#### PARTIALLY UNOBSERVED VARIABLES

- Certain variables 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.

## MISSING OUTPUTS

- 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.
- Let's focus on the idea of unobserved variables...

#### LATENT VARIABLES

- What to do when a variable 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 y, x fit the model p(z, y|x) = p(z|y)p(y|x, w)p(w).
- But if 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 (e.g. mixtures).

# Lecture 8:

## Unsupervised Learning & EM Algorithm

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#### Why is Learning Harder?

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

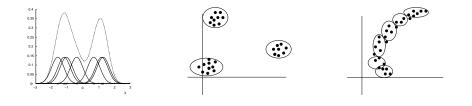
$$\ell(\theta; \mathcal{D}) = \sum_{n} \log p(\mathbf{y}_{n}, \mathbf{x}_{n} | \theta)$$
$$= \sum_{n} \log p(\mathbf{x}_{n} | \theta_{x}) + \sum_{n} \log p(\mathbf{y}_{n} | \mathbf{x}_{n}, \theta_{y})$$

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

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

#### MIXTURE MODELS

- $\bullet$  Most basic latent variable model with a single discrete node z.
- Allows different submodels (experts) to contribute to the (conditional) density model in different parts of the space.
- Divide and conquer idea: use simple parts to build complex models. (e.g. multimodal densities, or piecewise-linear regressions).



## LEARNING WITH LATENT VARIABLES

- 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.

## MIXTURE DENSITIES

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

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

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!

#### LEARNING WITH MIXTURES

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

$$\begin{split} \ell(\theta) &= \log p(\mathbf{x}|\theta) = \log \sum_{k} \alpha_{k} p_{k}(\mathbf{x}|\theta_{k}) \\ \frac{\partial \ell}{\partial \theta} &= \frac{1}{p(\mathbf{x}|\theta)} \sum_{k} \alpha_{k} \frac{\partial p_{k}(\mathbf{x}|\theta_{k})}{\partial \theta} \\ &= \sum_{k} \alpha_{k} \frac{1}{p(\mathbf{x}|\theta)} p_{k}(\mathbf{x}|\theta_{k}) \frac{\partial \log p_{k}(\mathbf{x}|\theta_{k})}{\partial \theta} \\ &= \sum_{k} \alpha_{k} \frac{p_{k}(\mathbf{x}|\theta_{k})}{p(\mathbf{x}|\theta)} \frac{\partial \ell_{k}}{\partial \theta_{k}} = \sum_{k} \alpha_{k} r_{k} \frac{\partial \ell_{k}}{\partial \theta_{k}} \end{split}$$

• In other words, the gradient is the *responsibility weighted sum* of the individual log likelihood gradients.

#### MIXTURE OF LINEAR REGRESSION EXPERTS

• Each expert generates data according to a linear function of the input plus additive Gaussian noise:

$$p(y|\mathbf{x}, \theta) = \sum_{k} \alpha_{k}(\mathbf{x}) \mathcal{N}(y|\beta_{k}^{\top} \mathbf{x}, \sigma_{k}^{2})$$

• The "gate" function can be a softmax classification machine:

$$\alpha_k(\mathbf{x}) = p(z = k | \mathbf{x}) = \frac{e^{\eta_k^\top \mathbf{x}}}{\sum_j e^{\eta_j^\top \mathbf{x}}}$$

- Remember: we are not modeling the density of the inputs x.
- Learning? Gradient descent is one option. You have seen the gradients for this example before.
- In a minute you will see another one...

## CONDITIONAL MIXTURES: MOES REVISITED

• 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:

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

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

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- 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:

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

## CLUSTERING EXAMPLE: GAUSSIAN MIXTURE MODELS

• 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.

#### MIXURE OF GAUSSIANS LEARNING

• 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  $\alpha_k$  are positive and sum to unity and that covariance matrices are positive definite.

#### BE CAREFUL: LOGSUM

- 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 maximum 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  $\log p(x) = \log [p(x|z=1) + p(x|z=2)]$ ? Answer:  $\log [2e^{-420}] = -420 + \log 2$ .

## PARAMETER CONSTRAINTS

- 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.  $\sum_k \alpha_k = 1$ ,  $\Sigma_k$  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:

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

#### RECAP: LEARNING WITH LATENT VARIABLES

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

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

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

#### 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:  $\ell(\theta) \ge \ell_q(\theta) + \mathcal{H}(q)$  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:  $\sum q(\mathbf{z}) = 1$ ;  $q(\mathbf{z}) > 0$ .)

### Complete & Incomplete Log Likelihoods

• Observed variables  $\mathbf{x}$ , latent variables  $\mathbf{z}$ , parameters  $\theta$ :

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

is the complete log likelihood.

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

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

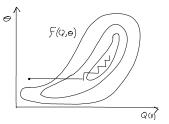
which is the incomplete log likelihood.

## LOWER BOUNDS AND FREE ENERGY

• For fixed data x, define a functional called the *free energy*:

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

• The EM algorithm is coordinate-ascent on F: E-step:  $q^{t+1} = \operatorname{argmax}_{q} F(q, \theta^{t})$ M-step:  $\theta^{t+1} = \operatorname{argmax}_{\theta} F(q^{t+1}, \theta^{t})$ 



#### M-step: maximization of expected $\ell_c$

• Note that the free energy breaks into two terms:

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

(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  $\theta$ , is the entropy.
- Thus, in the M-step, maximizing with respect to  $\theta$  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:

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

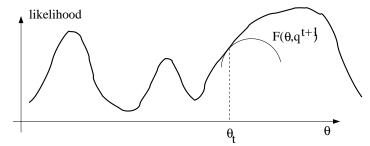
- This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform classification).
- $\bullet$  Proof (easy): this setting saturates the bound  $\ell(\theta;\mathbf{x})\geq F(q,\theta)$

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

• 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  $F(q^{t+1}, \cdot)$ .



## Partially Hidden Data

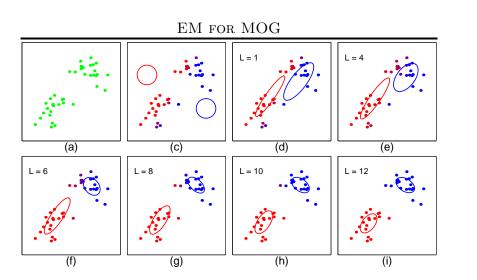
- Of course, we can learn when there are missing (hidden) variables on some cases and not on others.
- In this case the cost function was:

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

- 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.

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

$$\begin{split} \mathbf{E} - \mathbf{step} : \qquad p_{kn}^t &= \mathcal{N}(\mathbf{x}^n | \boldsymbol{\mu}_k^t, \boldsymbol{\Sigma}_k^t) \\ q_{kn}^{t+1} &= p(z \!=\! k | \mathbf{x}^n, \boldsymbol{\theta}^t) = \frac{\alpha_k^t p_{kn}^t}{\sum_j \alpha_j^t p_{kn}^t} \\ \mathbf{M} - \mathbf{step} : \qquad \boldsymbol{\mu}_k^{t+1} &= \frac{\sum_n q_{kn}^{t+1} \mathbf{x}^n}{\sum_n q_{kn}^{t+1}} \\ \boldsymbol{\Sigma}_k^{t+1} &= \frac{\sum_n q_{kn}^{t+1} (\mathbf{x}^n - \boldsymbol{\mu}_k^{t+1}) (\mathbf{x}^n - \boldsymbol{\mu}_k^{t+1})^\top}{\sum_n q_{kn}^{t+1}} \\ \alpha_k^{t+1} &= \frac{1}{M} \sum_n q_{kn}^{t+1} \end{split}$$

#### DERIVATION OF M-STEP

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

$$\sum_{n}\sum_{k}q_{kn}\left[\log\alpha_{k}-\frac{1}{2}(\mathbf{x}^{n}-\boldsymbol{\mu}_{k}^{t+1})^{\top}\boldsymbol{\Sigma}_{k}^{-1}(\mathbf{x}^{n}-\boldsymbol{\mu}_{k}^{t+1})-\frac{1}{2}\log|2\pi\boldsymbol{\Sigma}_{k}|\right]$$

• For fixed q we can optimize the parameters:

$$\begin{split} & \frac{\partial \ell_q}{\partial \mu_k} = \Sigma_k^{-1} \sum_n q_{kn} (\mathbf{x}^n - \mu_k) \\ & \frac{\partial \ell_q}{\partial \Sigma_k^{-1}} = \frac{1}{2} \sum_n q_{kn} \left[ \Sigma_k^\top - (\mathbf{x}^n - \mu_k^{t+1}) (\mathbf{x}^n - \mu_k^{t+1})^\top \right] \\ & \frac{\partial \ell_q}{\partial \alpha_k} = \frac{1}{\alpha_k} \sum_n q_{kn} - \lambda \qquad (\lambda = M) \end{split}$$
  
• Fact:  $\frac{\partial \log |A^{-1}|}{\partial A^{-1}} = A^\top$  and  $\frac{\partial \mathbf{x}^\top A \mathbf{x}}{\partial A} = \mathbf{x} \mathbf{x}^\top$ 

#### VARIANTS

## Compare: K-Means

- 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.

$$\begin{split} \mathbf{E} - \mathbf{step} : \qquad d_{kn}^t &= \frac{1}{2} (\mathbf{x}^n - \boldsymbol{\mu}_k^t)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}^n - \boldsymbol{\mu}_k^t) \\ q_{kn}^{t+1} &= \frac{\exp(-d_{kn}^t)}{\sum_j \exp(-d_{jn}^t)} = p(c_n^t = k | \mathbf{x}^n, \boldsymbol{\mu}^t) \\ \mathbf{M} - \mathbf{step} : \qquad \boldsymbol{\mu}_k^{t+1} &= \frac{\sum_n q_{kn}^{t+1} \mathbf{x}^n}{\sum_n q_{kn}^{t+1}} \end{split}$$

## A Report Card for EM

- Some good things about EM:
  - no learning rate parameter
  - very fast for low dimensions
  - $-\operatorname{each}$  iteration guaranteed to improve likelihood
  - $-\operatorname{adapts}$  unused units rapidly
- Some bad things about EM:
  - $-\operatorname{can}$  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  $\theta$
- 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,  $\ldots$

## • 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).