Exercises for the tutorials: Jupyter notebook at https://github.com/vsimkus/pmr2022-vae.

The other exercises are for self-study and exam preparation. All material is examinable unless otherwise mentioned.

Exercise 1. *Mean field variational inference I*

Let $\mathcal{L}_{\mathbf{x}}(q)$ be the evidence lower bound for the marginal $p(\mathbf{x})$ of a joint pdf/pmf $p(\mathbf{x}, \mathbf{y})$,

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right]. \tag{1}$$

Mean field variational inference assumes that the variational distribution $q(\mathbf{y}|\mathbf{x})$ fully factorises, i.e.

$$q(\mathbf{y}|\mathbf{x}) = \prod_{i=1}^{d} q_i(y_i|\mathbf{x}), \tag{2}$$

when $\mathbf{y}$ is d-dimensional. An approach to learning the q_i for each dimension is to update one at a time while keeping the others fixed. We here derive the corresponding update equations.

(a) Show that the evidence lower bound $\mathcal{L}_{\mathbf{x}}(q)$ can be written as

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q_1(y_1|\mathbf{x})}\mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x}, \mathbf{y})\right] - \sum_{i=1}^{d} \mathbb{E}_{q_i(y_i|\mathbf{x})}\left[\log q_i(y_i|\mathbf{x})\right] \tag{3}$$

where $q(\mathbf{y}_{\setminus 1}|\mathbf{x}) = \prod_{i=2}^{d} q_i(y_i|\mathbf{x})$ is the variational distribution without $q_1(y_1|\mathbf{x})$.

Solution. This follows directly from the definition of the ELBO and the assumed factorisation of $q(\mathbf{y}|\mathbf{x})$. We have

$$\begin{aligned}
\mathcal{L}_{\mathbf{x}}(q) &= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \log p(\mathbf{x}, \mathbf{y}) - \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \log q(\mathbf{y}|\mathbf{x}) && \text{(S.1)}\\
&= \mathbb{E}_{\prod_{i=1}^{d} q_i(y_i|\mathbf{x})} \log p(\mathbf{x}, \mathbf{y}) - \mathbb{E}_{\prod_{i=1}^{d} q_i(y_i|\mathbf{x})} \sum_{i=1}^{d} \log q_i(y_i|\mathbf{x}) && \text{(S.2)}\\
&= \mathbb{E}_{\prod_{i=1}^{d} q_i(y_i|\mathbf{x})} \log p(\mathbf{x}, \mathbf{y}) - \sum_{i=1}^{d} \mathbb{E}_{q_i(y_i|\mathbf{x})} \log q_i(y_i|\mathbf{x}) && \text{(S.3)}\\
&= \mathbb{E}_{q_1(y_1|\mathbf{x})}\mathbb{E}_{\prod_{i=2}^{d} q_i(y_i|\mathbf{x})} \log p(\mathbf{x}, \mathbf{y}) - \sum_{i=1}^{d} \mathbb{E}_{q_i(y_i|\mathbf{x})} \log q_i(y_i|\mathbf{x}) && \text{(S.4)}\\
&= \mathbb{E}_{q_1(y_1|\mathbf{x})}\mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x}, \mathbf{y})\right] - \sum_{i=1}^{d} \mathbb{E}_{q_i(y_i|\mathbf{x})}\left[\log q_i(y_i|\mathbf{x})\right] && \text{(S.5)}
\end{aligned}$$

(b) Assume that we would like to update $q_1(y_1|\mathbf{x})$ and that the variational marginals of the other dimensions are kept fixed. Show that

$$\operatorname*{argmax}_{q_1(y_1|\mathbf{x})} \mathcal{L}_{\mathbf{x}}(q) = \operatorname*{argmin}_{q_1(y_1|\mathbf{x})} KL(q_1(y_1|\mathbf{x})||\bar{p}(y_1|\mathbf{x})) \tag{4}$$

with

$$\log \bar{p}(y_1|\mathbf{x}) = \mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x}, \mathbf{y})\right] + const, \tag{5}$$

where const refers to terms not depending on y_1. That is, $\bar{p}(y_1|\mathbf{x}) = \frac{1}{Z} \exp\left[\mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x}, \mathbf{y})\right]\right]$, where Z is the normalising constant. Note that variables $y_2, \ldots, y_d$ are marginalised out due to the expectation with respect to $q(\mathbf{y}_{\setminus 1}|\mathbf{x})$.

Solution. Starting from

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q_1(y_1|\mathbf{x})}\mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x},\mathbf{y})\right] - \sum_{i=1}^{d}\mathbb{E}_{q_i(y_i|\mathbf{x})}\left[\log q_i(y_i|\mathbf{x})\right] \tag{S.6}$$

we drop terms that do not depend on q_1. We then obtain

$$\begin{aligned} J(q_1) &= \mathbb{E}_{q_1(y_1|\mathbf{x})}\mathbb{E}_{q(\mathbf{y}_{\setminus 1}|\mathbf{x})}\left[\log p(\mathbf{x},\mathbf{y})\right] - \mathbb{E}_{q_1(y_1|\mathbf{x})}\left[\log q_1(y_1|\mathbf{x})\right] && \text{(S.7)}\\ &= \mathbb{E}_{q_1(y_1|\mathbf{x})}\log\bar{p}(y_1|\mathbf{x}) - \mathbb{E}_{q_1(y_1|\mathbf{x})}\left[\log q_1(y_1|\mathbf{x})\right] + \text{const} && \text{(S.8)}\\ &= \mathbb{E}_{q_1(y_1|\mathbf{x})}\left[\log\frac{\bar{p}(y_1|\mathbf{x})}{q_1(y_1|\mathbf{x})}\right] && \text{(S.9)}\\ &= -\mathrm{KL}(q_1(y_1|\mathbf{x})||\bar{p}(y_1|\mathbf{x})) && \text{(S.10)} \end{aligned}$$

Hence

$$\operatorname*{argmax}_{q_1(y_1|\mathbf{x})}\mathcal{L}_{\mathbf{x}}(q) = \operatorname*{argmin}_{q_1(y_1|\mathbf{x})}\mathrm{KL}(q_1(y_1|\mathbf{x})||\bar{p}(y_1|\mathbf{x})) \tag{S.11}$$

(c) Conclude that given $q_i(y_i|\mathbf{x})$, $i = 2,\ldots,d$, the optimal $q_1(y_1|\mathbf{x})$ equals $\bar{p}(y_1|\mathbf{x})$.
This then leads to an iterative updating scheme where we cycle through the different dimensions, each time updating the corresponding marginal variational distribution according to:

$$q_i(y_i|\mathbf{x}) = \bar{p}(y_i|\mathbf{x}), \qquad \bar{p}(y_i|\mathbf{x}) = \frac{1}{Z}\exp\left[\mathbb{E}_{q(\mathbf{y}_{\setminus i}|\mathbf{x})}\left[\log p(\mathbf{x},\mathbf{y})\right]\right] \tag{6}$$

where $q(\mathbf{y}_{\setminus i}|\mathbf{x}) = \prod_{j\neq i} q(y_j|\mathbf{x})$ is the product of all marginals without marginal $q_i(y_i|\mathbf{x})$.

Solution. This follows immediately from the fact that the KL divergence is minimised when $q_1(y_1|\mathbf{x}) = \bar{p}(y_1|\mathbf{x})$. Side-note: The iterative update rule can be considered to be coordinate ascent optimisation in function space, where each "coordinate" corresponds to a $q_i(y_i|\mathbf{x})$.

Exercise 2. *Mean field variational inference II*

Assume random variables y_1, y_2, x are generated according to the following process

$$\begin{aligned} y_1 &\sim \mathcal{N}(y_1; 0, 1) & y_2 &\sim \mathcal{N}(y_2; 0, 1) && \text{(7)}\\ n &\sim \mathcal{N}(n; 0, 1) & x &= y_1 + y_2 + n && \text{(8)} \end{aligned}$$

where y_1, y_2, n are statistically independent.

(a) y_1, y_2, x are jointly Gaussian. Determine their mean and their covariance matrix.

Solution. The expected value of y_1 and y_2 is zero. By linearity of expectation, the expected value of x is

$$\mathbb{E}(x) = \mathbb{E}(y_1) + \mathbb{E}(y_2) + \mathbb{E}(n) = 0 \tag{S.12}$$

The variance of y_1 and y_2 is 1. Since y_1, y_2, n are statistically independent,

$$\mathbb{V}(x) = \mathbb{V}(y_1) + \mathbb{V}(y_2) + \mathbb{V}(n) = 1 + 1 + 1 = 3. \tag{S.13}$$

The covariance between y_1 and x is

$$\begin{aligned}\operatorname{cov}(y_1, x) &= \mathbb{E}((y_1 - \mathbb{E}(y_1))(x - \mathbb{E}(x))) = \mathbb{E}(y_1 x) && \text{(S.14)}\\ &= \mathbb{E}(y_1(y_1 + y_2 + n)) = \mathbb{E}(y_1^2) + \mathbb{E}(y_1 y_2) + \mathbb{E}(y_1 n) && \text{(S.15)}\\ &= 1 + \mathbb{E}(y_1)\mathbb{E}(y_2) + \mathbb{E}(y_1)\mathbb{E}(n) && \text{(S.16)}\\ &= 1 + 0 + 0 && \text{(S.17)}\end{aligned}$$

where we have used that y_1 and x have zero mean and the independence assumptions.
The covariance between y_2 and x is computed in the same way and equals 1 too.
We thus obtain the covariance matrix $\mathbf{\Sigma}$,

$$\mathbf{\Sigma} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 3 \end{pmatrix} \tag{S.18}$$

(b) The conditional $p(y_1, y_2|x)$ is Gaussian with mean $\mathbf{m}$ and covariance $\mathbf{C}$,

$$\mathbf{m} = \frac{x}{3}\begin{pmatrix}1\\1\end{pmatrix} \qquad\qquad \mathbf{C} = \frac{1}{3}\begin{pmatrix}2 & -1\\ -1 & 2\end{pmatrix} \tag{9}$$

Since x is the sum of three random variables that have the same distribution, it makes intuitive sense that the mean assigns $1/3$ of the observed value of x to y_1 and y_2. Moreover, y_1 and y_2 are negatively corrected since an increase in y_1 must be compensated with a decrease in y_2.

Let us now approximate the posterior $p(y_1, y_2|x)$ with mean field variational inference. Determine the optimal variational distribution using the method and results from Exercise 1. You may use that

$$p(y_1, y_2, x) = \mathcal{N}\left((y_1, y_2, x); \mathbf{0}, \mathbf{\Sigma}\right) \qquad \mathbf{\Sigma} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 3 \end{pmatrix} \qquad \mathbf{\Sigma}^{-1} = \begin{pmatrix} 2 & 1 & -1 \\ 1 & 2 & -1 \\ -1 & -1 & 1 \end{pmatrix} \tag{10}$$

Solution. The mean field assumption means that the variational distribution is assumed to factorise as

$$q(y_1, y_2|x) = q_1(y_1|x)q_2(y_2|x) \tag{S.19}$$

From Exercise 1, the optimal $q_1(y_1|x)$ and $q_2(y_2|x)$ satisfy

$$q_1(y_1|x) = \bar{p}(y_1|x), \qquad \bar{p}(y_1|x) = \frac{1}{Z}\exp\left[\mathbb{E}_{q_2(y_2|x)}\left[\log p(y_1, y_2, x)\right]\right] \tag{S.20}$$

$$q_2(y_2|x) = \bar{p}(y_2|x), \qquad \bar{p}(y_2|x) = \frac{1}{Z}\exp\left[\mathbb{E}_{q_1(y_1|x)}\left[\log p(y_1, y_2, x)\right]\right] \tag{S.21}$$

Note that these are coupled equations: q_2 features in the equation for q_1 via $\bar{p}(y_1|x)$, and q_1 features in the equation for q_2 via $\bar{p}(y_2|x)$. But we have two equations for two unknowns, which for the Gaussian joint model $p(x, y_1, y_2)$ can be solved in closed form.
Given the provided equation for $p(y_1, y_2, x)$, we have that

$$\log p(y_1, y_2, x) = -\frac{1}{2}\begin{pmatrix}y_1\\y_2\\x\end{pmatrix}^\top \begin{pmatrix} 2 & 1 & -1 \\ 1 & 2 & -1 \\ -1 & -1 & 1 \end{pmatrix} \begin{pmatrix}y_1\\y_2\\x\end{pmatrix} + \text{const} \tag{S.22}$$

$$= -\frac{1}{2}\left(2y_1^2 + 2y_2^2 + x^2 + 2y_1 y_2 - 2y_1 x - 2y_2 x\right) + \text{const} \tag{S.23}$$

Let us start with the equation for $\bar{p}(y_1|x)$. It is easier to work in the logarithmic domain, where we obtain:

$$\log \bar{p}(y_1|x) = \mathbb{E}_{q_2(y_2|x)} \left[\log p(y_1, y_2, x)\right] + \text{const} \tag{S.24}$$

$$= -\frac{1}{2}\mathbb{E}_{q_2(y_2|x)} \left[2y_1^2 + 2y_2^2 + x^2 + 2y_1y_2 - 2y_1x - 2y_2x\right] + \text{const} \tag{S.25}$$

$$= -\frac{1}{2}\left(2y_1^2 + 2y_1\mathbb{E}_{q_2(y_2|x)}[y_2] - 2y_1x\right) + \text{const} \tag{S.26}$$

$$= -\frac{1}{2}\left(2y_1^2 + 2y_1m_2 - 2y_1x\right) + \text{const} \tag{S.27}$$

$$= -\frac{1}{2}\left(2y_1^2 - 2y_1(x - m_2)\right) + \text{const} \tag{S.28}$$

where we have absorbed all terms not involving y_1 into the constant. Moreover, we set $\mathbb{E}_{q_2(y_2|x)}[y_2] = m_2$.

Note that an arbitrary Gaussian density $\mathcal{N}(y; m, \sigma^2)$ with mean m and variance σ^2 can be written in the log-domain as

$$\log \mathcal{N}(y; m, \sigma^2) = -\frac{1}{2}\frac{(y-m)^2}{\sigma^2} + \text{const} \tag{S.29}$$

$$= -\frac{1}{2}\left(\frac{y^2}{\sigma^2} - 2y\frac{m}{\sigma^2}\right) + \text{const} \tag{S.30}$$

Comparison with (S.28) shows that $\bar{p}(y_1|x)$, and hence $q_1(y_1|x)$, is Gaussian with variance and mean equal to

$$\sigma_1^2 = \frac{1}{2} \qquad\qquad m_1 = \frac{1}{2}(x - m_2) \tag{S.31}$$

Note that we have not made a Gaussianity assumption on $q_1(y_1|x)$. The optimal $q_1(y_1|x)$ turns out to be Gaussian because the model $p(y_1, y_2, x)$ is Gaussian.

The equation for $\bar{p}(y_2|x)$ gives similarly

$$\log \bar{p}(y_2|x) = \mathbb{E}_{q_1(y_1|x)} \left[\log p(y_1, y_2, x)\right] + \text{const} \tag{S.32}$$

$$= -\frac{1}{2}\mathbb{E}_{q_1(y_1|x)} \left[2y_1^2 + 2y_2^2 + x^2 + 2y_1y_2 - 2y_1x - 2y_2x\right] + \text{const} \tag{S.33}$$

$$= -\frac{1}{2}\left(2y_2^2 + 2\mathbb{E}_{q_1(y_1|x)}[y_1]y_2 - 2y_2x\right) + \text{const} \tag{S.34}$$

$$= -\frac{1}{2}\left(2y_2^2 + 2m_1y_2 - 2y_2x\right) + \text{const} \tag{S.35}$$

$$= -\frac{1}{2}\left(2y_2^2 - 2y_2(x - m_1)\right) + \text{const} \tag{S.36}$$

where we have absorbed all terms not involving y_2 into the constant. Moreover, we set $\mathbb{E}_{q_1(y_1|x)}[y_1] = m_1$. With (S.30), this is defines a Gaussian distribution with variance and mean equal to

$$\sigma_2^2 = \frac{1}{2} \qquad\qquad m_2 = \frac{1}{2}(x - m_1) \tag{S.37}$$

Hence the optimal marginal variational distributions $q_1(y_1|x)$ and $q_2(y_2|x)$ are both Gaussian with variance equal to $1/2$. Their means satisfy

$$m_1 = \frac{1}{2}(x - m_2) \qquad\qquad m_2 = \frac{1}{2}(x - m_1) \tag{S.38}$$

These are two equations for two unknowns. We can solve them as follows

$$2m_1 = x - m_2 \tag{S.39}$$
$$= x - \frac{1}{2}(x - m_1) \tag{S.40}$$
$$4m_1 = 2x - x + m_1 \tag{S.41}$$
$$3m_1 = x \tag{S.42}$$
$$m_1 = \frac{1}{3}x \tag{S.43}$$

Hence

$$m_2 = \frac{1}{2}x - \frac{1}{6}x = \frac{2}{6}x = \frac{1}{3}x \tag{S.44}$$

In summary, we find

$$q_1(y_1|x) = \mathcal{N}\left(y_1; \frac{x}{3}, \frac{1}{2}\right) \qquad q_2(y_2|x) = \mathcal{N}\left(y_2; \frac{x}{3}, \frac{1}{2}\right) \tag{S.45}$$

and the optimal variational distribution $q(y_1, y_2|x) = q_1(y_1|x)q_2(y_2|x)$ is Gaussian. We have made the mean field (independence) assumption but not the Gaussianity assumption. Gaussianity of the variational distribution is a consequence of the Gaussianity of the model $p(y_1, y_2, x)$.

Comparison with the true posterior shows that the mean field variational distribution $q(y_1, y_2|x)$ has the same mean but ignores the correlation and underestimates the marginal variances. The true posterior and the mean field approximation are shown in Figure 1.

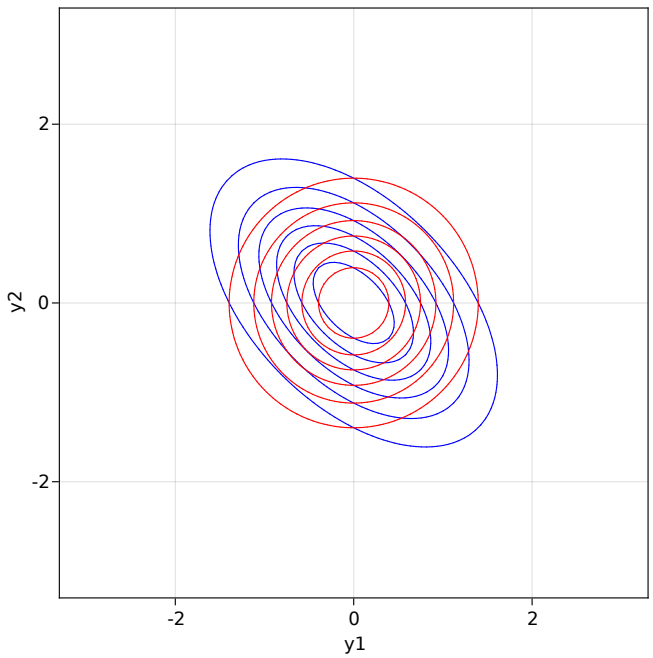


Figure 1: In blue: correlated true posterior. In red: mean field approximation.

Exercise 3. ***Variational posterior approximation I***

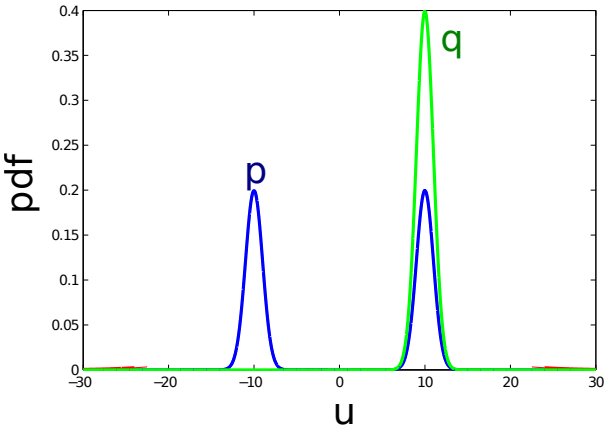
We have seen that maximising the evidence lower bound (ELBO) with respect to the variational distribution q minimises the Kullback-Leibler divergence to the true posterior p. We here assume that q and p

are probability density functions so that the Kullback-Leibler divergence between them is defined as

$$KL(q||p) = \int q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} \mathrm{d}\mathbf{x} = \mathbb{E}_q \left[\log \frac{q(\mathbf{x})}{p(\mathbf{x})} \right]. \tag{11}$$

(a) You can here assume that $\mathbf{x}$ *is one-dimensional so that* p *and* q *are univariate densities. Consider the case where* p *is a bimodal density but the variational densities* q *are unimodal. Sketch a figure that shows* p *and a variational distribution* q *that has been learned by minimising* $KL(q||p)$*. Explain qualitatively why the sketched* q *minimises* $KL(q||p)$*.*

Solution. A possible sketch is shown in the figure below.



Explanation: We can divide the domain of p and q into the areas where p is small (zero) and those where p has significant mass. Since the objective features q in the numerator while p is in the denominator, an optimal q needs to be zero where p is zero. Otherwise, it would incur a large penalty (division by zero). Since we take the expectation with respect to q, however, regions where $p > 0$ do not need to be covered by q; cutting them out does not incur a penalty. Hence, optimal unimodal q only cover one peak of the bimodal p.

(b) Assume that the true posterior $p(\mathbf{x}) = p(x_1, x_2)$ *factorises into two Gaussians of mean zero and variances* σ_1^2 *and* σ_2^2*,*

$$p(x_1, x_2) = \frac{1}{\sqrt{2\pi\sigma_1^2}} \exp\left[-\frac{x_1^2}{2\sigma_1^2} \right] \frac{1}{\sqrt{2\pi\sigma_2^2}} \exp\left[-\frac{x_2^2}{2\sigma_2^2} \right]. \tag{12}$$

Assume further that the variational density $q(x_1, x_2; \lambda^2)$ *is parametrised as*

$$q(x_1, x_2; \lambda^2) = \frac{1}{2\pi\lambda^2} \exp\left[-\frac{x_1^2 + x_2^2}{2\lambda^2} \right] \tag{13}$$

where λ^2 *is the variational parameter that is learned by minimising* $KL(q||p)$*. If* σ_2^2 *is much larger than* σ_1^2*, do you expect* λ^2 *to be closer to* σ_2^2 *or to* σ_1^2*? Provide an explanation.*

Solution. The learned variational parameter will be closer to σ_1^2 (the smaller of the two σ_i^2).

Explanation: First note that the σ_i^2 are the variances along the two different axes, and that λ^2 is the single variance for both x_1 and x_2. The objective penalises q if it is non-zero where p is zero (see above). The variational parameter λ^2 thus will get adjusted during learning so that the variance of q is close to the smallest of the two σ_i^2.

Exercise 4. ***Variational posterior approximation II***

We have seen that maximising the evidence lower bound (ELBO) with respect to the variational distribution minimises the Kullback-Leibler divergence to the true posterior. We here investigate the nature of the approximation if the family of variational distributions does not include the true posterior.

(a) Assume that the true posterior for $\mathbf{x} = (x_1, x_2)$ *is given by*

$$p(\mathbf{x}) = \mathcal{N}(x_1; \sigma_1^2)\mathcal{N}(x_2; \sigma_2^2) \tag{14}$$

and that our variational distribution $q(\mathbf{x}; \lambda^2)$ *is*

$$q(\mathbf{x}; \lambda^2) = \mathcal{N}(x_1; \lambda^2)\mathcal{N}(x_2; \lambda^2), \tag{15}$$

where $\lambda > 0$ *is the variational parameter. Provide an equation for* $J(\lambda) = KL(q(\mathbf{x}; \lambda^2)||p(\mathbf{x}))$*, where you can omit additive terms that do not depend on* λ*.*

Solution. We write

$$\begin{aligned}
\mathrm{KL}(q(\mathbf{x}; \lambda^2)||p(\mathbf{x})) &= \mathbb{E}_q\left[\log \frac{q(\mathbf{x}; \lambda^2)}{p(\mathbf{x})}\right] && \text{(S.46)}\\
&= \mathbb{E}_q \log q(\mathbf{x}; \lambda^2) - \mathbb{E}_q \log p(\mathbf{x}) && \text{(S.47)}\\
&= \mathbb{E}_q \log \mathcal{N}(x_1; \lambda^2) + \mathbb{E}_q \log \mathcal{N}(x_2; \lambda^2)\\
&\quad - \mathbb{E}_q \log \mathcal{N}(x_1; \sigma_1^2) - \mathbb{E}_q \log \mathcal{N}(x_2; \sigma_2^2) && \text{(S.48)}
\end{aligned}$$

We further have

$$\begin{aligned}
\mathbb{E}_q \log \mathcal{N}(x_i; \lambda^2) &= \mathbb{E}_q \log\left[\frac{1}{\sqrt{2\pi\lambda^2}} \exp\left[-\frac{x_i^2}{2\lambda^2}\right]\right] && \text{(S.49)}\\
&= \log\left[\frac{1}{\sqrt{2\pi\lambda^2}}\right] - \mathbb{E}_q\left[\frac{x_i^2}{2\lambda^2}\right] && \text{(S.50)}\\
&= -\log\lambda - \frac{\lambda^2}{2\lambda^2} + \text{const} && \text{(S.51)}\\
&= -\log\lambda - \frac{1}{2} + \text{const} && \text{(S.52)}\\
&= -\log\lambda + \text{const} && \text{(S.53)}
\end{aligned}$$

where we have used that for zero mean x_i, $\mathbb{E}_q[x_i^2] = \mathbb{V}(x_i) = \lambda^2$.
We similarly obtain

$$\begin{aligned}
\mathbb{E}_q \log \mathcal{N}(x_i; \sigma_i^2) &= \mathbb{E}_q \log\left[\frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{x_i^2}{2\sigma_i^2}\right]\right] && \text{(S.54)}\\
&= -\log\left[\frac{1}{\sqrt{2\pi\sigma_i^2}}\right] - \mathbb{E}_q\left[\frac{x_i^2}{2\sigma_i^2}\right] && \text{(S.55)}\\
&= -\log\sigma_i - \frac{\lambda^2}{2\sigma_i^2} + \text{const} && \text{(S.56)}\\
&= -\frac{\lambda^2}{2\sigma_i^2} + \text{const} && \text{(S.57)}
\end{aligned}$$

We thus have

$$\mathrm{KL}(q(\mathbf{x};\lambda^2||p(\mathbf{x})) = -2\log\lambda + \lambda^2\left(\frac{1}{2\sigma_1^2}+\frac{1}{2\sigma_2^2}\right) + \text{const} \tag{S.58}$$

(b) Determine the value of λ that minimises $J(\lambda) = KL(q(\mathbf{x};\lambda^2)||p(\mathbf{x}))$. Interpret the result and relate it to properties of the Kullback-Leibler divergence.

Solution. Taking derivatives of $J(\lambda)$ with respect to λ gives

$$\frac{\partial J(\lambda)}{\partial\lambda} = -\frac{2}{\lambda} + \lambda\left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right) \tag{S.59}$$

Setting it zero yields

$$\frac{1}{\lambda^2} = \frac{1}{2}\left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right) \tag{S.60}$$

so that

$$\lambda^2 = 2\frac{\sigma_1^2\sigma_2^2}{\sigma_1^2+\sigma_2^2} \tag{S.61}$$

or

$$\lambda = \sqrt{2}\sqrt{\frac{\sigma_1^2\sigma_2^2}{\sigma_1^2+\sigma_2^2}} \tag{S.62}$$

This is a minimum because the second derivative of $J(\lambda)$

$$\frac{\partial^2 J(\lambda)}{\partial\lambda^2} = \frac{2}{\lambda^2} + \left(\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}\right) \tag{S.63}$$

is positive for all $\lambda > 0$.

The result has an intuitive explanation: the optimal variance λ^2 is the harmonic mean of the variances σ_i^2 of the true posterior. In other words, the optimal precision $1/\lambda^2$ is given by the average of the precisions $1/\sigma_i^2$ of the two dimensions.

If the variances are not equal, e.g. if $\sigma_2^2 > \sigma_1^2$, we see that the optimal variance of the variational distribution strikes a compromise between two types of penalties in the KL-divergence: the penalty of having a bad fit because the variational distribution along dimension two is too narrow; and along dimension one, the penalty for the variational distribution to be nonzero when p is small.