Lecture 8:

Unsupervised Learning & EM Algorithm

November 1, 2005

Recall: Missing Outputs 1

- Remember that you can think of unsupervised learning as supervised learning in which all the outputs are *missing*:
  - Clustering == classification with missing labels.
  - Dimensionality reduction == regression with missing targets.
- Density estimation is actually very general and encompasses the two problems above and a whole lot more.
- Today, let's focus on the idea of missing (unobserved) variables...

Partially Unobserved Variables 2

- Certain variables $\mathbf{q}$ in our models may be *unobserved*, either at training time or at test time or both.
- If the are occasionally unobserved they are *missing data*. e.g. undefinied inputs, missing class labels, erroneous target values
- In this case, we define a new cost function in which we *integrate out* the missing values at training or test time:

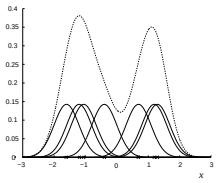
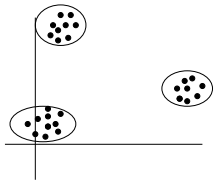
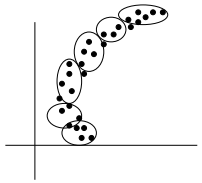
$$\ell(\theta;\mathcal{D}) = \sum_{\text{complete}} \log p(\mathbf{x}^c,\mathbf{y}^c|\theta) + \sum_{\text{missing}} \log p(\mathbf{x}^m|\theta)$$
$$= \sum_{\text{complete}} \log p(\mathbf{x}^c,\mathbf{y}^c|\theta) + \sum_{\text{missing}} \log \sum_{\mathbf{y}} p(\mathbf{x}^m,\mathbf{y}|\theta)$$

- Variables which are *always* unobserved are called *latent variables* or sometimes *hidden variables*.

Latent Variables 3

- What should we do when a variable $\mathbf{z}$ is *always* unobserved? Depends on where it appears in our model. If we never condition on it when computing the probability of the variables we *do* observe, then we can just forget about it and integrate it out. e.g. given $\mathbf{y},\mathbf{x}$ fit the model $p(\mathbf{z},\mathbf{y}|\mathbf{x}) = p(\mathbf{z}|\mathbf{y})p(\mathbf{y}|\mathbf{x},\mathbf{w})p(\mathbf{w})$.
- But if $\mathbf{z}$ is conditioned on, we need to model it: e.g. given $\mathbf{y},\mathbf{x}$ fit the model $p(\mathbf{y}|\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{y}|\mathbf{x},\mathbf{z})p(\mathbf{z})$
- Latent variables may appear naturally, from the structure of the problem. But also, we may want to *intentionally* introduce latent variables to model complex dependencies between variables without looking at the dependencies between them directly.
- This can actually simplify the model, and the most common example of this is in *mixture modeling*.

- Mixture models are the most basic possible latent variable model, having only a single discrete latent variable z.
- Idea: allow different submodels (experts) to contribute to the (conditional) density model in different parts of the space.
- Divide and conquer: use simple parts to build complex models. (e.g. multimodal densities, or piecewise-linear regressions).

- Exactly like a class-conditional model but the class is unobserved and so we sum it out. What we get is a perfectly valid density:

$$p(\mathbf{x}|\theta) = \sum_{k=1}^{K} p(z=k|\theta_z)p(\mathbf{x}|z=k,\theta_k)$$
$$= \sum_{k} \alpha_k p_k(\mathbf{x}|\theta_k)$$

  where the "mixing proportions" add to one: $\sum_k \alpha_k = 1$.
- We can use Bayes' rule to compute the posterior probability of the mixture component given some data:

$$r_k(\mathbf{x}) = p(z=k|\mathbf{x},\theta) = \frac{\alpha_k p_k(\mathbf{x}|\theta_k)}{\sum_j \alpha_j p_j(\mathbf{x}|\theta_j)}$$

  these quantities are called *responsibilities*.
  You've seen them many times before; now you know their names!

- In fully observed settings, the probability model is a product, thus the log likelihood is a sum where terms decouple.

$$\ell(\theta;\mathcal{D}) = \sum_n \log p(\mathbf{y}_n, \mathbf{x}_n|\theta)$$
$$= \sum_n \log p(\mathbf{x}_n|\theta_x) + \sum_n \log p(\mathbf{y}_n|\mathbf{x}_n,\theta_y)$$

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

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

- Likelihood $\ell(\theta) = \log \sum_{\mathbf{z}} p(\mathbf{z}|\theta_z)p(\mathbf{x}|\mathbf{z},\theta_x)$ couples parameters:
- We can treat this as a black box probability function and just try to optimize the likelihood as a function of θ.
  We did this many times before by taking gradients.
- However, sometimes taking advantage of the latent variable structure can make parameter estimation easier.
- Good news: today we will see the *EM algorithm* which allows us to treat learning with latent variables using fully observed tools.
- Basic trick: guess the values you don't know.
  Basic math: use convexity to lower bound the likelihood.

- We can learn mixture densities using gradient descent on the likelihood as usual. The gradients are quite interesting:

$$\ell(\theta) = \log p(\mathbf{x}|\theta) = \log \sum_k \alpha_k p_k(\mathbf{x}|\theta_k)$$

$$\frac{\partial \ell}{\partial \theta} = \frac{1}{p(\mathbf{x}|\theta)} \sum_k \alpha_k \frac{\partial p_k(\mathbf{x}|\theta_k)}{\partial \theta}$$

$$= \sum_k \alpha_k \frac{1}{p(\mathbf{x}|\theta)} p_k(\mathbf{x}|\theta_k) \frac{\partial \log p_k(\mathbf{x}|\theta_k)}{\partial \theta}$$

$$= \sum_k \alpha_k \frac{p_k(\mathbf{x}|\theta_k)}{p(\mathbf{x}|\theta)} \frac{\partial \ell_k}{\partial \theta_k} = \sum_k \alpha_k r_k \frac{\partial \ell_k}{\partial \theta_k}$$

- In other words, the gradient is the *responsibility weighted sum* of the individual log likelihood gradients. (cf. MOEs)

- Mixtures of Experts are also called conditional mixtures. Exactly like a class-conditional classification model, except the class is unobserved and so we sum it out:

$$p(\mathbf{y}|\mathbf{x}, \theta) = \sum_{k=1}^{K} p(z = k|\mathbf{x}, \theta_z) p(\mathbf{y}|z = k, \mathbf{x}, \theta_k)$$

$$= \sum_k \alpha_k(\mathbf{x}|\theta_z) p_k(\mathbf{y}|\mathbf{x}, \theta_k)$$

where $\sum_k \alpha_k(\mathbf{x}) = 1 \quad \forall \mathbf{x}$.

- Harder: must learn $\alpha_k(\mathbf{x})$ (unless chose z independent of $\mathbf{x}$). The $\alpha_k(\mathbf{x})$ are exactly what we called the *gating function*.
- We can still use Bayes' rule to compute the posterior probability of the mixture component given some data:

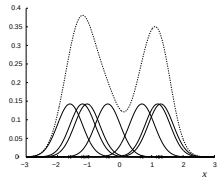
$$p(z = k|\mathbf{x}, \mathbf{y}, \theta) = \frac{\alpha_k(\mathbf{x}) p_k(\mathbf{y}|\mathbf{x}, \theta_k)}{\sum_j \alpha_j(\mathbf{x}) p_j(\mathbf{y}|\mathbf{x}, \theta_j)}$$

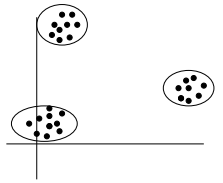
- Consider a mixture of K Gaussian components:

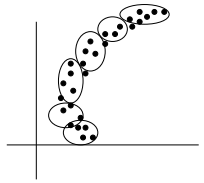
$$p(\mathbf{x}|\theta) = \sum_k \alpha_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

$$p(z = k|\mathbf{x}, \theta) = \frac{\alpha_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}{\sum_j \alpha_j \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}$$

$$\ell(\theta; \mathcal{D}) = \sum_n \log \sum_k \alpha_k \mathcal{N}(\mathbf{x}^n|\mu_k, \Sigma_k)$$







- Density model: $p(x|\theta)$ is a familiarity signal.
  Clustering: $p(z|\mathbf{x}, \theta)$ is the assignment rule, $-\ell(\theta)$ is the cost.

- We can learn mixtures of Gaussians using gradient descent. For example, the gradients of the means:

$$\ell(\theta) = \log p(\mathbf{x}|\theta) = \log \sum_k \alpha_k p_k(\mathbf{x}|\theta_k)$$

$$\frac{\partial \ell}{\partial \theta} = \sum_k \alpha_k r_k \frac{\partial \ell_k}{\partial \theta_k} = \sum_k \alpha_k r_k \frac{\partial \log p_k(\mathbf{x}|\theta_k)}{\partial \theta}$$

$$\frac{\partial \ell}{\partial \mu_k} = -\sum_k \alpha_k r_k \Sigma_k^{-1}(\mathbf{x} - \mu_k)$$

- Gradients of covariance matrices are harder: require derivatives of log determinants and quadratic forms.
- Must ensure that mixing proportions α_k are positive and sum to unity and that covariance matrices are positive definite.

- If we want to use general optimizations (e.g. conjugate gradient) to learn latent variable models, we often have to make sure parameters respect certain constraints. (e.g. $\sum_k \alpha_k = 1$, Σ_k pos.definite).
- A good trick is to reparameterize these quantities in terms of unconstrained values. For mixing proportions, use the softmax:

$$\alpha_k = \frac{\exp(q_k)}{\sum_j \exp(q_j)}$$

- For covariance matrices, use the Cholesky decomposition:

$$\Sigma^{-1} = A^\top A$$
$$|\Sigma|^{-1/2} = \prod_i A_{ii}$$

where A is upper diagonal with positive diagonal:

$$A_{ii} = \exp(r_i) > 0 \qquad A_{ij} = a_{ij} \quad (j > i) \qquad A_{ij} = 0 \quad (j < i)$$

- 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.

- 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 $\theta^{t+1} \leftarrow \operatorname{argmax} \ell(\theta; \mathbf{x}, \hat{\mathbf{z}}^t)$.
- 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".

- 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:

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

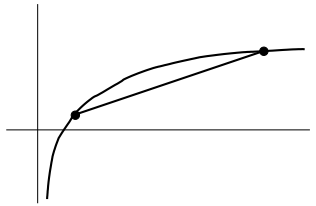
which is the *incomplete log likelihood*.

- 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: $\sum q(\mathbf{z}) = 1;\ q(\mathbf{z}) > 0$.)

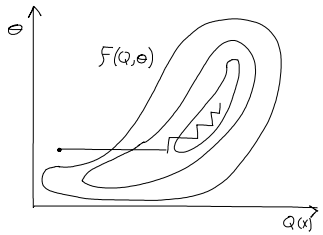
- For fixed data $\mathbf{x}$, define a functional called the *free energy*:

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

- The EM algorithm is coordinate-ascent on F:

  E-step: $q^{t+1} = \operatorname{argmax}_q \ F(q, \theta^t)$

  M-step: $\theta^{t+1} = \operatorname{argmax}_\theta \ F(q^{t+1}, \theta^t)$



- Note that the free energy breaks into two terms:

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

  (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:

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

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

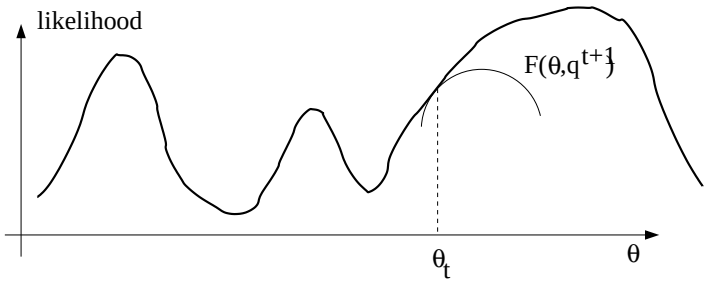
$$q^{t+1} = p(\mathbf{z}|\mathbf{x}, \theta^t)$$

- 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 $\ell(\theta) - F(q, \theta) = \mathrm{KL}[q || p(\mathbf{z}|\mathbf{x}, \theta)]$

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



- Often you can easily compute $b_k = \log p(\mathbf{x}|z=k, \theta_k)$, but it will be very negative, say -10^6 or smaller.
- Now, to compute $\ell = \log p(\mathbf{x}|\theta)$ you need to compute $\log \sum_k e^{b_k}$.
- Careful! Do not compute this by doing `log(sum(exp(b)))`. You will get underflow and an incorrect answer.
- Instead do this:
  - Add a constant exponent B to all the values b_k such that the largest value comes close to the maxiumum exponent allowed by machine precision: `B = MAXEXPONENT-log(K)-max(b)`.
  - Compute `log(sum(exp(b+B)))-B`.
- Example: if $\log p(x|z=1) = -420$ and $\log p(x|z=2) = -420$, what is $\log p(x) = \log\left[p(x|z=1) + p(x|z=2)\right]$? Answer: $\log[2e^{-420}] = -420 + \log 2$.

- 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:

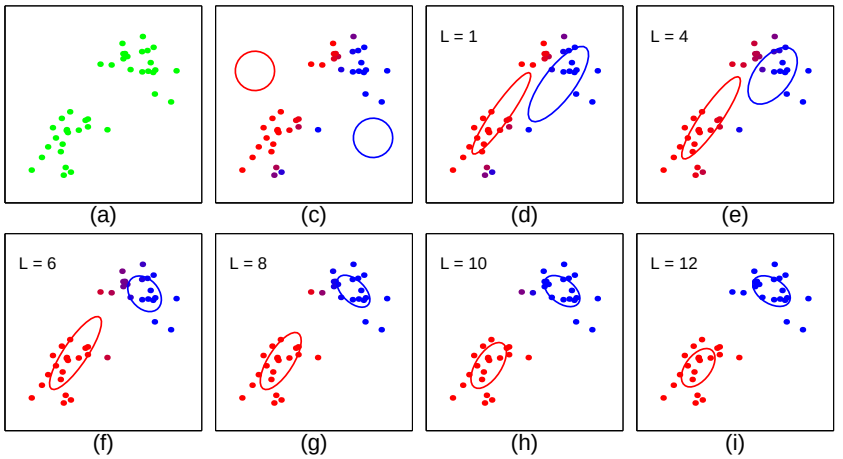
$$\mathbf{E-step}: \quad p_{kn}^t = \mathcal{N}(\mathbf{x}^n|\mu_k^t, \Sigma_k^t)$$

$$q_{kn}^{t+1} = p(z=k|\mathbf{x}^n, \theta^t) = \frac{\alpha_k^t p_{kn}^t}{\sum_j \alpha_j^t p_{kn}^t}$$

$$\mathbf{M-step}: \quad \mu_k^{t+1} = \frac{\sum_n q_{kn}^{t+1} \mathbf{x}^n}{\sum_n q_{kn}^{t+1}}$$

$$\Sigma_k^{t+1} = \frac{\sum_n q_{kn}^{t+1} (\mathbf{x}^n - \mu_k^{t+1})(\mathbf{x}^n - \mu_k^{t+1})^\top}{\sum_n q_{kn}^{t+1}}$$

$$\alpha_k^{t+1} = \frac{1}{M} \sum_n q_{kn}^{t+1}$$



- 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 $\frac{\partial \mathbf{x}^\top A \mathbf{x}}{\partial A} = \mathbf{x}\mathbf{x}^\top$

- The EM algorithm for mixtures of Gaussians is just like a soft version of the K-means algorithm with fixed priors and covariance.
- Instead of "hard assignment" in the E-step, we do "soft assignment" based on the softmax of the squared distance from each point to each cluster.
- Each centre is then moved to the *weighted mean* of the data, with weights given by soft assignments. In K-means, the weights are 0 or 1.

$$\mathbf{E-step}: \qquad d_{kn}^t = \frac{1}{2}(\mathbf{x}^n - \mu_k^t)^\top \Sigma^{-1} (\mathbf{x}^n - \mu_k^t)$$

$$q_{kn}^{t+1} = \frac{\exp(-d_{kn}^t)}{\sum_j \exp(-d_{jn}^t)} = p(c_n^t = k | \mathbf{x}^n, \mu^t)$$

$$\mathbf{M-step}: \qquad \mu_k^{t+1} = \frac{\sum_n q_{kn}^{t+1} \mathbf{x}^n}{\sum_n q_{kn}^{t+1}}$$

- 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: $\theta^{t+1} = \text{argmax}_\theta \sum_\mathbf{z} q(\mathbf{z}|\mathbf{x}) \log p(\mathbf{x}, \mathbf{z}|\theta)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

- 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, ...

- 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.

- 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).