} \operatorname{KL}(q||p) = -\int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X})}{q(\mathbf{Z})} \right\} d\mathbf{Z}.$$

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



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

where

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

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

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



- 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:

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



• 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.



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

$$\begin{split} \mathcal{L}(q) &= \int \prod_{i} q_{i} \left\{ \ln p(\mathbf{X}, \mathbf{Z}) - \sum_{i} \ln q_{i} \right\} d\mathbf{Z} \\ &= \iint q_{j} \prod_{i \neq j} q_{i} \left\{ \ln p(\mathbf{X}, \mathbf{Z}) - \sum_{i} \ln q_{i} - \ln q_{j} \right\} d\mathbf{Z}_{i} d\mathbf{Z}_{j} \\ &= \iint q_{j} \prod_{i \neq j} q_{i} \ln p(\mathbf{X}, \mathbf{Z}) d\mathbf{Z}_{i} d\mathbf{Z}_{j} - \iint q_{j} \prod_{i \neq j} q_{i} \sum_{i} \ln q_{i} d\mathbf{Z}_{i} d\mathbf{Z}_{j} - \iint q_{j} \prod_{i \neq j} q_{i} \ln q_{j} d\mathbf{Z}_{i} d\mathbf{Z}_{j} \end{split}$$



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

$$\mathcal{L}(q) = \iint q_{j} \prod_{i \neq j} q_{i} \ln p(\mathbf{X}, \mathbf{Z}) \, d\mathbf{Z}_{i} d\mathbf{Z}_{j} - \iint q_{j} \prod_{i \neq j} q_{i} \sum_{i} \ln q_{i} \, d\mathbf{Z}_{i} d\mathbf{Z}_{j} - \iint q_{j} \prod_{i \neq j} q_{i} \ln q_{j} \, d\mathbf{Z}_{i} d\mathbf{Z}_{j}$$

$$= \int q_{j} \left\{ \iint \prod_{i \neq j} q_{i} \ln p(\mathbf{X}, \mathbf{Z}) \, d\mathbf{Z}_{i} \right\} d\mathbf{Z}_{j} - \iint q_{j} d\mathbf{Z}_{j} \prod_{i \neq j} q_{i} \sum_{i} \ln q_{i} \, d\mathbf{Z}_{i} - \iint q_{j} \ln q_{j} \int \prod_{i \neq j} q_{i} \, d\mathbf{Z}_{i} \, d\mathbf{Z}_{j} \right\} d\mathbf{Z}_{j}$$



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

$$\mathcal{L}(q) = \int q_j \left\{ \int \ln p(\mathbf{X}, \mathbf{Z}) \prod_{i \neq j} q_i \, d\mathbf{Z}_i \right\} d\mathbf{Z}_j - \int q_j \ln q_j \, d\mathbf{Z}_j + \text{const}$$

$$= \int q_j \left[\ln \widetilde{p}(\mathbf{X}, \mathbf{Z}_j) \right] d\mathbf{Z}_j - \int q_j \ln q_j \, d\mathbf{Z}_j + \text{const}$$

We want to maximize w.r.t. each of the $q_i(z_i)$!



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

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

where

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

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

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

$$= \int q_j \ln \frac{\widetilde{p}(\mathbf{x}, \mathbf{z}_j)}{q_j} d\mathbf{Z}_j + \text{const}$$

$$= -KL(q_j \parallel \widetilde{p}(\mathbf{x}, \mathbf{z}_j)) + \text{const}$$

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

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



Proof:

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

Taking exponential on both sides, we get:

$$q_j^* = \exp\{\mathbb{E}_{i\neq j} \ln p(X, Z)\} \exp(\text{const.}) = \frac{\tilde{p}(\mathbf{x}, \mathbf{z}_j)}{z},$$

$$\ln \tilde{p}(\mathbf{x}, \mathbf{z}_j)$$

where we write

exp(const.) =
$$\frac{1}{z} = \frac{1}{\int \tilde{p}(\mathbf{x}, \mathbf{z}_i) d\mathbf{z}_i}$$

such that z is the partition function.



Proof:

Putting q_i^* back into the lower-bound, i.e.

$$\mathcal{L}(q) = -KL\left(\frac{\tilde{p}(\mathbf{x}, \mathbf{z}_j)}{z} \parallel \tilde{p}(\mathbf{x}, \mathbf{z}_j)\right) + \text{const}.$$

We can see that the $-KL(. \parallel .) \le 0$ term becomes 0.

This implies that the lower-bound $\mathcal{L}(q)$ is maximized!



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

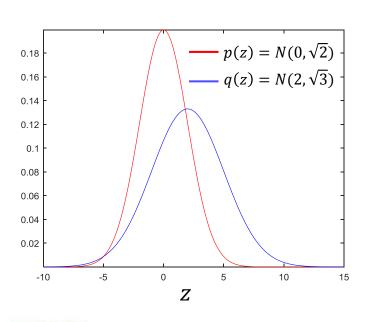
• The additive constant is set by normalizing the distribution $q_j^*(z_j)$, taking the exponential of both sides and normalize, we have

$$egin{aligned} & \widetilde{p}(\mathbf{x}, \mathbf{z}_j) \ q_j^\star(\mathbf{Z}_j) &= \dfrac{\exp\left(\mathbb{E}_{i
eq j}[\ln p(\mathbf{X}, \mathbf{Z})]
ight)}{\int \exp\left(\mathbb{E}_{i
eq j}[\ln p(\mathbf{X}, \mathbf{Z})]
ight) \mathrm{d}\mathbf{Z}_j}. \end{aligned}$$

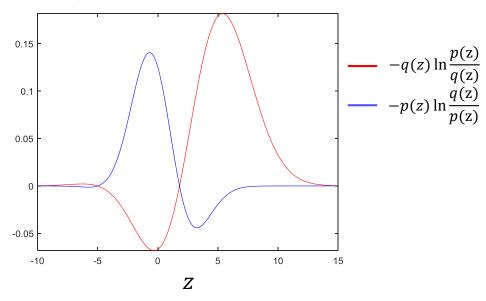


• KL-divergence is not symmetrical, minimizing $KL(q \parallel p)$ and $KL(p \parallel q)$ will give different results.

$$KL(q \parallel p) = -\sum_{z} q(z) \ln \frac{p(z)}{q(z)}, \quad KL(p \parallel q) = -\sum_{z} p(z) \ln \frac{q(z)}{p(z)}$$



 $KL(. \parallel .)$ = area under curve



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

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

- 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.



 Next, consider the forward KL, also known as an Mprojection or moment projection:

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

- 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.



Blue contours: Bimodal distribution p(Z)

Red contours: q(Z) that best approximates p(Z)

Minimizing $KL(q \parallel p)$ 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

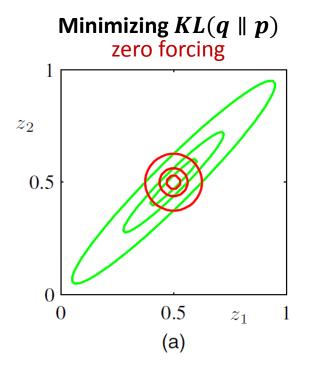


Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

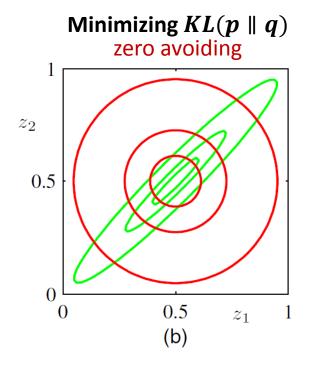
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Red contours: approximating distribution q(z)

Green contours: Gaussian distribution p(z)



Under-estimation



Over-estimation



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

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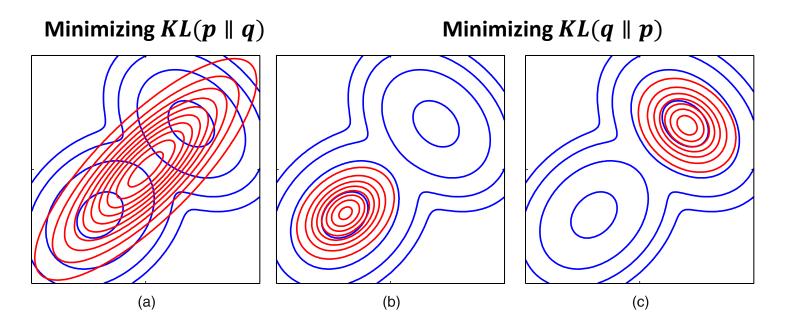
• We use Backward KL-divergence $KL(q \parallel p)$ because it leads to a tractable lower-bound:

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

• Compared to forward KL-divergence $KL(p \parallel q)$ which leads to an 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 $p(\mathbf{Z}|\mathbf{X})$



 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

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- **Given**: a data set $\mathcal{D} = \{x_1, ..., x_N\}$ 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:

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



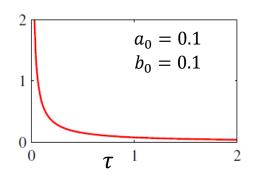
• The conjugate prior distributions (Gaussian-Gamma) for μ and τ given by:

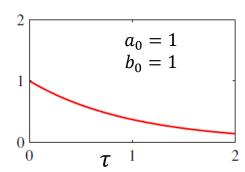
$$p(\mu|\tau) = \mathcal{N}\left(\mu|\mu_0, (\lambda_0\tau)^{-1}\right) \longleftarrow (\mu_0, \lambda_0)$$
: hyperparameters $p(\tau) = \operatorname{Gam}(\tau|a_0, b_0)$

Gamma distribution:

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

where a_0 and b_0 are the hyperparameters.





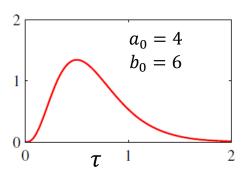


Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

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



 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:

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



• The optimal solution for $q_u(\mu)$ is given by:

$$\ln q_{\mu}^{\star}(\mu) = \mathbb{E}_{\tau} \left[\ln p(\mathcal{D}|\mu, \tau) + \ln p(\mu|\tau) \right] + \text{const}$$

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

• 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:

$$\mu_N = \frac{\lambda_0 \mu_0 + N\overline{x}}{\lambda_0 + N}$$

$$\lambda_N = (\lambda_0 + N)\mathbb{E}[\tau].$$

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



• Similarly, the optimal solution for the factor $q_{ au}(au)$ is given by:

$$\ln q_{\tau}^{\star}(\tau) = \mathbb{E}_{\mu} \left[\ln p(\mathcal{D}|\mu, \tau) + \ln p(\mu|\tau) \right] + \ln p(\tau) + \text{const}$$

$$= (a_0 - 1) \ln \tau - b_0 \tau + \frac{N}{2} \ln \tau$$

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

• Hence, $q_{\tau}(\tau)$ is a gamma distribution $\operatorname{Gam}(\tau \mid a_N, b_N)$ with parameters:

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

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



• 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
$$\begin{cases} \mu_N&=&\frac{\lambda_0\mu_0+N\overline{x}}{\lambda_0+N} \\ \lambda_N&=&(\lambda_0+N)\mathbb{E}[au]. \end{cases}$$
 Depends on $q_{ au}(au)!$

 $q_{\tau}(\tau) = \operatorname{Gam}(\tau \mid a_N, b_N)$, where

$$a_{N} = a_{0} + \frac{N}{2}$$

$$b_{N} = b_{0} + \frac{1}{2} \mathbb{E}_{\mu} \left[\sum_{n=1}^{N} (x_{n} - \mu)^{2} + \lambda_{0} (\mu - \mu_{0})^{2} \right].$$



Example 1: The Univariate Gaussian

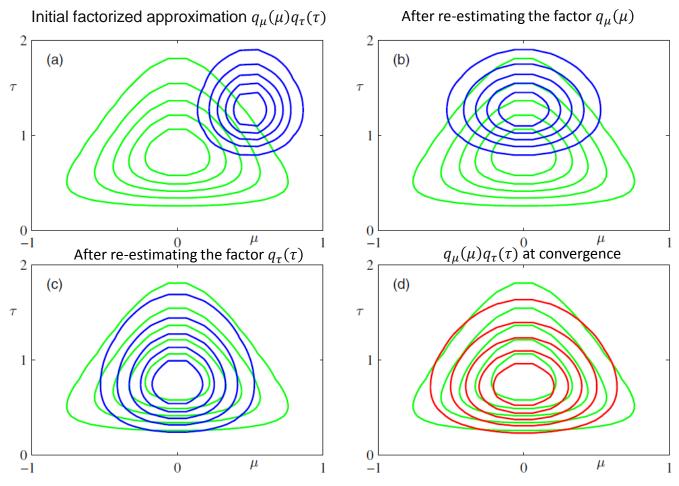
Solution: an iterative approach

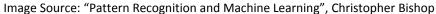
- 1. Make an initial guess for $\mathbb{E}[\tau]$ and use this to recompute $q_{\mu}(\mu)$.
- 2. Use the revised $q_{\mu}(\mu)$ to extracted the moments $\mathbb{E}[\mu]$ and $\mathbb{E}[\mu^2]$, and use these to re-compute $q_{\tau}(\tau)$.
- 3. Use the revised $q_{\tau}(\tau)$ to extract the moment $\mathbb{E}[\tau]$ and use this to re-compute $q_{\mu}(\mu)$.
- 4. Repeat until convergence.



Example 1: The Univariate Gaussian

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







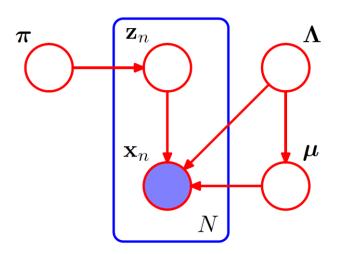


Plate denotes a set of N i.i.d. observations μ denotes $\{\mu_k\}$ and Λ denotes $\{\Lambda_k\}$.

 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

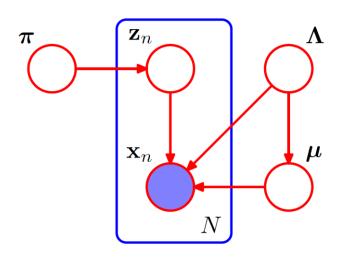


Plate denotes a set of N i.i.d. observations μ denotes $\{\mu_k\}$ and Λ denotes $\{\Lambda_k\}$.

- 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 $X = \{X_1, ..., X_N\}$, and similarly we denote the latent variables set by $Z = \{Z_1, ..., Z_N\}$.



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

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

• Dirichlet distribution conjugate prior over the mixing coefficients π :

Normalizing constant (see Lecture 1)

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

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



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

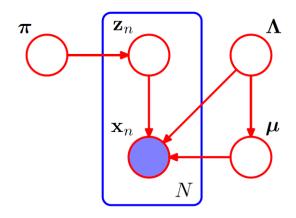
$$p(\mathbf{X}|\mathbf{Z}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mathcal{N}\left(\mathbf{x}_{n} | \boldsymbol{\mu}_{k}, \boldsymbol{\Lambda}_{k}^{-1}\right)^{z_{nk}}$$

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

$$p(\boldsymbol{\mu}, \boldsymbol{\Lambda}) = p(\boldsymbol{\mu}|\boldsymbol{\Lambda})p(\boldsymbol{\Lambda})$$

$$= \prod_{k=1}^{K} \mathcal{N}\left(\boldsymbol{\mu}_{k}|\mathbf{m}_{0}, (\beta_{0}\boldsymbol{\Lambda}_{k})^{-1}\right) \mathcal{W}(\boldsymbol{\Lambda}_{k}|\mathbf{W}_{0}, \nu_{0})$$

• Where m_0 , W_0 , v_0 are the hyperparameters.



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

• The log of the optimized factor for q(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 ${\cal Z}$ into the additive constant, we get:

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



• 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

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



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:

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)!



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

$$N_k = \sum_{n=1}^{N} r_{nk}$$

$$\overline{\mathbf{x}}_k = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} \mathbf{x}_n$$

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

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



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

Depends only on π

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



Further factorizes into

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



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

$$\mathbb{E}[z_{nk}] = \sum_{Z} z_{nk} q(Z)$$

$$= \sum_{Z} z_{nk} \prod_{n} \prod_{k} r_{nk}^{z_{nk}}$$

$$= r_{nk}$$

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

Taking exponential of both sides, we get:

$$q^{\star}(\boldsymbol{\pi}) = \operatorname{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha})$$
 Dirichlet distribution!

where α has components α_k given by:

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



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

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

$$\mathcal{N}\left(\boldsymbol{\mu}_{k} | \mathbf{m}_{0}, (\beta_{0} \boldsymbol{\Lambda}_{k})^{-1}\right) \mathcal{W}(\boldsymbol{\Lambda}_{k} | \mathbf{W}_{0}, \nu_{0})$$

Proof:

$$\mathbb{E}[z_{nk}] = \sum_{z} q(z) z_{nk}$$
 where $q^\star(\mathbf{Z}) = \prod_{n=1}^N \prod_{k=1}^K r_{nk}^{z_{nk}}$ $= \sum_{z} z_{nk} \prod_n \prod_k r_{nk}^{z_{nk}}$ $= r_{nk}$



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

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

with:

$$\begin{array}{lll} \beta_k & = & \beta_0 + N_k \\ \mathbf{m}_k & = & \frac{1}{\beta_k} \left(\beta_0 \mathbf{m}_0 + N_k \overline{\mathbf{x}}_k\right) & \text{algorithm for mixture of Gaussians!} \\ \mathbf{W}_k^{-1} & = & \mathbf{W}_0^{-1} + N_k \overline{\mathbf{S}}_k + \frac{\beta_0 N_k}{\beta_0 + N_k} (\overline{\mathbf{x}}_k - \mathbf{m}_0) (\overline{\mathbf{x}}_k - \mathbf{m}_0)^\mathrm{T} \\ \nu_k & = & \nu_0 + N_k. & \text{Dependent on responsibility } \mathbb{E}[z_{nk}] \end{array}$$



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

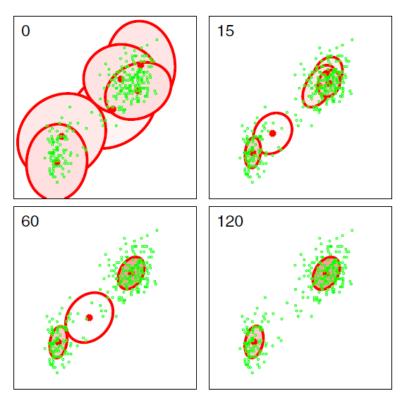
$$\ln q^{\star}(\mathbf{Z}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \ln \rho_{nk} + \text{const}$$
 Depends on $q(\pi, \mu, \Lambda)$ where
$$\ln \rho_{nk} = \mathbb{E}[\ln \pi_k] + \frac{1}{2} \mathbb{E}[\ln |\Lambda_k|] - \frac{D}{2} \ln(2\pi) - \frac{1}{2} \mathbb{E}[\mu_k, \Lambda_k \left[(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}} \boldsymbol{\Lambda}_k (\mathbf{x}_n - \boldsymbol{\mu}_k) \right]]$$

$$\ln q^{\star}(\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Lambda}) = \ln p(\boldsymbol{\pi}) + \sum_{k=1}^{K} \ln p(\boldsymbol{\mu}_{k},\boldsymbol{\Lambda}_{k}) + \mathbb{E}_{\mathbf{Z}} \left[\ln p(\mathbf{Z}|\boldsymbol{\pi})\right] \qquad \text{Depends on } q(\mathbf{Z})$$

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



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

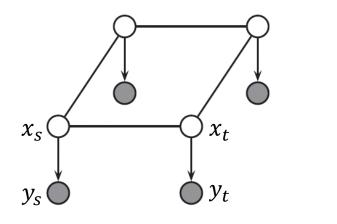


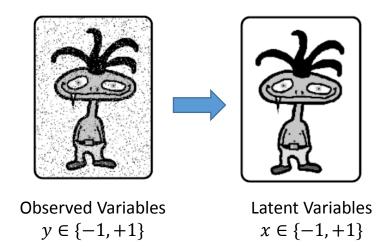
Model selection!



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

Image denoising problem: Get the "clean" image!





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

• The prior has the form:

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

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

Ising prior normally set to 1

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

The likelihood has the form:

High energy
$$L(x_i)$$
 when $x_i \neq y_i$, and vice-versa.
$$p(\mathbf{y}|\mathbf{x}) = \prod_i p(\mathbf{y}_i|x_i) = \exp\left(\sum_i L_i(x_i)\right))$$

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

• Therefore, the joint probability has the form:

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

where

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

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



We will now approximate this by a fully factored approximation:

$$q(\mathbf{x}) = \prod_{i} q(x_i)$$

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

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

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

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



• 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_i !



• 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:

$$L_i^+ \triangleq L_i(+1)$$
 and $L_i^- \triangleq L_i(-1)$.

The approximate marginal posterior is given by

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

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

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



• we can compute the new mean for site *i*:

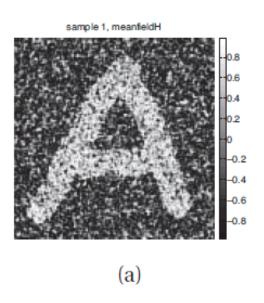
$$\mu_{i} = \mathbb{E}_{q_{i}}[x_{i}] = q_{i}(x_{i} = +1) \cdot (+1) + q_{i}(x_{i} = -1) \cdot (-1)$$

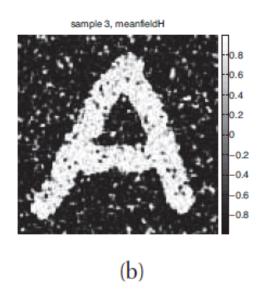
$$= \frac{1}{1 + e^{-2a_{i}}} - \frac{1}{1 + e^{2a_{i}}} = \frac{e^{a_{i}}}{e^{a_{i}} + e^{-a_{i}}} - \frac{e^{-a_{i}}}{e^{-a_{i}} + e^{a_{i}}} = \tanh(a_{i})$$

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

Iterate until convergence!







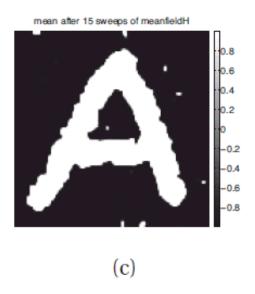


Image source: "Machine Learning: A probabilistic Perspective", Kevin Murphy



 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).



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!



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

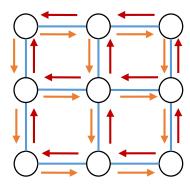
$$\int m_{s \to t}(x_t) = 1$$
$$bel_s(x_s) = 1$$

Algorithm: Loopy belief propagation for a pairwise MRF

- 1 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 $bel_s(x_s) = 1$ for all nodes s;
- 4 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 $\operatorname{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \operatorname{nbr}_s} m_{t \to s}(x_s);$
- 7 **until** beliefs don't change significantly;
- 8 Return marginal beliefs $bel_s(x_s)$;





Algorithm: Loopy belief propagation for a pairwise MRF

- 1 Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
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- Initialize beliefs $bel_s(x_s) = 1$ for all nodes s;
- 4 repeat

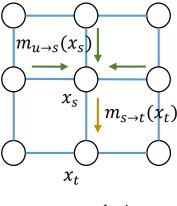
Message passing

Sand massage

$$m_{s \to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s) \right);$$
Update belief of each node bel $(x_s) \propto \psi_s(x_s) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s)$

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 $u \in nbr_s \setminus t$

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



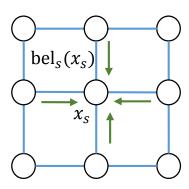
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- Initialize beliefs $bel_s(x_s) = 1$ for all nodes s;
- 4 repeat
 - Send message on each edge

Belief is updated at every iteration!

$$m_{s \to t}(x_t) = \sum_{x_s} \Big(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s) \Big);$$
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;
- 8 Return marginal beliefs $bel_s(x_s)$;





Algorithm: Loopy belief propagation for a pairwise MRF

- 1 Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
- 2 Initialize messages $m_{s\to t}(x_t)=1$ for all edges s-t;
- 3 Initialize beliefs $bel_s(x_s) = 1$ for all nodes s;
- 4 repeat

Send message on each edge

Can be asynchronous or synchronous!

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

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

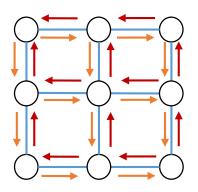


Source: "Machine Learning: A probabilistic Perspective", Kevin Murphy

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Loopy Belief Propagation: Synchronous

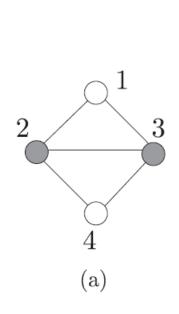
All messages are passed concurrently!

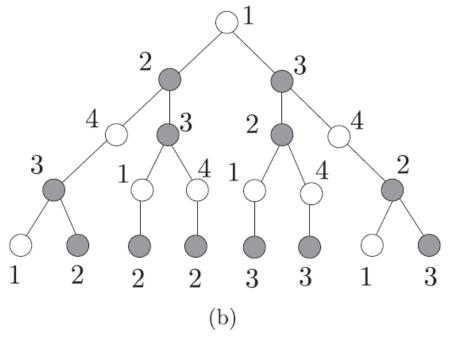


$$m_{s\to t}^{(k)}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u\to s}^{(k-1)}(x_s) \right);$$

• 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





- 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.

