CSC412 – Probabilistic Learning & Reasoning — Sam Roweis

Lecture 9:

The EM Algorithm

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Reminder: Learning with Latent Variables

- With latent variables, the probability contains a sum, so the log likelihood has all parameters coupled together:

$$\ell(\theta; \mathcal{D}) = \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta) = \log \sum_{\mathbf{z}} p(\mathbf{z}|\theta_z) p(\mathbf{x}|\mathbf{z}, \theta_x)$$

  (we can also consider continuous $\mathbf{z}$ and replace $\sum$ with $\int$)
- If the latent variables were observed, parameters would decouple again and learning would be easy:

$$\ell(\theta; \mathcal{D}) = \log p(\mathbf{x}, \mathbf{z}|\theta) = \log p(\mathbf{z}|\theta_z) + \log p(\mathbf{x}|\mathbf{z}, \theta_x)$$

- One idea: ignore this fact, compute $\partial\ell/\partial\theta$, and do learning with a smart optimizer like conjugate gradient.
- Another idea: what if we use our current parameters to *guess* the values of the latent variables, and then do fully-observed learning? This back-and-forth trick might make optimization easier.

Expectation-Maximization (EM) Algorithm

- Iterative algorithm with two linked steps:
  E-step: fill in values of $\hat{\mathbf{z}}^t$ using $p(\mathbf{z}|\mathbf{x}, \theta^t)$.
  M-step: update parameters using $\theta^{t+1} \leftarrow \text{argmax}\ \ell(\theta; \mathbf{x}, \hat{\mathbf{z}}^t)$.
- E-step involves inference, which we need to do at runtime anyway. M-step is no harder than in fully observed case.
- We will prove that this procedure monotonically improves ℓ (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood (as any optimizer should).
- Note: EM is an optimization strategy for objective functions that can be interpreted as likelihoods in the presence of missing data.
- EM is *not* a cost function such as "maximum-likelihood". EM is *not* a model such as "mixture-of-Gaussians".

Complete & Incomplete Log Likelihoods

- Observed variables $\mathbf{x}$, latent variables $\mathbf{z}$, parameters θ:

$$\ell_c(\theta; \mathbf{x}, \mathbf{z}) = \log p(\mathbf{x}, \mathbf{z}|\theta)$$

  is the *complete log likelihood*.
- Usually optimizing $\ell_c(\theta)$ given both $\mathbf{z}$ and $\mathbf{x}$ is straightforward. (e.g. class conditional Gaussian fitting, linear regression)
- With $\mathbf{z}$ unobserved, we need the log of a marginal probability:

$$\ell(\theta; \mathbf{x}) = \log p(\mathbf{x}|\theta) = \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta)$$

  which is the *incomplete log likelihood*.

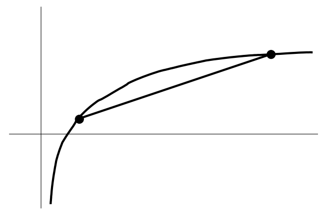
Expected Complete Log Likelihood

- For *any* distribution $q(\mathbf{z})$ define *expected complete log likelihood*:

$$\ell_q(\theta; \mathbf{x}) = \langle \ell_c(\theta; \mathbf{x}, \mathbf{z}) \rangle_q \equiv \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$$

- Amazing fact: $\ell(\theta) \geq \ell_q(\theta) + \mathcal{H}(q)$ because of concavity of $\log$:

$$\begin{aligned} \ell(\theta; \mathbf{x}) &= \log p(\mathbf{x}|\theta) \\ &= \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta) \\ &= \log \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \\ &\geq \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \end{aligned}$$



- Where the inequality is called *Jensen's inequality*.
  (It is only true for distributions: $\sum q(\mathbf{z}) = 1$; $q(\mathbf{z}) > 0$.)

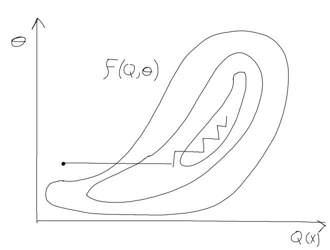
Lower Bounds and Free Energy

- For fixed data $\mathbf{x}$, define a functional called the *free energy*:

$$F(q, \theta) \equiv \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \quad \leq \ell(\theta)$$

- The EM algorithm is coordinate-ascent on F:

$$\begin{aligned} \textbf{E-step}: \quad q^{t+1} &= \operatorname{argmax}_q \; F(q, \theta^t) \\ \textbf{M-step}: \quad \theta^{t+1} &= \operatorname{argmax}_\theta \; F(q^{t+1}, \theta^t) \end{aligned}$$



M-step: maximization of expected ℓ_c

- Note that the free energy breaks into two terms:

$$\begin{aligned} F(q, \theta) &= \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log \frac{p(\mathbf{x}, \mathbf{z}|\theta)}{q(\mathbf{z}|\mathbf{x})} \\ &= \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta) - \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log q(\mathbf{z}|\mathbf{x}) \\ &= \ell_q(\theta; \mathbf{x}) + \mathcal{H}(q) \end{aligned}$$

  (this is where its name comes from)
- The first term is the expected complete log likelihood (energy) and the second term, which does not depend on θ, is the entropy.
- Thus, in the M-step, maximizing with respect to θ for fixed q we only need to consider the first term:

$$\theta^{t+1} = \operatorname{argmax}_\theta \ell_q(\theta; \mathbf{x}) = \operatorname{argmax}_\theta \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$$

E-step: inferring latent posterior

- Claim: the optimim setting of q in the E-step is:

$$q^{t+1} = p(\mathbf{z}|\mathbf{x}, \theta^t)$$

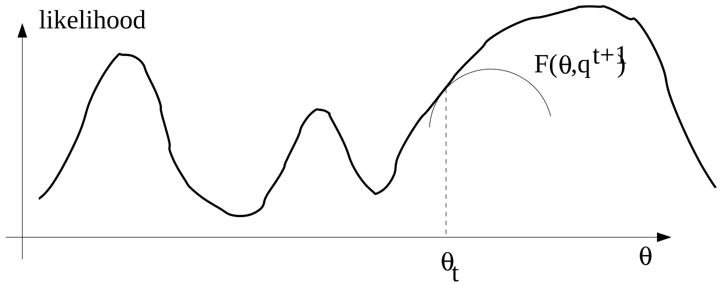
- This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform classification).
- Proof (easy): this setting saturates the bound $\ell(\theta; \mathbf{x}) \geq F(q, \theta)$

$$\begin{aligned} F(p(\mathbf{z}|\mathbf{x}, \theta^t), \theta^t) &= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \log \frac{p(\mathbf{x}, \mathbf{z}|\theta^t)}{p(\mathbf{z}|\mathbf{x}, \theta^t)} \\ &= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \log p(\mathbf{x}|\theta^t) \\ &= \log p(\mathbf{x}|\theta^t) \textstyle\sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}, \theta^t) \\ &= \ell(\theta; \mathbf{x}) \cdot 1 \end{aligned}$$

- Can also show this result using variational calculus or the fact that $\ell(\theta) - F(q, \theta) = \mathrm{KL}[q||p(\mathbf{z}|\mathbf{x}, \theta)]$

EM Constructs Sequential Convex Lower Bounds

- Consider the likelihood function and the function $F(q^{t+1},\cdot)$.



Recap: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds ML parameters when the original (hard) problem can be broken up into two (easy) pieces:
  1. Estimate some "missing" or "unobserved" data from observed data and current parameters.
  2. Using this "complete" data, find the maximum likelihood parameter estimates.
- Alternate between filling in the latent variables using our best guess (posterior) and updating the paramters based on this guess:
  E-step: $q^{t+1} = p(\mathbf{z}|\mathbf{x}, \theta^t)$
  M-step: $\theta^{t+1} = \mathrm{argmax}_\theta \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

Example: Mixtures of Gaussians

- Recall: a mixture of K Gaussians:
  $p(\mathbf{x}|\theta) = \sum_k \alpha_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$
  $\ell(\theta; \mathcal{D}) = \sum_n \log \sum_k \alpha_k \mathcal{N}(\mathbf{x}^n|\mu_k, \Sigma_k)$
- Learning with EM algorithm:

$$\mathbf{E-step}: \quad p^t_{kn} = \mathcal{N}(\mathbf{x}^n|\mu^t_k, \Sigma^t_k)$$

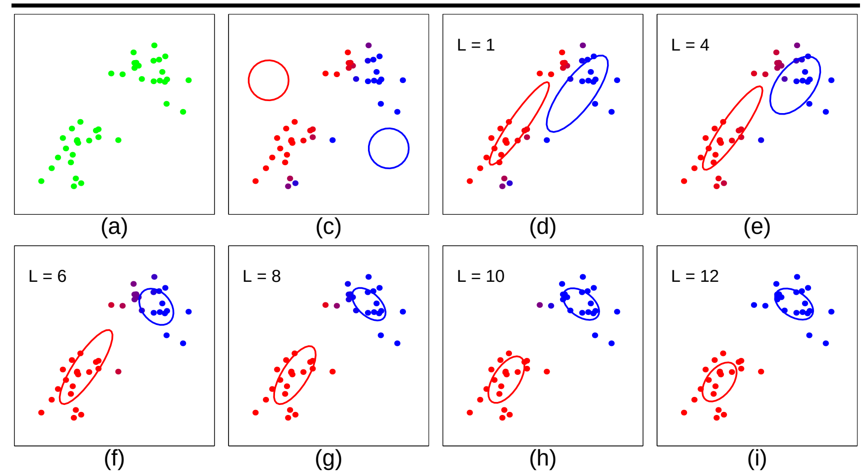
$$q^{t+1}_{kn} = p(z=k|\mathbf{x}^n, \theta^t) = \frac{\alpha^t_k p^t_{kn}}{\sum_j \alpha^t_j p^t_{kn}}$$

$$\mathbf{M-step}: \quad \mu^{t+1}_k = \frac{\sum_n q^{t+1}_{kn} \mathbf{x}^n}{\sum_n q^{t+1}_{kn}}$$

$$\Sigma^{t+1}_k = \frac{\sum_n q^{t+1}_{kn} (\mathbf{x}^n - \mu^{t+1}_k)(\mathbf{x}^n - \mu^{t+1}_k)^\top}{\sum_n q^{t+1}_{kn}}$$

$$\alpha^{t+1}_k = \frac{1}{M} \sum_n q^{t+1}_{kn}$$

EM for MOG



Derivation of M-step

- Expected complete log likelihood $\ell_q(\theta; \mathcal{D})$:

$$\sum_n \sum_k q_{kn} \left[\log \alpha_k - \frac{1}{2}(\mathbf{x}^n - \mu_k^{t+1})^\top \Sigma_k^{-1} (\mathbf{x}^n - \mu_k^{t+1}) - \frac{1}{2} \log |2\pi\Sigma_k| \right]$$

- For fixed q we can optimize the parameters:

$$\frac{\partial \ell_q}{\partial \mu_k} = \Sigma_k^{-1} \sum_n q_{kn}(\mathbf{x}^n - \mu_k)$$

$$\frac{\partial \ell_q}{\partial \Sigma_k^{-1}} = \frac{1}{2} \sum_n q_{kn} \left[\Sigma_k^\top - (\mathbf{x}^n - \mu_k^{t+1})(\mathbf{x}^n - \mu_k^{t+1})^\top \right]$$

$$\frac{\partial \ell_q}{\partial \alpha_k} = \frac{1}{\alpha_k} \sum_n q_{kn} - \lambda \qquad (\lambda = M)$$

- Fact: $\frac{\partial \log |A^{-1}|}{\partial A^{-1}} = A^\top$ and $\frac{\partial \mathbf{x}^\top A \mathbf{x}}{\partial A} = \mathbf{x}\mathbf{x}^\top$

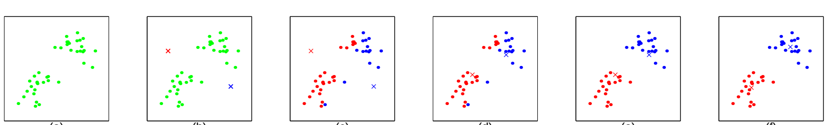
Compare: K-means

- The EM algorithm for mixtures of Gaussians is just like a soft version of the K-means algorithm.
- In the K-means "E-step" we do hard assignment:

$$c_n^{t+1} = \text{argmin}_k (\mathbf{x}^n - \mu_k^t)^\top \Sigma_k^{-1} (\mathbf{x}^n - \mu_k^t)$$

- In the K-means "M-step" we update the means as the weighted sum of the data, but now the weights are 0 or 1:

$$\mu_k^{t+1} = \frac{\sum_n [c_k^{t+1} = n] \mathbf{x}^n}{\sum_n [c_k^{t+1} = n]}$$



(a) (b) (c) (d) (e) (f)

Partially Hidden Data

- Of course, we can learn when there are missing (hidden) variables on some cases and not on others.
- In this case the cost function was:

$$\ell(\theta; \mathcal{D}) = \sum_{\text{complete}} \log p(\mathbf{x}^c, \mathbf{y}^c | \theta) + \sum_{\text{missing}} \log \sum_{\mathbf{y}} \log p(\mathbf{x}^m, \mathbf{y} | \theta)$$

- Now you can think of this in a new way: in the E-step we estimate the hidden variables on the incomplete cases only.
- The M-step optimizes the log likelihood on the complete data plus the expected likelihood on the incomplete data using the E-step.

A Report Card for EM

- Some good things about EM:
  - no learning rate parameter
  - very fast for low dimensions
  - each iteration guaranteed to improve likelihood
  - adapts unused units rapidly
- Some bad things about EM:
  - can get stuck in local minima
  - both steps require considering *all* explanations of the data which is an exponential amount of work in the dimension of θ
- EM is typically used with mixture models, for example mixtures of Gaussians or mixtures of experts. The "missing" data are the labels showing which sub-model generated each datapoint.
  Very common: also used to train HMMs, Boltzmann machines, ...

- Sparse EM:
  Do not recompute exactly the posterior probability on each data point under all models, because it is almost zero.
  Instead keep an "active list" which you update every once in a while.
- Generalized (Incomplete) EM: It might be hard to find the ML parameters in the M-step, even given the completed data. We can still make progress by doing an M-step that improves the likelihood a bit (e.g. gradient step).