

Variational Inference and Learning

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Recap

- ▶ Learning and inference often involves intractable integrals
- ▶ For example: marginalisation

$$p(\mathbf{x}) = \int_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$

- ▶ For example: likelihood in case of unobserved variables

$$L(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta}) = \int_{\mathbf{u}} p(\mathbf{u}, \mathcal{D}; \boldsymbol{\theta}) d\mathbf{u}$$

- ▶ We can use Monte Carlo integration and sampling to approximate the integrals.
- ▶ Alternative: 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.

Program

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

Program

1. Preparations

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

2. The variational principle

3. Application to inference and learning

log is concave

- ▶ $\log(u)$ is concave

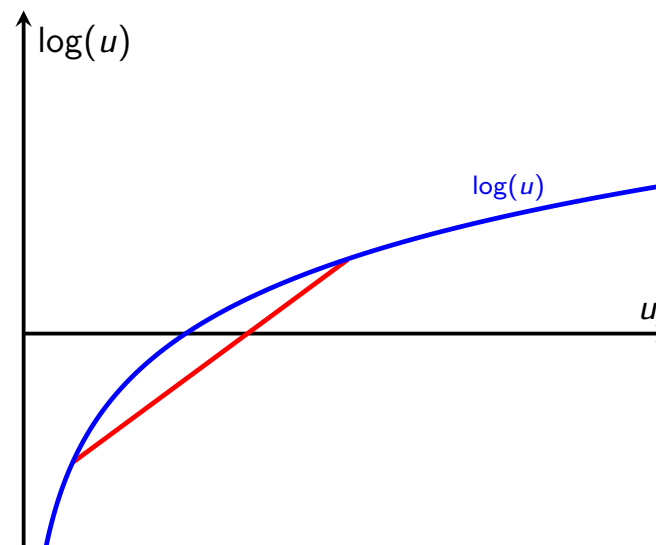
$$\log(au_1 + (1-a)u_2) \geq a \log(u_1) + (1-a) \log(u_2) \quad a \in [0, 1]$$

- ▶ $\log(\text{average}) \geq \text{average}(\log)$

- ▶ Generalisation

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

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



- ▶ Jensen's inequality for concave functions.

Kullback-Leibler divergence

- ▶ Kullback Leibler divergence $KL(p||q)$

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

- ▶ Properties

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

Non-negativity of the KL divergence

Non-negativity follows from the concavity of the logarithm.

$$\begin{aligned}\mathbb{E}_{p(\mathbf{x})} \left[\log \frac{q(\mathbf{x})}{p(\mathbf{x})} \right] &\leq \log \mathbb{E}_{p(\mathbf{x})} \left[\frac{q(\mathbf{x})}{p(\mathbf{x})} \right] \\ &= \log \int p(\mathbf{x}) \frac{q(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x} \\ &= \log \int q(\mathbf{x}) d\mathbf{x} \\ &= \log 1 = 0.\end{aligned}$$

From

$$\mathbb{E}_{p(\mathbf{x})} \left[\log \frac{q(\mathbf{x})}{p(\mathbf{x})} \right] \leq 0$$

it follows that

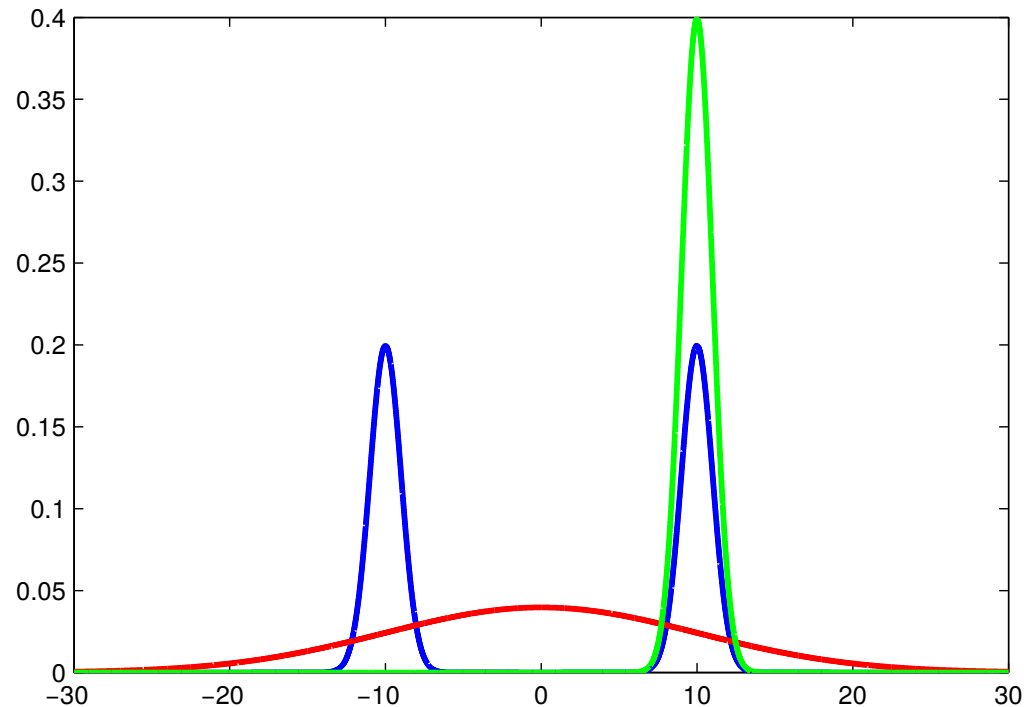
$$\text{KL}(p||q) = \mathbb{E}_{p(\mathbf{x})} \left[\log \frac{p(\mathbf{x})}{q(\mathbf{x})} \right] = -\mathbb{E}_{p(\mathbf{x})} \left[\log \frac{q(\mathbf{x})}{p(\mathbf{x})} \right] \geq 0$$

Asymmetry of the KL divergence

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

Green: (unimodal) Gaussian q that minimises $KL(q||p)$

Red: (unimodal) Gaussian q that minimises $KL(p||q)$



Barber Figure 28.1, Section 28.3.4

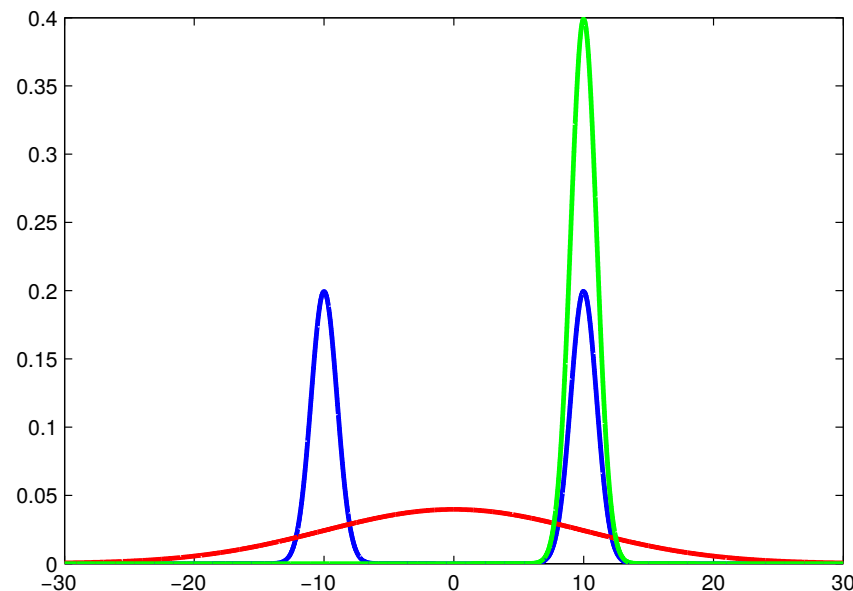
Asymmetry of the KL divergence

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

- ▶ Optimal q avoids regions where p is small.
- ▶ Produces good local fit, “mode seeking”

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

- ▶ 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

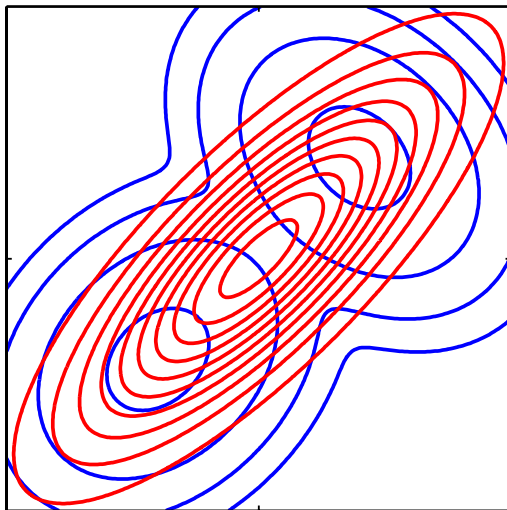


Asymmetry of the KL divergence

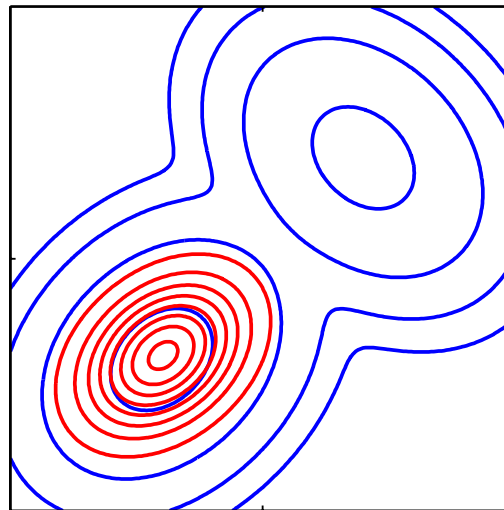
Blue: mixture of Gaussians $p(\mathbf{x})$ (fixed)

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

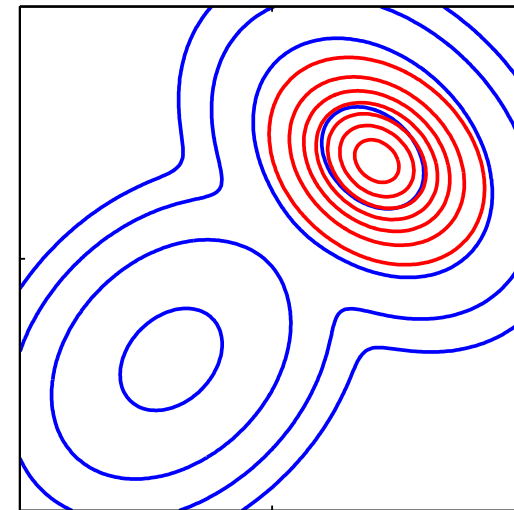
Global moment matching (left) versus mode seeking (middle and right). (two local minima are shown)



$\min_q \text{KL}(p \parallel q)$



$\min_q \text{KL}(q \parallel p)$



$\min_q \text{KL}(q \parallel p)$

Bishop Figure 10.3

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1. Preparations

- Concavity of the logarithm and Jensen's inequality
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2. The variational principle

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1. Preparations

2. The variational principle

- Variational lower bound
- Free energy and the decomposition of the log marginal
- Free energy maximisation to compute the marginal and conditional from the joint

3. Application to inference and learning

Variational lower bound: auxiliary distribution

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

- ▶ Like for importance sampling, we can write

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

where $q(\mathbf{y})$ is an auxiliary distribution (called the variational distribution in the context of variational inference/learning)

- ▶ Log marginal is

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

- ▶ Instead of approximating the expectation with a sample average, use now the concavity of the logarithm.

Variational lower bound: concavity of the logarithm

- ▶ Concavity of the log gives

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

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

- ▶ Right-hand side is called the (variational) free energy

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

It depends on \mathbf{x} through the joint $p(\mathbf{x}, \mathbf{y})$, and on the auxiliary distribution $q(\mathbf{y})$

(since q is a function, the free energy is called a functional, which is a mapping that depends on a function)

Decomposition of the log marginal

- ▶ We can re-write the free energy as

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

- ▶ Hence: $\log p(\mathbf{x}) = \text{KL}(q(\mathbf{y})||p(\mathbf{y}|\mathbf{x})) + \mathcal{F}(\mathbf{x}, q)$
- ▶ $\text{KL} \geq 0$ implies the bound $\log p(\mathbf{x}) \geq \mathcal{F}(\mathbf{x}, q)$.
- ▶ $\text{KL}(q||p) = 0$ iff $q = p$ implies that for $q(\mathbf{y}) = p(\mathbf{y}|\mathbf{x})$, the free energy is maximised and equals $\log p(\mathbf{x})$.

Variational principle

- ▶ By maximising the free energy

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

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

$$\log p(\mathbf{x}) = \max_{q(\mathbf{y})} \mathcal{F}(\mathbf{x}, q)$$

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

- ▶ You can think of free energy maximisation as a “function” that takes as input a joint $p(\mathbf{x}, \mathbf{y})$ and returns as output the (log) marginal and the conditional.

Variational principle

- ▶ Given $p(\mathbf{x}, \mathbf{y})$, consider inference tasks
 1. compute $p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}$
 2. compute $p(\mathbf{y}|\mathbf{x})$
- ▶ Variational principle: we can formulate the marginal inference problems as an optimisation problem.
- ▶ Maximising the free energy

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

gives

1. $\log p(\mathbf{x}) = \max_{q(\mathbf{y})} \mathcal{F}(\mathbf{x}, q)$
 2. $p(\mathbf{y}|\mathbf{x}) = \operatorname{argmax}_{q(\mathbf{y})} \mathcal{F}(\mathbf{x}, q)$
- ▶ Inference becomes optimisation.
 - ▶ Note: while we use $q(\mathbf{y})$ to denote the variational distribution, it depends on (fixed) \mathbf{x} . Better (and rarer) notation is $q(\mathbf{y}|\mathbf{x})$.

Solving the optimisation problem

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

- ▶ Difficulties when maximising the free energy:
 - ▶ optimisation with respect to pdf/pmf $q(\mathbf{y})$
 - ▶ computation of the expectation
- ▶ Restrict search space to family of variational distributions $q(\mathbf{y})$ for which $\mathcal{F}(\mathbf{x}, q)$ is computable.
- ▶ Family \mathcal{Q} specified by
 - ▶ independence assumptions, e.g. $q(\mathbf{y}) = \prod_i q(y_i)$, which corresponds to “mean-field” variational inference
 - ▶ parametric assumptions, e.g. $q(y_i) = \mathcal{N}(y_i; \mu_i, \sigma_i^2)$
- ▶ Optimisation is generally challenging: lots of research on how to do it (keywords: stochastic variational inference, black-box variational inference)

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2. The variational principle

- Variational lower bound
- Free energy and the decomposition of the log marginal
- Free energy maximisation to compute the marginal and conditional from the joint

3. Application to inference and learning

Program

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
 - Learning with statistical models and unobs variables: 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

$$\hat{p}(\mathbf{y}|\mathbf{x}_o) = \operatorname{argmax}_{q(\mathbf{y}) \in \mathcal{Q}} \mathcal{F}(\mathbf{x}, q)$$

\mathcal{Q} is the set of pdfs in which we search for the solution

- ▶ The decomposition of the log marginal gives

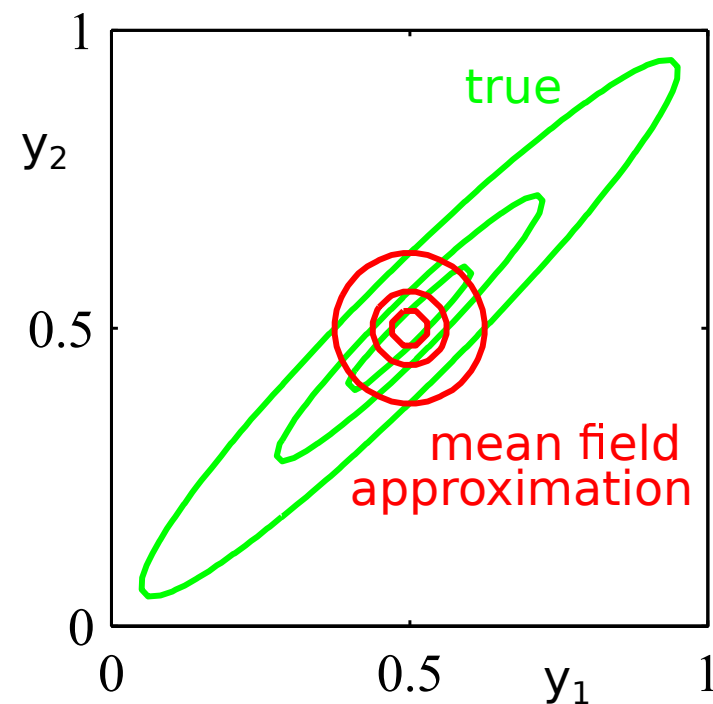
$$\log p(\mathbf{x}_o) = \operatorname{KL}(q(\mathbf{y})||p(\mathbf{y}|\mathbf{x})) + \mathcal{F}(\mathbf{x}, q) = \text{const}$$

- ▶ Because the sum of the KL and free energy term is constant we have

$$\operatorname{argmax}_{q(\mathbf{y}) \in \mathcal{Q}} \mathcal{F}(\mathbf{x}, q) = \operatorname{argmin}_{q(\mathbf{y}) \in \mathcal{Q}} \operatorname{KL}(q(\mathbf{y})||p(\mathbf{y}|\mathbf{x}))$$

Nature of the approximation

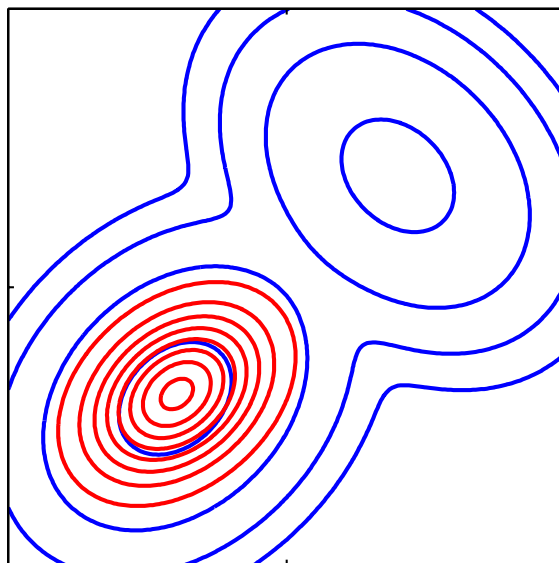
- ▶ When minimising $\text{KL}(q||p)$ with respect to q , q will try to be zero where p is small.
- ▶ Assume true posterior is correlated bivariate Gaussian and we work with $\mathcal{Q} = \{q(\mathbf{y}) : q(\mathbf{y}) = q(y_1)q(y_2)\}$
(independence but no parametric assumptions)
- ▶ $\hat{p}(\mathbf{y}|\mathbf{x}_o)$, i.e. $q(\mathbf{y})$ that minimises $\text{KL}(q||p)$, is Gaussian.
- ▶ Mean is correct but variances dictated by the marginal variances along the y_1 and y_2 axes.
- ▶ **Posterior variance is underestimated.**



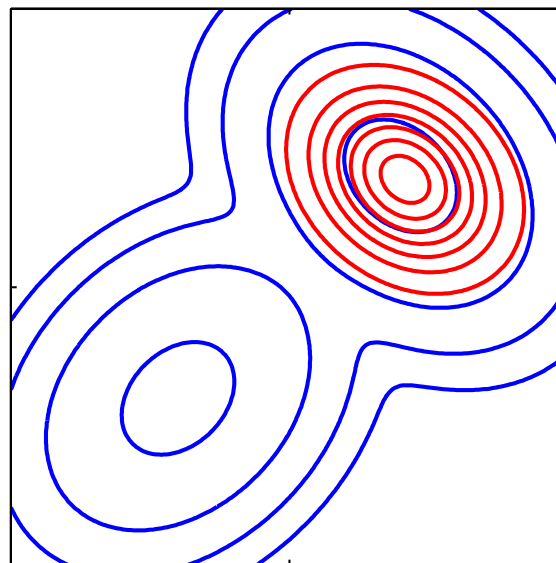
(Bishop, Figure 10.2)

Nature of the approximation

- ▶ Assume that true posterior is multimodal, but that the family of variational distributions \mathcal{Q} only includes unimodal distributions.
- ▶ The learned approximate posterior $\hat{p}(\mathbf{y}|\mathbf{x}_o)$ 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.
- ▶ But the variational distribution $q(\mathbf{y})$ becomes $q(\mathbf{h}, \boldsymbol{\theta})$.
- ▶ Often: assume $q(\mathbf{h}, \boldsymbol{\theta})$ factorises as $q(\mathbf{h})q(\boldsymbol{\theta})$ (see Barber Section 11.5)

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} about the visibles \mathbf{v} .
- ▶ See slides on *Intractable Likelihood Functions*: the log likelihood function $\ell(\boldsymbol{\theta})$ is implicitly defined by the integral

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

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

- ▶ Foundational result that we derived

$$\log p(\mathbf{x}) = \text{KL}(q(\mathbf{y})||p(\mathbf{y}|\mathbf{x})) + \mathcal{F}(\mathbf{x}, q) \quad \mathcal{F}(\mathbf{x}, q) = \mathbb{E}_{q(\mathbf{y})} \left[\log \frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y})} \right]$$
$$\log p(\mathbf{x}) = \max_{q(\mathbf{y})} \mathcal{F}(\mathbf{x}, q) \quad p(\mathbf{y}|\mathbf{x}) = \operatorname{argmax}_{q(\mathbf{y})} \mathcal{F}(\mathbf{x}, q)$$

- ▶ With correspondence

$$\mathbf{v} \equiv \mathbf{x} \quad \mathbf{h} \equiv \mathbf{y} \quad p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}) \equiv p(\mathbf{x}, \mathbf{y})$$

we obtain

$$\log p(\mathbf{v}; \boldsymbol{\theta}) = \text{KL}(q(\mathbf{h})||p(\mathbf{h}|\mathbf{v})) + \mathcal{F}(\mathbf{v}, q; \boldsymbol{\theta}) \quad \mathcal{F}(\mathbf{v}, q; \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{h})} \left[\log \frac{p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h})} \right]$$
$$\log p(\mathbf{v}; \boldsymbol{\theta}) = \max_{q(\mathbf{h})} \mathcal{F}(\mathbf{v}, q; \boldsymbol{\theta}) \quad p(\mathbf{h}|\mathbf{v}; \boldsymbol{\theta}) = \operatorname{argmax}_{q(\mathbf{h})} \mathcal{F}(\mathbf{v}, q; \boldsymbol{\theta})$$

- ▶ Plug in \mathcal{D} for \mathbf{v} : $\log p(\mathcal{D}; \boldsymbol{\theta})$ equals $\ell(\boldsymbol{\theta})$

Approximate MLE by free energy maximisation

- ▶ With $\mathbf{v} = \mathcal{D}$ and $\ell(\boldsymbol{\theta}) = p(\mathcal{D}; \boldsymbol{\theta})$, the equations become

$$\ell(\boldsymbol{\theta}) = \text{KL}(q(\mathbf{h})||p(\mathbf{h}|\mathcal{D})) + \overbrace{\mathcal{F}(\mathcal{D}, q; \boldsymbol{\theta})}^{J_{\mathcal{F}}(q, \boldsymbol{\theta})} \quad J_{\mathcal{F}}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{h})} \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h})} \right]$$
$$\ell(\boldsymbol{\theta}) = \max_{q(\mathbf{h})} J_{\mathcal{F}}(q, \boldsymbol{\theta}) \quad p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}) = \operatorname{argmax}_{q(\mathbf{h})} J_{\mathcal{F}}(q, \boldsymbol{\theta})$$

Write $J_{\mathcal{F}}(q, \boldsymbol{\theta})$ for $\mathcal{F}(\mathcal{D}, q; \boldsymbol{\theta})$ when data \mathcal{D} are fixed.

- ▶ Maximum likelihood estimation (MLE)

$$\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \max_{\boldsymbol{\theta}} \max_{q(\mathbf{h})} J_{\mathcal{F}}(q, \boldsymbol{\theta})$$

MLE = maximise the free energy with respect to $\boldsymbol{\theta}$ and $q(\mathbf{h})$

- ▶ Restricting the search space \mathcal{Q} for the variational distribution $q(\mathbf{h})$ due to computational reasons leads to an approximation.

Free energy as sum of completed log likelihood and entropy

- ▶ We can write the free energy as

$$J_{\mathcal{F}}(q, \theta) = \mathbb{E}_{q(\mathbf{h})} \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \theta)}{q(\mathbf{h})} \right] = \mathbb{E}_{q(\mathbf{h})} [\log p(\mathcal{D}, \mathbf{h}; \theta)] - \mathbb{E}_{q(\mathbf{h})} [\log q(\mathbf{h})]$$

- ▶ $-\mathbb{E}_{q(\mathbf{h})} [\log q(\mathbf{h})]$ is the entropy of $q(\mathbf{h})$
(entropy is a measure of randomness or variability, see e.g. Barber Section 8.2)
- ▶ $\log p(\mathcal{D}, \mathbf{h}; \theta)$ is the log-likelihood for the filled-in data $(\mathcal{D}, \mathbf{h})$
- ▶ $\mathbb{E}_{q(\mathbf{h})} [\log p(\mathcal{D}, \mathbf{h}; \theta)]$ is the weighted average of these “completed” log-likelihoods, with the weighting given by $q(\mathbf{h})$.

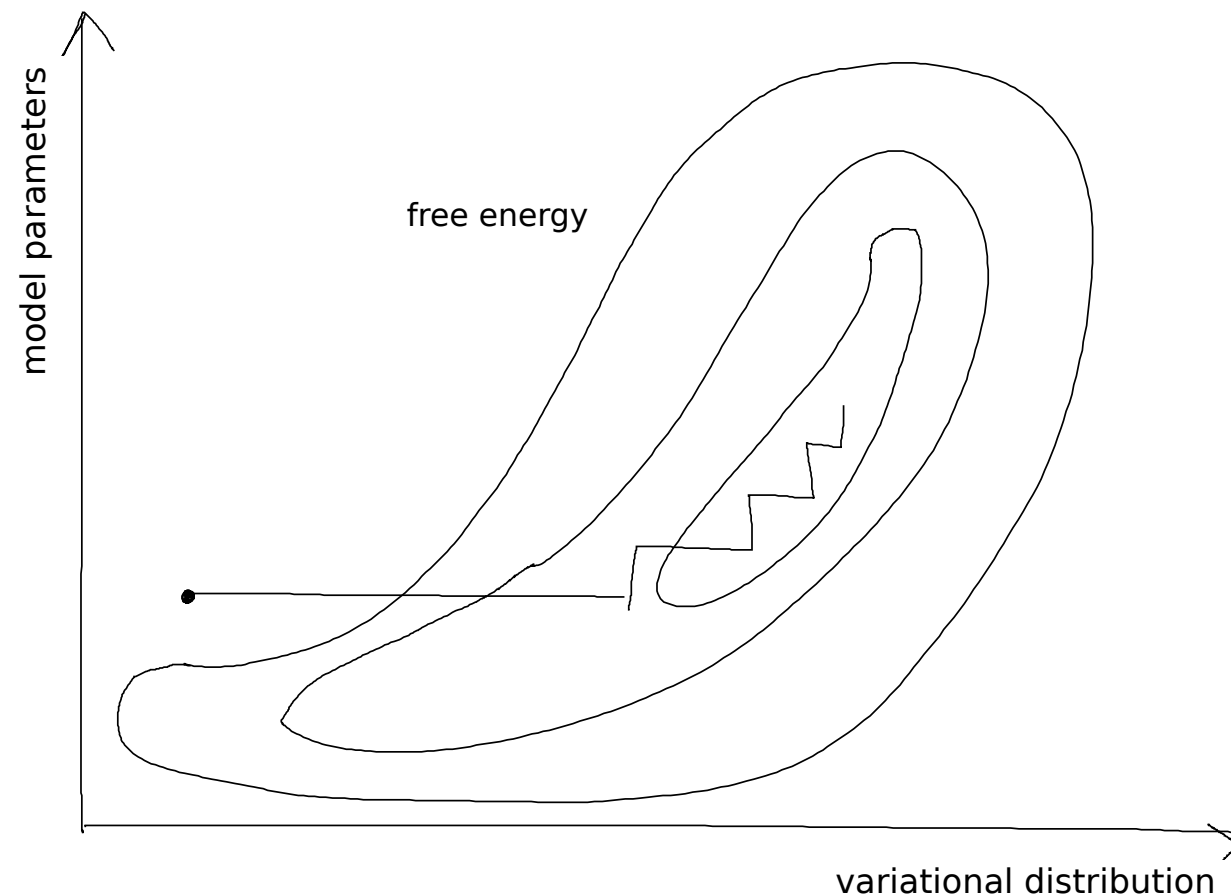
Free energy as sum of completed log likelihood and entropy

$$J_{\mathcal{F}}(q, \theta) = \mathbb{E}_{q(\mathbf{h})} [\log p(\mathcal{D}, \mathbf{h}; \theta)] - \mathbb{E}_{q(\mathbf{h})} [\log q(\mathbf{h})]$$

- ▶ When maximising $J_{\mathcal{F}}(q, \theta)$ with respect to q we look for random variables \mathbf{h} (filled-in data) that
 - ▶ are maximally variable (large entropy)
 - ▶ are maximally compatible with the observed data (according to the model $p(\mathcal{D}, \mathbf{v}; \theta)$)
- ▶ If included in the search space \mathcal{Q} , $p(\mathbf{h}|\mathcal{D}; \theta)$ is the optimal q , which means that the posterior fulfils the two desiderata best.

Variational EM algorithm

Variational expectation maximisation (EM): maximise $J_{\mathcal{F}}(q, \theta)$ by iterating between maximisation with respect to q and maximisation with respect to θ .



(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”

$$\max_{q \in \mathcal{Q}} J_{\mathcal{F}}(q, \boldsymbol{\theta}) = \max_{q \in \mathcal{Q}} \mathbb{E}_q \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h})} \right]$$

- ▶ Denote the best q by q^* so that $\max_{q \in \mathcal{Q}} J_{\mathcal{F}}(q, \boldsymbol{\theta}) = J_{\mathcal{F}}(q^*, \boldsymbol{\theta})$
- ▶ When we maximise with respect to $\boldsymbol{\theta}$, we need to know $J_{\mathcal{F}}(q^*, \boldsymbol{\theta})$,

$$J_{\mathcal{F}}(q^*, \boldsymbol{\theta}) = \mathbb{E}_{q^*} \left[\log \frac{p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})}{q^*(\mathbf{h})} \right],$$

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

Classical EM algorithm

- ▶ From

$$\ell(\boldsymbol{\theta}_k) = \text{KL}(q(\mathbf{h}) || p(\mathbf{h}|\mathcal{D})) + J_{\mathcal{F}}(q, \boldsymbol{\theta}_k)$$

We know that the optimal $q(\mathbf{h})$ is given by $p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}_k)$

- ▶ If we can compute the posterior $p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}_k)$, we obtain the (classical) EM algorithm that iterates between:

Expectation step

$$J_{\mathcal{F}}(q^*, \boldsymbol{\theta}) = \mathbb{E}_{p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}_k)}[\log p(\mathcal{D}, \mathbf{h}; \boldsymbol{\theta})] - \underbrace{\mathbb{E}_{p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}_k)} \log p(\mathbf{h}|\mathcal{D}; \boldsymbol{\theta}_k)}_{\text{does not depend on } \boldsymbol{\theta} \text{ and does not need to be computed}}$$

Maximisation step

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

Classical EM algorithm never decreases the log likelihood

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

$$\max_q J_{\mathcal{F}}(q, \boldsymbol{\theta}_{k-1})$$

- ▶ Optimal solution q_k^* is the posterior so that

$$\ell(\boldsymbol{\theta}_{k-1}) = J_{\mathcal{F}}(q_k^*, \boldsymbol{\theta}_{k-1})$$

- ▶ Optimise with respect to the $\boldsymbol{\theta}$ while keeping q fixed at q_k^*

$$\max_{\boldsymbol{\theta}} J_{\mathcal{F}}(q_k^*, \boldsymbol{\theta})$$

- ▶ Because of **maximisation**, optimiser $\boldsymbol{\theta}_k$ is such that

$$J_{\mathcal{F}}(q_k^*, \boldsymbol{\theta}_k) \geq J_{\mathcal{F}}(q_k^*, \boldsymbol{\theta}_{k-1}) = \ell(\boldsymbol{\theta}_{k-1})$$

- ▶ From variational lower bound: $\ell(\boldsymbol{\theta}) \geq J_{\mathcal{F}}(q, \boldsymbol{\theta})$

$$\ell(\boldsymbol{\theta}_k) \geq J_{\mathcal{F}}(q_k^*, \boldsymbol{\theta}_k) \geq \ell(\boldsymbol{\theta}_{k-1})$$

Hence: EM yields non-decreasing sequence $\ell(\boldsymbol{\theta}_1), \ell(\boldsymbol{\theta}_2), \dots$

Examples

- ▶ Work through the examples in Barber Section 11.2 for the classical EM algorithm.
- ▶ Example 11.4 treats the cancer-asbestos-smoking example that we had in an earlier lecture.

Program recap

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- Free energy maximisation 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
- Learning with statistical models and unobs variables: EM algorithm