Variational Inference and Learning

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Recap

- Learning and inference often involves intractable integrals.

  - For example: marginalisation
    \[ p(x) = \int_y p(x, y) \, dy \]
  
  - For example: likelihood in case of unobserved variables
    \[ L(\theta) = p(D; \theta) = \int_u p(u, D; \theta) \, du \]

- We can use Monte Carlo integration and sampling to approximate the integrals.
- Alternative: variational approach to (approximate) inference and learning.
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- For example: marginalisation

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Learning and inference often involves intractable integrals. For example: marginalisation

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Recap

- Learning and inference often involves intractable integrals
- For example: marginalisation
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  p(x) = \int_y p(x, y) \, dy
  \]
- For example: likelihood in case of unobserved variables
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  L(\theta) = p(D; \theta) = \int_u p(u, D; \theta) \, du
  \]
- We can use Monte Carlo integration and sampling to approximate the integrals.
- Alternative: variational approach to (approximate) inference and learning.
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)
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- **Principle of least action** in classical mechanics and beyond (see e.g. http://www.feynmanlectures.caltech.edu/II_19.html)
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.
1. Preparations

2. The variational principle

3. Application to inference and learning
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

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

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

- **Generalisation**

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

with \(g(x) > 0\)

- **Jensen’s inequality for concave functions.**
Kullback-Leibler divergence

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

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

- 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.

\[
\mathbb{E}_{p(x)} \left[ \log \frac{q(x)}{p(x)} \right] \leq \log \mathbb{E}_{p(x)} \left[ \frac{q(x)}{p(x)} \right] \\
= \log \int p(x) \frac{q(x)}{p(x)} \, dx \\
= \log \int q(x) \, dx \\
= \log 1 = 0.
\]

From

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

it follows that

\[
KL(p\|q) = \mathbb{E}_{p(x)} \left[ \log \frac{p(x)}{q(x)} \right] = - \mathbb{E}_{p(x)} \left[ \log \frac{q(x)}{p(x)} \right] \geq 0
\]
Asymmetry of the KL divergence

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

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

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

Barber Figure 28.1, Section 28.3.4
Asymmetry of the KL divergence

\[
\arg\min_q \text{KL}(q \| p) = \arg\min_q \int q(x) \log \frac{q(x)}{p(x)} \, dx
\]

▷ Optimal \( q \) avoids regions where \( p \) is small.

▷ Produces good local fit, “mode seeking”
Asymmetry of the KL divergence

$$\text{argmin}_q \text{KL}(q||p) = \text{argmin}_q \int q(x) \log \frac{q(x)}{p(x)} \, dx$$

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

$$\text{argmin}_q \text{KL}(p||q) = \text{argmin}_q \int p(x) \log \frac{p(x)}{q(x)} \, dx$$

- 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 $p(x)$ (fixed)

Red: optimal (unimodal) Gaussians $q(x)$

Global moment matching (left) versus mode seeking (middle and right). (two local minima are shown)
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   - Kullback-Leibler divergence and its properties

2. The variational principle

3. Application to inference and learning
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 $p(x, y)$ with marginal $p(x) = \int p(x, y) dy$

- Like for importance sampling, we can write

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

where $q(y)$ is an auxiliary distribution (called the variational distribution in the context of variational inference/learning)
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- Log marginal is

$$\log p(x) = \log \mathbb{E}_{q(y)} \left[ \frac{p(x, y)}{q(y)} \right]$$
Variational lower bound: auxiliary distribution

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- Log marginal is

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

- 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

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

This is the variational lower bound for \( \log p(x) \).
Variational lower bound: concavity of the logarithm

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This is the variational lower bound for \( \log p(x) \).

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

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

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

(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

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

\[ = \mathbb{E}_{q(y)} \left[ \log \frac{p(y|x)}{q(y)} + \log p(x) \right] \]

\[ = \mathbb{E}_{q(y)} \left[ \log \frac{p(y|x)}{q(y)} \right] + \log p(x) \]

\[ = -KL(q(y) \Vert p(y|x)) + \log p(x) \]
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\[
= \mathbb{E}_{q(y)} \left[ \log \frac{p(y|x)}{q(y)} + \log p(x) \right]
\]

\[
= \mathbb{E}_{q(y)} \left[ \log \frac{p(y|x)}{q(y)} \right] + \log p(x)
\]

\[
= - \text{KL}(q(y) \| p(y|x)) + \log p(x)
\]

Hence: \( \log p(x) = \text{KL}(q(y) \| p(y|x)) + \mathcal{F}(x, q) \)
Decomposition of the log marginal

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\[ = -KL(q(y) \| p(y|x)) + \log p(x) \]

Hence: \( \log p(x) = KL(q(y) \| p(y|x)) + \mathcal{F}(x, q) \)

KL \( \geq 0 \) implies the bound \( \log p(x) \geq \mathcal{F}(x, q) \).
Decomposition of the log marginal

- We can re-write the free energy as

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

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\[ = -\text{KL}(q(y) \| p(y|x)) + \log p(x) \]

- Hence: \( \log p(x) = \text{KL}(q(y) \| p(y|x)) + \mathcal{F}(x, q) \)

- \( \text{KL} \geq 0 \) implies the bound \( \log p(x) \geq \mathcal{F}(x, q) \).

- \( \text{KL}(q\|p) = 0 \) iff \( q = p \) implies that for \( q(y) = p(y|x) \), the free energy is maximised and equals \( \log p(x) \).
By maximising the free energy

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

we can split the joint \( p(x, y) \) into \( p(x) \) and \( p(y|x) \)

\[
\log p(x) = \max_{q(y)} \mathcal{F}(x, q)
\]

\[
p(y|x) = \arg\max_{q(y)} \mathcal{F}(x, q)
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By maximising the free energy

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

we can split the joint $p(x, y)$ into $p(x)$ and $p(y|x)$

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

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

You can think of free energy maximisation as a “function” that takes as input a joint $p(x, y)$ and returns as output the (log) marginal and the conditional.
Variational principle

- Given \( p(x, y) \), consider inference tasks

\[
\begin{align*}
\text{1. compute } & \quad p(x) = \int p(x, y) \, dy \\
\text{2. compute } & \quad p(y | x) = \arg\max_q F(x, q)
\end{align*}
\]

Variational principle: we can formulate the marginal inference problems as an optimisation problem.

\[\text{Maximising the free energy } F(x, q) = \mathbb{E}_q(y) \left[ \log p(x, y) q(y) \right]\]

gives

1. \( \log p(x) = \max_q F(x, q) \)
2. \( p(y | x) = \arg\max_q F(x, q) \)

Inference becomes optimisation.

Note: while we use \( q(y) \) to denote the variational distribution, it depends on (fixed) \( x \). Better (and rarer) notation is \( q(y | x) \).
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- Given \( p(x, y) \), consider inference tasks
  1. compute \( p(x) = \int p(x, y) \, dy \)
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Maximising the free energy

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

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- Inference becomes optimisation.
Variational principle

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- Inference becomes optimisation.

- Note: while we use $q(y)$ to denote the variational distribution, it depends on (fixed) $x$. Better (and rarer) notation is $q(y|x)$. 
Solving the optimisation problem

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

- Difficulties when maximising the free energy:

  - Optimisation with respect to pdf/pmf \( q(y) \)
  - Computation of the expectation

Restrict search space to family of variational distributions \( q(y) \) for which \( \mathcal{F}(x, q) \) is computable.

- Family \( Q \) specified by:
  - Independence assumptions, e.g. \( q(y) = \prod_i q(y_i) \), which corresponds to "mean-field" variational inference.
  - Parametric assumptions, e.g. \( q(y_i) = N(y_i; \mu_i, \sigma^2_i) \).

Optimisation is generally challenging: lots of research on how to do it (keywords: stochastic variational inference, black-box variational inference).
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   • 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

2. The variational principle

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 $x = x_o$ and joint pdf/pmf $p(x, y)$, compute $p(y|x_o)$.

Variational approach: estimate the posterior by solving an optimisation problem

\[ \hat{p}(y|x_o) = \arg\max_{q(y) \in Q} F(x, q) \]

$Q$ is the set of pdfs in which we search for the solution

The decomposition of the log marginal gives

\[ \log p(x_o) = KL(q(y)||p(y|x)) + F(x, q) = \text{const} \]

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

\[ \arg\max_{q(y) \in Q} F(x, q) = \arg\min_{q(y) \in Q} KL(q(y)||p(y|x)) \]
Approximate posterior inference

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

$\mathcal{Q}$ is the set of pdfs in which we search for the solution.
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- The decomposition of the log marginal gives

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

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

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

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

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

$$
\arg\max_{q(\mathbf{y}) \in \mathcal{Q}} \mathcal{F}(\mathbf{x}, q) = \arg\min_{q(\mathbf{y}) \in \mathcal{Q}} \text{KL}(q(\mathbf{y})||p(\mathbf{y}|\mathbf{x}))
$$
Nature of the approximation

- When minimising $\text{KL}(q||p)$ with respect to $q$, $q$ will try to be zero where $p$ is small.
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 $\mathcal{Q} = \{q(y) : q(y) = q(y_1)q(y_2)\}$ (independence but no parametric assumptions)

\[
\hat{p}(y|x_0), \text{ i.e. } q(y) \text{ that minimises } \text{KL}(q\|p), \text{ is Gaussian.}
\]

\[
\text{Mean is correct but variances dictated by the marginal variances along the } y_1 \text{ and } y_2 \text{ axes.}
\]

\[
\text{Posterior variance is underestimated.}
\]
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- $\hat{p}(y \mid x_o)$, i.e. $q(y)$ that minimises $\text{KL}(q \| p)$, is Gaussian.
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- Posterior variance is underestimated.
Nature of the approximation

- Assume that true posterior is multimodal, but that the family of variational distributions $Q$ only includes unimodal distributions.
Nature of the approximation

- Assume that true posterior is multimodal, but that the family of variational distributions $Q$ only includes unimodal distributions.
- The learned approximate posterior $\hat{p}(y|x_o)$ only covers one mode ("mode-seeking" behaviour)
Learning by Bayesian inference

- Task 1: For a Bayesian model $p(x|\theta)p(\theta) = p(x, \theta)$, compute the posterior $p(\theta|\mathcal{D})$
Learning by Bayesian inference

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- Formally the same problem as before: \( D = x_0 \) and \( \theta \equiv y \).
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- Task 2: For a Bayesian model \( p(v, h|\theta)p(\theta) = p(v, h, \theta) \), compute the posterior \( p(\theta|D) \) where the data \( D \) are for the visibles \( v \) only.
Learning by Bayesian inference

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▶ With the equivalence \( D = x_o \) and \( (h, \theta) \equiv y \), we are formally back to the problem just studied.
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With the equivalence \( D = x_o \) and \((h, \theta) \equiv y\), we are formally back to the problem just studied.

But the variational distribution \( q(y) \) becomes \( q(h, \theta) \).

Often: assume \( q(h, \theta) \) factorises as \( q(h)q(\theta) \) (see Barber Section 11.5)
Task: For the model $p(v, h; \theta)$, estimate the parameters $\theta$ from data $D$ about the visibles $v$. 
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See slides on *Intractable Likelihood Functions*: the log likelihood function $\ell(\theta)$ is implicitly defined by the integral

$$\ell(\theta) = \log p(D; \theta) = \log \int_h p(D, h; \theta) dh,$$

which is generally intractable.
Task: For the model $p(v, h; \theta)$, estimate the parameters $\theta$ from data $\mathcal{D}$ about the visibles $v$.

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We could approximate $\ell(\theta)$ and its gradient using Monte Carlo integration.
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which is generally intractable.

We could approximate $\ell(\theta)$ and its gradient using Monte Carlo integration.

Here: use the variational approach.
Foundational result that we derived

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

\[
\log p(x) = \max_{q(y)} \mathcal{F}(x, q) \\
p(y|x) = \arg \max_{q(y)} \mathcal{F}(x, q)
\]
Parameter estimation in presence of unobserved variables

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\log p(x) = \text{KL}(q(y) \| p(y|x)) + \mathcal{F}(x, q) \quad \mathcal{F}(x, q) = \mathbb{E}_{q(y)} \left[ \log \frac{p(x, y)}{q(y)} \right]
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- With correspondence

\[
v \equiv x \quad h \equiv y \quad p(v, h; \theta) \equiv p(x, y)
\]

we obtain

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

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

$$\log p(v; \theta) = \max_{q(h)} \mathcal{F}(v, q; \theta) \quad p(h|v; \theta) = \arg\max_{q(h)} \mathcal{F}(v, q; \theta)$$

- Plug in $\mathcal{D}$ for $v$: $\log p(\mathcal{D}; \theta)$ equals $\ell(\theta)$
Approximate MLE by free energy maximisation

With $v = D$ and $\ell(\theta) = p(D; \theta)$, the equations become

\[
\ell(\theta) = \text{KL}(q(h) \| p(h|D)) + J_F(q, \theta)
\]

\[
J_F(q, \theta) = \mathbb{E}_{q(h)} \left[ \log \frac{p(D, h; \theta)}{q(h)} \right]
\]

\[
\ell(\theta) = \max_{q(h)} J_F(q, \theta)
\]

\[
p(h|D; \theta) = \arg\max_{q(h)} J_F(q, \theta)
\]

Write $J_F(q, \theta)$ for $F(D, q; \theta)$ when data $D$ are fixed.
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Write \( J_F(q, \theta) \) for \( F(D, q; \theta) \) when data \( D \) are fixed.

- Maximum likelihood estimation (MLE)

\[
\max_\theta \ell(\theta) = \max_\theta \max_{q(h)} J_F(q, \theta)
\]

\( \text{MLE} = \text{maximise the free energy with respect to } \theta \text{ and } q(h) \)
Approximate MLE by free energy maximisation

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

\[
\ell(\theta) = \text{KL}(q(h)||p(h|\mathcal{D})) + \mathcal{F}(\mathcal{D}, q; \theta) \\
J_{\mathcal{F}}(q, \theta) = \mathbb{E}_{q(h)} \left[ \log \frac{p(\mathcal{D}, h; \theta)}{q(h)} \right]
\]

\[
\ell(\theta) = \max_{q(h)} J_{\mathcal{F}}(q, \theta) \\
p(h|\mathcal{D}; \theta) = \arg\max_{q(h)} J_{\mathcal{F}}(q, \theta)
\]

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

Maximum likelihood estimation (MLE)

\[
\max_{\theta} \ell(\theta) = \max_{\theta} \max_{q(h)} J_{\mathcal{F}}(q, \theta)
\]

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

Restricting the search space \( Q \) for the variational distribution \( q(h) \) due to computational reasons leads to an approximation.
We can write the free energy as

\[ J_F(q, \theta) = \mathbb{E}_{q(h)} \left[ \log \frac{p(D, h; \theta)}{q(h)} \right] = \mathbb{E}_{q(h)} \left[ \log p(D, h; \theta) \right] - \mathbb{E}_{q(h)} \left[ \log q(h) \right] \]
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\[ -\mathbb{E}_{q(h)} \left[ \log q(h) \right] \text{ is the entropy of } q(h) \]

(entropy is a measure of randomness or variability, see e.g. Barber Section 8.2)
We can write the free energy as

\[
J_F(q, \theta) = \mathbb{E}_{q(h)} \left[ \log \frac{p(D, h; \theta)}{q(h)} \right] = \mathbb{E}_{q(h)} [\log p(D, h; \theta)] - \mathbb{E}_{q(h)} [\log q(h)]
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- \( -\mathbb{E}_{q(h)} [\log q(h)] \) is the entropy of \( q(h) \)
  (entropy is a measure of randomness or variability, see e.g. Barber Section 8.2)
- \( \log p(D, h; \theta) \) is the log-likelihood for the filled-in data \( (D, h) \)
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- \( \log p(D, h; \theta) \) is the log-likelihood for the filled-in data \((D, h)\)
- \( \mathbb{E}_{q(h)} [\log p(D, h; \theta)] \) is the weighted average of these “completed” log-likelihoods, with the weighting given by \( q(h) \).
Free energy as sum of completed log likelihood and entropy

\[ J_F(q, \theta) = \mathbb{E}_{q(h)} [\log p(D, h; \theta)] - \mathbb{E}_{q(h)} [\log q(h)] \]

- When maximising \( J_F(q, \theta) \) with respect to \( q \) we look for random variables \( h \) (filled-in data) that
- are maximally variable (large entropy)
- are maximally compatible with the observed data (according to the model \( p(D, h; \theta) \))
- If included in the search space \( Q \), \( p(h|D; \theta) \) is the optimal \( q \), which means that the posterior fulfils the two desiderata best.
Free energy as sum of completed log likelihood and entropy

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Free energy as sum of completed log likelihood and entropy

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

- When maximising $J_{\mathcal{F}}(q, \theta)$ with respect to $q$ we look for random variables $h$ (filled-in data) that
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Free energy as sum of completed log likelihood and entropy

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- If included in the search space \( Q \), \( p(h|D; \theta) \) is the optimal \( q \), which means that the posterior fulfils the two desiderata best.
Variational EM algorithm

Variational expectation maximisation (EM): maximise $J_F(q, \theta)$ by iterating between maximisation with respect to $q$ and maximisation with respect to $\theta$.

(Adapted from http://www.cs.cmu.edu/~tom/10-702/Zoubin-702.pdf)
The optimisation with respect to $q$ is called the “expectation step”

$$\max_{q \in Q} J_F(q, \theta) = \max_{q \in Q} \mathbb{E}_q \left[ \log \frac{p(D, h; \theta)}{q(h)} \right]$$
The optimisation with respect to $q$ is called the “expectation step”

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

Denote the best $q$ by $q^*$ so that $\max_{q \in Q} J_{\mathcal{F}}(q, \theta) = J_{\mathcal{F}}(q^*, \theta)$
The optimisation with respect to \( q \) is called the “expectation step”

\[
\max_{q \in Q} J_F(q, \theta) = \max_{q \in Q} \mathbb{E}_q \left[ \log \frac{p(D, h; \theta)}{q(h)} \right]
\]

Denote the best \( q \) by \( q^* \) so that \( \max_{q \in Q} J_F(q, \theta) = J_F(q^*, \theta) \)

When we maximise with respect to \( \theta \), we need to know \( J_F(q^*, \theta) \),

\[
J_F(q^*, \theta) = \mathbb{E}_{q^*} \left[ \log \frac{p(D, h; \theta)}{q^*(h)} \right],
\]

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

- From

\[ \ell(\theta_k) = \text{KL}(q(h) \| p(h|D)) + J_F(q, \theta_k) \]

We know that the optimal \( q(h) \) is given by \( p(h|D; \theta_k) \)
Classical EM algorithm

- From

\[ \ell(\theta_k) = KL(q(h)\|p(h|\mathcal{D})) + J_F(q, \theta_k) \]

We know that the optimal \( q(h) \) is given by \( p(h|\mathcal{D}; \theta_k) \)

- If we can compute the posterior \( p(h|\mathcal{D}; \theta_k) \), we obtain the (classical) EM algorithm that iterates between:

**Expectation step**

\[
J_F(q^*, \theta) = \mathbb{E}_{p(h|\mathcal{D};\theta_k)}[\log p(\mathcal{D}, h; \theta)] - \mathbb{E}_{p(h|\mathcal{D};\theta_k)} \log p(h|\mathcal{D}; \theta_k)
\]

\( \text{does not depend on } \theta \text{ and does not need to be computed} \)

**Maximisation step**

\[
\arg\max_{\theta} J_F(q^*, \theta) = \arg\max_{\theta} \mathbb{E}_{p(h|\mathcal{D};\theta_k)}[\log p(\mathcal{D}, h; \theta)]
\]
Classical EM algorithm never decreases the log likelihood

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

\[
\max_q J_{\mathcal{F}}(q, \theta_{k-1})
\]
Classical EM algorithm never decreases the log likelihood

- Assume you have updated the parameters and start iteration $k$ with optimisation with respect to $q$
  
  $$\max_q J_F(q, \theta_{k-1})$$

- Optimal solution $q_k^*$ is the posterior so that
  
  $$\ell(\theta_{k-1}) = J_F(q_k^*, \theta_{k-1})$$

Hence: EM yields non-decreasing sequence $\ell(\theta_1), \ell(\theta_2), \ldots$.
Classical EM algorithm never decreases the log likelihood

- Assume you have updated the parameters and start iteration $k$ with optimisation with respect to $q$
  \[
  \max_q J_F(q, \theta_{k-1})
  \]
- Optimal solution $q_{k}^*$ is the posterior so that
  \[
  \ell(\theta_{k-1}) = J_F(q_{k}^*, \theta_{k-1})
  \]
- Optimise with respect to the $\theta$ while keeping $q$ fixed at $q_{k}^*$
  \[
  \max_\theta J_F(q_{k}^*, \theta)
  \]
Classical EM algorithm never decreases the log likelihood

- Assume you have updated the parameters and start iteration $k$ with optimisation with respect to $q$
  \[
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  \]
- Optimal solution $q^*_k$ is the posterior so that
  \[
  \ell(\theta_{k-1}) = J_F(q^*_k, \theta_{k-1})
  \]
- Optimise with respect to the $\theta$ while keeping $q$ fixed at $q^*_k$
  \[
  \max_{\theta} J_F(q^*_k, \theta)
  \]
- Because of maximisation, optimiser $\theta_k$ is such that
  \[
  J_F(q^*_k, \theta_k) \geq J_F(q^*_k, \theta_{k-1}) = \ell(\theta_{k-1})
  \]
Classical EM algorithm never decreases the log likelihood

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  \]

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  \[
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  \]

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  \[
  J_F(q_k^*, \theta_k) \geq J_F(q_k^*, \theta_{k-1}) = \ell(\theta_{k-1})
  \]

- From variational lower bound: $\ell(\theta) \geq J_F(q, \theta)$
  \[
  \ell(\theta_k) \geq J_F(q_k^*, \theta_k) \geq \ell(\theta_{k-1})
  \]

Hence: EM yields non-decreasing sequence $\ell(\theta_1), \ell(\theta_2), \ldots$. 
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

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

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
   - Inference: approximating posteriors
   - Learning with Bayesian models
   - Learning with statistical models and unobserved variables
   - Learning with statistical models and unobs variables: EM algorithm