Statistical Approaches to Learning and Discovery

Variational Approximations

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Review: The EM algorithm

Given a set of observed (visible) variables V, a set of unobserved (hidden / latent / missing) variables H, and model parameters θ, optimize the log likelihood:

$$\mathcal{L}(\theta) = \log p(V|\theta) = \log \int p(H, V|\theta) dH,$$

Using Jensen's inequality, for any distribution of hidden variables $q(H)$ we have:

$$\mathcal{L}(\theta) = \log \int q(H) \frac{p(H, V|\theta)}{q(H)} \, dH \geq \int q(H) \log \frac{p(H, V|\theta)}{q(H)} \, dH = \mathcal{F}(q, \theta),$$

defining the $\mathcal{F}(q, \theta)$ functional, which is a lower bound on the log likelihood.

In the EM algorithm, we alternately optimize $\mathcal{F}(q, \theta)$ wrt q and θ, and we can prove that this will never decrease $\mathcal{L}$.

The E and M steps of EM

The lower bound on the log likelihood:

$$\mathcal{F}(q,\theta) = \int q(H) \log \frac{p(H,V|\theta)}{q(H)} dH = \int q(H) \log p(H,V|\theta) dH + \mathcal{H}(q),$$

where $\mathcal{H}(q) = -\int q(H) \log q(H) dH$ is the entropy of q. We iteratively alternate:

E step: maximize $\mathcal{F}(q,\theta)$ wrt the distribution over hidden variables given the parameters:

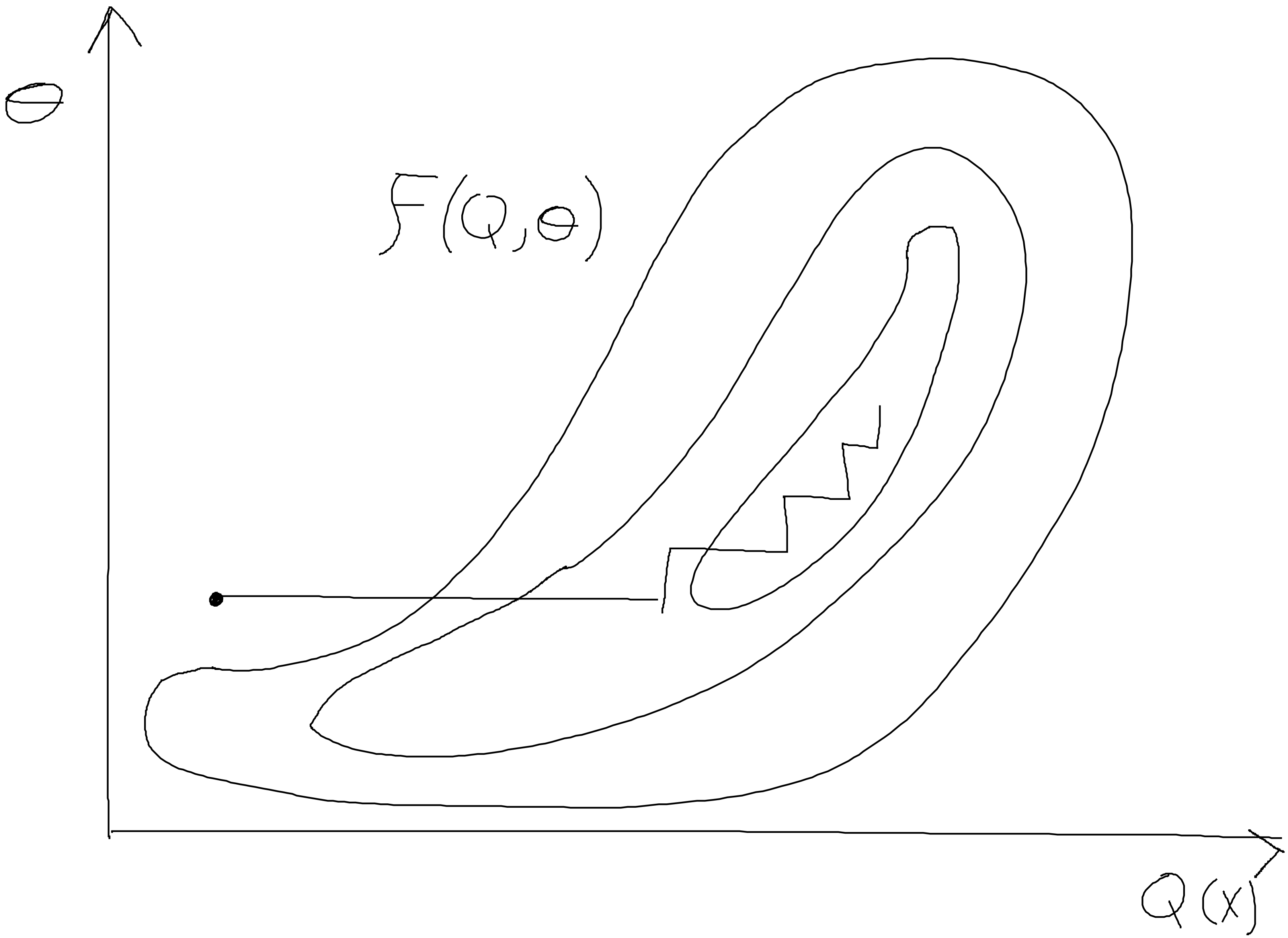
$$q^{(k)}(H) := \underset{q(H)}{\operatorname{argmax}} \ \mathcal{F}\big(q(H), \theta^{(k-1)}\big).$$

M step: maximize $\mathcal{F}(q,\theta)$ wrt the parameters given the hidden distribution:

$$\theta^{(k)} := \underset{\theta}{\operatorname{argmax}} \ \mathcal{F}\big(q^{(k)}(H), \theta\big) = \underset{\theta}{\operatorname{argmax}} \ \int q^{(k)}(H) \log p(H,V|\theta) dH,$$

which is equivalent to optimizing the expected complete-data likelihood $p(H,V|\theta)$, since the entropy of $q(H)$ does not depend on θ.

EM as Coordinate Ascent in $\mathcal{F}$



Variational Approximations to the EM algorithm

Often $p(H|V, \theta)$ is computationally intractable, so an exact E step is out of the question.

Assume some simpler form for $q(H)$, e.g. $q \in \mathcal{Q}$, the set of fully-factorized distributions over the hidden variables: $q(H) = \prod_i q(H_i)$

E step (approximate): maximize $\mathcal{F}(q, \theta)$ wrt the distribution over hidden variables given the parameters:

$$q^{(k)}(H) := \underset{q(H) \in \mathcal{Q}}{\operatorname{argmax}} \; \mathcal{F}\big(q(H), \theta^{(k-1)}\big).$$

M step : maximize $\mathcal{F}(q, \theta)$ wrt the parameters given the hidden distribution:

$$\theta^{(k)} := \underset{\theta}{\operatorname{argmax}} \; \mathcal{F}\big(q^{(k)}(H), \theta\big) = \underset{\theta}{\operatorname{argmax}} \; \int q^{(k)}(H) \log p(H, V|\theta) dH,$$

This maximizes a lower bound on the log likelihood.
Using the fully factorized form of q is sometimes called a **mean-field approximation**.

Example: A Multiple Cause Model

Model with binary latent variables s_i, real-valued observed vector $\mathbf{y}$ and parameters $\boldsymbol{\theta} = \{\{\boldsymbol{\mu}_i, \pi_i\}_{i=1}^K, \sigma^2\}$

$$p(s_1, \ldots, s_K|\boldsymbol{\pi}) = \prod_{i=1}^{K} p(s_i) = \prod_{i=1}^{K} \pi_i^{s_i}(1 - \pi_i)^{(1-s_i)}$$

$$p(\mathbf{y}|s_1, \ldots, s_K|\boldsymbol{\mu}, \sigma^2) = \mathcal{N}(\sum_i s_i \boldsymbol{\mu}_i, \sigma^2 I)$$

EM optimizes lower bound on likelihood:

$$\mathcal{F}(q, \boldsymbol{\theta}) = \langle \log p(\mathbf{s}, \mathbf{y}|\boldsymbol{\theta}) \rangle_{q(\mathbf{s})} - \langle \log q(\mathbf{s}) \rangle_{q(\mathbf{s})}$$

where $\langle \rangle_q$ is expectation under q.

Optimum E step: $q(\mathbf{s}) = p(\mathbf{s}|\mathbf{y}, \boldsymbol{\theta})$ is **exponential** in K.

Example: A Multiple Cause Model (cont)

$$\mathcal{F}(q, \boldsymbol{\theta}) = \langle \log p(\mathbf{s}, \mathbf{y}|\boldsymbol{\theta}) \rangle_{q(\mathbf{s})} - \langle \log q(\mathbf{s}) \rangle_{q(\mathbf{s})}$$

$$\begin{aligned}
\log \quad & p(\mathbf{s}, \mathbf{y}|\boldsymbol{\theta}) + c \\
= \quad & \textstyle\sum_{i=1}^{K} s_i \log \pi_i \quad + (1 - s_i) \log(1 - \pi_i) - D \log \sigma - \frac{1}{2\sigma^2} (\mathbf{y} - \sum_i s_i \boldsymbol{\mu}_i)^\top (\mathbf{y} - \sum_i s_i \boldsymbol{\mu}_i) \\
= \quad & \textstyle\sum_{i=1}^{K} s_i \log \pi_i \quad + (1 - s_i) \log(1 - \pi_i) - D \log \sigma \\
& \qquad - \frac{1}{2\sigma^2} (\mathbf{y}^\top \mathbf{y} - 2 \sum_i s_i \boldsymbol{\mu}_i{}^\top \mathbf{y} + \sum_i \sum_j s_i s_j \boldsymbol{\mu}_i{}^\top \boldsymbol{\mu}_j)
\end{aligned}$$

we therefore need $\langle s_i \rangle$ and $\langle s_i s_j \rangle$ to compute $\mathcal{F}$.

These are the expected sufficient statistics of the hidden variables.

Example: A Multiple Cause Model (cont)

Variational approximation:

$$q(\mathbf{s}) = \prod_i q_i(s_i) = \prod_{i=1}^{K} \lambda_i^{s_i}(1-\lambda_i)^{(1-s_i)}$$

Under this approximation we know $\langle s_i \rangle = \lambda_i$ and $\langle s_i s_j \rangle = \lambda_i \lambda_j + \delta_{ij}(\lambda_i - \lambda_i^2)$.

$$\begin{aligned}\mathcal{F}(\boldsymbol{\lambda}, \boldsymbol{\theta}) = & \sum_i \lambda_i \log \frac{\pi_i}{\lambda_i} + (1-\lambda_i) \log \frac{(1-\pi_i)}{(1-\lambda_i)} \\ & - D \log \sigma - \frac{1}{2\sigma^2}(\mathbf{y} - \sum_i \lambda_i \boldsymbol{\mu}_i)^\top (\mathbf{y} - \sum_i \lambda_i \boldsymbol{\mu}_i) + C(\boldsymbol{\lambda}, \boldsymbol{\mu})\end{aligned}$$

where $C(\boldsymbol{\lambda}, \boldsymbol{\mu}) = -\frac{1}{2\sigma^2} \sum_i (\lambda_i - \lambda_i^2) {\boldsymbol{\mu}_i}^\top \boldsymbol{\mu}_i$

Fixed point equations for multiple cause model

Taking derivatives w.r.t. λ_i:

$$\frac{\partial \mathcal{F}}{\partial \lambda_i} = \log \frac{\pi_i}{1-\pi_i} - \log \frac{\lambda_i}{1-\lambda_i} + \frac{1}{\sigma^2}(\mathbf{y} - \sum_{j \neq i} \lambda_j \boldsymbol{\mu}_j)^\top \boldsymbol{\mu}_i - \frac{1}{2\sigma^2} \boldsymbol{\mu}_i{}^\top \boldsymbol{\mu}_i$$

Setting to zero we get fixed point equations:

$$\lambda_i = f\left(\log \frac{\pi_i}{1-\pi_i} + \frac{1}{\sigma^2}(\mathbf{y} - \sum_{j \neq i} \lambda_j \boldsymbol{\mu}_j)^\top \boldsymbol{\mu}_i - \frac{1}{2\sigma^2} \boldsymbol{\mu}_i{}^\top \boldsymbol{\mu}_i \right)$$

where $f(x) = 1/(1 + \exp(-x))$ is the logistic (sigmoid) function.

Learning algorithm:

E step: run fixed point equations until convergence of $\boldsymbol{\lambda}$ for each data point.
M step: re-estimate $\boldsymbol{\theta}$ given $\boldsymbol{\lambda}$s.

KL divergence

Note that

E step maximize $\mathcal{F}(q, \theta)$ wrt the distribution over hidden variables, given the parameters:

$$q^{(k)}(H) := \underset{q(H) \in \mathcal{Q}}{\operatorname{argmax}} \; \mathcal{F}\big(q(H), \theta^{(k-1)}\big).$$

is equivalent to:

E step minimize $\mathcal{KL}(q \| p(H|V, \theta))$ wrt the distribution over hidden variables, given the parameters:

$$q^{(k)}(H) := \underset{q(H) \in \mathcal{Q}}{\operatorname{argmin}} \int q(H) \log \frac{q(H)}{p(H|V, \theta^{(k-1)})} dH$$

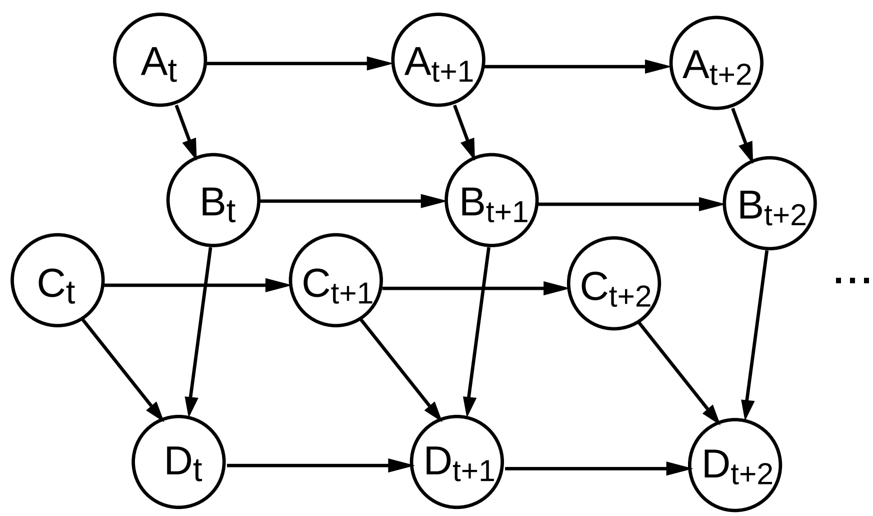
So, at each E step, the variational approximation is trying to find the best approximation to p in $\mathcal{Q}$.
This is related to ideas in information geometry.

Structured Variational Approximations

$q(H)$ need not be completely factorized.

For example, suppose you can partition H into sets H_1 and H_2 such that computing the expected sufficient statistics under $q(H_1)$ and $q(H_2)$ is tractable.
Then $q(H) = q(H_1)q(H_2)$ is tractable.

If you have a graphical model, you may want to factorize $q(H)$ into a product of trees, which are tractable distributions.



More about this later (after we study graphical models).

Variational Approximations to Bayesian Learning

$$\begin{aligned}\log p(V) &= \log \int\int p(V,H|\boldsymbol{\theta})p(\boldsymbol{\theta})\; dH\; d\boldsymbol{\theta} \\ &\geq \int\int q(H,\boldsymbol{\theta}) \log \frac{p(V,H,\boldsymbol{\theta})}{q(H,\boldsymbol{\theta})}\; dH\; d\boldsymbol{\theta}\end{aligned}$$

Constrain $q \in \mathcal{Q}$ s.t. $q(H,\boldsymbol{\theta}) = q(H)q(\boldsymbol{\theta})$.

This results in the **variational Bayesian EM algorithm**.

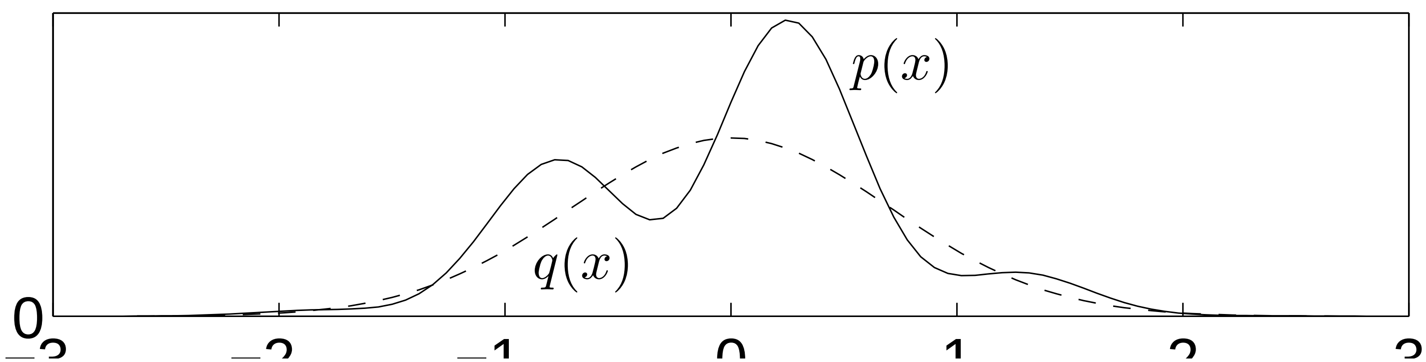
More about this later (when we study model selection).

How tight is the lower bound?

It is hard to compute a nontrivial general upper bound.

To determine how tight the bound is, one can approximate the true likelihood by a variety of other methods.

One approach is to use the variational approximation as as a proposal distribution for **importance sampling** (but we know how hard importance sampling can be in high dimensions).



Readings

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