Variational Inference

A/Prof Richard Yi Da Xu
Yida.Xu@uts.edu.au
Wechat: aubedata
https://github.com/roboticcam/machine-learning-notes

University of Technology Sydney (UTS)

February 18, 2018

Log-likelihood and Evidence Lower Bound (ELOB)

- It is universally true that:

$$\ln(p(X)) = \ln(p(X,Z)) - \ln(p(Z|X))$$

- It's also true (a bit silly) that:

$$\ln(p(X)) = [\ln(p(X,Z)) - \ln(q(Z))] - [\ln(p(Z|X)) - \ln(q(Z))]$$

- The above is so that we can insert an arbitrary pdf $q(Z)$ into, now we get:

$$\ln(p(X)) = \ln\left(\frac{p(X,Z)}{q(Z)}\right) - \ln\left(\frac{p(Z|X)}{q(Z)}\right)$$

- Taking the expectation on both sides, given $q(Z)$:

$$\begin{aligned}
\ln(p(X)) &= \int q(Z)\ln\left(\frac{p(X,Z)}{q(Z)}\right)dZ - \int q(Z)\ln\left(\frac{p(Z|X)}{q(Z)}\right)dZ \\
&= \underbrace{\int q(Z)\ln(p(X,Z))dZ - \int q(Z)\ln(q(Z))dZ}_{\mathcal{L}(q)} + \underbrace{\left(-\int q(Z)\ln\left(\frac{p(Z|X)}{q(Z)}\right)dZ\right)}_{\mathbb{KL}(q\|p)} \\
&= \mathcal{L}(q) + \mathbb{KL}(q\|p)
\end{aligned}$$

Alternative Evidence Lower Bound (ELOB)

We often see the following alternative derivation:

$$
\begin{aligned}
\ln\left(p(X)\right) &= \log \int_Z p(X,Z)\mathrm{d}z \\
&= \log \int_Z p(X,Z)\frac{q(Z)}{q(Z)}\mathrm{d}z \\
&= \log\left(\mathbb{E}_q\left[\frac{p(X,Z)}{q(Z)}\right]\right) \\
&\geq \mathbb{E}_q\left[\log\left(\frac{p(X,Z)}{q(Z)}\right)\right] \text{ using Jensen's inequality} \\
&= \mathbb{E}_q\left[\log(p(X,Z))\right] - \mathbb{E}_q\left[\log(q(Z))\right] \\
&\triangleq \mathcal{L}(q)
\end{aligned}
$$

It can be proven easily that the “missing” part, i.e., $\ln\left(p(X)\right) - \mathcal{L}(q) = \mathbb{KL}(q\|p)$.

Maximize Evidence Lower Bound (ELOB)

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

- We can give a name to both terms:

$$\text{Evidence Lower Bound (ELOB):} \quad \mathcal{L}(q) = \int q(Z)\ln(p(X,Z))\mathrm{d}Z - \int q(Z)\ln(q(Z))\mathrm{d}Z$$

$$\text{KL divergence:} \quad \mathbb{KL}(q\|p) = \int q(Z)\ln\left(\frac{p(Z|X)}{q(Z)}\right)dZ$$

- Notice $p(X)$ is fixed with respect to the choice of $q(Z)$. We wanted to choose a $q(Z)$ function that minimize KL divergence, so that $q(Z)$ becomes closer and closer to $p(Z|X)$. Of course, let's see what happens when $q(Z) = p(Z|X)$:

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

- We know that $p(X) = \mathcal{L}(q) + \mathbb{KL}(q\|p)$. Minimizing $\mathbb{KL}(q\|p)$ is the same as maximizing the Evidence Lower Bound $\mathcal{L}(q)$.

Approach One

- Arbitrary (i.e., non Exponential Family) distributions
- No maximizing variational distribution parameters

The choice of $q(Z)$

- Suppose let's choose $q(Z)$, such that:

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

- Substitute this choice into Evidence Lower Bound (ELOB):

$$\begin{aligned}
\mathcal{L}(q) &= \int q(Z)\ln(p(X,Z))\mathrm{d}Z - \int q(Z)\ln(q(Z))\mathrm{d}Z \\
&= \underbrace{\int \prod_{i=1}^{M} q_i(Z_i)\ln\left(p(X,Z)\right)\mathrm{d}Z}_{\text{part (1)}} - \underbrace{\int \prod_{i=1}^{M} q_i(Z_i)\sum_{i=1}^{M}\ln\left(q_i(Z_i)\right)\mathrm{d}Z}_{\text{part (2)}}
\end{aligned}$$

Simplification of (Part 1):

$$\text{(Part 1)} = \int \prod_{i=1}^{M} q_i(Z_i) \ln\left(p(X,Z)\right) \mathrm{d}Z$$

$$\int_{Z_1}\int_{Z_2}\dots\int_{Z_M} \prod_{i=1}^{M} q_i(Z_i) \ln\left(p(X,Z)\right) \mathrm{d}Z_1, \mathrm{d}Z_2, \dots, \mathrm{d}Z_M$$

- Rearrange the expression by taking a particular $q_j(Z_j)$ out of the integral:

$$\text{(Part 1)} = \int_{Z_j} q_j(Z_j) \left(\int_{Z_{i\neq j}} \cdots \int \prod_{i\neq j}^{M} q_i(Z_i) \ln\left(p(X,Z)\right) \prod_{i\neq j}^{M} dZ_i \right) dZ_j$$

- or, more compactly:

$$\text{(Part 1)} = \int_{Z_j} q_j(Z_j) \left(\int_{Z_{i\neq j}} \cdots \int \ln\left(p(X,Z)\right) \prod_{i\neq j}^{M} q_i(Z_i) dZ_i \right) dZ_j$$

- or, even more meaningfully, it can be put into an expectation function, and since $\prod_{i\neq j}^{M} q_i(Z_i)$ is a joint probability density

$$\text{(Part 1)} = \int_{Z_j} q_j(Z_j) \left[\mathbb{E}_{i\neq j} \left[\ln\left(p(X,Z)\right) \right] \right] dZ_j$$

Simplification of (Part 2):

$$
\text{(Part 2)} = \int \prod_{i=1}^{M} q_i(Z_i) \sum_{i=1}^{M} \ln\left(q_i(Z_i)\right) dZ
$$

- Note that the above needs to integrate out all $Z = \{z_1, \ldots, z_M\}$, which is quite daunting. However, notice that each term in the sum, $\sum_{i=1}^{M} \ln\left(q_i(Z_i)\right)$ involves only a single i, therefore, we are able to simplify the above into the following:

$$
\text{(Part 2)} = \sum_{i=1}^{M} \left(\int_{Z_i} q_i(Z_i) \ln\left(q_i(Z_i)\right) dZ_i \right)
$$

- For a particular $p_j(Z_j)$, the rest of the sum can be treated like a constant, part 2 can be written as:

$$
\text{(Part 2)} = \int_{Z_j} q_i(Z_i) \ln\left(q_i(Z_i)\right) dZ_j + \text{const.}
$$

where const. are the term does not involve Z_j.

Putting Part (1) and Part (2) together:

$$\mathcal{L}(q) = \text{Part (1)} - \text{Part (2)} = \int_{Z_j} q_j(Z_j)\mathbb{E}_{i\neq j}\Big[\ln\left(p(X,Z)\right)\Big]\mathrm{d}Z_j - \int_{Z_j} q_j(Z_j)\ln\left(q_j(Z_j)\right)\mathrm{d}Z_j + \text{const.}$$

- Note that $\mathbb{E}_{i\neq j}\left[\ln\left(p(X,Z)\right)\right]$ would be some $\ln[p(Z_i)]$, we name it $\ln(\tilde{p}_j(X,Z_j))$, i.e.,:

$$\ln(\tilde{p}_j(X,Z_j)) = \mathbb{E}_{i\neq j}\left[\ln\left(p(X,Z)\right)\right]$$

- Or equivalently we can express Evidence Lower Bound (ELOB) in terms of:

$$\mathcal{L}(q_j) = \int_{Z_j} q_j(Z_j)\ln\left[\frac{\tilde{p}_j(X,Z_j)}{q_j(Z_j)}\right] + \text{const..}$$

  This is the same as $-\mathbb{KL}\left(\mathbb{E}_{i\neq j}\left[\ln\left(p(X,Z)\right)\right] \| q_i(Z_i)\right)$

- **This is the key**: We can maximize ELOB, or $\mathcal{L}(q)$, by minimizing this special KL divergence, where we can find approximate and optimal $q_i^*(Z_i)$, such that:

$$\ln\left(q_i^*(Z_i)\right) = \mathbb{E}_{i\neq j}\left[\ln\left(p(X,Z)\right)\right]$$

Example: Gaussian-Gamma Conjugate prior

- Let $\mathcal{D} = \{x_1, \dots x_n\}$:

$$
\begin{aligned}
p(\mathcal{D}|\mu,\tau) &= \prod_{i=1}^{n} \left(\frac{\tau}{2\pi}\right)^{\frac{1}{2}} \exp\left(\frac{-\tau}{2}(x_i - \mu)^2\right) \\
&= \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \exp\left(\frac{-\tau}{2}\sum_{i=1}^{n}(x_i - \mu)^2\right)
\end{aligned}
$$

$$
\begin{aligned}
p(\mu|\tau) &= \mathcal{N}(\mu_0, (\lambda_0\tau)^{-1}) \propto \exp\left(\frac{-\lambda_0\tau}{2}(\mu - \mu_0)^2\right) \\
p(\tau) &= \text{Gamma}(\tau|a_0, b_0) \propto \tau^{a_0 - 1} \exp^{-b_0\tau}
\end{aligned}
$$

- Complete data-likelihood is:

$$
p(\mathcal{D},\mu,\tau) = p(\mathcal{D}|\mu,\tau)p(\mu|\tau)p(\tau)
$$

Of course, due to conjugacy, the solution can be found exactly:

$$p(\mu, \tau|\mathrm{d}) \propto p(\mathcal{D}|\mu, \tau)p(\mu|\tau)p(\tau) = \mathcal{N}(\mu_n, (\lambda_n \tau)^{-1})\mathrm{Gamma}(\tau|a_n, b_n)$$

where:

$$\begin{aligned}
\mu_n &= \frac{\lambda_0 \mu_0 + n\bar{x}}{\lambda_0 + n} \\
\lambda_n &= \lambda_0 + n \\
a_n &= a_0 + n/2 \\
b_n &= b_0 + \frac{1}{2}\sum_{i=1}^{n}(x_i - \bar{x})^2 + \frac{\lambda_0 n(\bar{x} - \mu_0)^2}{2(\lambda_0 + n)}
\end{aligned}$$

However, for demo purpose, we assume $q(\mu, \tau)$:

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

$$
\begin{aligned}
\ln(q^*_\mu(\mu)) &= \mathbb{E}_{q_\tau}[\ln(p(\mu,\tau|\mathcal{D}))] \\
&= \mathbb{E}_{q_\tau}[\ln(p(\mathcal{D}|\mu,\tau)) + \ln p(\mu|\tau)] + \text{const.} \qquad \text{remove terms do NOT contain } \mu \\
&= \mathbb{E}_{q_\tau}\left[\underbrace{-\frac{\tau}{2}\sum_{i=1}^n (x_i-\mu)^2}_{\ln(p(\mathcal{D}|\mu,\tau))} + \underbrace{\frac{\lambda_0\tau}{2}(\mu-\mu_0)^2}_{\ln p(\mu|\gamma)}\right] + \text{const.} \\
&= -\frac{\mathbb{E}_{q_\tau}[\tau]}{2}\underbrace{\left[\sum_{i=1}^n (x_i-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right]}_{\text{terms contain } \mu \text{ but does not contain } \tau} + \text{const.}
\end{aligned}
$$

Completing the square for the μ terms:

$$
\begin{aligned}
&\sum_{i=1}^n (x_i-\mu)^2 + \lambda_0(\mu-\mu_0)^2 = n\mu^2 - 2n\mu\bar{x} + \lambda_0\mu^2 - 2\lambda_0\mu_0\mu + \text{const.} \\
=&(n+\lambda_0)\mu^2 - 2\mu(n\bar{x}+\lambda_0\mu_0) = (n+\lambda_0)\left(\mu^2 - \frac{2\mu(n\bar{x}+\lambda_0\mu_0)}{(n+\lambda_0)}\right) \\
=&(n+\lambda_0)\left(\mu - \frac{(n\bar{x}+\lambda_0\mu_0)}{(n+\lambda_0)}\right)^2 + \text{const.}
\end{aligned}
$$

Computing $\ln(q^*_\mu(\mu)) = \mathbb{E}_{q_\tau(\tau)}[\ln(p(\mu,\tau|\mathcal{D}))]$ (2)

Therefore, we have:

$$
\begin{aligned}
\ln(q^*_\mu(\mu)) &= -\frac{\mathbb{E}_{q_\tau}[\tau]}{2}\left[\sum_{i=1}^{n}(x_i-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right] + \text{const.}\\
&= -\frac{\mathbb{E}_{q_\tau}[\tau](n+\lambda_0)}{2}\left(\mu - \frac{(n\bar{x}+\lambda_0\mu_0)}{(n+\lambda_0)}\right)^2 + \text{const.}\\
&= \mathcal{N}\left(\frac{n\bar{x}+\lambda_0\mu_0}{n+\lambda_0}, \mathbb{E}_{q_\tau}[\tau](n+\lambda_0)\right)
\end{aligned}
$$

Computing $\ln(q_i^*(\tau)) = \mathbb{E}_{q_\mu(\mu)}[\ln(p(\mu, \tau|\mathcal{D}))]$ (1)

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

Bring terms without μ outside of the integral:

$$
\begin{aligned}
&= \frac{n}{2}\ln(\tau) + (a_0 - 1)\ln(\tau) - b_0\tau - \frac{\tau}{2}\mathbb{E}_{q_\mu(\mu)}\left[\sum_{i=1}^{n}(x_i - \mu)^2 + \lambda_0(\mu - \mu_0)^2\right] + \text{const.} \\
&= \left(\underbrace{\frac{n}{2} + a_0}_{a_n} - 1\right)\ln(\tau) - \tau\left(\underbrace{b_0 + \frac{1}{2}\mathbb{E}_{q_\mu(\mu)}\left[\sum_{i=1}^{n}(x_i - \mu)^2 + \lambda_0(\mu - \mu_0)^2\right]}_{b_n}\right) + \text{const.}
\end{aligned}
$$

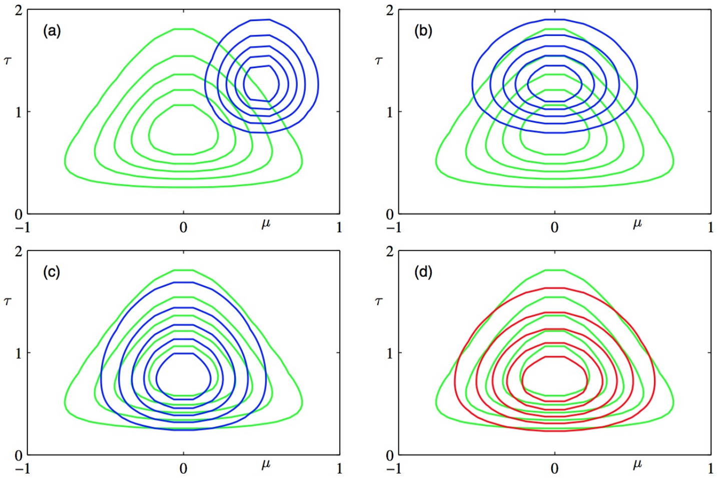
Computing $\ln(q_i^*(\tau)) = \mathbb{E}_{q_\mu(\mu)}[\ln(p(\mu,\tau|\mathcal{D}))]$ (2)

We can rewrite,

$$\begin{aligned}
b_n &= b_0 + \frac{1}{2}\mathbb{E}_{q_\mu}\left[\sum_{i=1}^{n}(x_i-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right] \\
&= b_0 + \frac{1}{2}\mathbb{E}_{q_\mu}\left[-2\mu n\bar{x} + n\mu^2 + \lambda_0\mu^2 - 2\lambda_0\mu_0\mu\right] + \sum_{i=1}^{n}(x_i)^2 + \lambda_0\mu_0^2 \\
&= b_0 + \frac{1}{2}\left[(n+\lambda_0)\mathbb{E}_{q_\mu}[\mu^2] - 2\left(n\bar{x}+\lambda_0\mu_0\right)\mathbb{E}_{q_\mu}[\mu] + \sum_{i=1}^{n}(x_i)^2 + \lambda_0\mu_0^2\right]
\end{aligned}$$

We will compute $\mathbb{E}_{q_\mu}[\mu]$ and $\mathbb{E}_{q_\mu}[\mu^2]$ since we know of $q_\mu(\mu)$ from previously.

Figure and Demo



Also see Matlab Demo!

Approach Two

- Perform direct maximisation over $q(Z)$ using variational calculus

Functional identity

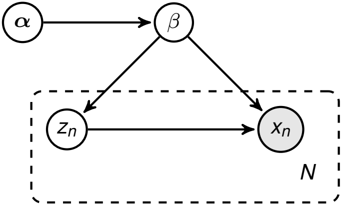
$$
\begin{aligned}
G(f_x(x), f_y(y)) &= \int_x \int_y f_x(x) f_y(y) \ln p(x, y) \mathrm{d}x\mathrm{d}y \implies \\
\frac{\delta G(f_x(x), f_y(y))}{\delta f_x(x')} &= \int_x \int_y \frac{\delta f_x(x)}{\delta f_x(x')} f_y(y) \ln p(x, y) \mathrm{d}x\mathrm{d}y \\
&= \int_x \int_y \delta(x - x') f_y(y) \ln p(x, y) \mathrm{d}x\mathrm{d}y \\
&= \int_y f_y(y) \ln p(x', y) \mathrm{d}y
\end{aligned}
$$

Let $Z \triangleq (z, \theta)$ $\quad p(X, Z, \theta) = p(X, Z|\theta)p(\theta)$ $\quad q(Z, \theta) = q_z(Z)q_\theta(\theta)$:
Evidence Lower Bound (ELBO) can be written as:

Approach Three

- Exponential Family distributions
- Maximizing variational distribution parameters
- Introduction to Stochastic Variational Inference (SVI)

Problem to consider:



$$p(X, Z, \beta|\alpha) = p(\beta|\alpha) \prod_{n=1}^{N} p(x_n, z_n|\beta)$$

$$p(x_n, z_n|x_{-n}, z_{-n}, \beta, \alpha) = p(x_n, z_n|\beta, \alpha)$$

All posterior is based on Exponential family:

$$p(\beta|X, Z, \alpha) = h(\beta) \exp\left\{\eta_g(X, Z, \alpha)^T t(\beta) - A_g(\eta_g(X, Z, \alpha))\right\}$$

$$p(z_{n,j}|x_n, z_{n,-j}, \beta) = h(z_{n,j}) \exp\left\{\eta_l(x_n, z_{n,-j}, \beta)^T t(z_{n,j}) - A_l(\eta_l(x_n, z_{n,-j}, \beta))\right\}$$

Most of the distributions we are going to look at are from **exponential family**
exponential family can be expressed in terms of its natural parameters:

$$h(x) \exp\left(T(x)^T \eta - A(\eta)\right)$$

Think about why is this representation useful?

Always have in mind ask yourself where are the **support** of these distributions, i.e., where $p(X) > 0$?

More about Gaussian 1-d: Natural Parameter Representation

$$
\begin{aligned}
\mathcal{N}(x;\mu,\sigma^2) &= (2\pi\sigma^2)^{-1/2}\exp^{-\frac{(x-\mu)^2}{2\sigma^2}}\\
&= \exp\left(-\frac{x^2-2x\mu+\mu^2}{2\sigma^2}-\frac{1}{2}\ln(2\pi\sigma^2)\right)\\
&= \exp\left(-\frac{1}{2\sigma^2}x^2+\frac{\mu}{\sigma^2}x-\frac{\mu^2}{2\sigma^2}-\frac{1}{2}\ln(2\pi\sigma^2)\right)\\
&= \exp\left(\underbrace{\begin{bmatrix} x \\ x^2 \end{bmatrix}^T}_{T(X)}\begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix}-\frac{\mu^2}{2\sigma^2}-\frac{1}{2}\ln(2\pi\sigma^2)\right)
\end{aligned}
$$

- $\eta = \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} = \begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} \; A(\eta) = \frac{-\eta_1^2}{4\eta_2} - \frac{1}{2}\ln(-2\eta_2)$
- $\eta_2 = -\frac{1}{2\sigma^2} \implies \sigma^2 = -\frac{1}{2\eta_2} \qquad \mu = \eta_1\sigma^2 = \eta_1\frac{-1}{2\eta_2} = \frac{-\eta_1}{2\eta_2}$

- Reverse is: $\theta = \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} \frac{-\eta_1}{2\eta_2} \\ \frac{-1}{2\eta_2} \end{bmatrix}$

$$
\begin{aligned}
\tilde{\mathcal{N}}(x, \eta) &= \exp\left(\begin{bmatrix} x \\ x^2 \end{bmatrix}^T \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} - \frac{\mu^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2) \right) \\
&= \exp\left(\begin{bmatrix} x \\ x^2 \end{bmatrix}^T \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} - \frac{\left(\frac{-\eta_1}{2\eta_2}\right)^2}{2\left(\frac{-1}{2\eta_2}\right)} - \frac{1}{2}\ln\left(2\pi\left(\frac{-1}{2\eta_2}\right)\right) \right) \\
&= \exp\left(T(x)^T\eta + \frac{\eta_1^2}{4\eta_2} - \frac{1}{2}\ln\left(\frac{2\pi}{-2\eta_2}\right) \right) \\
&= \exp\left(T(x)^T\eta + \frac{\eta_1^2}{4\eta_2} + \frac{1}{2}\ln(-2\eta_2) - \frac{1}{2}\ln(2\pi) \right)
\end{aligned}
$$

$$
\mathcal{N}_{\text{nat}}(x, \eta) = \exp\left(T(x)^T\eta - \underbrace{\left(\frac{-\eta_1^2}{4\eta_2} - \frac{1}{2}\ln(-2\eta_2) \right)}_{A(\eta)} - \frac{1}{2}\ln(2\pi) \right)
$$

- Prior:

$$p(\beta) = h(\beta)\exp\{\alpha^T t(\beta) - A_g(\alpha)\} = \underbrace{\exp(-A_g(\alpha))}_{\text{normalization}} h(\beta)\exp\{\alpha^T t(\beta)\}$$

$$\implies \int_\beta h(\beta)\exp\{\alpha^T t(\beta)\} = \exp(A_g(\alpha))$$

Let sufficient statistics $t(\beta) = [\beta, \underbrace{-A_l(\beta)}_{\text{same}}]^T \implies \alpha = [\alpha_1 \ \alpha_2]^T$:

$$p(\beta) = h(\beta)\exp\left\{[\alpha_1, \alpha_2]^T[\beta, \underbrace{-A_l(\beta)}_{\text{same}}] - A_g(\alpha)\right\}$$

- Likelihood density per (x_n, z_n) is:

$$p(x_n, z_n|\beta) = h(x_n, z_n)\exp\left\{t(x_n, z_n)\beta \underbrace{-A_l(\beta)}_{\text{same}}\right\}$$

- Posterior is:

$$\begin{aligned}
p(\beta|x_n, z_n, \alpha) &\propto \underbrace{h(\beta)\exp\{\alpha^T t(\beta)\}}\,\underbrace{\exp\{t(x_n, z_n)\beta - A_l(\beta)\}} \\
&= h(\beta)\exp\{(\alpha_1 + t(x_n, z_n))\beta - \alpha_2 A_l(\beta) - A_l(\beta)\} \\
&= h(\beta)\exp\{(\alpha_1 + t(x_n, z_n))\beta - (\alpha_2 + 1)A_l(\beta)\} \\
&= h(\beta)\exp\{[\alpha_1 + t(x_n, z_n) \quad \alpha_2 + 1]^T t(\beta)\}
\end{aligned}$$

The complete posterior

- Complete likelihood:

$$p(X, Z|\beta) = \prod_{n=1}^{N} h(x_n, z_n) \exp\{\beta^T t(x_n, z_n) - A_l(\beta)\} = h(X, Z) \exp\left\{ \sum_{n=1}^{N} \beta^T t(x_n, z_n) - N \times A_l(\beta) \right\}$$

- Complete posterior:
  Since: $p(\beta|x_n, z_n, \alpha) \propto h(\beta) \exp\{[\alpha_1 + t(x_n, z_n) \quad \alpha_2 + 1]^T t(\beta)\}$:

$$\Longrightarrow \quad p(\beta|X, Z, \alpha) \propto h(\beta) \exp\left\{ \left[\alpha_1 + \sum_{n=1}^{N} t(x_n, z_n) \quad \alpha_2 + N \right]^T t(\beta) \right\}$$

When we use the expression:

$$p(\beta|X, Z, \alpha) = h(\beta) \exp\{\eta_g(X, Z, \alpha)^T t(\beta) - A_g(\eta_g(X, Z, \alpha))\}$$

$$\Longrightarrow \quad \eta_g(X, Z, \alpha) = \left[\alpha_1 + \sum_{n=1}^{N} t(x_n, z_n) \quad \alpha_2 + N \right]$$

$$\Longrightarrow \quad A_g(\eta_g(X, Z, \alpha)) = \int_{\beta} h(\beta) \exp\{\eta_g(X, Z, \alpha)^T t(\beta)\}$$

Example: Posterior of Gaussian mean (1)

To summarise:

$$
\begin{aligned}
p(\beta|X, Z, \alpha) &\propto h(\beta) \exp\left\{[\hat{\alpha_1} \quad \hat{\alpha_2}]^T \, [\beta \quad - A_l(\beta)]\right\} \\
&= h(\beta) \exp\left\{ \left[\underbrace{\alpha_1 + \sum_{n=1}^{N} t(x_n, z_n)}_{\hat{\alpha}_1} \quad \underbrace{\alpha_2 + N}_{\hat{\alpha}_2} \right]^T t(\beta) \right\}
\end{aligned}
$$

- Example: suppose data x_i come from unit variance Gaussian:

$$
p(x|\mu) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x-\mu)^2\right\} = \underbrace{\frac{\exp\left(-x^2/2\right)}{\sqrt{2\pi}}}_{h(x)} \exp\left\{ \underbrace{\mu}_{\beta} \underbrace{x}_{t(x)} - \underbrace{\frac{\mu^2}{2}}_{A_l(\beta)} \right\}
$$

- So we have:

$$
\begin{aligned}
\beta &= \mu & t(x) &= x \\
A_l(\beta) &= \frac{\beta^2}{2} & h(x) &= \frac{\exp\left(-x^2/2\right)}{\sqrt{2\pi}}
\end{aligned}
$$

Example: Posterior of Gaussian mean (2)

$$p(x|\mu) = \frac{\exp\left(-x^2/2\right)}{\sqrt{2\pi}} \exp\left\{\mu x - \frac{\mu^2}{2}\right\} = \frac{\exp\left(-x^2/2\right)}{\sqrt{2\pi}} \exp\left\{\beta x + \underbrace{-\frac{\beta^2}{2}}_{A_l(\beta)}\right\}$$

- For the above likelihood, its conjugate prior MUST be in the form of:

$$\begin{aligned} p(\beta|\alpha) &= h(\beta) \exp\left\{\alpha_1 \beta + \alpha_2 \underbrace{(-\beta^2/2)}_{A_l(\beta)} - A_g(\alpha)\right\} \\ &= h(\beta) \exp\left\{\begin{bmatrix}\alpha_1 & -\frac{\alpha_2}{2}\end{bmatrix}^T \begin{bmatrix}\beta & \beta^2\end{bmatrix} - A_g(\alpha)\right\} \end{aligned}$$

- Since we know,

$$p(\beta|\alpha) = h(\beta)\exp\left\{[\alpha_1 \quad \alpha_2/2]^T \begin{bmatrix}\beta & \beta^2\end{bmatrix} - A_g(\alpha)\right\}$$

  From our knowledge, a distribution with $t(\beta) = [\beta \quad \beta^2]$ is a Gaussian.
- Suppose the data come from an exponential family. Every exponential family has a conjugate prior in theory.
- The natural parameter $\alpha = [\alpha_1, \alpha_2]$ has dimension dim(β) + 1.
- The sufficient statistics of the prior are $[\beta, -A_l(\beta)]$

For exponential family distribution: $\mathbb{E}_q[t(\beta)] = \nabla_\lambda A_g(\lambda)$

Given $\quad q(\beta|\lambda) = h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\} = \frac{1}{\exp(A_g(\lambda))} h(\beta)\exp\{\lambda^T t(\beta)\}$

Why $\quad \mathbb{E}_q[t(\beta)] = \nabla_\lambda A_g(\lambda)$

$$
\begin{aligned}
&\int_\beta q(\beta|\lambda)\mathrm{d}\beta = \int_\beta h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\mathrm{d}\beta = 0\\
\Longrightarrow\ & \nabla_\lambda \left(\int_\beta h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\mathrm{d}\beta\right) = 0\\
\Longrightarrow\ & \int_\beta \nabla_\lambda \left(h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\right)\mathrm{d}\beta = 0\\
\Longrightarrow\ & \int_\beta \left(h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\right)(t(\beta) - \nabla_\lambda A_g(\lambda)) = 0\\
\Longrightarrow\ & \int_\beta \left(h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\right) t(\beta) - \int_\beta \left(h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}\right)\nabla_\lambda A_g(\lambda) = 0\\
\Longrightarrow\ & \mathbb{E}_q[t(\beta)] - \nabla_\lambda A_g(\lambda) = 0
\end{aligned}
$$

The choice of $q(\beta, Z)$

We choose $q(\beta, Z)$ to decouple β and Z completely:

$$q(\beta, Z) = q(\beta|\lambda) \prod_{n=1}^{N} \prod_{j=1}^{J} q(z_{n,j}|\phi_{n,j})$$

- $q(\beta|\lambda)$ is the SAME distribution type as $p(\beta|X, Z, \alpha)$, they only differ in parameter

$$q(\beta|\lambda) = h(\beta) \exp\{\lambda^T t(\beta) - A_g(\lambda)\}$$

compare with: $$p(\beta|X, Z, \alpha) = h(\beta) \exp\left\{\eta_g(X, Z, \alpha)^T t(\beta) - A_g(\eta_g(X, Z, \alpha))\right\}$$

- $q(z_{n,j}|\phi_{n,j})$ is the SAME distribution type as $p(z_{n,j}|x_n, z_{n,-j}, \beta)$, they only differ in parameter

$$q(z_{n,j}|\phi_{n,j}) = h(z_{n,j}) \exp\left\{\phi_{n,j}^T t(z_{n,j}) - A_l(\phi_{n,j})\right\}$$

compare with: $$p(z_{n,j}|x_n, z_{n,-j}, \beta) = h(z_{n,j}) \exp\left\{\eta_l(x_n, z_{n,-j}, \beta)^T t(z_{n,j}) - A_l(\eta_l(x_n, z_{n,-j}, \beta))\right\}$$

Update for $\mathcal{L}(\lambda)$

We need to maximize the ELBO, i.e.,

$$\mathcal{L}(q) \triangleq \mathbb{E}_q[\log p(X, Z, \beta|\alpha)] - \mathbb{E}_q[\log q(Z, \beta)]$$

Note that q used here is $q(\beta, Z)$ not just $q(\beta|\lambda)$

$$\begin{aligned}
\mathcal{L}(\lambda) &= \mathbb{E}_q[\log p(\beta|X, Z, \alpha)] + \mathbb{E}_q[\log p(X, Z)] - \mathbb{E}_q[\log q(\beta)] \\
&= \mathbb{E}_q[\log p(\beta|X, Z, \alpha)] - \mathbb{E}_q[\log q(\beta)] + \text{const.} \\
&= \mathbb{E}_q\left[\log\left(h(\beta)\exp\{\eta_g(x, z, \alpha)^T t(\beta) - A_g(\eta_g(x, z, \alpha))\}\right)\right] - \mathbb{E}_q[\log q(\beta)] + \text{const.} \\
&= \mathbb{E}_q[\log(h(\beta))] + \underbrace{\mathbb{E}_q[\eta_g(x, z, \alpha)^T t(\beta)]} - \mathbb{E}_q[\log h(\beta)\exp\{\lambda^T t(\beta) - A_g(\lambda)\}] + \text{const.} \\
&= \mathbb{E}_q[\log(h(\beta))] + \underbrace{\mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \mathbb{E}_{q(\beta|\lambda)}[t(\beta)]} - \mathbb{E}_q[\log h(\beta)] - \mathbb{E}_q[\lambda^T t(\beta)] + A_g(\lambda) + \text{const.} \\
&= \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \mathbb{E}_q[t(\beta)] - \lambda^T \mathbb{E}_q[t(\beta)] + A_g(\lambda) + \text{const.}
\end{aligned}$$

Substitute $\mathbb{E}_q[t(\beta)] = \nabla_\lambda A_g(\lambda)$:

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \nabla_\lambda A_g(\lambda) - \lambda^T \nabla_\lambda A_g(\lambda) + A_g(\lambda) + \text{const.}$$

Update for $\mathcal{L}(\lambda)$

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \nabla_\lambda A_g(\lambda) - \lambda^T \nabla_\lambda A_g(\lambda) + A_g(\lambda) + \text{const.}$$

Maximize $\mathcal{L}(\lambda)$ we get:

$$\begin{aligned}
\nabla_\lambda \mathcal{L}(\lambda) &= \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \nabla^2_\lambda A_g(\lambda) \underbrace{- \nabla_\lambda A_g(\lambda) - \lambda^T \nabla^2_\lambda A_g(\lambda)} + \nabla_\lambda A_g(\lambda) = 0 \\
&= \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T \nabla^2_\lambda A_g(\lambda) - \lambda^T \nabla^2_\lambda A_g(\lambda) = 0 \\
&\implies \nabla^2_\lambda A_g(\lambda) \left(\mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]^T - \lambda^T \right) = 0
\end{aligned}$$

$$\lambda = \mathbb{E}_{q(Z|\Phi)}[\eta_g(x, z, \alpha)]$$

Update for $\mathcal{L}(\phi_{n,j})$

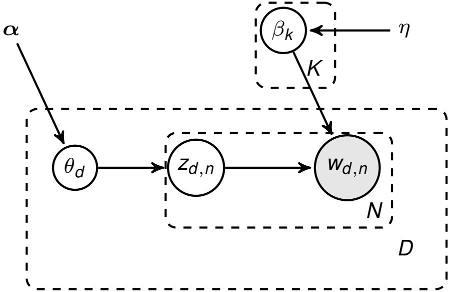
In a very similar fashion to $\mathcal{L}(\lambda)$, we can prove:

$$\nabla_{\phi_{n,j}} \mathcal{L}(\phi_{n,j}) = \nabla^2_{\phi_{n,j}} A_l(\phi_{n,j}) \left(\mathbb{E}_{q(\lambda)}[\eta_l(x_n, z_{n,-j}, \beta)]^T - \phi_{n,j}^T \right) = 0$$

$$\phi_{n,j} = \mathbb{E}_{q(\lambda)}[\eta_l(x_n, z_{n,-j}, \beta)]$$

Continue next time for Stochastic Maximization . . .

Latent Dirichlet Allocation



- $\beta_k \sim \text{Dir}(\eta, \dots \eta)$ for $k \in \{1, ..., K\}$.
- For each document d:

  $\theta \sim \text{Dir}(\alpha, \dots, \alpha)$

  For each word $w \in \{1, ..., N\}$:

  $z_{dn} \sim \text{Mult}(\theta_d)$

  $w_{dn} \sim \text{Mult}(\beta_{z_{dn}})$

Updating $q(z_{d,n}|\phi_{d,n})$: posterior conditional in Exponential Family form

$$
\begin{aligned}
p(z_{dn} = k|\theta_d, \beta_{1:K}, w_{d,n}) &\propto p(z_{d,n} = k|\theta_d) p(w_{d,n}|z_{d,n} = k, \beta_{1:K}) \\
&= \text{Mult}(\theta_{d,k}) \times \text{Mult}(\beta_{k,w_{d,n}}) \\
&\propto \exp\left(\underbrace{\log(\theta_{d,k}) + \log(\beta_{k,w_{d,n}})}_{\eta_l(\theta_d,\beta_{1:K},w_{d,n})} \times \underbrace{1}_{t(z_{d,n})} \right)
\end{aligned}
$$

Updating $q(z_{d,n}|\phi_{d,n})$: optimize $\phi_{d,n}$

- $q(z_{d,n}) = \text{Mult}(\phi_{d,n})$ or $q(z_{d,n} = k) = \phi_{d,n}^k$ $\qquad q(\beta_k) = \text{Dir}(\lambda_k)$ $\qquad q(\theta_d) = \text{Dir}(\gamma_d)$
- Fact about Dirichlet Distribution $\theta \sim \text{Dir}(\gamma_1, \dots \gamma_K) \implies \mathbb{E}[\log(\theta_k)|\gamma] = \Psi(\gamma_k) - \Psi\left(\sum_{i=1}^K \gamma_i\right)$
- In terms of natural parameter:

$$\begin{aligned}
\eta\left(\phi_{d,n}^k\right) = \log\left(\phi_{d,n}^k\right) &\propto \mathbb{E}_{q(\theta_d)q(\beta_k)}\left[\eta_l\left(\theta_d, \beta_{1:K}, w_{d,n}\right)\right] \\
&= \mathbb{E}_{q(\theta_d)}\left[\log(\theta_{d,k})\right] + \mathbb{E}_{q(\beta_k)}\left[\log(\beta_{k,w_{d,n}})\right] \\
&= \Psi(\gamma_{d,k}) - \Psi\left(\sum_{k=1}^K \gamma_{d,k}\right) + \Psi\left(\lambda_{k,w_{d,n}}\right) - \Psi\left(\sum_v \lambda_{k,v}\right)
\end{aligned}$$

- Change it back to traditional parameter:

$$\begin{aligned}
\implies \phi_{d,n}^k &\propto \exp\left[\Psi(\gamma_{d,k}) - \underbrace{\Psi\left(\sum_{k=1}^K \gamma_{d,k}\right)}_{\text{irrelevant in proportionality}} + \Psi\left(\lambda_{k,w_{d,n}}\right) - \Psi\left(\sum_v \lambda_{k,v}\right)\right] \\
&\propto \exp\left[\Psi(\gamma_{d,k}) + \Psi\left(\lambda_{k,w_{d,n}}\right) - \Psi\left(\sum_v \lambda_{k,v}\right)\right]
\end{aligned}$$

Updating $q(\theta_d|\gamma_d)$: posterior conditional in Exponential Family form

$$
\begin{aligned}
p(\theta_d|z_d) &= p(\theta_d|\alpha)\prod_{n=1}^{N} p(z_{d,n}|\theta_d) = \text{Dir}(\alpha) \times \prod_{n=1}^{N} \text{Mult}(z_{d,n}|\theta_d) \\
&= \prod_k \left(\theta_{d,k}^{\alpha_k - 1} \prod_{n=1}^{N} \theta_{d,k}^{\delta(z_{d,n},k)} \right) \\
&= \exp\left[\log \left(\prod_k \left(\theta_{d,k}^{\alpha_k - 1} \prod_{n=1}^{N} \theta_{d,k}^{\delta(z_{d,n},k)} \right) \right) \right] \\
&= \exp\left[\sum_k \log \left(\theta_{d,k}^{\alpha_k - 1} \prod_{n=1}^{N} \theta_{d,k}^{\delta(z_{d,n},k)} \right) \right] = \exp\left[\sum_k \left(\log \theta_{d,k}^{\alpha_k - 1} + \sum_{n=1}^{N} \log \left(\theta_{d,k}^{\delta(z_{d,n},k)} \right) \right) \right] \\
&= \exp\left[\sum_k \left((\alpha_k - 1) \log \theta_{d,k} + \sum_{n=1}^{N} \delta(z_{d,n}, k) \log \theta_{d,k} \right) \right] \\
&= \exp\left[\sum_k \left(\alpha_k - 1 + \sum_{n=1}^{N} \delta(z_{d,n}, k) \right) \log \left(\theta_{d,k} \right) \right] \\
&= \exp\left(\underbrace{[(\alpha_1 - 1 + n_1) \dots (\alpha_K - 1 + n_K)]^T}_{\eta_l(\alpha, z_d)} \underbrace{[\log(\theta_{d,1}) \dots \log(\theta_{d,K})]}_{t(\theta_d)} \right) \quad \text{by letting } n_k = \sum_{n=1}^{N} \delta(z_{d,n}, k)
\end{aligned}
$$

Updating $q(\theta_d|\gamma_d)$: optimize γ_d

- $q(z_{d,n}) = \text{Mult}(\phi_{d,n})$ or $q(z_{d,n} = k) = \phi_{d,n}^k$ $\quad q(\beta_k) = \text{Dir}(\lambda_k)$ $\quad q(\theta_d) = \text{Dir}(\gamma_d)$
- In terms of natural parameter:

$$
\begin{aligned}
\eta(\gamma_d) &= \mathbb{E}_{q(z_{d,n}|\phi_{d,n})}\left[\eta_l\,(\alpha, z_d)\right] \\
&= \mathbb{E}_{q(z_{d,n}|\phi_{d,n})}\left[\left[(\alpha_1 - 1 + n_1)\dots(\alpha_K - 1 + n_K)\right]\right] \\
&= \left[\left(\alpha_1 - 1 + \sum_{n=1}^{N} \delta(z_{d,n}, 1)\phi_{d,n}^1\right)\dots\left(\alpha_K - 1 + \sum_{n=1}^{N} \delta(z_{d,n}, K)\phi_{d,n}^K\right)\right]
\end{aligned}
$$

- Change it back to traditional parameter:

$$
\begin{aligned}
\gamma_d &= \left[\left(\alpha_1 + \sum_{n=1}^{N} \delta(z_{d,n}, 1)\phi_{d,n}^1\right)\dots\left(\alpha_K + \sum_{n=1}^{N} \delta(z_{d,n}, K)\phi_{d,n}^K\right)\right] \\
&= \alpha + \sum_{n=1}^{N} \phi_{d,n}
\end{aligned}
$$

Updating $q(\beta_k|\lambda_k)$ posterior conditional in Exponential Family form:

$$p(\beta_k|Z,W) = p(\beta_k|\eta)\prod_{d=1}^{D}\prod_{n=1}^{N} p\left(w_{d,n}|\beta_k\right)^{\delta(z_{d,n},k)} = \text{Dir}(\eta)\times\prod_{d=1}^{D}\prod_{n=1}^{N}\beta_k^{w_{d,n}\delta(z_{d,n},k)}$$

$$\propto \exp\left(\underbrace{\left(\eta - 1 + \sum_{d=1}^{D}\sum_{n=1}^{N} w_{d,n}\delta(z_{d,n},k)\right)}_{\eta_l(\eta,Z,W)}\times\underbrace{\log(\beta_k)}_{t(\beta_k)}\right)$$

Updating $q(\beta_k|\lambda_k)$ optimize λ_k

- $q(z_{d,n}) = \text{Mult}(\phi_{d,n})$ or $q(z_{d,n} = k) = \phi_{d,n}^k$ $\qquad q(\beta_k) = \text{Dir}(\lambda_k)$ $\qquad q(\theta_d) = \text{Dir}(\gamma_d)$
- In terms of natural parameter:

$$\begin{aligned}
\eta(\lambda_k) &= \mathbb{E}_{\prod_{d=1}^{D} \prod_{n=1}^{N} q(z_{d,n})} \left[\eta_l\left(\eta, Z, W\right)\right] \\
&= \mathbb{E}_{\prod_{d=1}^{D} \prod_{n=1}^{N} q(z_{d,n})} \left[\eta - 1 + \sum_{d=1}^{D} \sum_{n=1}^{N} w_{d,n} \delta(z_{d,n}, k)\right] \\
&= \eta - 1 + \sum_{d=1}^{D} \sum_{n=1}^{N} w_{d,n} \phi_{d,n}^k
\end{aligned}$$

- Change it back to traditional parameter:

$$\lambda_k = \eta + \sum_{d=1}^{D} \sum_{n=1}^{N} w_{d,n} \phi_{d,n}^k$$

Collapsed Variational Inference

$$q(z_{d,n}) = \text{Mult}(\phi_{d,n}) \text{ or } q(z_{d,n} = k) = \phi_{d,n}^k \qquad q(\beta_k) = \text{Dir}(\lambda_k) \qquad q(\theta_d) = \text{Dir}(\gamma_d)$$

$$\begin{aligned}
\implies q(Z, \theta_1 \dots \theta_D, \beta_1 \dots \beta_K) &= \left(\prod_{d=1}^{d=D} \prod_{n=1}^{N} q(z_{d,n}|\phi_{d,n}) \right) \prod_{d=1}^{D} q(\theta_d|\gamma_d) \prod_{k=1}^{K} q(\theta_k|\lambda_k) \\
\text{now change to: } &= \underbrace{\left(\prod_{d=1}^{d=D} \prod_{n=1}^{N} q(z_{d,n}|\phi_{d,n}) \right)}_{q(Z)} q(\Theta, \beta|Z)
\end{aligned}$$

Maximize ELOB, it becomes: (remove X for clarity)
Let $U = \{\Theta, \beta\}$:

$$\begin{aligned}
\mathcal{L}(q) &\triangleq \mathbb{E}_{q(U,Z)}[\log p(Z, U)] - \mathbb{E}_{q(U,Z)}[\log q(Z, U)] \\
&= \mathbb{E}_{q(U,Z)}[\log p(Z, U)] - \mathbb{E}_{q(U,Z)}[\log q(U|Z) - \log q(Z)] \\
&= \mathbb{E}_{q(Z)} \left(\mathbb{E}_{q(U|Z)}[\log p(Z, U)] \right) - \mathbb{E}_{q(Z)} \left(\mathbb{E}_{q(U|Z)}[\log q(U|Z)] \right) - \mathbb{E}_{q(Z,U)}[\log q(Z)] \\
&= \mathbb{E}_{q(Z)} \left(\underbrace{\mathbb{E}_{q(U|Z)} ([\log p(Z, U)] - [\log q(U|Z)])}_{\mathcal{L}(q(U|Z))} \right) - \mathbb{E}_{q(Z)}[\log q(Z)]
\end{aligned}$$

Think this as treating Z as X.

Collapsed Variational Inference (2)

(removed X for clarity)

$$
\begin{aligned}
\arg\max_{q(U|Z)}(\mathcal{L}(q)) &= \arg\max_{q(U|Z)}\left[\mathbb{E}_{q(Z)}\left(\underbrace{\mathbb{E}_{q(U|Z)}\left([\log p_X(Z,U)] - [\log q(U|Z)]\right)}_{\mathcal{L}(q(U|Z))}\right) - \mathbb{E}_{q(Z)}[\log q(Z)]\right] \\
&= \mathbb{E}_{q(Z)}\left(\underbrace{\arg\max_{q(U|Z)}\left[\mathbb{E}_{q(U|Z)}\left([\log p(Z,U)] - [\log q(U|Z)]\right)\right]}\right) - \mathbb{E}_{q(Z)}[\log q(Z)] \\
&= \mathbb{E}_{q(Z)}[\underbrace{p(Z)}] - \mathbb{E}_{q(Z)}[\log q(Z)]
\end{aligned}
$$

$$
\arg\max_{q(U|Z)}\left[\mathbb{E}_{q(U|Z)}\left([\log p(Z,U)] - [\log q(U|Z)]\right)\right] = p(Z)
$$

maximum occur when $q(U|Z) = p(U|Z) \implies \mathbb{KL}\left(q(U|Z)\|p(U|Z)\right) = 0$