Lecture 10, 11: Variational Approximations

4F13: Machine Learning

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Motivation

Many statistical inference problems result in intractable computations...

• Bayesian posterior over model parameters:

$$P(\theta|\mathcal{D}) = \frac{P(\mathcal{D}|\theta)P(\theta)}{P(\mathcal{D})}$$

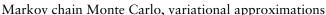
• Computing posterior over hidden variables (e.g. for E step of EM):

$$P(H|V,\theta) = \frac{P(V|H,\theta)P(H|\theta)}{P(V|\theta)}$$

• Computing marginals in a multiply-connected graphical models:

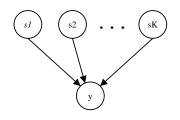
$$P(x_i|x_j=e) = \sum_{\mathbf{x} \setminus \{x_i, x_j\}} P(\mathbf{x}|x_j=e)$$







Example: Binary latent factor model



Model with K binary latent variables, $s_i \in \{0, 1\}$, organised into a vector $\mathbf{s} = (s_1, \dots, s_K)$ real-valued observation vector v parameters $\theta = \{\{\mu_i, \pi_i\}_{i=1}^K, \sigma^2\}$

s ~ Bernoulli $\mathbf{y}|\mathbf{s} \sim \text{Gaussian}$

$$\begin{split} p(s|\pi) &= p(s_1, \dots, s_K|\pi) &= \prod_{i=1}^K p(s_i|\pi_i) = \prod_{i=1}^K \pi_i^{s_i} (1 - \pi_i)^{(1 - s_i)} \\ p(y|s_1, \dots, s_K, \mu, \sigma^2) &= \mathcal{N}\left(\sum_{i=1}^K s_i \mu_i, \sigma^2 I\right) \end{split}$$

EM optimizes bound on likelihood:
$$\mathcal{F}(q,\theta) = \langle \log p(s,y|\theta) \rangle_{q(s)} - \langle \log q(s) \rangle_{q(s)}$$
 where $\langle \rangle_q$ is expectation under q:
$$\langle f(s) \rangle_q \stackrel{\text{def}}{=} \sum_s f(s) q(s)$$

Exact E step: $q(s) = p(s|y, \theta)$ distribution over 2^K states: intractable for large K

Example: Binary latent factor model

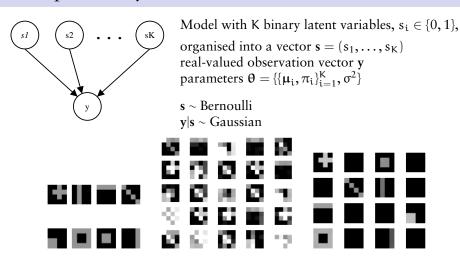


Figure 2: Left panel: Original source images used to generate data. Middle panel: Observed images resulting from mixture of sources. Right panel: Recovered sources

from Lu et al (2004)

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:

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

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:

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

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

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

$$q^{[k]}(H) := \underset{q(H)}{\text{argmax}} \ \mathcal{F}\big(q(H), \theta^{[k-1]}\big) = p(H|V, \theta^{[k-1]}).$$

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

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

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

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. $q \in \Omega$, 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:

$$q^{[k]}(H) := \underset{q(H) \in \mathbb{Q}}{argmax} \ \mathfrak{F}\big(q(H), \textcolor{red}{\theta^{[k-1]}}\big).$$

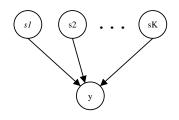
M step: maximize $\mathcal{F}(q,\theta)$ wrt the parameters given the hidden distribution:

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

This maximizes a lower bound on the log likelihood.

Using the fully-factorized q is sometimes called a mean-field approximation.

Example: Binary latent factor model



Model with K binary latent variables, $s_i \in \{0, 1\}$, organised into a vector $\mathbf{s} = (s_1, \dots, s_K)$ real-valued observation vector \mathbf{y} parameters $\mathbf{\theta} = \{\{\mu_i, \pi_i\}_{i=1}^K, \sigma^2\}$

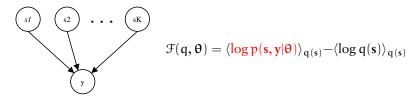
s ~ Bernoulli y|s ~ Gaussian

$$\begin{split} p(s|\pi) &= p(s_1, \dots, s_K|\pi) &= \prod_{i=1}^K p(s_i|\pi_i) = \prod_{i=1}^K \pi_i^{s_i} (1 - \pi_i)^{(1 - s_i)} \\ p(y|s_1, \dots, s_K, \mu, \sigma^2) &= \mathcal{N}\left(\sum_{i=1}^K s_i \mu_i, \sigma^2 I\right) \end{split}$$

EM optimizes bound on likelihood: $\mathfrak{F}(q,\theta) = \langle \log p(s,y|\theta) \rangle_{q(s)} - \langle \log q(s) \rangle_{q(s)}$ where $\langle \rangle_q$ is expectation under q: $\langle f(s) \rangle_q \stackrel{\text{def}}{=} \sum_s f(s) q(s)$

Exact E step: $q(s) = p(s|y, \theta)$ distribution over 2^K states: intractable for large K

Example: Binary latent factors model (cont.)



$$\begin{split} \log & & p(\boldsymbol{s}, \boldsymbol{y}|\boldsymbol{\theta}) + c \\ & = & \sum_{i=1}^K s_i \log \pi_i & + (1-s_i) \log(1-\pi_i) - D \log \sigma - \frac{1}{2\sigma^2} (\boldsymbol{y} - \sum_i s_i \mu_i)^\top (\boldsymbol{y} - \sum_i s_i \mu_i) \\ & = & \sum_{i=1}^K s_i \log \pi_i & + (1-s_i) \log(1-\pi_i) - D \log \sigma \\ & & - \frac{1}{2\sigma^2} \left(\boldsymbol{y}^\top \boldsymbol{y} - 2 \sum_i s_i \mu_i^\top \boldsymbol{y} + \sum_i \sum_i s_i s_j \mu_i^\top \mu_j \right) \end{split}$$

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

These are the expected *sufficient statistics* of the hidden variables.

Example: Binary latent factors model (cont.)

Variational approximation:

$$q(s) = \prod_{\mathfrak{i}} q_{\mathfrak{i}}(s_{\mathfrak{i}}) = \prod_{\mathfrak{i}=1}^K \lambda_{\mathfrak{i}}^{s_{\mathfrak{i}}} (1-\lambda_{\mathfrak{i}})^{(1-s_{\mathfrak{i}})}$$

where λ_i is a parameter of the variational approximation modelling the posterior mean of s_i (compare to π_i which models the *prior* mean of s_i).

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

$$\begin{split} \mathcal{F}(\pmb{\lambda},\pmb{\theta}) &= \sum_i \lambda_i \log \frac{\pi_i}{\lambda_i} + (1-\lambda_i) \log \frac{(1-\pi_i)}{(1-\lambda_i)} \\ &- D \log \sigma - \frac{1}{2\sigma^2} (y - \sum_i \lambda_i \mu_i)^\top (y - \sum_i \lambda_i \mu_i) \\ &- \frac{1}{2\sigma^2} \sum_i (\lambda_i - \lambda_i^2) {\mu_i}^\top \mu_i - \frac{D}{2} \log(2\pi) \end{split}$$

Fixed point equations for the binary latent factor model

Taking derivatives w.r.t. λ_i :

$$\frac{\partial \mathcal{F}}{\partial \lambda_i} = log \frac{\pi_i}{1-\pi_i} - log \frac{\lambda_i}{1-\lambda_i} + \frac{1}{\sigma^2} (y - \sum_{j \neq i} \lambda_j \mu_j)^\top \mu_i - \frac{1}{2\sigma^2} {\mu_i}^\top \mu_i$$

Setting to zero we get fixed point equations:

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

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

Learning algorithm:

E step: run fixed point equations until convergence of λ *for each data point*. **M step:** re-estimate θ given λ s.

KL divergence

Note that

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

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

is equivalent to:

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

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

So, in each E step, the algorithm tries to find the best approximation to p in Q. This is related to ideas in *information geometry*.

Variational Approximations to Bayesian Learning

$$\begin{split} \log p(V) &= \log \iint p(V, H|\theta) p(\theta) \; dH \; d\theta \\ &\geqslant \iint q(H, \theta) \log \frac{p(V, H, \theta)}{q(H, \theta)} \; dH \; d\theta \end{split}$$

Constrain $q \in \Omega$ s.t. $q(H, \theta) = q(H)q(\theta)$.

This results in the variational Bayesian EM algorithm.

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

Variational Approximations and Graphical Models I

Let $q(H) = \prod_i q_i(H_i)$.

Variational approximation maximises \mathfrak{F} :

$$\mathfrak{F}(q) = \int q(H) \log p(H,V) dH - \int q(H) \log q(H) dH$$

Focusing on one term, q_j , we can write this as:

$$\mathcal{F}(q_j) \ = \ \int q_j(H_j) \Big\langle \log p(H,V) \Big\rangle_{\sim q_j(H_j)} dH_j - \int q_j(H_j) \log q_j(H_j) dH_j + const$$

Where $\langle \cdot \rangle_{\sim \mathfrak{q}_{\mathfrak{i}}(H_{\mathfrak{i}})}$ denotes averaging w.r.t. $\mathfrak{q}_{\mathfrak{i}}(H_{\mathfrak{i}})$ for all $\mathfrak{i} \neq \mathfrak{j}$

Optimum occurs when:

$$q_{\mathfrak{j}}^{*}(H_{\mathfrak{j}}) = \frac{1}{Z} \exp \left\langle \log p(H,V) \right\rangle_{\sim q_{\mathfrak{j}}(H_{\mathfrak{j}})}$$

Variational Approximations and Graphical Models II

Optimum occurs when:

$$q_{j}^{*}(H_{j}) = \frac{1}{Z} \exp \left\langle \log p(H, V) \right\rangle_{\sim q_{j}(H_{j})}$$

Assume graphical model: $p(H, V) = \prod_i p(X_i|pa_i)$

$$\begin{split} \log q_j^*(H_j) &= \left\langle \left. \sum_i \log p(X_i|pa_i) \right\rangle_{\sim q_j(H_j)} + const \right. \\ &= \left. \left\langle \log p(H_j|pa_j) \right\rangle_{\sim q_j(H_j)} + \sum_{k \in Ch_j} \left\langle \log p(X_k|pa_k) \right\rangle_{\sim q_j(H_j)} + const \end{split}$$

This defines messages that get passed between nodes in the graph. Each node receives messages from its Markov boundary: parents, children and parents of children.

Variational Message Passing (Winn and Bishop, 2004)

Expectation Propagation (EP)

Data (iid) $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}\$, model $\mathfrak{p}(\mathbf{x}|\theta)$, with parameter prior $\mathfrak{p}(\theta)$.

The parameter posterior is:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{p(\mathcal{D})} p(\boldsymbol{\theta}) \prod_{i=1}^{N} p(\mathbf{x}^{(i)}|\boldsymbol{\theta})$$
$$p(\boldsymbol{\theta}) \prod_{i=1}^{N} p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) = \prod_{i=1}^{N} f_{i}(\boldsymbol{\theta})$$

We can write this as product of factors over θ :

$$p(\boldsymbol{\theta}) \prod_{i=1}^{N} p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) = \prod_{i=0}^{N} f_{i}(\boldsymbol{\theta})$$

where $f_0(\theta) \stackrel{\text{def}}{=} p(\theta)$ and $f_i(\theta) \stackrel{\text{def}}{=} p(\mathbf{x}^{(i)}|\theta)$ and we will ignore the constants.

We wish to approximate this by a product of *simpler* terms:

$$q(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \prod_{i=1}^{N} \tilde{f}_{i}(\boldsymbol{\theta})$$

$$\begin{split} & \underset{q(\theta)}{\text{min}} \, \mathcal{KL} \Big(\prod_{i=0}^{N} f_i(\theta) \Big\| \prod_{i=0}^{N} \tilde{f}_i(\theta) \Big) & \text{(intractable)} \\ & \underset{\tilde{f}_i(\theta)}{\text{min}} \, \mathcal{KL} \left(f_i(\theta) \| \tilde{f}_i(\theta) \right) & \text{(simple, non-iterative, inaccurate)} \\ & \underset{\tilde{f}_i(\theta)}{\text{min}} \, \mathcal{KL} \Big(f_i(\theta) \prod_{i \neq j} \tilde{f}_j(\theta) \Big\| \tilde{f}_i(\theta) \prod_{i \neq j} \tilde{f}_j(\theta) \Big) & \text{(simple, iterative, accurate)} \leftarrow EP \end{split}$$

Expectation Propagation II

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\begin{split} & \text{Input } f_0(\theta) \dots f_N(\theta) \\ & \text{Initialize } \tilde{f}_0(\theta) = f_0(\theta), \, \tilde{f}_i(\theta) = 1 \text{ for } i > 0, \, q(\theta) = \prod_i \tilde{f}_i(\theta) \\ & \text{repeat} \\ & \text{ for } i = 0 \dots N \text{ do} \\ & \text{Deletion: } q_{\setminus i}(\theta) \leftarrow \frac{q(\theta)}{\tilde{f}_i(\theta)} = \prod_{j \neq i} \tilde{f}_j(\theta) \\ & \text{Projection: } \tilde{f}_i^{new}(\theta) \leftarrow \arg\min_{f(\theta)} \mathcal{KL}(f_i(\theta)q_{\setminus i}(\theta) \| f(\theta)q_{\setminus i}(\theta)) \\ & \text{Inclusion: } q(\theta) \leftarrow \tilde{f}_i^{new}(\theta) \, q_{\setminus i}(\theta) \\ & \text{ end for } \\ & \text{until convergence} \end{split}
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The EP algorithm. Some variations are possible: here we assumed that f_0 is in the exponential family, and we updated sequentially over i.

- Tries to minimize the opposite KL to variational methods
- $\tilde{f}_i(\theta)$ in exponential family \rightarrow projection step is moment matching
- No convergence guarantee (although convergent forms can be developed)

Some Further Readings

- MacKay, D.J.C. (2003) Information Theory, Inference, and Learning Algorithms. Chapter 33.
- Bishop, C.M. (2006) Pattern Recognition and Machine Learning.
- Winn, J. and Bishop, C.M. (2005) Variational Message Passing. J. Machine Learning Research. http://johnwinn.org/Publications/papers/VMP2005.pdf
- Lu, X., Hauskrecht, M., and Day, R.S. (2004) Modeling cellular processes with variational Bayesian cooperative vector quantizer. In the Proceedings of the Pacific Symposium on Biocomputing (PSB) 9:533-544.
 - http://psb.stanford.edu/psb-online/proceedings/psb04/lu.pdf
- Minka, T.P. (2004) Roadmap to EP: http://research.microsoft.com/~minka/papers/ep/roadmap.html
- Ghahramani, Z. (1995) Factorial learning and the EM algorithm. In Adv Neur Info Proc Syst 7.
 - http://learning.eng.cam.ac.uk/zoubin/zoubin/factorial.abstract.html
- Jordan, M.I., Ghahramani, Z., Jaakkola, T.S. and Saul, L.K. (1999) An Introduction to Variational Methods for Graphical Models. Machine Learning 37:183-233. Available at: http://learning.eng.cam.ac.uk/zoubin/papers/varintro.pdf

Appendix: Binary latent factor model for i.i.d. data

Assume data set $\mathcal{D} = \{y^{(1)}...,y^{(N)}\}$ of N points and params $\theta = \{\{\mu_i, \pi_i\}_{i=1}^K, \sigma^2\}$. Use a factorised distribution:

$$q(s) = \prod_{n=1}^N q_n(s^{(n)}) = \prod_{n=1}^N \prod_{i=1}^K q_n(s^{(n)}_i) = \prod_n \prod_i (\lambda^{(n)}_i)^{s^{(n)}_i} (1-\lambda^{(n)}_i)^{(1-s^{(n)}_i)}$$

$$\begin{array}{lll} & & & \\ p(\mathcal{D}|\theta) & = & \displaystyle \prod_{n=1}^{N} p(y^{(n)}|\theta) \\ & & p(y^{(n)}|\theta) & = & \displaystyle \sum_{s} p(y^{(n)}|s,\mu,\sigma) p(s|\pi) \\ & & \mathcal{F}(q(s),\theta) & = & \displaystyle \sum_{n} \mathcal{F}_{n}(q_{n}(s^{(n)}),\theta) \leqslant \log p(\mathcal{D}|\theta) \\ & & \\ \mathcal{F}_{n}(q_{n}(s^{(n)}),\theta) & = & \left\langle \log p(s^{(n)},y^{(n)}|\theta) \right\rangle_{q_{n}(s^{(n)})} - \left\langle \log q_{n}(s^{(n)}) \right\rangle_{q_{n}(s^{(n)})} \end{array}$$

We need to optimise w.r.t. $q_n(s^{(n)})$ for each data point, so

E step: optimize $q_n(s^{(n)})$ (i.e. $\lambda^{(n)}$) for each n.

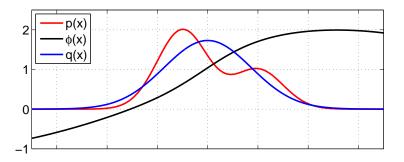
M step: re-estimate θ given $q_n(s^{(n)})$'s.

Appendix: 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 this will generally not work well. See exercise 33.6 in David MacKay's textbook.