Lecture 12:

Parameter Learning for BNs with hidden nodes

Kevin Murphy

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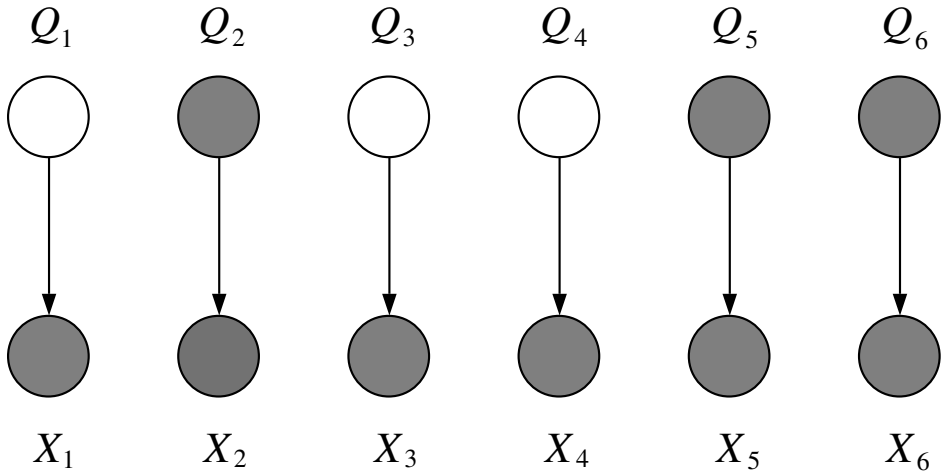
Outline

- Latent variable models
- Maximum likelihood learning
  - Gradient ascent
  - EM
- (Bayesian learning)

Unobserved Variables

- Certain variables Q in our models may be *unobserved*,
  either some of the time or always,
  either at training time or at test time.



  Graphically, we will use shading to indicate observation.

- We shall assume values are *missing at random*; if not, we need to model the *data censoring mechanism* explicitly.

- e.g., probability we observe a medical record may depend on values of the other attributes.

Partially Unobserved (Missing) Variables

- If variables are occasionally unobserved they are *missing data*.
  e.g. undefinied inputs, missing class labels, erroneous target values
- Variables which are always unobserved are called *latent variables*.
- Now we maximize the likelihood of the observed data; we have to *sum out* or *marginalize* the missing values at training or test time:

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

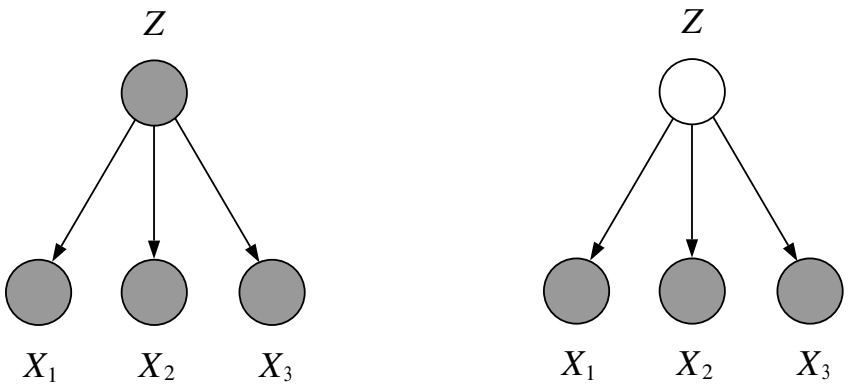
Why is Learning Harder?

- In fully observed iid settings, the log likelihood decomposes into a sum of local terms (at least for directed models).

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

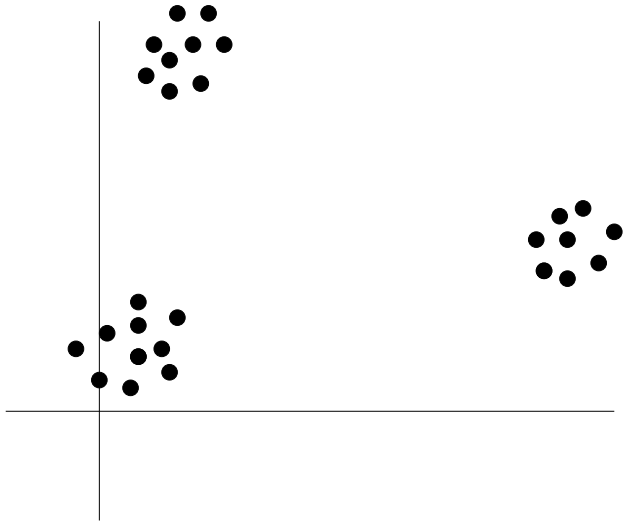
- With latent variables, all the parameters become coupled together via $\log \sum()$:

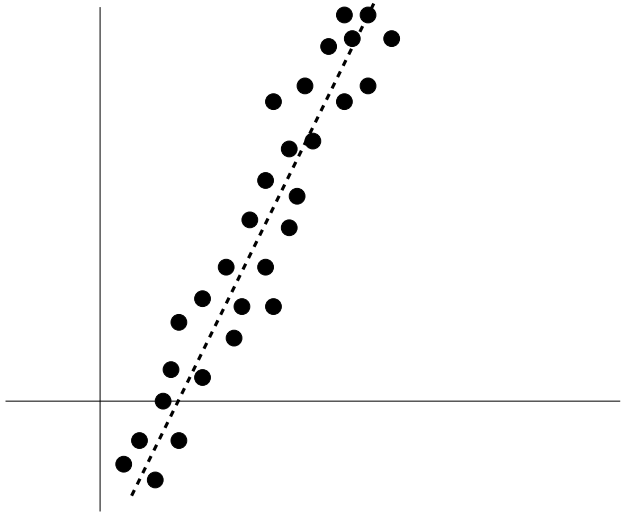
$$\ell(\theta; \mathcal{D}) = \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}|\theta) = \log \sum_{\mathbf{z}} p(\mathbf{z}|\theta_z) p(\mathbf{x}|\mathbf{z}, \theta_x)$$



Where Do Latent Variables Come From?

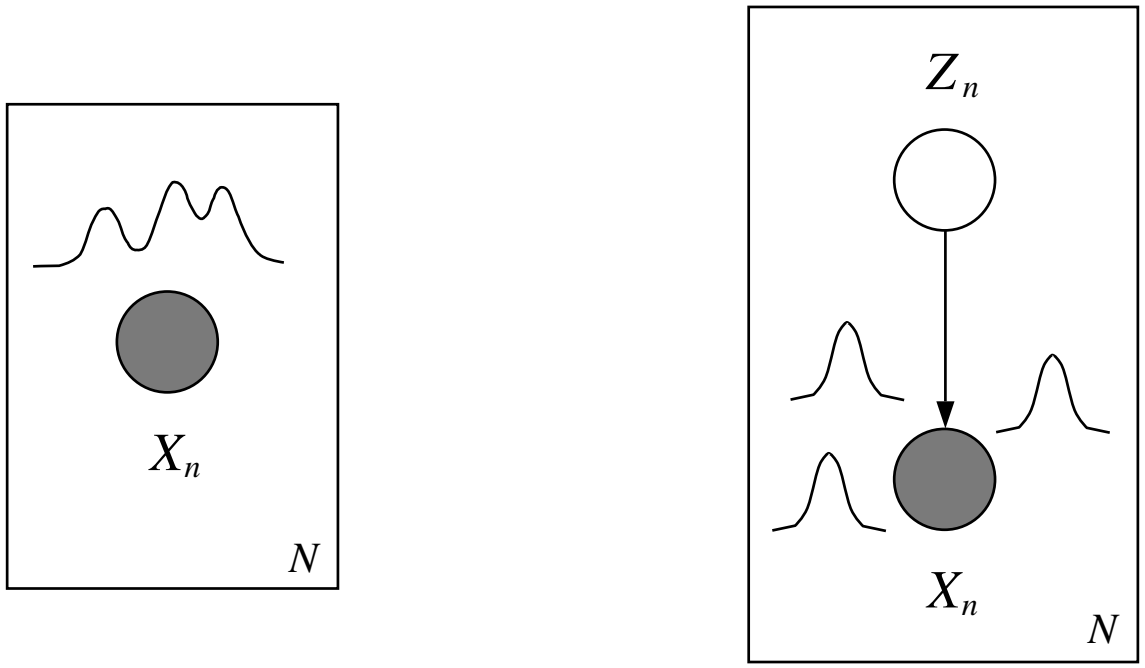
- Missing values can arise because something wasn't measured, because of faulty sensors, etc.
- But we may also *intentionally* introduce latent variables to simplify a model.
- Discrete latent variables can be used to partition/ cluster data into sub-groups.
- Continuous latent variables (factors) can be used for dimensionality reduction (PCA, etc).





Mixture models

- A density model $p(x)$ may be multi-modal.
- We may be able to model it as a mixture of uni-modal distributions (e.g., Gaussians).
- Each mode may correspond to a different sub-population (e.g., male and female).

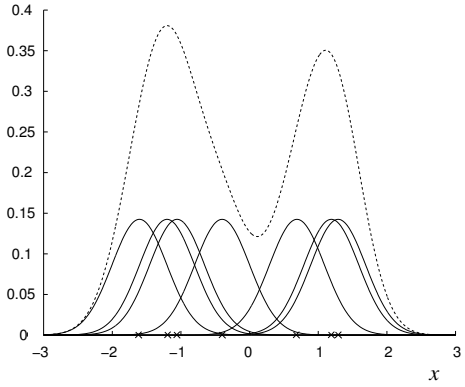


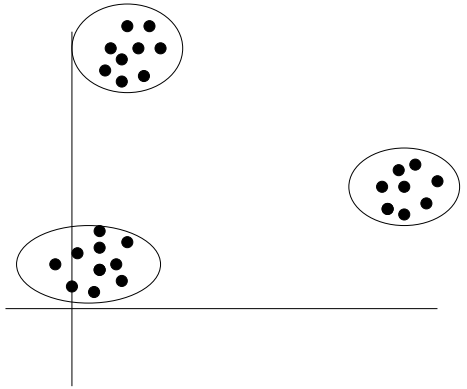
(a) (b)

Gaussian Mixture Models (GMMs)

- Consider a mixture of K Gaussian components:

$$p(Z = k) = \alpha_k \text{ mixing weights}$$
$$p(\mathbf{x}|z = k) = \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k) \text{ class-conditional densities}$$





- This can be used for *unsupervised clustering*.
- This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

Gaussian Mixture Models

- The posterior probability that a data point x is assigned to cluster k is given by

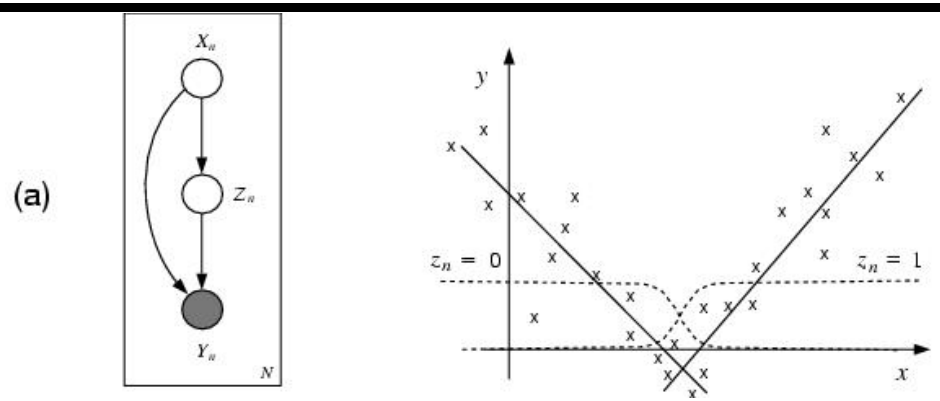
$$p(z = k|\mathbf{x}, \theta) = \frac{\alpha_k p_k(\mathbf{x}|\theta_k)}{\sum_j \alpha_j p_j(\mathbf{x}|\theta_j)} = r_k(x)$$

- These quantities are called *responsibilities* or *soft assignments*.
- *Vector quantization (VQ)* = hard assignment of x to the most probable cluster.
- The log-likelihood is

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

- We will discuss how to maximize this later.

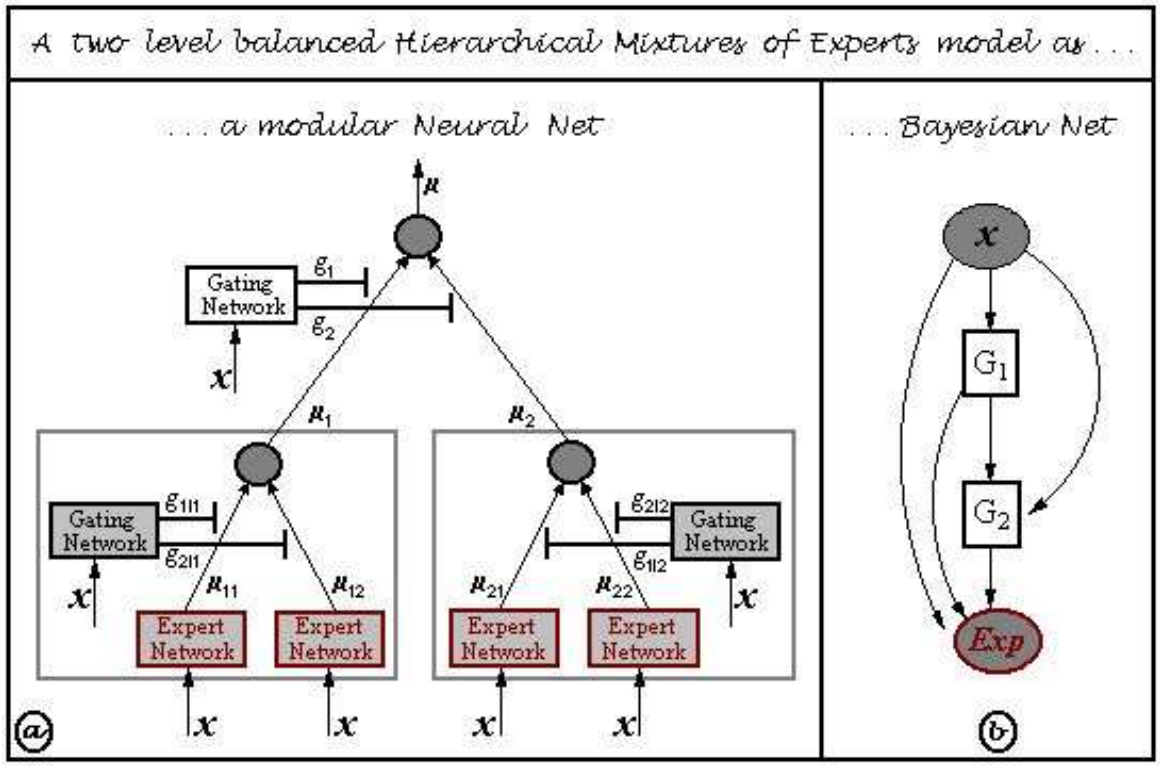
Conditional mixture model: Mixture of experts



- We will model $P(Y|X)$ using different experts, each responsible for different regions of the input space.
- Latent variable Z chooses expert using softmax gating function: $P(Z = k|x) = \sigma(\theta_k^T x)$.
- Each expert can be a linear regression model: $p(y|x, Z = k) = \mathcal{N}(y; \beta_k^T x, \sigma_k^2)$.
- The posterior expert responsibilities are

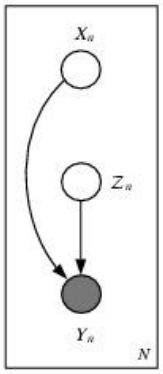
$$p(z = k|\mathbf{x}, \mathbf{y}, \theta) = \frac{\alpha_k(\mathbf{x}) p_k(\mathbf{y}|\mathbf{x}, \theta_k)}{\sum_j \alpha_j(\mathbf{x}) p_j(\mathbf{y}|\mathbf{x}, \theta_j)}$$

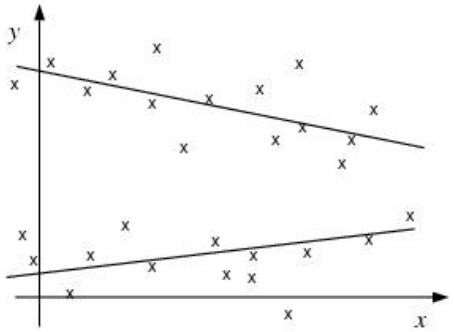
Hierarchical mixture of experts



- This is like a soft version of a depth-2 classification/ regression tree.
- $P(Y|X, Z_1, Z_2)$ can be modelled as a GLIM, with parameters dependent on the values of Z_1 and Z_2 (which specify the path to a given leaf in the tree).

Mixture of overlapping experts





- By removing the $X \rightarrow Z$ arc, we can make the partitions independent of the input, thus allowing overlap.
- This is a mixture of linear regressors; each subpopulation has a different conditional mean.

Gradient Learning for mixture models

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

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

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

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

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

- In other words, the gradient is the *responsibility weighted sum* of the individual log likelihood gradients.
- Can pass this to a conjugate gradient routine.

Parameter Constraints

- Often we have constraints on the parameters, e.g. $\sum_k \alpha_k = 1$, Σ symmetric positive definite (hence $\Sigma_{ii} > 0$).
- We can use constrained optimization, or we can reparameterize in terms of unconstrained values.
- For discrete variables, use the softmax transform: $\alpha_k = \frac{\exp(q_k)}{\sum_j \exp(q_j)}$
- For covariance matrices, use the Cholesky decomposition:

$$\Sigma^{-1} = A^\top A$$

  where A is upper diagonal with positive diagonal:

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

- The variables $q_i, r_i, a_{ij} \in \mathbb{R}$ are unconstrained.
- Use chain rule to compute $\frac{\partial \ell}{\partial \alpha}$, $\frac{\partial \ell}{\partial A}$.

Logsum

- You may encounter numerical problems when computing the log-likelihood:

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

  since $p_k(\mathbf{x}|\theta_k)$ may be extremely small.

- The class conditional *log* likelihoods are well-behaved: $b_k = \log p_k(\mathbf{x}|\theta_k)$.

- But the following will underflow:

$$\log \sum_k e^{b_k}$$

Logsum

- You should use

$$\begin{aligned}
\log \sum_k e^{b_k} &= \log \left[(\sum_k e^{b_k}) e^{-B} e^{B} \right] \\
&= \log \left[(\sum_k e^{b_k - B}) e^{B} \right] \\
&= \left[\log (\sum_k e^{b_k - B}) \right] + B
\end{aligned}$$

  where $B = \max_k b_k$

- Example

$$\log(e^{-120} + e^{-121}) = \log \left(e^{-120} (e^{0} + e^{-1}) \right) = \log(e^{0} + e^{-1}) - 120$$

Gradient learning for BNs with tabular CPDs

- Let $\theta_{ijk} = P(X_i = j | X_{\pi_i} = k)$.
- For a fully observed case, the gradient of the likelihood is

$$\begin{aligned}
\frac{\partial}{\partial \theta_{ijk}} P(x_{1:N}) &= \frac{\partial}{\partial \theta_{ijk}} \prod_{i'} \theta_{i', x'_i, x_{\pi_{i'}}} \\
&= \delta(x_i = j, x_{\pi_i} = k) \theta_{ijk} \prod_{i' \neq i} \theta_{i', x_{i'}, x_{\pi_{i'}}} \\
&= \delta(x_i = j, x_{\pi_i} = k) \frac{\prod_{i'} \theta_{i', x_{i'}, x_{\pi_{i'}}}}{\theta_{ijk}} \\
&= \delta(x_i = j, x_{\pi_i} = k) \frac{P(x_{1:N})}{\theta_{ijk}}
\end{aligned}$$

Gradient learning for BNs with tabular CPDs

- For a partially observed case,

$$\begin{aligned}\frac{\partial}{\partial \theta_{ijk}} P(e) &= \frac{\partial}{\partial \theta_{ijk}} \sum_{x:x(E)=e} P(x) \\ &= \sum_{x} \delta(x_E = e)\delta(x_i = j, x_{\pi_i} = k)\frac{P(x_{1:N})}{\theta_{ijk}} \\ &= \frac{P(x_i = j, x_{\pi_i} = k, e)}{\theta_{ijk}}\end{aligned}$$

- A more complex expression can be used if $\theta_{ijk} = 0$.
- The numerator can be computed using probabilistic inference.
- A junction tree will always contain X_i and X_{π_i} in the same clique.
- For batch learning, we need to do inference for every training case for every iteration of gradient ascent (slow!).

Gradient learning for BNs with general CPDs

- Consider CPD $P(X = x|X_\pi = u; \phi)$.
- We have

$$\frac{\partial P(e)}{\partial P(X = x|X_\pi = u)} = \frac{P(X = x, X_\pi = u, e)}{P(X = x|X_\pi = u)}$$

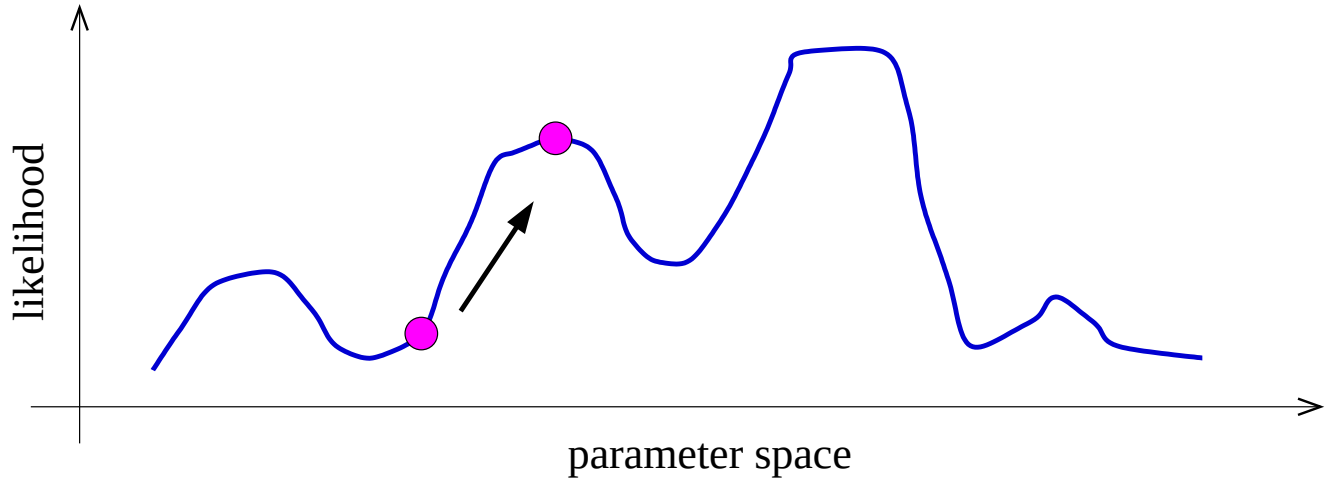
- By the chain rule

$$\frac{\partial P(e)}{\partial \phi} = \sum_{x,u} \frac{\partial P(e)}{\partial P(X = x, X_\pi = u)} \frac{\partial P(X = x|X_\pi = u)}{\partial \phi}$$

- This can be used to learn noisy-OR, sigmoids, etc.

Identifiability

- A mixture model induces a multi-modal likelihood.
- Hence gradient ascent can only find a local maximum.
- Mixture models are unidentifiable, since we can always switch the hidden labels without affecting the likelihood.
- Hence we should be careful in trying to interpret the "meaning" of latent variables.



Expectation-Maximization (EM) Algorithm

- EM is an optimization strategy for objective functions that can be interpreted as likelihoods in the presence of missing data.
- It is much simpler than gradient methods:
  - No need to choose step size.
  - Enforces constraints automatically.
  - Calls inference and fully observed learning as subroutines.
- EM is an Iterative algorithm with two linked steps:
  - E-step: fill-in hidden values using inference, $p(\mathbf{z}|\mathbf{x}, \theta^t)$.
  - M-step: update parameters θ^{t+1} using standard MLE/MAP method applied to completed data
- We will prove that this procedure monotonically improves ℓ (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.

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*.

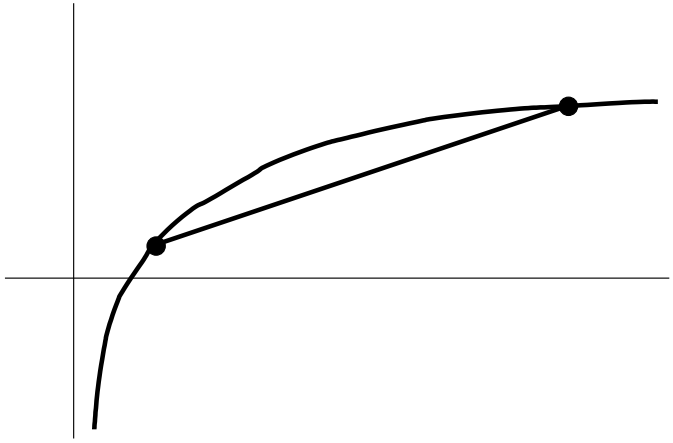
Expected Complete Log Likelihood

- 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

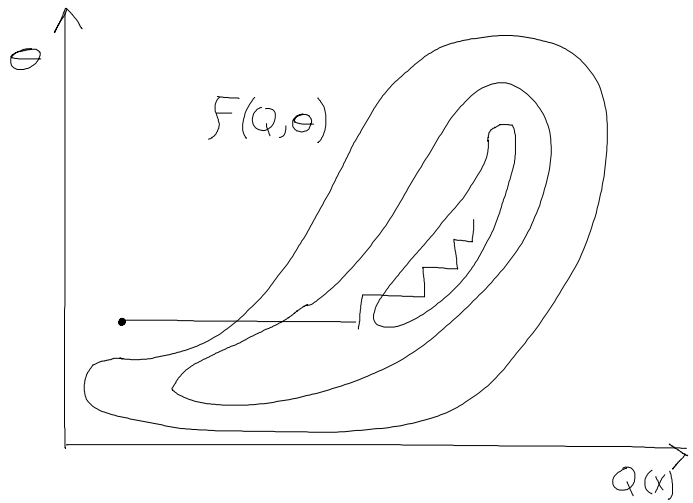
- For fixed data $\mathbf{x}$, define a functional called the *free energy*:

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

- The EM algorithm is coordinate-ascent on F:

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

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



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:

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

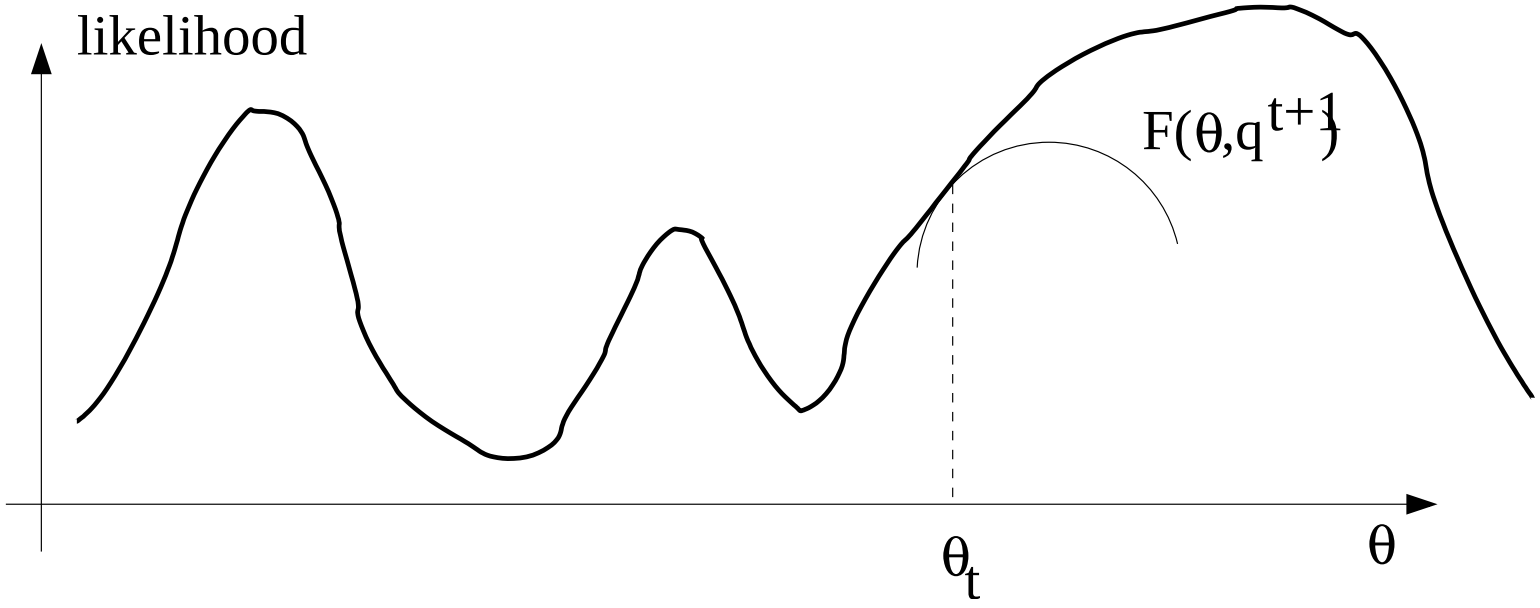
- This is the posterior distribution over the latent variables given the data and the parameters. Often we need this at test time anyway (e.g. to perform classification).
- Proof (easy): this setting saturates the bound $\ell(\theta; \mathbf{x}) \geq F(q, \theta)$

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

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

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:

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

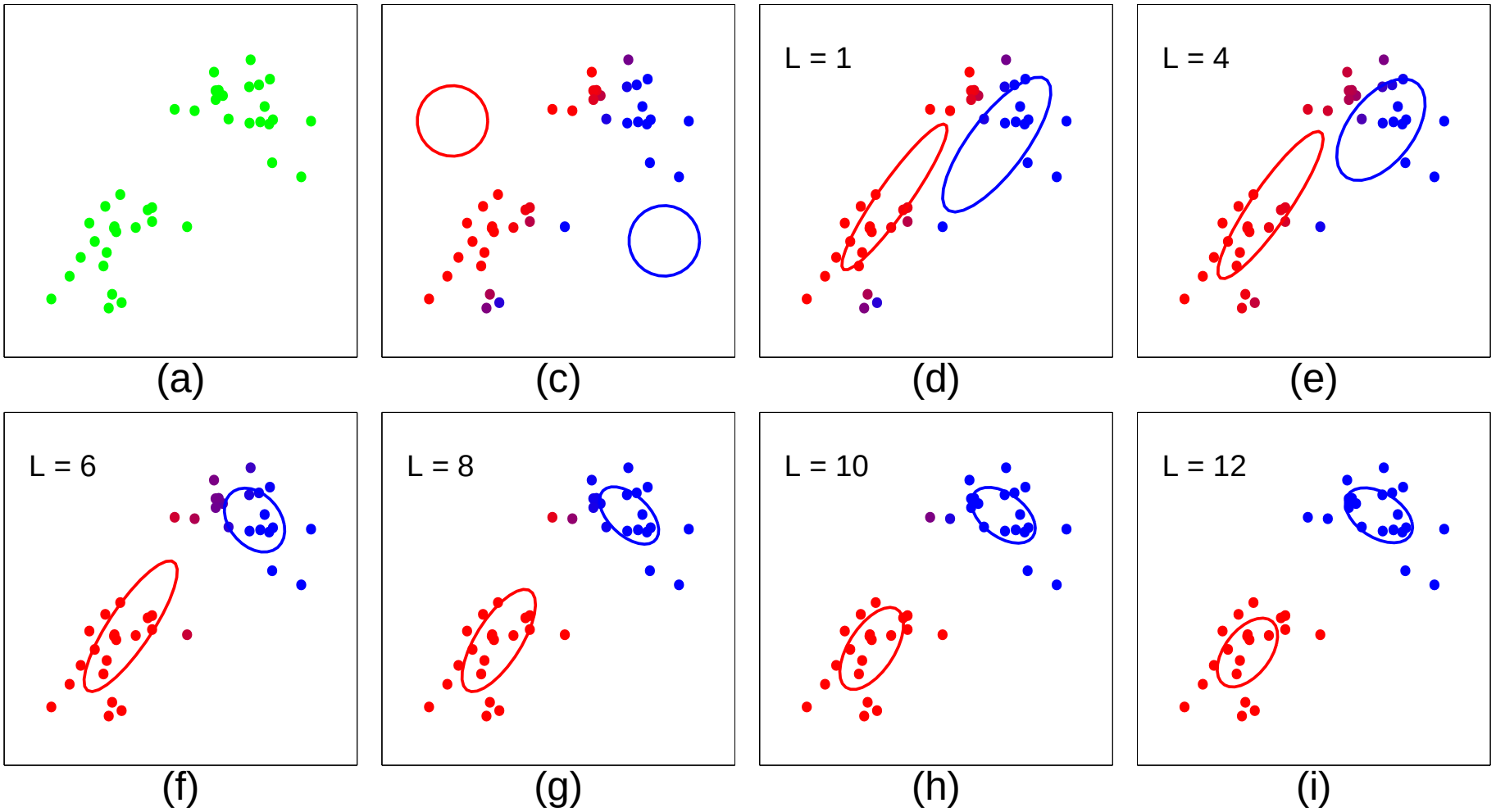
$$q_{kn}^{t+1} = p(z=k|\mathbf{x}^n, \theta^t) = \frac{\alpha_k^t p_{kn}^t}{\sum_j \alpha_j^t p_{kn}^t}$$

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

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

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

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

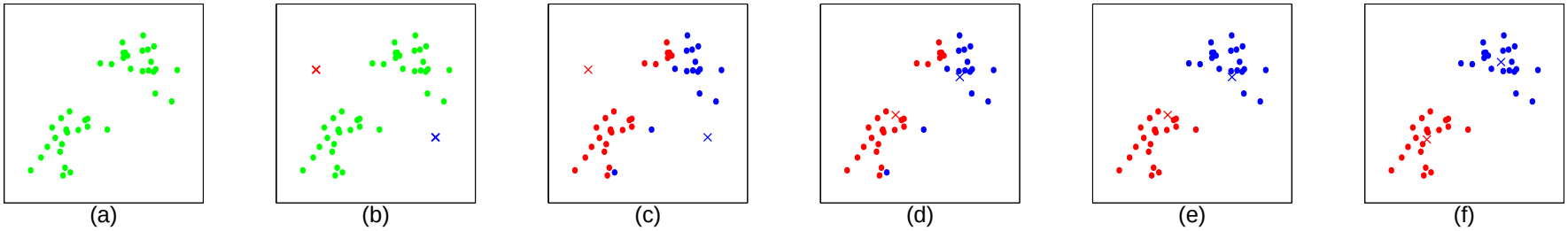
Compare: K-means

- 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:

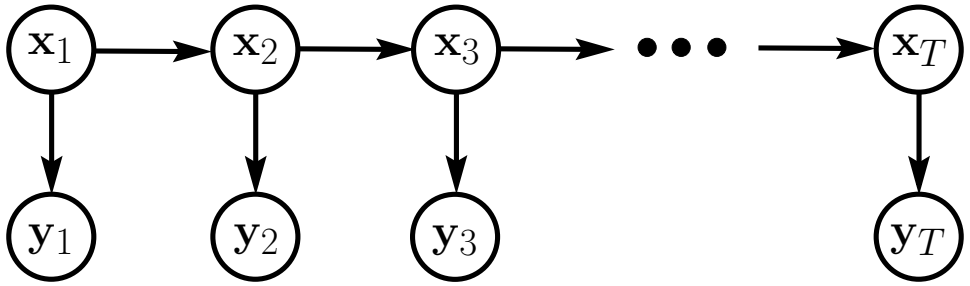
$$c_n^{t+1} = \text{argmin}_k (\mathbf{x}^n - \mu_k^t)^\top \Sigma_k^{-1} (\mathbf{x}^n - \mu_k^t)$$

- 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:

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



Reminder: HMM Graphical Model



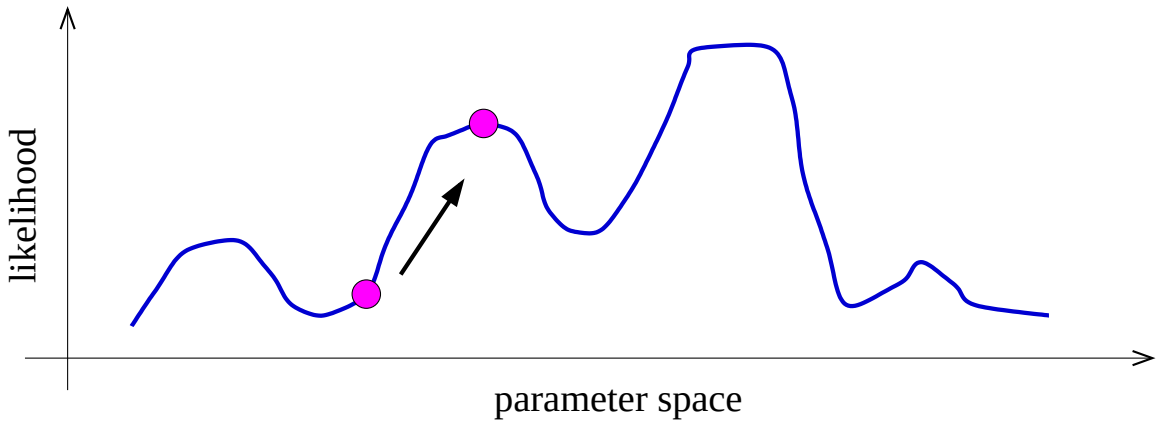
- Hidden states $\{x_t\}$, outputs $\{\mathbf{y}_t\}$
  Joint probability factorizes:

$$\mathsf{P}(\{\mathbf{x}\},\{\mathbf{y}\}) = \prod_{t=1}^{T} \mathsf{P}(x_t|\mathbf{x}_{t-1})\mathsf{P}(\mathbf{y}_t|x_t)$$
$$= \pi_{\mathbf{x}_1} \prod_{t=1}^{T-1} S_{x_t,x_{t+1}} \prod_{t=1}^{T} A_{x_t}(\mathbf{y}_t)$$

- We saw efficient recursions for computing
  $L = \mathsf{P}(\{\mathbf{y}\}) = \sum_{\{\mathbf{x}\}} \mathsf{P}(\{\mathbf{x}\},\{\mathbf{y}\})$ and $\gamma_i(t) = \mathsf{P}(x_t = i|\{\mathbf{y}\})$.

Baum-Welch Algorithm: EM Training

1. Intuition: if only we *knew* the true state path then ML parameter estimation would be trivial (MM1 on x, conditional on y).
2. But: can *estimate* state path using inference recursions.
3. *Baum-Welch algorithm* (special case of EM): estimate the states, then compute params, then re-estimate states, and so on ...
4. This works and we can *prove* that it always improves likelihood.
5. However: finding the ML parameters is NP complete, so initial conditions matter a lot and convergence is hard to tell.



Parameter Estimation using EM

- S_{ij} are transition probs; state j has output distribution $B_j(\mathbf{y})$

$$\mathsf{P}(x_{t+1} = j | x_t = i) = S_{ij} \qquad \mathsf{P}(x_1 = j) = \pi_j$$
$$\mathsf{P}(\mathbf{y}_t = y | x_t = j) = B_j(y)$$

- Complete log likelihood:

$$\log p(x, y) = \log\{\pi_{\mathbf{x}_1} \prod_{t=1}^{T-1} S_{x_t, x_{t+1}} \prod_{t=1}^{T} B_{x_t}(\mathbf{y}_t)\}$$
$$= \log\{\prod_i \pi_i^{[\mathbf{x}_1^i]} \prod_{t=1}^{T-1} \prod_{ij} S_{ij}^{[x_t^i, x_{t+1}^j]} \prod_{t=1}^{T} \prod_k B_k(\mathbf{y}_t)^{[\mathbf{x}_t^k]}\}$$
$$= \sum_i [\mathbf{x}_1^i] \log \pi_i + \sum_{t=1}^{T-1} \sum_{ij} [x_t^i, x_{t+1}^j] \log S_{ij} + \sum_{t=1}^{T} \sum_k [x_t^k] \log B_k(\mathbf{y}_t)$$

  where the indicator $[x_t^i] = 1$ if $x_t = i$ and 0 otherwise

- For EM, we need to compute the *expected complete log likelihood*.

State expectations required from the E-Step

- The expected complete log likelihood requires
  $\gamma_i(t) =< [x_t^i] >$ *and* $\xi_{ij}(t) =< [x_t^i, x_{t+1}^j] >$
- So in the E-step we need to compute both
  $\gamma_i(t) = p(x_t = i|\{\mathbf{y}\})$ and $\xi_{ij}(t) = p(x_t = i, x_{t+1} = j|\{\mathbf{y}\})$.
- We can use the forwards-backwards (Shafer-Shenoy) or Lauritzen-Spiegelhalter algorithms.

M-step: New Parameters are just Ratios of Frequency Counts

- Initial state distribution: expected #times in state i at time 1:

$$\hat{\pi}_i = \gamma_i(1)$$

- Expected #transitions from state i to j which begin at time t:

$$\xi_{ij}(t) = \alpha_i(t) S_{ij} B_j(\mathbf{y}_{t+1}) \beta_j(t+1)/L$$

so the estimated transition probabilities are:

$$\hat{S}_{ij} = \sum_{t=1}^{T-1} \xi_{ij}(t) \Big/ \sum_{t=1}^{T-1} \gamma_i(t)$$

- The output distributions are the expected number of times we observe a particular symbol in a particular state:

$$\hat{B}_j(y) = \sum_{t:\mathbf{y}_t=y} \gamma_j(t) \Big/ \sum_{t=1}^{T} \gamma_j(t)$$

HMM Practicalities

- Multiple observation sequences: can be dealt with by averaging numerators and averaging denominators in the ratios given above.
- Initialization: mixtures of Naive Bayes or mixtures of Gaussians for the output (observation) models, left-to-right for the transition matrix (if appropriate).
- Numerical scaling: the probability values $P(X_t, y_{1:t})$ can get very small, so normalize to get $P(X_t|y_{1:t})$ or use `logsum` trick.

EM for general BNs

while not converged

// E-step

for each node i

$ESS_i = 0$ // reset expected sufficient statistics

for each case m

do inference with $e(m)$

for each node i

$ESS_i += SS(P(X_i, X_{\pi_i}|e_m))$

// M-step

for each node i

$\theta_i := MLE(ESS_i)$

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.

EM Variants

- 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).

A Report Card for EM

- Some good things about EM:
  - no learning rate (step-size) parameter
  - automatically enforces parameter constraints
  - very fast for low dimensions
  - each iteration guaranteed to improve likelihood
- Some bad things about EM:
  - can get stuck in local minima
  - can be slower than conjugate gradient (especially near convergence)
  - requires expensive inference step
  - is a maximum likelihood/MAP method