Notes: Pattern Recognition and Machine Learning – Ch10 Variational Inference

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10/27/2020

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Definitions

- Variational inference is also called variational Bayes, thus
  - all parameters are viewed as random variables, and
  - they will have prior distributions.
- We denote the set of all latent variables and parameters by $\mathbf{Z}$
  - Note: the parameter vector $\boldsymbol{\theta}$ no long appears, because it's now a part of $\mathbf{Z}$
- Goal: find approximation for
  - posterior distribution $p(\mathbf{Z} \mid \mathbf{X})$, and
  - marginal likelihood $p(\mathbf{X})$, also called the model evidence

Model evidence equals lower bound plus KL divergence

- **Goal**: We want to find a distribution $q(\mathbf{Z})$ that approximates the posterior distribution $p(\mathbf{Z} \mid \mathbf{X})$. In other word, we want to minimize the KL divergence $\mathsf{KL}(q \| p)$.
- Note the decomposition of the marginal likelihood

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

- Thus, maximizing the lower bound (also called ELBO) $\mathcal{L}(q)$ is equivalent to minimizing the KL divergence $\mathsf{KL}(q \| p)$.

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

$$\mathsf{KL}(q \| p) = -\int q(\mathbf{Z}) \log \left\{ \frac{p(\mathbf{Z} \mid \mathbf{X})}{q(\mathbf{Z})} \right\} d\mathbf{Z}$$

Mean field family

- **Goal**: restrict the family of distribution $q(\mathbf{Z})$ so that they comprise only tractable distributions, while allow the family to be sufficiently flexible so that it can approximate the posterior distribution well
- Mean field family : partition the elements of $\mathbf{Z}$ into disjoint groups denoted by $\mathbf{Z}_j$, for $j = 1, \ldots, M$, and assume q factorizes wrt these groups:

$$q(\mathbf{Z}) = \prod_{j=1}^{M} q_j(\mathbf{Z}_j)$$

  – Note: we place no resitriction on the functional forms of the individual factors $q_j(\mathbf{Z}_j)$

Solution for mean field families: derivation

- We will optimize wrt each $q_j(\mathbf{Z}_j)$ in turn.
- For q_j, the lower bound (to be maximized) can be decomposed as

$$\mathcal{L}(q) = \int \prod_k q_k \left\{ \log p(\mathbf{X}, \mathbf{Z}) - \sum_k \log q_k \right\} d\mathbf{Z}$$

$$= \int q_j \underbrace{\left\{ \int \log p(\mathbf{X}, \mathbf{Z}) \prod_{k \neq j} q_k d\mathbf{Z}_k \right\}}_{\mathbb{E}_{k \neq j}[\log p(\mathbf{X}, \mathbf{Z})]} d\mathbf{Z}_j - \int q_j \log q_j d\mathbf{Z}_j + \text{const}$$

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

  - Here the new distribution $\tilde{p}(\mathbf{X}, \mathbf{Z}_j)$ is defined as

$$\log \tilde{p}(\mathbf{X}, \mathbf{Z}_j) = \mathbb{E}_{k \neq j}\left[\log p(\mathbf{X}, \mathbf{Z})\right] + \text{const}$$

Solution for mean field families

- A general expression for the optimal solution $q_j^*(\mathbf{Z}_j)$ is

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

  – We can only use this solution in an iterative manner, because the expectations should be computed wrt other factors $q_k(\mathbf{Z}_k)$ for $k \neq j$.
  – Convergence is guaranteed because bound is convex wrt each factor q_j
  – On the right hand side we only need to retain those terms that have some functional dependence on $\mathbf{Z}_j$

Example: approximate a bivariate Gaussian using two independent distributions

- Target distribution: a bivariate Gaussian

$$p(\mathbf{z}) = \mathsf{N}\left(\mathbf{z} \mid \boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1}\right), \quad \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \boldsymbol{\Lambda} = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{12} & \lambda_{22} \end{pmatrix}$$

- We use a factorized form to approximate $p(\mathbf{z})$:

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

- Note: we do not assume any functional forms for q_1 and q_2

VI solution to the bivariate Gaussian problem

$$\begin{aligned}
\log q_1^*(z_1) &= \mathbb{E}_{z_2}\left[\log p(\mathbf{z})\right] + \text{const} \\
&= \mathbb{E}_{z_2}\left[-\frac{1}{2}(z_1-\mu_1)^2\Lambda_{11} - (z_1-\mu_1)\Lambda_{12}(z_2-\mu_2)\right] + \text{const} \\
&= -\frac{1}{2}z_1^2\Lambda_{11} + z_1\mu_1\Lambda_{11} - (z_1-\mu_1)\Lambda_{12}\left(\mathbb{E}[z_2]-\mu_2\right) + \text{const}
\end{aligned}$$

- Thus we identify a normal, with mean depending on $\mathbb{E}[z_2]$:

$$q^*(z_1) = \mathrm{N}\left(z_1 \mid m_1, \Lambda_{11}^{-1}\right), \quad m_1 = \mu_1 - \Lambda_{11}^{-1}\Lambda_{12}\left(\mathbb{E}[z_2]-\mu_2\right)$$

- By symmetry, $q^*(z_2)$ is also normal; its mean depends on $\mathbb{E}[z_1]$

$$q^*(z_2) = \mathrm{N}\left(z_2 \mid m_2, \Lambda_{22}^{-1}\right), \quad m_2 = \mu_2 - \Lambda_{22}^{-1}\Lambda_{12}\left(\mathbb{E}[z_1]-\mu_1\right)$$

- We treat the above variational solutions as re-estimation equations, and cycle through the variables in turn updating them until some convergence criterion is satisfied

Visualize VI solution to bivariate Gaussian

- Variational inference minimizes $\mathrm{KL}(q\|p)$: mean of the approximation is correct, but variance (along the orthogonal direction) is significantly under-estimated
- Expectation propagation minimizes $\mathrm{KL}(p\|q)$: solution equals marginal distributions

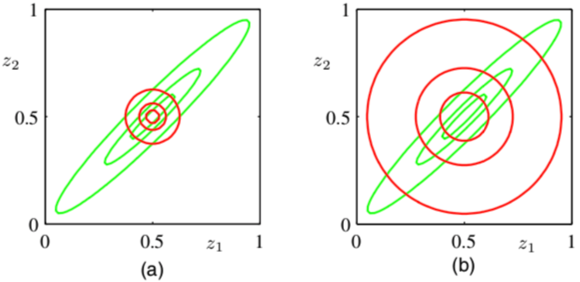
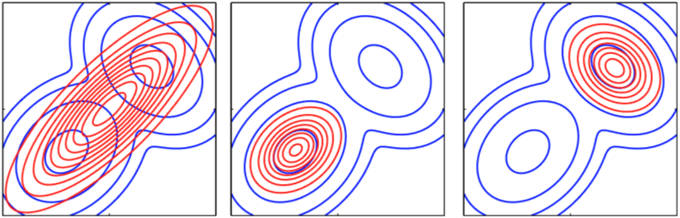


Figure 1: Left: variational inference. Right: expectation propagation

Another example to compare KL$(q\|p)$ and KL$(p\|q)$

- To approximate a mixture of two Gaussians p (blue contour)
- Use a single Gaussian q (red contour) to approximate p
  - By minimizing KL$(p\|q)$: figure (a)
  - By minimizing KL$(q\|p)$: figure (b) and (c) show two local minimum



(a) (b) (c)

- For multimodal distribution
  - a variational solution will tend to find one of the modes,
  - but an expectation propagation solution would lead to poor predictive distribution (because the average of the two good parameter values is typically itself not a good parameter value)

Example: univariate Gaussian

- Suppose the data $D = \{x_1, \ldots, x_N\}$ follows iid normal distribution

$$x_i \sim \mathsf{N}\left(\mu, \tau^{-1}\right)$$

- The prior distributions are

$$\mu \mid \tau \sim \mathsf{N}\left(\mu_0, (\lambda_0 \tau)^{-1}\right)$$
$$\tau \sim \mathsf{Gam}(a_0, b_0)$$

- Factorized variational approximation

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

Variational solution for μ

$$
\begin{aligned}
\log q^*(\mu) &= \mathbb{E}_\tau\left[\log p(D \mid \mu, \tau) + \log p(\mu \mid \tau)\right] + \text{const} \\
&= -\frac{\mathbb{E}[\tau]}{2}\left\{\lambda_0(\mu - \mu_0)^2 + \sum_{i=1}^{N}(x_i - \mu)^2\right\} + \text{const}
\end{aligned}
$$

Thus, the variational solution for μ is

$$
\begin{aligned}
q(\mu) &= \mathsf{N}\left(\mu \mid \mu_N, \lambda_N^{-1}\right) \\
\mu_N &= \frac{\lambda_0\mu_0 + N\bar{x}}{\lambda_0 + N} \\
\lambda_N &= (\lambda_0 + N)\,\mathbb{E}[\tau]
\end{aligned}
$$

Variational solution for τ

$$\log q^*(\tau) = \mathbb{E}_\mu \left[\log p(D \mid \mu, \tau) + \log p(\mu \mid \tau) + \log p(\tau)\right] + \text{const}$$
$$= (a_0 - 1)\log\tau - b_0\tau + \frac{N}{2}\log\tau$$
$$- \frac{\tau}{2}\mathbb{E}_\mu\left[\lambda_0(\mu-\mu_0)^2 + \sum_{i=1}^{N}(x_i-\mu)^2\right] + \text{const}$$

Thus, the variational solution for τ is

$$q(\tau) = \text{Gam}\left(\tau \mid a_N, b_N\right)$$
$$a_N = a_0 + + \frac{N}{2}$$
$$b_N = b_0 + \frac{1}{2}\mathbb{E}_\mu\left[\lambda_0(\mu-\mu_0)^2 + \sum_{i=1}^{N}(x_i-\mu)^2\right]$$

Visualization of VI solution to univariate normal

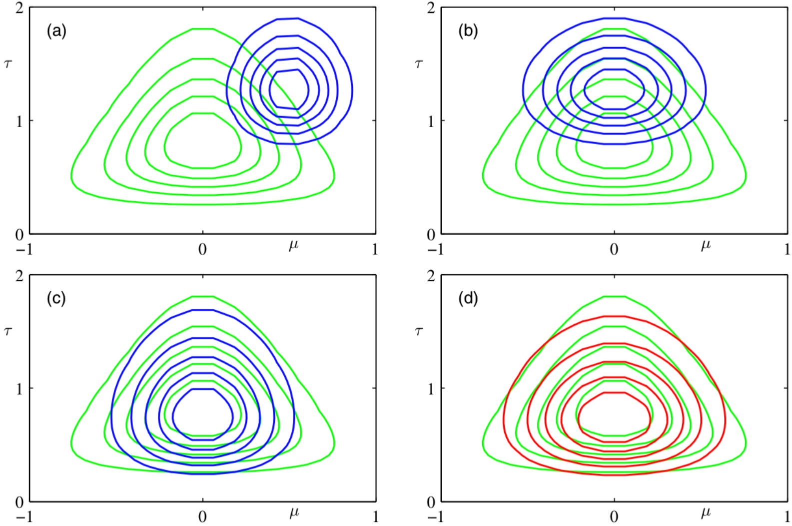


Figure 10.4 Illustration of variational inference for the mean μ and precision τ of a univariate Gaussian distribution. Contours of the true posterior distribution $p(\mu, \tau|D)$ are shown in green. (a) Contours of the initial factorized approximation $q_\mu(\mu)q_\tau(\tau)$ are shown in blue. (b) After re-estimating the factor $q_\mu(\mu)$. (c) After re-estimating the factor $q_\tau(\tau)$. (d) Contours of the optimal factorized approximation, to which the iterative scheme converges, are shown in red.

Model selection (comparison) under variational inference

- In addition to making inference on the parameter $\mathbf{Z}$, we may also want to compare a set of candidate models, denoted by index m
- We should consider the factorization

$$q(\mathbf{Z}, m) = q(\mathbf{Z} \mid m) q(m)$$

to approximate the posterior $p(\mathbf{Z}, m \mid \mathbf{X})$

- We can maximize the information lower bound

$$\mathcal{L}_m = \sum_m \sum_{\mathbf{Z}} q(\mathbf{Z} \mid m) q(m) \log \left\{ \frac{p(\mathbf{Z}, \mathbf{X}, m)}{q(\mathbf{Z} \mid m) q(m)} \right\}$$

which is a lower bound of $\log p(\mathbf{X})$

- The maximized $q(m)$ can be used for model selection

Mixture of Gaussians

- For each observation $\mathbf{x}_n \in \mathbb{R}^D$, we have a corresponding latent variable $\mathbf{z}_n$, a 1-of-K binary group indicator vector
- Mixture of Gasussians joint likelihood, based on N observations

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

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

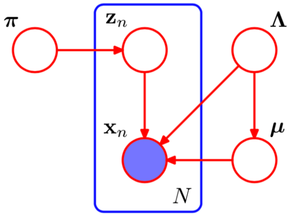


Figure 2: Graph representation of mixture of Gaussians

Conjugate priors

- Dirichlet for $\boldsymbol{\pi}$

$$p(\boldsymbol{\pi}) = \mathsf{Dir}(\boldsymbol{\pi} \mid \boldsymbol{\alpha}_0) \propto \prod_{k=1}^{K} \pi_k^{\alpha_{0k}-1}$$

- Independent Gaussian-Wishart for $\boldsymbol{\mu}, \boldsymbol{\Lambda}$

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

  – Usually, the prior mean $\mathbf{m}_0 = \mathbf{0}$

Variational distribution

- Joint posterior

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

- Variational distribution factorizes between the latent variables and the parameters

$$\begin{aligned} q(\mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) &= q(\mathbf{Z}) q(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) \\ &= q(\mathbf{Z}) q(\boldsymbol{\pi}) \prod_{k=1}^{K} q(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) \end{aligned}$$

Variational solution for $\mathbf{Z}$

- Optimized factor

$$\begin{aligned}\log q^*(\mathbf{Z}) &= \mathbb{E}_{\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Lambda}}\left[\log p(\mathbf{X},\mathbf{Z},\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Lambda})\right] \\ &= \mathbb{E}_{\boldsymbol{\pi}}\left[\log p(\mathbf{Z} \mid \boldsymbol{\pi})\right] + \mathbb{E}_{\boldsymbol{\mu},\boldsymbol{\Lambda}}\left[\log p(\mathbf{X} \mid \mathbf{Z},\boldsymbol{\mu},\boldsymbol{\Lambda})\right] \\ &= \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\log\rho_{nk} + \text{const}\end{aligned}$$

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

- Thus, the factor $q^*(\mathbf{Z})$ takes the same functional form as the prior $p(\mathbf{Z} \mid \boldsymbol{\pi})$

$$q^*(\mathbf{Z}) = \prod_{n=1}^{N}\prod_{k=1}^{K} r_{nk}^{z_{nk}}, \quad r_nk = \frac{\rho_{nk}}{\sum_{j=1}^{K}\rho_{nj}}$$

  - By $q^*(\mathbf{Z})$, the posterior mean (i.e., responsibility) $\mathbb{E}[z_{nk}] = r_{nk}$

Define three statistics wrt the responsibilities

- For each of group $k = 1, \ldots, K$, denote

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

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

$$\mathbf{S}_k = \frac{1}{N_k} \sum_{n=1}^{N} r_{nk} \left(\mathbf{x}_n - \bar{\mathbf{x}}_k\right) \left(\mathbf{x}_n - \bar{\mathbf{x}}_k\right)'$$

Variational solution for π

- Optimized factor

$$\log q^*(\boldsymbol{\pi}) = \log p(\boldsymbol{\pi}) + \mathbb{E}_{\mathbf{Z}}\left[p(\mathbf{Z} \mid \boldsymbol{\pi})\right]$$
$$= (\alpha_0 - 1)\sum_{k=1}^{K} \log \pi_k + \sum_{k=1}^{K}\sum_{n=1}^{N} r_{nk} \log \pi_{nk} + \text{const}$$

- Thus, $q^*(\boldsymbol{\pi})$ is a Dirichlet distribution

$$q^*(\boldsymbol{\pi}) = \text{Dir}(\boldsymbol{\alpha}), \quad \alpha_k = \alpha_0 + N_k$$

Variational solution for μ_k, Λ_k

- Optimized factor for $(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k)$

$$\log q^*(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k) = \mathbb{E}_{\mathbf{Z}}\left[\sum_{n=1}^{N} z_{nk} \log \mathsf{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k^{-1}\right)\right] + \log p(\boldsymbol{\mu}_k \mid \boldsymbol{\Lambda}_k) + \log p(\boldsymbol{\Lambda}_k)$$

- Thus, $q^*(\boldsymbol{\mu}_k, \boldsymbol{\Lambda}_k)$ is Gaussian-Wishart

$$q^*(\boldsymbol{\mu}_k \mid \boldsymbol{\Lambda}_k) = \mathsf{N}\left(\mathbf{m}_k, (\beta_k \boldsymbol{\Lambda}_k)^{-1}\right) \quad q^*(\boldsymbol{\Lambda}_k) \quad = \mathsf{W}(\boldsymbol{\Lambda}_k \mid \mathbf{W}_k, \nu_k)$$

- Parameters are updated by the data

$$\beta_k = \beta_0 + N_k, \quad \mathbf{m}_k = \frac{1}{\beta_k}\left(\beta_0 \mathbf{m}_0 + N_k \bar{\mathbf{x}}_k\right), \quad \nu_k = \nu_0 + N_k$$

$$\mathbf{W}_k^{-1} = \mathbf{W}_0^{-1} + N_k \mathbf{S}_k + \frac{\beta_0 N_k}{\beta_0 + N_k}\left(\bar{\mathbf{x}}_k - \mathbf{m}_0\right)\left(\bar{\mathbf{x}}_k - \mathbf{m}_0\right)'$$

Similarity between VI and EM solutions

- Optimization of the variational posterior distribution involves cycling between two stages analogous to the E and M steps of the maximum likelihood EM algorithm
  - Finding $q^*(\mathbf{Z})$: analogous to the E step, both need to compute the responsibilities
  - Finding $q^*(\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})$: analogous to the M step
- The VI solution (Bayesian approach) has little computational overhead, comparing with the EM solution (maximum likelihood approach). The dominant computational cost for VI are
  - Evaluation of the responsibilities
  - Evaluation and inversion of the weighted data covariance matrices

Advantage of the VI solution over the EM solution:

- Since our priors are conjugate, the variational posterior distributions have the same functional form as the priors

1. No singularity arises in maximum likelihood when a Gassuain component "collapses" onto a specific data point
   - This is actually the advantage of Bayesian solutions (with priors) over frequentist ones
2. No overfitting if we choose a large number K. This is helpful in determining the optimal number of components without performing cross validation
   - For $\alpha_0 < 1$, the prior favors soutions where some of the mixing coefficients $\boldsymbol{\pi}$ are zero, thus can result in some less than K number components having nonzero mixing coefficients

Computing variational lower bound

- To test for convergence, it is useful to monitor the bound during the re-estimation.
- At each step of the iterative re-estimation, the value of the lower bound should not decrease

$$
\begin{aligned}
\mathcal{L} = & \sum_{\mathbf{Z}} \iiint q^*(\mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) \log \left\{ \frac{p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})}{q^*(\mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})} \right\} d\boldsymbol{\pi} d\boldsymbol{\mu} d\boldsymbol{\Lambda} \\
= & \ \mathbb{E}\left[\log p(\mathbf{X}, \mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})\right] - \mathbb{E}\left[\log q^*(\mathbf{Z}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Lambda})\right] \\
= & \ \mathbb{E}\left[\log p(\mathbf{X} \mid \mathbf{Z}, \boldsymbol{\mu}, \boldsymbol{\Lambda})\right] + \mathbb{E}\left[\log p(\mathbf{Z} \mid \boldsymbol{\pi})\right] \\
& + \mathbb{E}\left[\log p(\boldsymbol{\pi})\right] + \mathbb{E}\left[\log p(\boldsymbol{\mu}, \boldsymbol{\Lambda})\right] \\
& - \mathbb{E}\left[\log q^*(\mathbf{Z})\right] - \mathbb{E}\left[\log q^*(\boldsymbol{\pi})\right] - \mathbb{E}\left[\log q^*(\boldsymbol{\mu}, \boldsymbol{\Lambda})\right]
\end{aligned}
$$

Label switching problem

- EM solution of maximum likelihood does not have label switching problem, because the initialization will lead to just one of the solutions
- In a Bayesian setting, label switching problem can be an issue, because the marginal posterior is multi-modal.
- Recall that for multi-modal posteriors, variational inference usually approximate the distribution in the neighborhood of one of the modes and ignore the others

Induced factorizations

- Induced factorizations: the additional factorizations that are a consequence of the interaction between
  - the assumed factorization, and
  - the conditional independence properties of the true distribution
- For example, suppose we have three variation groups $\mathbf{A}, \mathbf{B}, \mathbf{C}$
  - We assume the following factorization

$$q(\mathbf{A}, \mathbf{B}, \mathbf{C}) = q(\mathbf{A}, \mathbf{B}) q(\mathbf{C})$$

  - If $\mathbf{A}$ and $\mathbf{B}$ are conditional independent

$$\mathbf{A} \perp \mathbf{B} \mid \mathbf{X}, \mathbf{C} \Longleftrightarrow p(\mathbf{A}, \mathbf{B} \mid \mathbf{X}, \mathbf{C}) = p(\mathbf{A} \mid \mathbf{X}, \mathbf{C}) p(\mathbf{B} \mid \mathbf{X}, \mathbf{C})$$

    then we have induced factorization $q^*(\mathbf{A}, \mathbf{B}) = q^*(\mathbf{A}) q^*(\mathbf{B})$

$$\begin{aligned} \log q^*(\mathbf{A}, \mathbf{B}) &= \mathbb{E}_{\mathbf{C}}\left[\log p(\mathbf{A}, \mathbf{B} \mid \mathbf{X}, \mathbf{C})\right] + \text{const} \\ &= \mathbb{E}_{\mathbf{C}}\left[\log p(\mathbf{A} \mid \mathbf{X}, \mathbf{C})\right] + \mathbb{E}_{\mathbf{C}}\left[\log p(\mathbf{B} \mid \mathbf{X}, \mathbf{C})\right] + \text{const} \end{aligned}$$

Bayesian linear regression

- Here, I use a denotion system commonly used in statistics textbooks. So its different from the one used in this book.
- Likelihood function

$$p(\mathbf{y} \mid \boldsymbol{\beta}) = \prod_{n=1}^{N} \mathsf{N}\left(y_n \mid \mathbf{x}_n \boldsymbol{\beta}, \phi^{-1}\right)$$

  - $\phi = 1/\sigma^2$ is the precision parameter. We assume that it is known.
  - $\boldsymbol{\beta} \in \mathbb{R}^p$ includes the intercept

- Prior distributions: Normal Gamma

$$p(\boldsymbol{\beta} \mid \kappa) = \mathsf{N}\left(\boldsymbol{\beta} \mid \mathbf{0}, \kappa^{-1}\mathbf{I}\right)$$
$$p(\kappa) = \mathsf{Gam}(\kappa \mid a_0, b_0)$$

Variational solution for κ

- Variational posterior factorization

$$q(\boldsymbol{\beta}, \kappa) = q(\boldsymbol{\beta})q(\kappa)$$

- Varitional solution for κ

$$\begin{aligned} \log q^*(\kappa) &= \log p(\kappa) + \mathbb{E}_{\boldsymbol{\beta}}\left[\log p(\boldsymbol{\beta} \mid \kappa)\right] \\ &= (a_0 - 1)\log\kappa - b_0\kappa + \frac{p}{2}\log\kappa - \frac{\kappa}{2}\mathbb{E}\left[\boldsymbol{\beta}'\boldsymbol{\beta}\right] \end{aligned}$$

- Varitional posterior is a Gamma

$$\begin{aligned} \kappa &\sim \text{Gam}\left(a_N, b_N\right) \\ a_N &= a_0 + \frac{p}{2} \\ b_N &= b_0 + \frac{\mathbb{E}\left[\boldsymbol{\beta}'\boldsymbol{\beta}\right]}{2} \end{aligned}$$

Variational solution for β

- Variational solution for β

$$\begin{aligned}
\log q^*(\boldsymbol{\beta}) &= \log p(\mathbf{y} \mid \boldsymbol{\beta}) + \mathbb{E}_\kappa \left[\log p(\boldsymbol{\beta} \mid \kappa)\right] \\
&= -\frac{\phi}{2} \left(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\right)^2 - \frac{\mathbb{E}\left[\kappa\right]}{2} \boldsymbol{\beta}' \boldsymbol{\beta} \\
&= -\frac{1}{2} \boldsymbol{\beta}' \left(\mathbb{E}\left[\kappa\right] \mathbf{I} + \phi \mathbf{X}'\mathbf{X}\right) \boldsymbol{\beta} + \phi \boldsymbol{\beta}' \mathbf{X}' \mathbf{y}
\end{aligned}$$

- Variational posterior is a Normal

$$\begin{aligned}
\boldsymbol{\beta} &\sim \mathsf{N}\left(\mathbf{m}_N, \mathbf{S}_N\right) \\
\mathbf{S}_N &= \left(\mathbb{E}\left[\kappa\right] \mathbf{I} + \phi \mathbf{X}'\mathbf{X}\right)^{-1} \\
\mathbf{m}_N &= \phi \mathbf{S}_N \mathbf{X}' \mathbf{y}
\end{aligned}$$

Iteratively re-estimate the variational solutions

- Means of the variational posteriors

$$\mathbb{E}[\kappa] = \frac{a_N}{b_N}$$
$$\mathbb{E}[\beta'\beta] = \mathbf{m}_N \mathbf{m}_N' + \mathbf{S}_N$$

- Lower bound of $\log p(\mathbf{y})$ can be used in convergence monitoring, and also model selection

$$\begin{aligned}\mathcal{L} =& \ \mathbb{E}\left[\log p(\boldsymbol{\beta}, \kappa, \mathbf{y})\right] - \mathbb{E}\left[\log q^*(\boldsymbol{\beta}, \kappa)\right] \\ =& \ \mathbb{E}_{\boldsymbol{\beta}}\left[\log p(\mathbf{y} \mid \boldsymbol{\beta})\right] + \mathbb{E}_{\boldsymbol{\beta},\kappa}\left[\log p(\boldsymbol{\beta} \mid \kappa)\right] + \mathbb{E}_{\kappa}\left[\log p(\kappa)\right] \\ & - \mathbb{E}_{\boldsymbol{\beta}}\left[\log q^*(\boldsymbol{\beta})\right] - \mathbb{E}_{\kappa}\left[\log q^*(\kappa)\right]\end{aligned}$$

References

- Bishop, C. M. (2006). Pattern Recognition and Machine Learning. Springer.