11. Variational Inference

Motivation

- A major task in probabilistic reasoning is to evaluate the **posterior** distribution $p(Z \mid X)$ of a set of latent variables Z given data X **(inference)**

However: This is often not tractable, e.g. because the latent space is high-dimensional

- Two different solutions are possible: sampling methods and variational methods.
- In variational optimization, we seek a tractable distribution q that **approximates** the posterior.
- Optimization is done using **functionals**.

Motivation

- A major task in probabilistic reasoning is to evaluate the **posterior** distribution $p(Z \mid X)$ of a set of latent variables Z given data X **(inference)**
- **How** … beca … al
- Two … ng meth …

Careful: Different notation!
In Bishop (and in the following slides)
Z are hidden states
and X are observations

- In variational optimization, we seek a tractable distribution q that **approximates** the posterior.
- Optimization is done using **functionals**.

Variational Inference

In general, variational methods are concerned with mappings that take **functions** as input.

Example: the entropy of a distribution p

$$\mathbb{H}[p] = \int p(x) \log p(x) dx$$

"Functional"

Variational optimization aims at finding **functions** that minimize (or maximize) a given functional.

This is mainly used to find approximations to a given function by choosing from a family.

The aim is mostly tractability and simplification.

The KL-Divergence

Aim: define a functional that resembles a "difference" between distributions p and q

Idea: use the average additional amount of information:

$$-\int p(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x} - \left(-\int p(\mathbf{x}) \log p(\mathbf{x}) d\mathbf{x} \right) = -\int p(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x} \quad = \mathrm{KL}(p\|q)$$

This is known as the **Kullback-Leibler** divergence

It has the properties: $\mathrm{KL}(q\|p) \neq \mathrm{KL}(p\|q)$

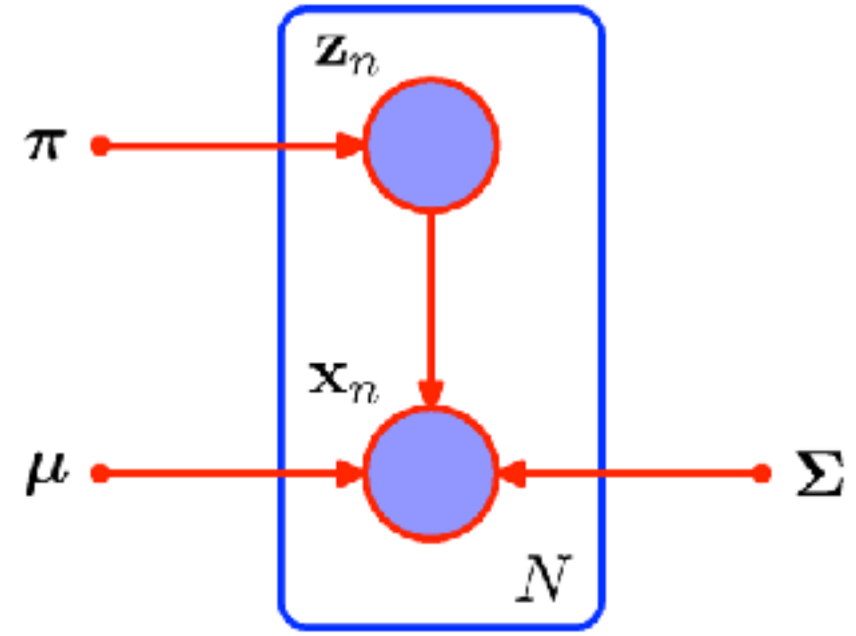
$$\mathrm{KL}(p\|q) \geq 0 \qquad \mathrm{KL}(p\|q) = 0 \Leftrightarrow p \equiv q$$

This follows from Jensen's inequality

Example: A Variational Formulation of EM

Assume for a moment that we observe X and the binary latent variables Z. The likelihood is then:

$$p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \prod_{n=1}^{N} p(\mathbf{z}_n \mid \boldsymbol{\pi}) p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\mu}, \Sigma)$$



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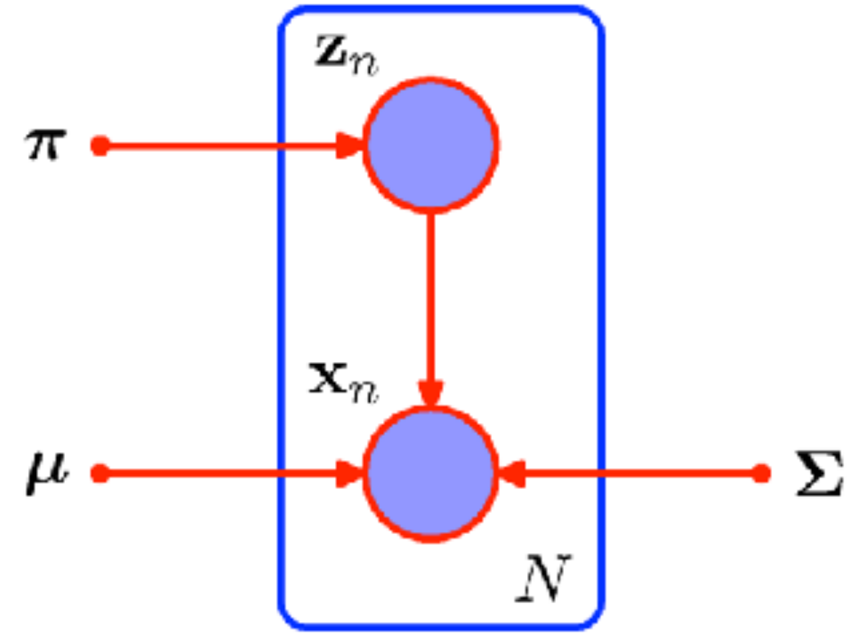
Remember:

$$z_{nk} \in \{0, 1\}, \quad \sum_{k=1}^{K} z_{nk} = 1$$

where $p(\mathbf{z}_n \mid \boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{z_{nk}}$ and

$$p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\mu}, \Sigma) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k)^{z_{nk}}$$



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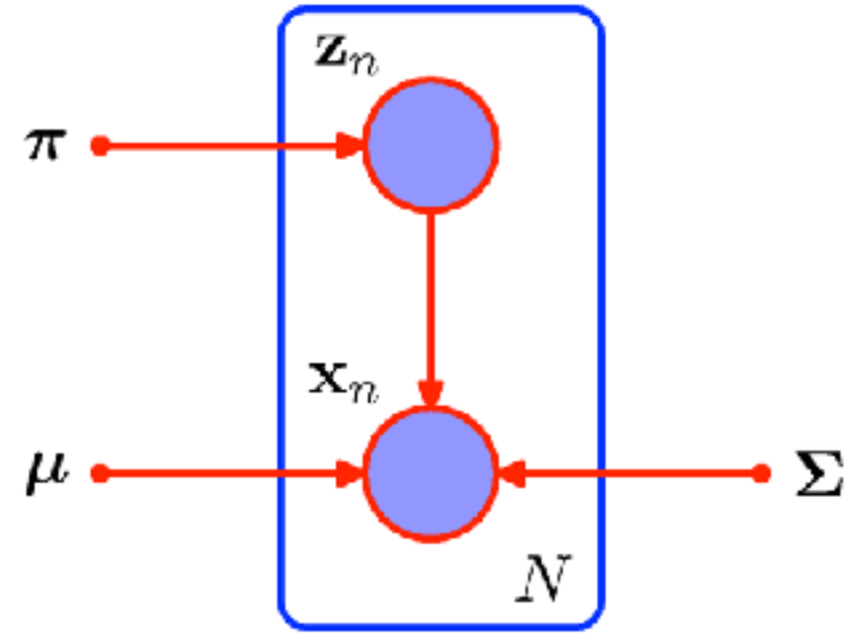

which leads to the log-formulation:

$$\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} (\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

The Complete-Data Log-Likelihood

$$\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} (\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

- This is called the **complete-data log-likelihood**
- Advantage: solving for the parameters $(\pi_k, \boldsymbol{\mu}_k, \Sigma_k)$ is much simpler, as the log is inside the sum!
- We could switch the sums and then for every mixture component k only look at the points that are associated with that component.
- This leads to simple closed-form solutions for the parameters
- However: the latent variables Z are not observed!

The Main Idea of EM

Instead of maximizing the joint log-likelihood, we maximize its **expectation** under the latent variable distribution:

$$\mathbb{E}_Z[\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \mathbb{E}_Z[z_{nk}](\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

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where the latent variable distribution per point is:

$$p(\mathbf{z}_n \mid \mathbf{x}_n, \boldsymbol{\theta}) = \frac{p(\mathbf{x}_n \mid \mathbf{z}_n, \boldsymbol{\theta}) p(\mathbf{z}_n \mid \boldsymbol{\theta})}{p(\mathbf{x}_n \mid \boldsymbol{\theta})} \qquad \boldsymbol{\theta} = (\boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)$$

$$= \frac{\prod_{l=1}^{K} (\pi_l \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_l, \Sigma_l))^{z_{nl}}}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \Sigma_j)}$$

The Main Idea of EM

The expected value of the latent variables is:

$$\mathbb{E}[z_{nk}] = \gamma(z_{nk})$$

Remember:

$$\gamma(z_{nk}) = p(z_{nk} = 1 \mid \mathbf{x}_n)$$

plugging in we obtain:

$$\mathbb{E}_Z[\log p(X, Z \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \Sigma)] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk})(\log \pi_k + \log \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \Sigma_k))$$

We compute this iteratively:

1. Initialize $i = 0, \quad (\pi_k^i, \boldsymbol{\mu}_k^i, \Sigma_k^i)$
2. Compute $\mathbb{E}[z_{nk}] = \gamma(z_{nk})$
3. Find parameters $(\pi_k^{i+1}, \boldsymbol{\mu}_k^{i+1}, \Sigma_k^{i+1})$ that maximize this
4. Increase i; if not converged, goto 2.

Why Does This Work?

- We have seen that EM maximizes the **expected complete-data log-likelihood**, but:
- Actually, we need to maximize the log-marginal

$$\log p(X \mid \boldsymbol{\theta}) = \log \sum_Z p(X, Z \mid \boldsymbol{\theta})$$

- It turns out that the log-marginal is maximized **implicitly!**

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- It turns out that the log-marginal is maximized **implicitly!**

$$\log p(X \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q \| p)$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_Z q(Z) \log \frac{p(X, Z \mid \boldsymbol{\theta})}{q(Z)} \qquad \mathrm{KL}(q \| p) = -\sum_Z q(Z) \log \frac{p(Z \mid X, \boldsymbol{\theta})}{q(Z)}$$

A Variational Formulation of EM

- Thus: The Log-likelihood consists of two functionals

$$\log p(X \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q \| p)$$

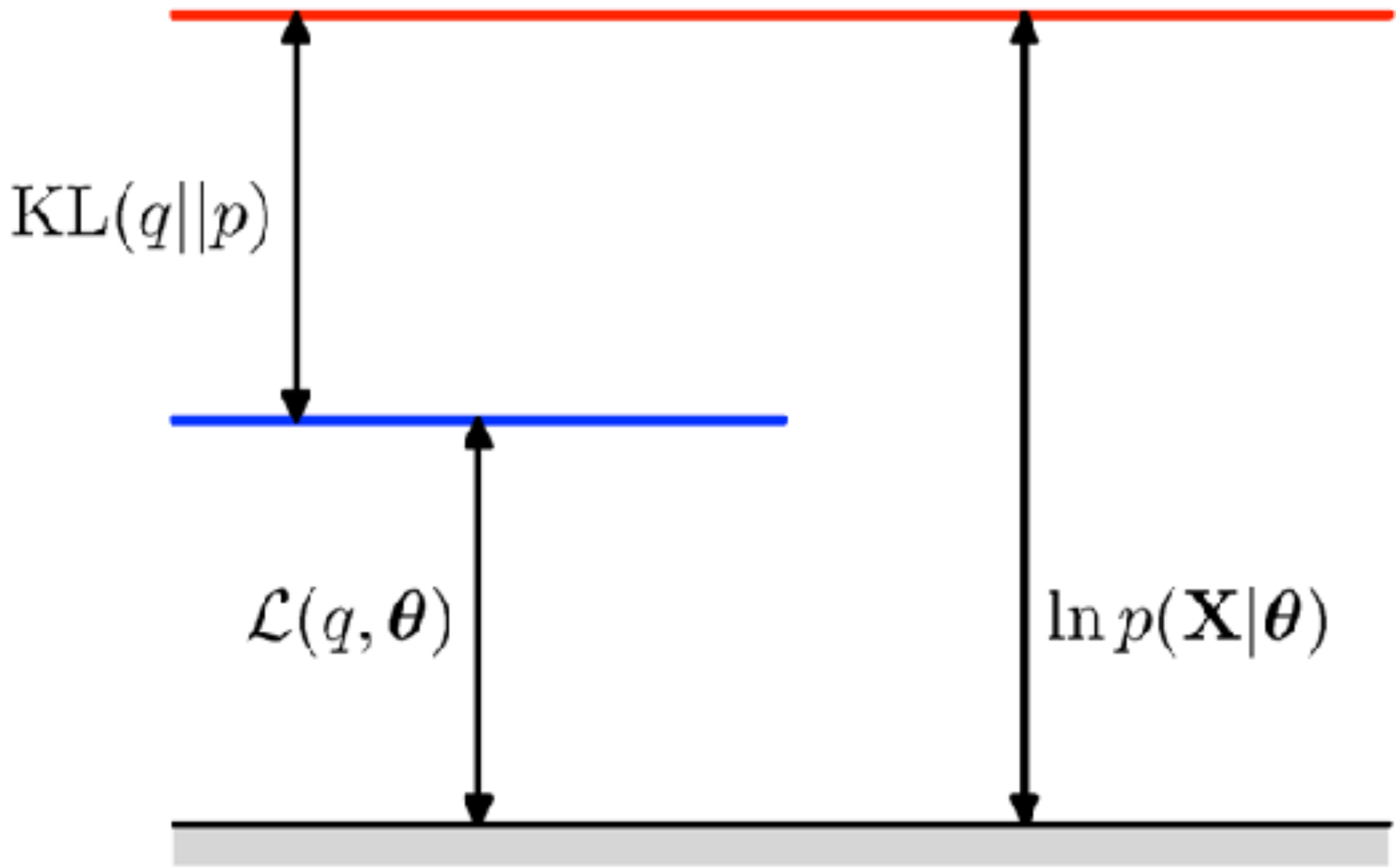
where the first is (proportional to) an **expected complete-data log-likelihood** under a distribution q

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_Z q(Z) \log \frac{p(X, Z \mid \boldsymbol{\theta})}{q(Z)}$$

and the second is the **KL-divergence** between p and q:

$$\mathrm{KL}(q \| p) = -\sum_Z q(Z) \log \frac{p(Z \mid X, \boldsymbol{\theta})}{q(Z)}$$

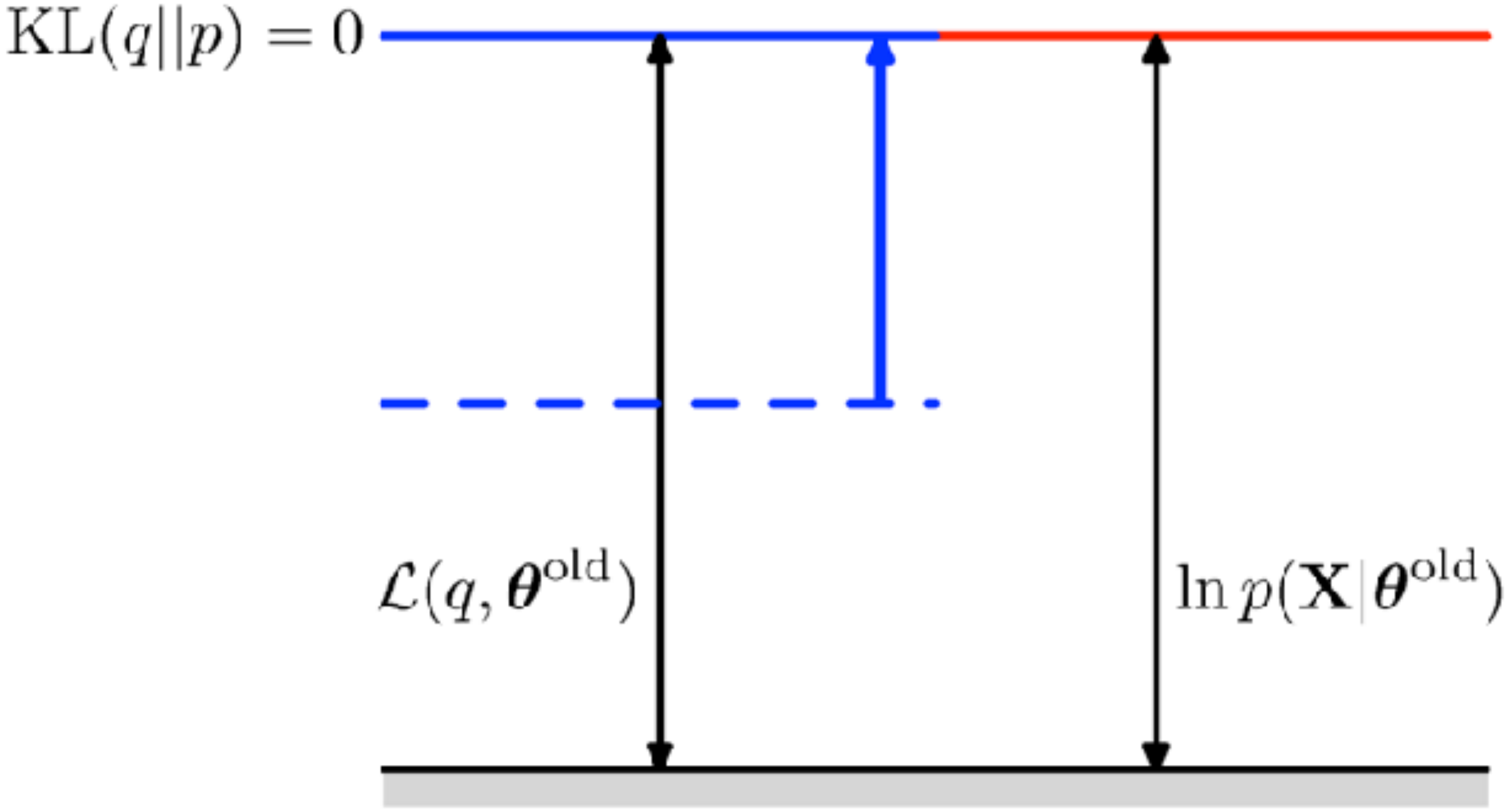
Visualization



- The KL-divergence is positive or 0
- Thus, the log-likelihood is at least as large as $\mathcal{L}$ or:
- $\mathcal{L}$ is a **lower bound** (ELBO) of the log-likelihood (evidence):

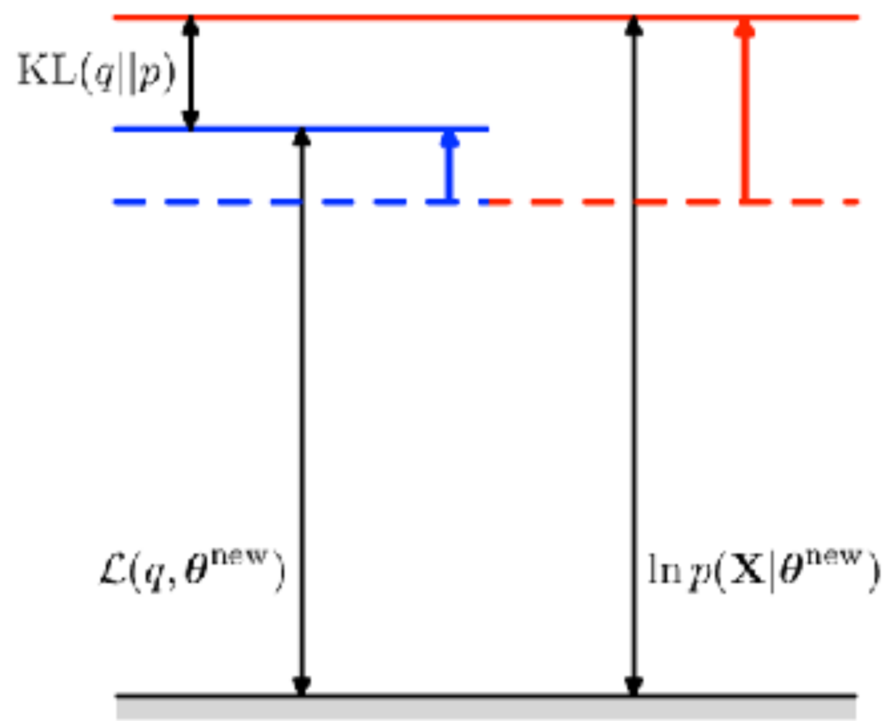
$$\log p(X \mid \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$$

What Happens in the E-Step?



- The log-likelihood is independent of q
- Thus: $\mathcal{L}$ is maximized iff KL divergence is minimal (=0)
- This is the case iff $q(Z) = p(Z \mid X, \boldsymbol{\theta})$

What Happens in the M-Step?

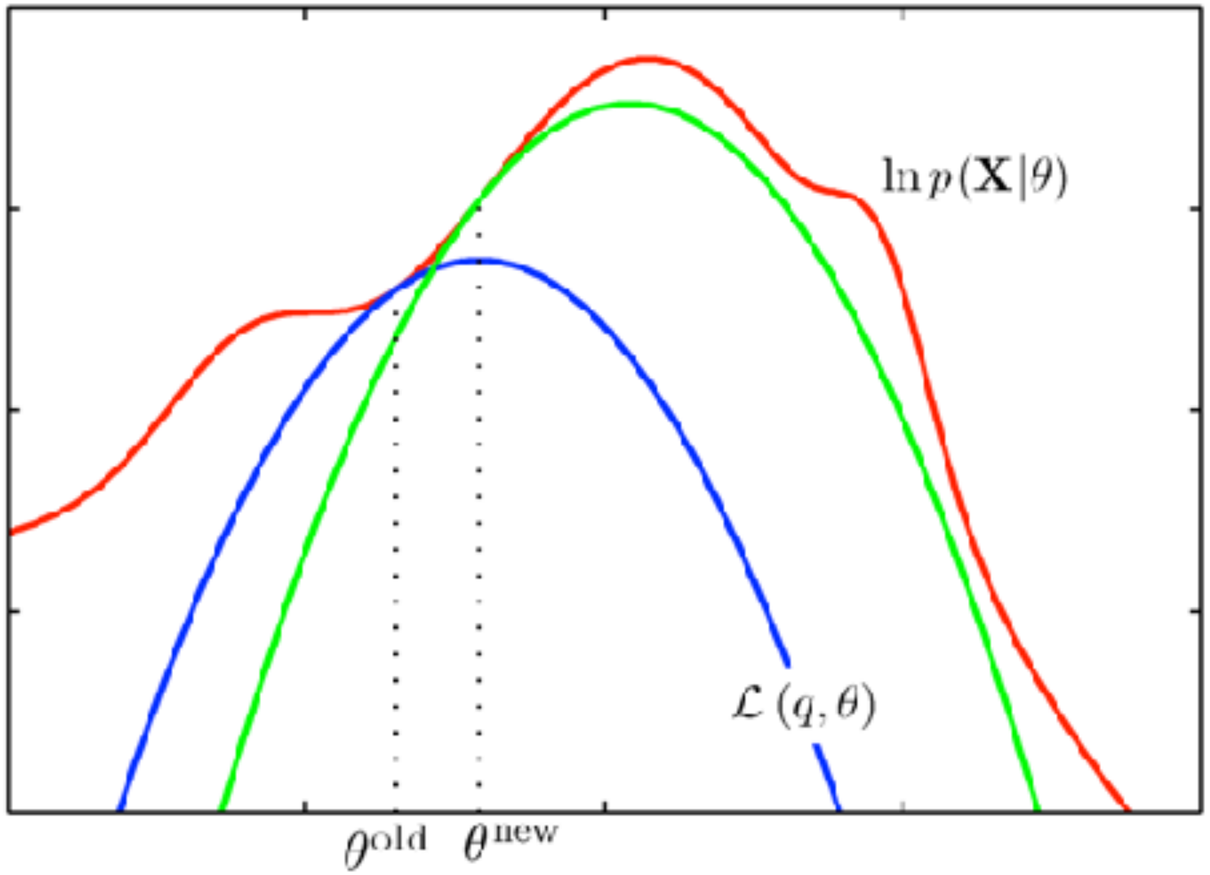


- In the M-step we keep q fixed and find new $\boldsymbol{\theta}$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_Z p(Z \mid X, \boldsymbol{\theta}^{\mathrm{old}}) \log p(X, Z \mid \boldsymbol{\theta}) - \sum_Z q(Z) \log q(Z)$$

- We maximize the first term, the second is indep.
- This implicitly makes KL non-zero
- The log-likelihood is maximized even more!

Visualization in Parameter-Space



- In the E-step we compute the concave lower bound for given old parameters θ^{old} (blue curve)
- In the M-step, we maximize this lower bound and obtain new parameters θ^{new}
- This is repeated (green curve) until convergence

VI in General

Analogue to the discussion about EM we have:

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

$$\mathcal{L}(q) = \int q(Z) \log \frac{p(X,Z)}{q(Z)} dZ \qquad \mathrm{KL}(q) = -\int q(Z) \log \frac{p(Z \mid X)}{q(Z)} dZ$$

Again, maximizing the lower bound is equivalent to minimizing the KL-divergence.

The maximum is reached when the KL-divergence vanishes, which is the case for $q(Z) = p(Z \mid X)$.

However: Often the true posterior is intractable and we restrict q to a tractable family of dist.

Generalizing the Idea

- In EM, we were looking for an optimal distribution q in terms of KL-divergence
- Luckily, we could compute q in closed form
- In general, this is not the case, but we can use an approximation instead: $q(Z) \approx p(Z \mid X)$
- Idea: make a simplifying assumption on q so that a good approximation can be found
- For example: Consider the case where q can be expressed as a **product** of simpler terms

Factorized Distributions

We can split up q by partitioning Z into disjoint sets and assuming that q factorizes over the sets:

$$q(Z) = \prod_{i=1}^{M} q_i(Z_i)$$

Shorthand:

$$q_i \leftarrow q_i(Z_i)$$

This is the only assumption about q!

Idea: Optimize $\mathcal{L}(q)$ by optimizing wrt. each of the factors of q in turn. Setting $q_i \leftarrow q_i(Z_i)$ we have

$$\mathcal{L}(q) = \int \prod_i q_i \left(\log p(X, Z) - \sum_i \log q_i \right) dZ$$

Mean Field Theory

This results in:

$$\mathcal{L}(q) = \int q_j \log \tilde{p}(X, Z_j) dZ_j - \int q_j \log q_j dZ_j + \text{const}$$

where

$$\log \tilde{p}(X, Z_j) = \mathbb{E}_{-j}\ [\log p(X, Z)] + \text{const}$$

Thus, we have $\mathcal{L}(q) = -\text{KL}(q_j \| \tilde{p}(X, Z_j)) + \text{const}$

I.e., maximizing the lower bound is equivalent to minimizing the KL-divergence of a single factor and a distribution that can be expressed in terms of an expectation:

$$\mathbb{E}_{-j}\ [\log p(X, Z)] = \int \log p(X, Z) \prod_{i \neq j} q_i dZ_{-j}$$

Mean Field Theory

Therefore, the optimal solution in general is

$$\log q_j^*(Z_j) = \mathbb{E}_{-j}\,[\log p(X, Z)] + \text{const}$$

In words: the log of the optimal solution for a factor q_j is obtained by taking the expectation with respect to **all other** factors of the log-joint probability of all observed and unobserved variables

The constant term is the normalizer and can be computed by taking the exponential and marginalizing over Z_j

This is not always necessary.

Variational Mixture of Gaussians

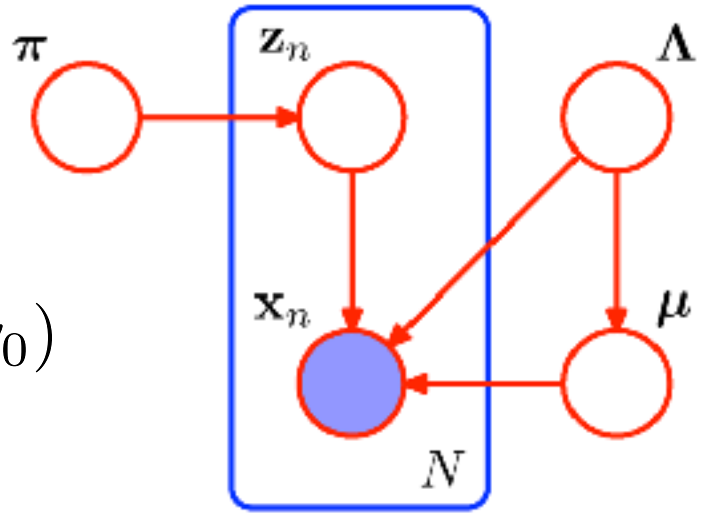
- Again, we have observed data $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and latent variables $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$
- Furthermore we have

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

- We introduce **priors** for all parameters, e.g.

$$p(\boldsymbol{\pi}) = \mathrm{Dir}(\boldsymbol{\pi} \mid \boldsymbol{\alpha}_0)$$

$$p(\boldsymbol{\mu}, \Lambda) = \prod_{k=1}^{K} \mathcal{N}(\boldsymbol{\mu}_k \mid \mathbf{m}_0, (\beta_0 \Lambda_k)^{-1}) \mathcal{W}(\Lambda_k \mid W_0, \nu_0)$$



Variational Mixture of Gaussians

- The joint probability is then:

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

- We consider a distribution q so that

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

- Using our general result:

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

- Plugging in:

$$\log q^*(Z) = \mathbb{E}_{\boldsymbol{\pi}}[\log p(Z \mid \boldsymbol{\pi})] + \mathbb{E}_{\boldsymbol{\mu}, \Lambda}[\log p(X \mid Z, \boldsymbol{\mu}, \Lambda)] + \text{const}$$

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- From this we can show that:

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

Variational Mixture of Gaussians

This means: the optimal solution to the factor $q(Z)$ has the same functional form as the prior of Z.

It turns out, this is true for all factors.

However: the factors q depend on moments computed with respect to the other variables, i.e. the computation has to be done iteratively.

This results again in an EM-style algorithm, with the difference, that here we use conjugate priors for all parameters. This reduces overfitting.

Example: Clustering

- 6 Gaussians
- After convergence, only two components left
- Complexity is traded off with data fitting
- This behaviour depends on a parameter of the Dirichlet prior