Variational Inference and Learning I

Basic Properties and Use

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Recap

- Learning and inference often involves integrals that are hard to compute.
- For example:
  - Marginalisation/inference: $p(\mathbf{x}) = \int_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y}$
  - Likelihood in case of unobserved variables: $L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta}) = \int_{\mathbf{u}} p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta}) \mathrm{d}\mathbf{u}$
- We here discuss a variational approach to (approximate) inference and learning.

History

Variational methods have a long history, in particular in physics. For example:

- Fermat's principle (1650) to explain the path of light: "light travels between two given points along the path of shortest time" (see e.g. http://www.feynmanlectures.caltech.edu/I_26.html)
- Principle of least action in classical mechanics and beyond (see e.g. http://www.feynmanlectures.caltech.edu/II_19.html)
- Finite elements methods to solve problems in fluid dynamics or civil engineering.

Loosely speaking: the general idea is to frame the original problem in terms of an optimisation problem.

Program

1. Preparations
2. The variational principle
3. Application to inference and learning

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1. Preparations
   - Concavity of the logarithm and Jensen's inequality
   - Kullback-Leibler divergence and its properties
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$\log(u)$ is a concave function

- $\log(u)$ is a concave function

  $$\log((1-a)u_1 + au_2) \geq (1-a)\log(u_1) + a\log(u_2) \qquad a \in [0,1]$$

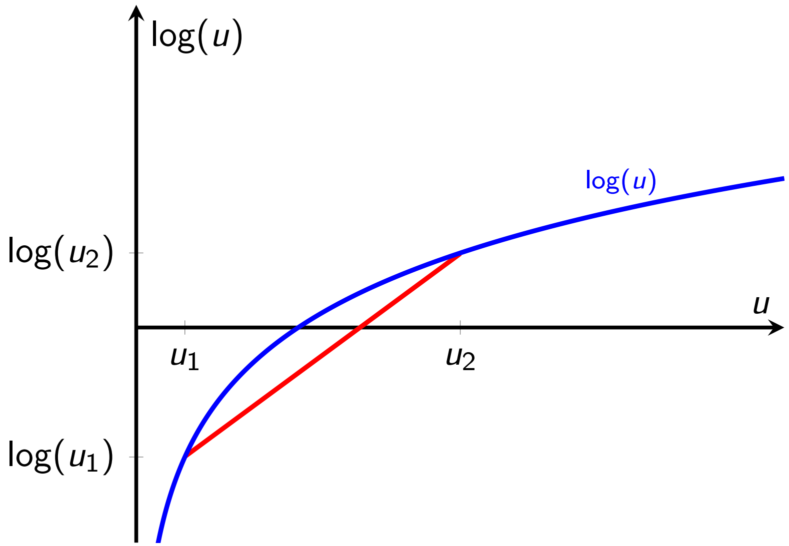
  $(1-a)x + ay$ with $a \in [0,1]$ linearly interpolates between x and y.

- log(average) $\geq$ average (log)

- Generalisation

  $$\log \mathbb{E}[g(\mathbf{x})] \geq \mathbb{E}[\log g(\mathbf{x})]$$

  with $g(\mathbf{x}) > 0$



- Called Jensen's inequality for concave functions.

Kullback-Leibler divergence

- Kullback Leibler divergence $\text{KL}(p||q)$

$$\text{KL}(p||q) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} \mathrm{d}\mathbf{x} = \mathbb{E}_{p(\mathbf{x})} \left[\log \frac{p(\mathbf{x})}{q(\mathbf{x})} \right] \qquad (1)$$

- Properties
  - $\text{KL}(p||q) = 0$ if and only if (iff) $p = q$
    (they may be different on sets of probability zero under p)
  - $\text{KL}(p||q) \neq \text{KL}(q||p)$
  - $\text{KL}(p||q) \geq 0$
- Non-negativity follows from the concavity of the logarithm.

Non-negativity of the KL divergence

Non-negativity follows from the concavity of the logarithm.

$$-\mathrm{KL}(p||q) = -\mathbb{E}_{p(\mathbf{x})}\left[\log \frac{p(\mathbf{x})}{q(\mathbf{x})}\right] \tag{2}$$

$$= \mathbb{E}_{p(\mathbf{x})}\left[\log \frac{q(\mathbf{x})}{p(\mathbf{x})}\right] \tag{3}$$

$$\leq \log \underbrace{\mathbb{E}_{p(\mathbf{x})}\left[\frac{q(\mathbf{x})}{p(\mathbf{x})}\right]}_{\int p(\mathbf{x})q(\mathbf{x})/p(\mathbf{x})d\mathbf{x}=1} \tag{4}$$

Hence $-\mathrm{KL}(p||q) \leq \log(1) = 0$ and thus

$$\mathrm{KL}(p||q) \geq 0 \tag{5}$$

KL divergence minimisation and MLE for iid data

- Assume your data $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is sampled iid from $p_*(\mathbf{x})$.
- Your model is $p(\mathbf{x}; \boldsymbol{\theta})$. Consider KL div $\mathrm{KL}(p_*(\mathbf{x})||p(\mathbf{x}; \boldsymbol{\theta}))$

$$\mathrm{KL}(p_*(\mathbf{x})||p(\mathbf{x}; \boldsymbol{\theta})) = \mathbb{E}_{p_*(\mathbf{x})}\left[\log \frac{p_*(\mathbf{x})}{p(\mathbf{x}; \boldsymbol{\theta})}\right] \tag{6}$$

$$= \mathbb{E}_{p_*(\mathbf{x})} \log p_*(\mathbf{x}) - \mathbb{E}_{p_*(\mathbf{x})} \log p(\mathbf{x}; \boldsymbol{\theta}) \tag{7}$$

- $\operatorname{argmin}_{\boldsymbol{\theta}} \mathrm{KL}(p_*(\mathbf{x})||p(\mathbf{x}; \boldsymbol{\theta})) = \operatorname{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{p_*(\mathbf{x})} \log p(\mathbf{x}; \boldsymbol{\theta})$
- Approximating the expectation $\mathbb{E}_{p_*(\mathbf{x})}$ with a sample average gives log-likelihood (scaled by $1/n$)

$$\frac{1}{n}\ell(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \log p(\mathbf{x}_i; \boldsymbol{\theta}) \tag{8}$$

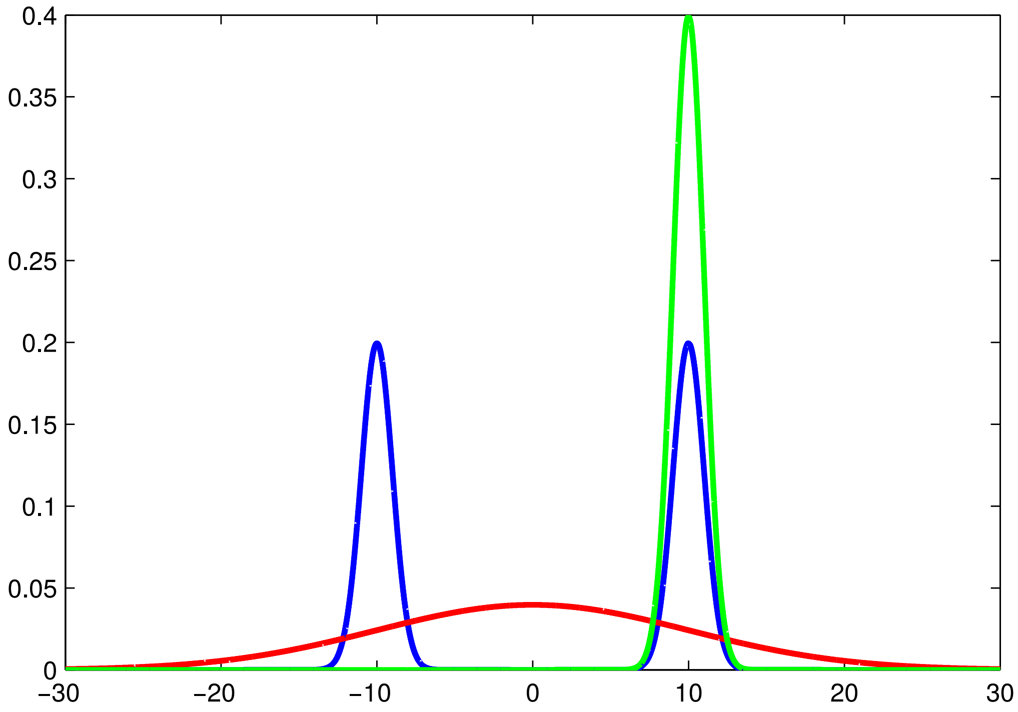
- Hence: $\hat{\boldsymbol{\theta}}_{\mathrm{MLE}} = \operatorname{argmax}_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) \approx \operatorname{argmin}_{\boldsymbol{\theta}} \mathrm{KL}(p_*(\mathbf{x})||p(\mathbf{x}; \boldsymbol{\theta}))$

Asymmetry of the KL divergence

Blue: mixture of Gaussians $p(x)$ (fixed)

Green: (unimodal) Gaussian q that minimises $\mathrm{KL}(q||p)$

Red: (unimodal) Gaussian q that minimises $\mathrm{KL}(p||q)$



Barber Figure 28.1, Section 28.3.4

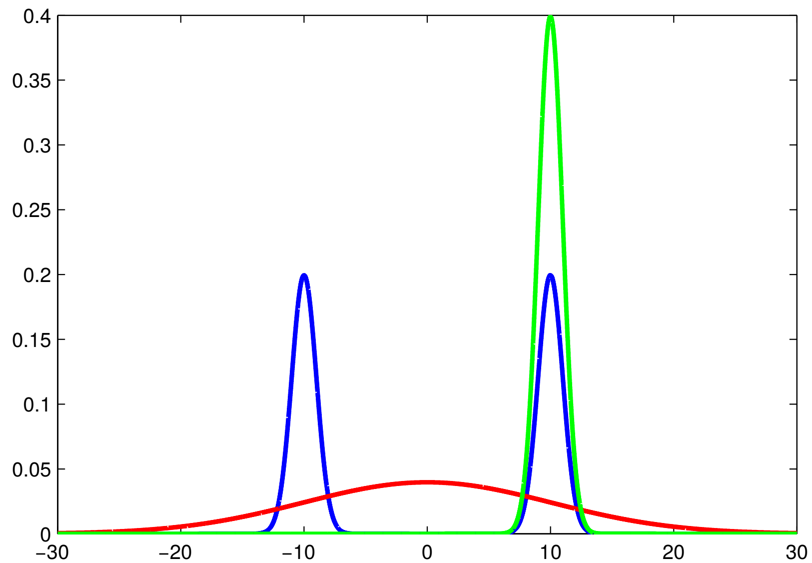
Asymmetry of the KL divergence

$\operatorname{argmin}_q \mathrm{KL}(q||p) = \operatorname{argmin}_q \int q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} \mathrm{d}\mathbf{x}$

- Optimal q avoids regions where p is small.
  (but can be small where p is large)
- Produces good local fit, "mode seeking"

$\operatorname{argmin}_q \mathrm{KL}(p||q) = \operatorname{argmin}_q \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} \mathrm{d}\mathbf{x}$

- Optimal q is nonzero where p is nonzero
  (and does not care about regions where p is small)
- Corresponds to MLE; produces global fit/moment matching

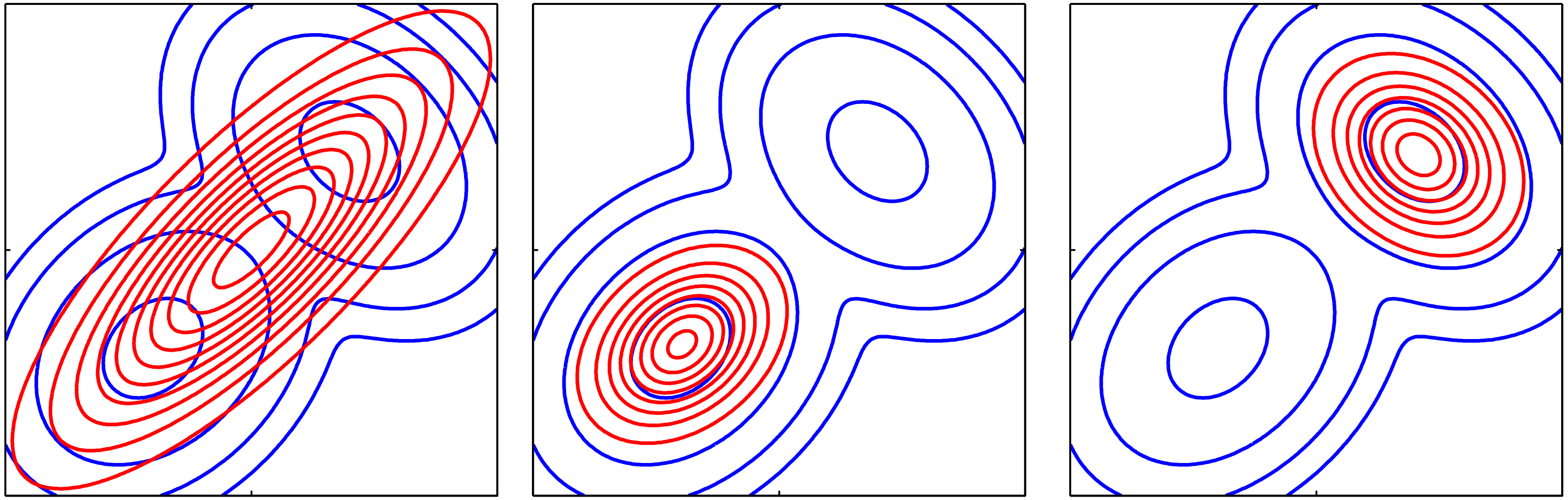


Asymmetry of the KL divergence

Blue: mixture of Gaussians $p(\mathbf{x})$ (fixed)

Red: optimal (unimodal) Gaussians $q(\mathbf{x})$

Global moment matching (left) versus mode seeking (middle and right). (two local minima are shown)



$\min_q \mathrm{KL}(p \,||\, q)$ $\min_q \mathrm{KL}(q \,||\, p)$ $\min_q \mathrm{KL}(q \,||\, p)$

Bishop Figure 10.3

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Variational lower bound: auxiliary distribution

Consider joint pdf /pmf $p(\mathbf{x}, \mathbf{y})$ with marginal $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y}$

- We can write $p(\mathbf{x})$ as

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) \frac{q(\mathbf{y}|\mathbf{x})}{q(\mathbf{y}|\mathbf{x})} \mathrm{d}\mathbf{y} = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \left[\frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y}|\mathbf{x})} \right] \tag{9}$$

  where $q(\mathbf{y}|\mathbf{x})$ is an auxiliary distribution (called the variational distribution in the context of variational inference/learning) for a given $\mathbf{x}$.

- Log marginal is

$$\log p(\mathbf{x}) = \log \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \left[\frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y}|\mathbf{x})} \right] \tag{10}$$

- Approximating the expectation with a sample average leads to importance sampling. Another approach is to work with the concavity of the logarithm instead.

Variational lower bound: concavity of the logarithm

- Concavity of the log gives

$$\log p(\mathbf{x}) = \log \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\frac{p(\mathbf{x},\mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] \geq \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x},\mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] \quad (11)$$

  This is the variational lower bound for $\log p(\mathbf{x})$.

- Right-hand side is called the (variational) free energy $\mathcal{F}_{\mathbf{x}}(q)$ or the evidence lower bound (ELBO) $\mathcal{L}_{\mathbf{x}}(q)$

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x},\mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] \quad (12)$$

- Since q is a function, the ELBO is a functional, which is a mapping that depends on a function.

Properties of the ELBO

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

- By manipulating the definition of the ELBO, we obtain the following equivalent forms

$$\mathcal{L}_{\mathbf{x}}(q) = \log p(\mathbf{x}) - \mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x})) \quad (13)$$

$$= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{y}) - \mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y})) \quad (14)$$

$$= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})} \log p(\mathbf{x},\mathbf{y}) + \mathcal{H}(q) \quad (15)$$

  where $p(\mathbf{y})$ is the marginal of $p(\mathbf{x},\mathbf{y})$ and $\mathcal{H}(q)$ is the entropy of q.

- Entropy is a measure of randomness/variability of a variable

$$\mathcal{H}(q) = -\mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log q(\mathbf{y}|\mathbf{x})\right] \quad (16)$$

  Larger entropy means more variability.

Properties of the ELBO (proof)

- First expression:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x},\mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] &= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{q(\mathbf{y}|\mathbf{x})}\right] \\
&= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{y}|\mathbf{x})}{q(\mathbf{y}|\mathbf{x})} + \log p(\mathbf{x})\right] \\
&= \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{y}|\mathbf{x})}{q(\mathbf{y}|\mathbf{x})}\right] + \log p(\mathbf{x}) \\
&= -\mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x})) + \log p(\mathbf{x})
\end{aligned}
$$

- Second expression is obtained similarly but using $p(\mathbf{x},\mathbf{y}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y})$ instead of $p(\mathbf{x},\mathbf{y}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$ above.
- Third expression from the definition of the entropy.

Tightness of the ELBO

- From $\mathcal{L}_{\mathbf{x}}(q) = \log p(\mathbf{x}) - \mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x}))$ and non-negativity of the KL divergence, we have
  1. $\log p(\mathbf{x}) \geq \mathcal{L}_{\mathbf{x}}(q)$ (as before)
  2. $\log p(\mathbf{x}) = \mathcal{L}_{\mathbf{x}}(q) \Leftrightarrow q(\mathbf{y}|\mathbf{x}) = p(\mathbf{y}|\mathbf{x})$
- Maximising $\mathcal{L}_{\mathbf{x}}(q)$ with respect to q yields both $\log p(\mathbf{x})$ and the conditional $p(\mathbf{y}|\mathbf{x})$ at the same time.
- Makes sense because if we know $p(\mathbf{x}, \mathbf{y})$ and $p(\mathbf{x})$, we know $p(\mathbf{y}|\mathbf{x})$, and vice versa, since $p(\mathbf{y}|\mathbf{x}) = p(\mathbf{x}, \mathbf{y})/p(\mathbf{x})$.

Alternative approach

- We started from the task of approximating the marginal

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} \tag{17}$$

- Alternative starting point is the task of approximating the conditional $p(\mathbf{y}|\mathbf{x})$ for some given $\mathbf{x}$ by a distribution $q(\mathbf{y}|\mathbf{x})$.
- Measuring the quality of the approximation $q(\mathbf{y}|\mathbf{x})$ by $\mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x}))$ gives

$$\mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x})) = \log p(\mathbf{x}) - \mathcal{L}_{\mathbf{x}}(q) \tag{18}$$

Same key result as before.

Variational principle

- By maximising the ELBO

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

  we can split the joint $p(\mathbf{x}, \mathbf{y})$ into $p(\mathbf{x})$ and $p(\mathbf{y}|\mathbf{x})$

$$\log p(\mathbf{x}) = \max_q \mathcal{L}_{\mathbf{x}}(q)$$

$$p(\mathbf{y}|\mathbf{x}) = \operatorname{argmax}_q \mathcal{L}_{\mathbf{x}}(q)$$

- Highlights the variational principle: Inference becomes optimisation.

Solving the optimisation problem

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

- Difficulties when maximising the ELBO:
  - Learning of a pdf/pmf $q(\mathbf{y}|\mathbf{x})$
  - Maximisation when objective involves $\mathbb{E}_{q(\mathbf{y}|\mathbf{x})}$ that depends on q
- Restrict search space to a family $\mathcal{Q}$ of variational distributions $q(\mathbf{y}|\mathbf{x})$ for which $\mathcal{L}_{\mathbf{x}}(q)$ is computable.
- Family $\mathcal{Q}$ specified by
  - independence assumptions, e.g. $q(\mathbf{y}|\mathbf{x}) = \prod_i q(y_i|\mathbf{x})$, which corresponds to "mean-field" variational inference
  - parametric assumptions, e.g. $q(y_i|\mathbf{x}) = \mathcal{N}(y_i; \mu_i(\mathbf{x}), \sigma_i^2(\mathbf{x}))$
- Discussed in more detail later.
- $\mathcal{L}_{\mathbf{x}}(q)$ can be computed analytically in closed form only in special cases.

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1. Preparations

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3. Application to inference and learning
   - Inference: approximating posteriors
   - Learning with Bayesian models
   - Learning with statistical models and unobserved variables
   - (Variational) EM algorithm

Approximate posterior inference

- Inference task: given value $\mathbf{x} = \mathbf{x}_o$ and joint pdf/pmf $p(\mathbf{x}, \mathbf{y})$, compute $p(\mathbf{y}|\mathbf{x}_o)$.
- Variational approach: estimate the posterior by solving an optimisation problem

$$\hat{p}(\mathbf{y}|\mathbf{x}_o) = \operatorname*{argmax}_{q \in \mathcal{Q}} \mathcal{L}_{\mathbf{x}_o}(q) \tag{19}$$

  $\mathcal{Q}$ is the set of pdfs/pmfs in which we search for the solution
- From the basic property of the ELBO in Equation (13)

$$\log p(\mathbf{x}_o) = \mathrm{KL}(q(\mathbf{y}|\mathbf{x}_o)||p(\mathbf{y}|\mathbf{x}_o)) + \mathcal{L}_{\mathbf{x}_o}(q) = \text{const} \tag{20}$$

- Because the sum of the KL and ELBO is constant, we have

$$\operatorname*{argmax}_{q \in \mathcal{Q}} \mathcal{L}_{\mathbf{x}_o}(q) = \operatorname*{argmin}_{q \in \mathcal{Q}} \mathrm{KL}(q(\mathbf{y}|\mathbf{x}_o)||p(\mathbf{y}|\mathbf{x}_o)) \tag{21}$$

Posterior as compromise between prior and fit

- Equivalent forms of the ELBO:

$$\mathcal{L}_{\mathbf{x}_o}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x}_o)} \log p(\mathbf{x}_o|\mathbf{y}) - \mathrm{KL}(q(\mathbf{y}|\mathbf{x}_o)||p(\mathbf{y})) \tag{22}$$

- By maximising $\mathcal{L}_{\mathbf{x}_o}(q)$ we find a q that
  - produces $\mathbf{y}$ which are likely explanations of $\mathbf{x}_o$
  - stays close to the prior $p(\mathbf{y})$
- If included in the search space $\mathcal{Q}$, $p(\mathbf{y}|\mathbf{x}_o)$ is the optimal q, which means that the posterior fulfils the two desiderata best.

As compromise between variable and likely imputations

- Equivalent forms of the ELBO:

$$\mathcal{L}_{\mathbf{x}_o}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x}_o)} \log p(\mathbf{x}_o, \mathbf{y}) + \mathcal{H}(q) \tag{23}$$

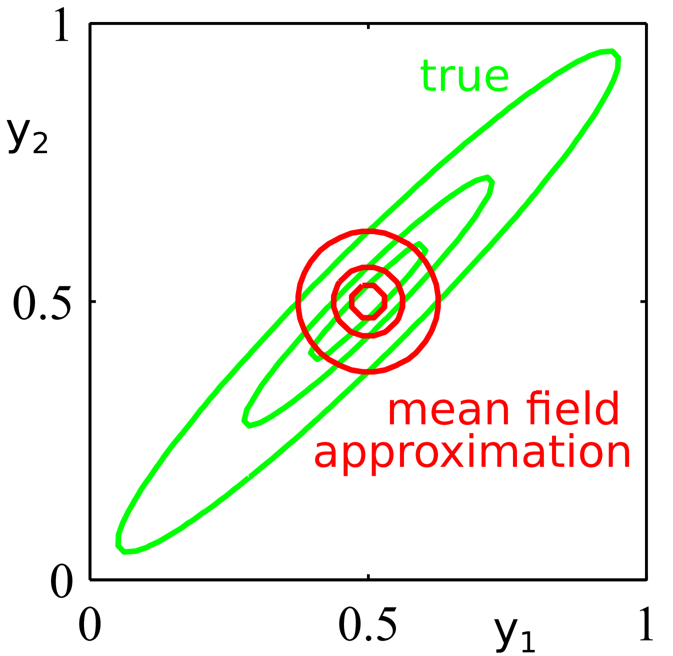
- By maximising $\mathcal{L}_{\mathbf{x}_o}(q)$ we find a q that
  - produces likely imputations (filled-in data) $\mathbf{y}$
  - is maximally variable
- If included in the search space $\mathcal{Q}$, $p(\mathbf{y}|\mathbf{x}_o)$ is the optimal q, which means that the posterior fulfils the two desiderata best.

Nature of the approximation

$$\mathrm{argmax}_{q \in \mathcal{Q}} \mathcal{L}_{\mathbf{x}_o}(q) = \mathrm{argmin}_{q \in \mathcal{Q}} \mathrm{KL}(q(\mathbf{y}|\mathbf{x}_o)||p(\mathbf{y}|\mathbf{x}_o))$$

- When minimising $\mathrm{KL}(q||p)$ with respect to q, q will try very hard to be zero where p is small.
- Assume true posterior is correlated bivariate Gaussian and we work with $\mathcal{Q} = \{q(\mathbf{y}|\mathbf{x}_o) : q(\mathbf{y}|\mathbf{x}_o) = q(y_1|\mathbf{x}_o)q(y_2|\mathbf{x}_o)\}$ (independence but no parametric assumptions)

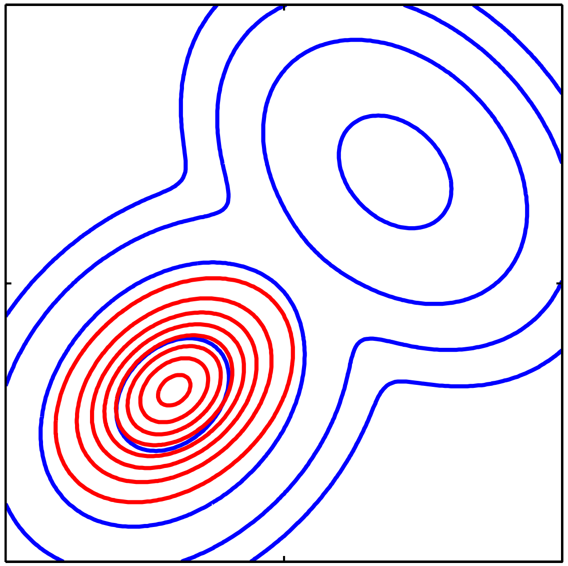
- Optimal q is Gaussian.
- Mean is correct but variances dictated by the variances of $p(\mathbf{y}|\mathbf{x}_o)$ along the y_1 and y_2 axes.
- Posterior variance is underestimated.

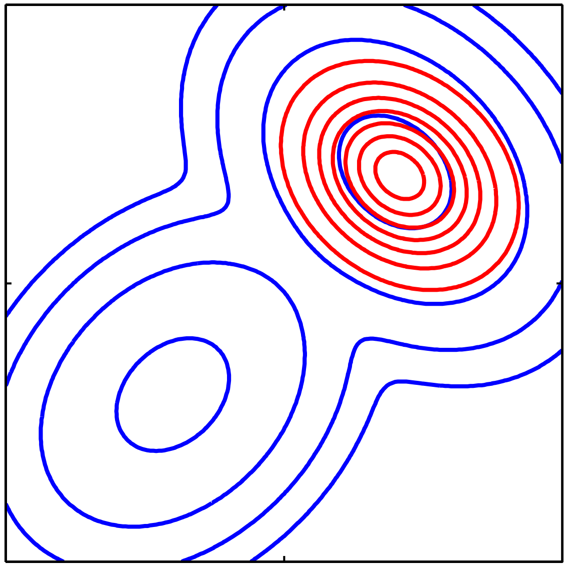


(Bishop, Figure 10.2)

Nature of the approximation

- Assume that true posterior is multimodal, but that the family of variational distributions $\mathcal{Q}$ only includes unimodal distributions.
- The optimal $q(\mathbf{y}|\mathbf{x}_o)$ only covers one mode: "mode-seeking behaviour".





local optimum local optimum

Blue: true posterior
Red: approximation

Bishop Figure 10.3 (adapted)

Learning by Bayesian inference

- Task 1: For a Bayesian model $p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) = p(\mathbf{x}, \boldsymbol{\theta})$, compute the posterior $p(\boldsymbol{\theta}|\mathcal{D})$
- Formally the same problem as before: $\mathcal{D} = \mathbf{x}_o$ and $\boldsymbol{\theta} \equiv \mathbf{y}$.
- Task 2: For a Bayesian model $p(\mathbf{v}, \mathbf{h}|\boldsymbol{\theta})p(\boldsymbol{\theta}) = p(\mathbf{v}, \mathbf{h}, \boldsymbol{\theta})$, compute the posterior $p(\boldsymbol{\theta}|\mathcal{D})$ where the data $\mathcal{D}$ are for the visibles $\mathbf{v}$ only.
- With the equivalence $\mathcal{D} = \mathbf{x}_o$ and $(\mathbf{h}, \boldsymbol{\theta}) \equiv \mathbf{y}$, we are formally back to the problem just studied.

Parameter estimation in presence of unobserved variables

- Task: For the model $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$, estimate the parameters $\boldsymbol{\theta}$ from data $\mathcal{D}$ on the visibles $\mathbf{v}$ only ($\mathbf{h}$ is unobserved).
- To evaluate the log likelihood function $\ell(\boldsymbol{\theta})$, we need to evaluate the integral

$$\ell(\boldsymbol{\theta}) = \log p(\mathcal{D}; \boldsymbol{\theta}) = \log \int_{\mathbf{h}} p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta}) \mathrm{d}\mathbf{h}, \tag{24}$$

  which is generally intractable.
- We could approximate $\ell(\boldsymbol{\theta})$ and its gradient using Monte Carlo integration.
- Here: use the variational approach.

Parameter estimation in presence of unobserved variables

- We had

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] \tag{25}$$

$$= \log p(\mathbf{x}) - \mathrm{KL}(q(\mathbf{y}|\mathbf{x})||p(\mathbf{y}|\mathbf{x})) \tag{26}$$

- Substitute

$$\mathbf{x} \to \mathcal{D}, \qquad \mathbf{y} \to \mathbf{h}, \qquad p(\mathbf{x}, \mathbf{y}) \to p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta}) \tag{27}$$

- We then have

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \mathbb{E}_{q(\mathbf{h}|\mathcal{D})}\left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h}|\mathcal{D})}\right] \tag{28}$$

$$= \log p(\mathcal{D}; \boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{h}|\mathcal{D})||p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta})) \tag{29}$$

- Notation $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q)$ highlights dependency on $\boldsymbol{\theta}$ and q.

MLE by maximising the ELBO

- Using $\ell(\boldsymbol{\theta})$ for the log-likelihood $\log p(\mathcal{D}; \boldsymbol{\theta})$, we have

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \ell(\boldsymbol{\theta}) - \mathrm{KL}(q(\mathbf{h}|\mathcal{D})||p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta})) \tag{30}$$

- If the search space $\mathcal{Q}$ is unrestricted or includes $p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta})$

$$\max_{q} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \ell(\boldsymbol{\theta}) \tag{31}$$

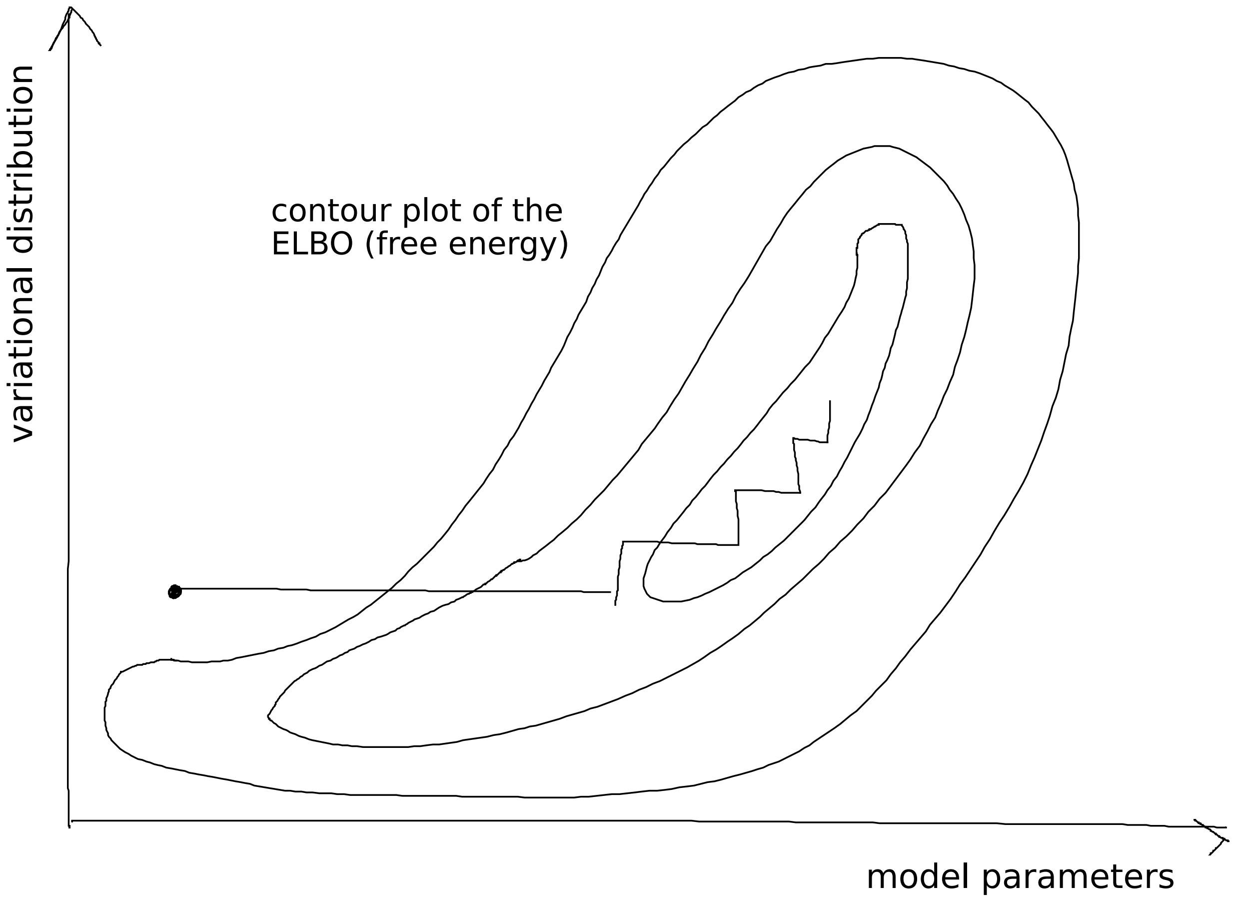
- Maximum likelihood estimation (MLE)

$$\max_{\boldsymbol{\theta}, q} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) \tag{32}$$

  MLE = maximise the ELBO $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q)$ with respect to $\boldsymbol{\theta}$ and q
- Restricted search space $\mathcal{Q}$ leads to approximate estimate of $\boldsymbol{\theta}$ and $p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta})$.

Variational EM algorithm

Variational expectation maximisation (EM): maximise $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q)$ by iterating between maximisation with respect to $\boldsymbol{\theta}$ and maximisation with respect to q (coordinate ascent).



(Adapted from `http://www.cs.cmu.edu/~tom/10-702/Zoubin-702.pdf`)

Where is the “expectation”?

- The optimisation with respect to q is called the “expectation step”

$$\max_{q \in \mathcal{Q}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \max_{q \in \mathcal{Q}} \mathbb{E}_{q(\mathbf{h}|\mathcal{D})} \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h}|\mathcal{D})} \right] \tag{33}$$

- Denote the best q by q^* so that

$$\max_{q \in \mathcal{Q}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q^*) = \mathbb{E}_{q^*(\mathbf{h}|\mathcal{D})} \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q^*(\mathbf{h}|\mathcal{D})} \right] \tag{34}$$

  which is defined in terms of an expectation and the reason for the name “expectation step”.

Classical EM algorithm

- Denote the parameters at iteration k by $\boldsymbol{\theta}_k$.
- We know that the optimal q for the expectation step is $q^*(\mathbf{h}|\mathcal{D}) = p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)$
- If we can compute the posterior $p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)$, we obtain the (classical) EM algorithm that iterates between:

E-step: compute the expectation

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q^*) = \underbrace{\mathbb{E}_{p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)}[\log p(\mathcal{D},\mathbf{h};\boldsymbol{\theta})]}_{\substack{\text{interpretation: expected} \\ \text{completed log-likelihood of } \boldsymbol{\theta}}} - \underbrace{\mathbb{E}_{p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)} \log p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)}_{\substack{\text{does not depend on } \boldsymbol{\theta} \text{ and} \\ \text{does not need to be computed}}}$$

M-step: maximise with respect to $\boldsymbol{\theta}$

$$\boldsymbol{\theta}_{k+1} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q^*) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \mathbb{E}_{p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)}[\log p(\mathcal{D},\mathbf{h};\boldsymbol{\theta})]$$

Classical EM algorithm never decreases the log likelihood

- Assume you have updated the parameters and start iteration $k+1$ with optimisation with respect to q

$$\max_q \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_k, q) \tag{35}$$

- Optimal solution q^*_{k+1} is the posterior $p(\mathbf{h}|\mathcal{D};\boldsymbol{\theta}_k)$ so that

$$\ell(\boldsymbol{\theta}_k) = \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_k, q^*_{k+1}) \tag{36}$$

- Optimise with respect to the $\boldsymbol{\theta}$ while keeping q fixed at q^*_{k+1}

$$\max_{\boldsymbol{\theta}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q^*_{k+1}) \tag{37}$$

- Due to maximisation, updated parameter $\boldsymbol{\theta}_{k+1}$ is such that

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_{k+1}, q^*_{k+1}) \geq \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_k, q^*_{k+1}) = \ell(\boldsymbol{\theta}_k) \tag{38}$$

- From variational lower bound: $\ell(\boldsymbol{\theta}) \geq \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q)$. Hence:

$$\ell(\boldsymbol{\theta}_{k+1}) \geq \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}_{k+1}, q^*_{k+1}) \geq \ell(\boldsymbol{\theta}_k)$$

$\Rightarrow$ EM yields non-decreasing sequence $\ell(\boldsymbol{\theta}_1), \ell(\boldsymbol{\theta}_2), \ldots$.

Program recap

1. Preparations
   - Concavity of the logarithm and Jensen's inequality
   - Kullback-Leibler divergence and its properties

2. The variational principle
   - Variational lower bound
   - Maximising the ELBO to compute the marginal and conditional from the joint

3. Application to inference and learning
   - Inference: approximating posteriors
   - Learning with Bayesian models
   - Learning with statistical models and unobserved variables
   - (Variational) EM algorithm