Carnegie Mellon University
School of Computer Science

10701: Introduction to Machine Learning

Mixture models and the Expectation Maximization algorithm

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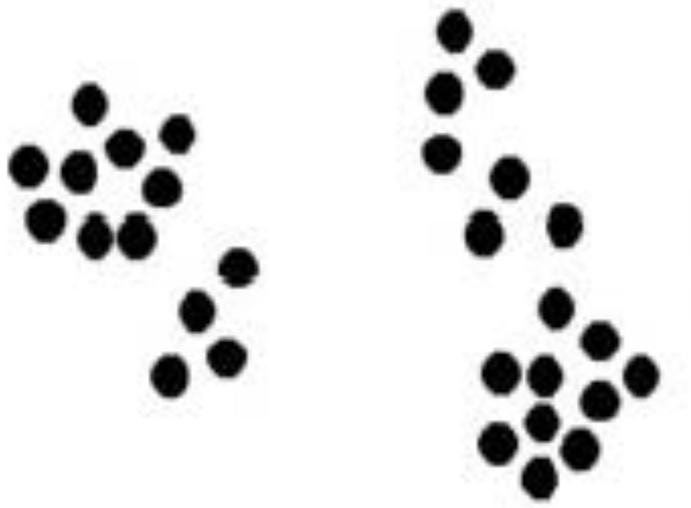
Lecture 14, October 21, 2020

Reading: Chap. 9, 13, C.B book

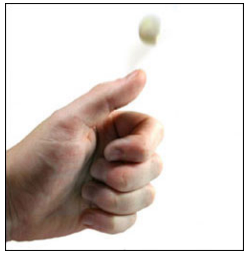
Clustering and partially observable probabilistic models



Recap: Indicator Variables and Discrete Distributions

- Bernoulli distribution: Ber(p)

$$P(x) = \begin{cases} 1-p & \text{for } x = 0 \\ p & \text{for } x = 1 \end{cases} \quad \Rightarrow \quad P(x) = p^x (1-p)^{1-x}$$



- Multinomial distribution: Mult($1, \theta$)
  - Multinomial (indicator) variable:

$$X = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix}, \quad \text{where} \quad \begin{array}{l} X_j = [0,1], \quad \text{and} \quad \sum_{j \in [1,\dots,6]} X_j = 1 \\ X_j = 1 \text{ w.p. } \theta_j, \quad \sum_{j \in [1,\dots,6]} \theta_j = 1 \ . \end{array}$$

$$P(x_i) = P(\{x_{n,k} = 1, \text{where } k \text{ index the die-side of the } n\text{th roll}\})$$

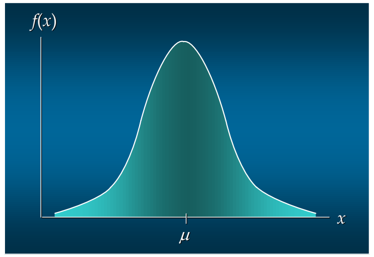
$$= \theta_k = \theta_1^{x_{n,1}} \times \theta_2^{x_{n,2}} \times \cdots \times \theta_K^{x_{n,K}} = \prod_{k=1}^{K} \theta_k^{x_{n,k}}$$

  - It can be shown that:

$$\hat{\theta}_{k,MLE} = \frac{n_k}{N} \quad \text{or} \quad \hat{\theta}_{k,MLE} = \frac{1}{N} \sum_n x_{n,k}$$

Recap: Continuous Variables and Gaussian Distributions

- Normal (Gaussian) Probability Density Function

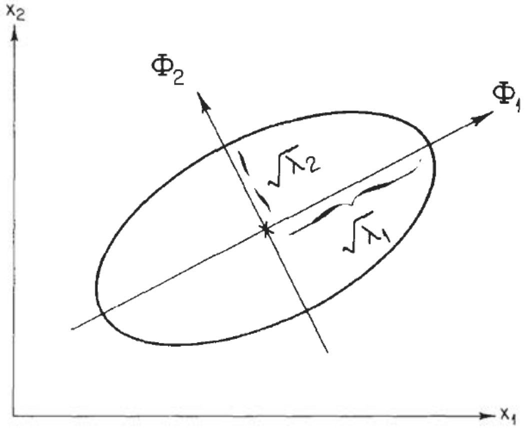


$$p(x)=\frac{1}{\sqrt{2\pi\sigma}}e^{-(x-\mu)^2/2\sigma^2}$$

  - The distribution is symmetric, and is often illustrated as a bell-shaped curve.
  - Two parameters, μ (mean) and σ (standard deviation), determine the location and shape of the distribution.
  - The highest point on the normal curve is at the mean, which is also the median and mode.
  - The mean can be any numerical value: negative, zero, or positive.

- Multivariate Gaussian

$$p(X;\vec{\mu},\Sigma)=\frac{1}{\left(\sqrt{2\pi}\right)^{n/2}|\Sigma|^{1/2}}\exp\left\{-\frac{1}{2}(X-\vec{\mu})^T\Sigma^{-1}(X-\vec{\mu})\right\}$$



Recap: MLE for a multivariate-Gaussian

- It can be shown that the MLE for μ *and* Σ is

$$\mu_{MLE} = \frac{1}{N}\sum_n (x_n)$$

$$\Sigma_{MLE} = \frac{1}{N}\sum_n (x_n - \mu_{ML})(x_n - \mu_{ML})^T = \frac{1}{N} S$$

$$x_n = \begin{pmatrix} x_{n,1} \\ x_{n,2} \\ \vdots \\ x_{n,K} \end{pmatrix}$$

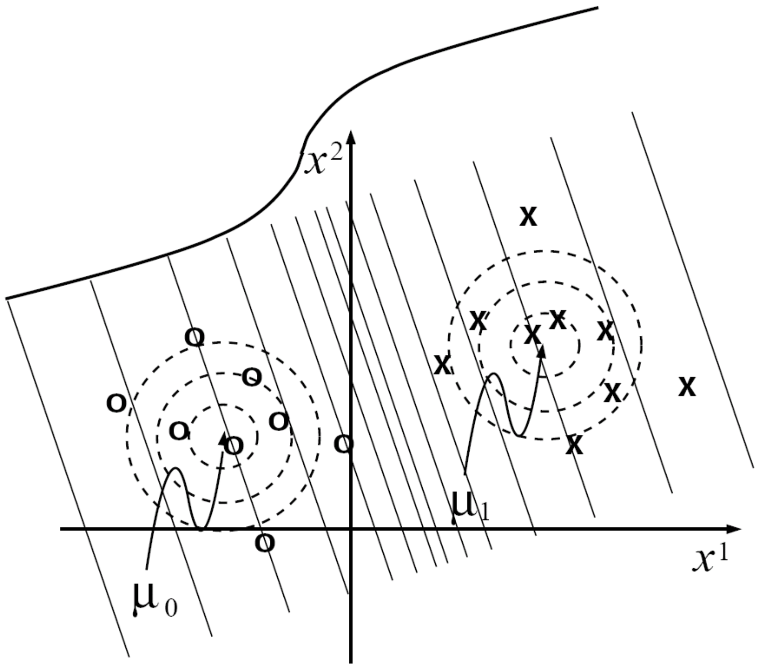
$$X = \begin{pmatrix} --- & x_1^T & --- \\ --- & x_2^T & --- \\ & \vdots & \\ --- & x_N^T & --- \end{pmatrix}$$

where the scatter matrix is

$$S = \sum_n (x_n - \mu_{ML})(x_n - \mu_{ML})^T = \left(\sum_n x_n x_n^T\right) - N\mu_{ML}\mu_{ML}^T$$

- The sufficient statistics are $\Sigma_n x_n$ and $\Sigma_n x_n x_n^T$.
- Note that $X^T X = \Sigma_n x_n x_n^T$ may not be full rank (eg. if $N < D$), in which case Σ_{ML} is not invertible

Recap: Conditional Gaussian



- The data:

$$\{(x_1, y_1), (x_2, y_2), (x_3, y_3), \cdots, (x_N, y_N)\}$$

- Both nodes are observed:
  - Y is a class indicator vector

$$p(y_n) = \mathrm{multi}(y_n : \pi) = \prod_k \pi_k^{y_{n,k}}$$

  - X is a conditional Gaussian variable with a class-specific mean

$$p(x_n \mid y_{n,k} = 1, \mu, \sigma) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{ -\frac{1}{2\sigma^2}(x_n - \mu_k)^2 \right\}$$

$$p(x \mid y, \mu, \sigma) = \prod_n \left(\prod_k N(x_n : \mu_k, \sigma)^{y_{n,k}} \right)$$

Recap: MLE of conditional Gaussian

- Data log-likelihood

$$\ell(\boldsymbol{\theta}; D) = \log \prod_n p(x_n, y_n) = \log \prod_n p(y_n \mid \pi) p(x_n \mid y_n, \mu, \sigma)$$

- MLE

$$\hat{\pi}_{k,MLE} = \arg\max_{\pi} \ell(\boldsymbol{\theta}; D), \qquad \hat{\pi}_{k,MLE} = \sum_n y_{n,k} \Big/ N = n_k \big/ N$$

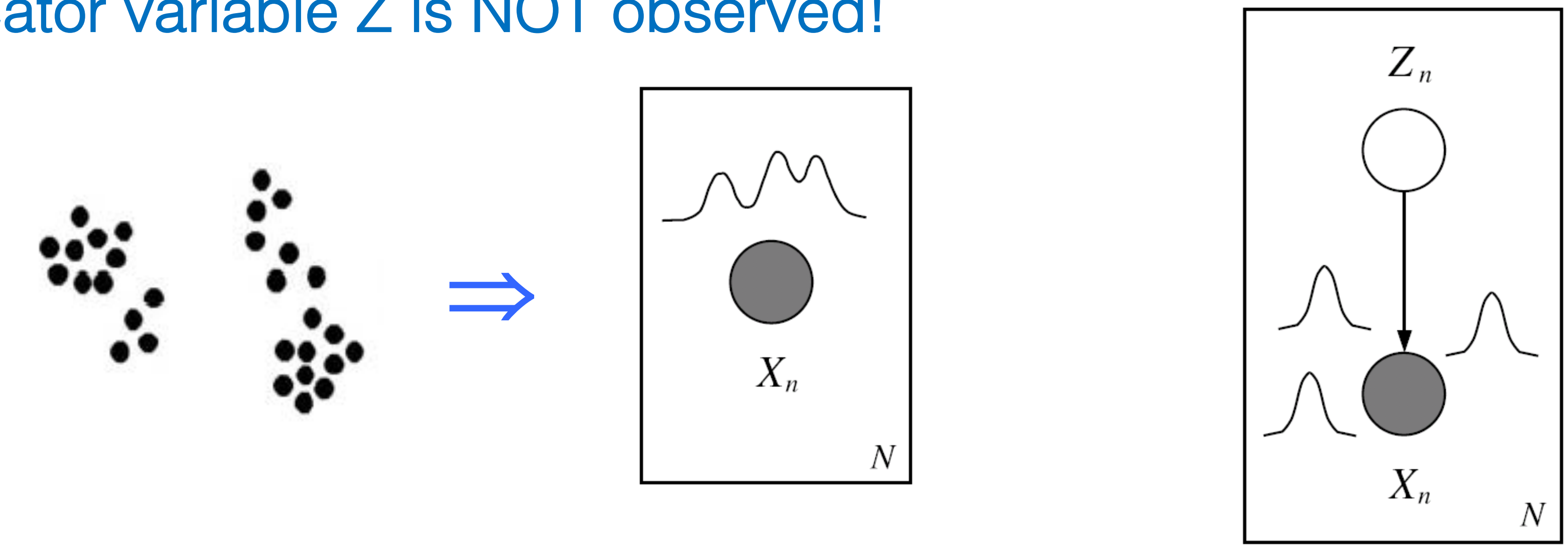
the fraction of samples of class *m*

$$\hat{\mu}_{k,MLE} = \arg\max \ell(\boldsymbol{\theta}; D), \qquad \hat{\mu}_{k,MLE} = \frac{\sum_n y_{n,k} x_n}{\sum_n y_{n,k}} = \frac{\sum_n y_{n,k} x_n}{n_k}$$

the average of samples of class *m*

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).
- Indicator variable Z is NOT observed!



(a) (b)

Unobserved Variables

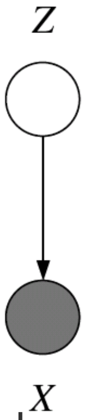
- A variable can be unobserved (latent) because:
  - it is an imaginary quantity meant to provide some simplified and abstractive view of the data generation process
    - e.g., speech recognition models, mixture models …
  - it is a real-world object and/or phenomena, but difficult or impossible to measure
    - e.g., the temperature of a star, causes of a disease, evolutionary ancestors …
  - it is a real-world object and/or phenomena, but sometimes wasn't measured, because of faulty sensors; or was measure with a noisy channel, etc.
    - e.g., traffic radio, aircraft signal on a radar screen,
- Discrete latent variables can be used to partition/cluster data into sub-groups (mixture models, forthcoming).
- Continuous latent variables (factors) can be used for dimensionality reduction (factor analysis, etc., later lectures).

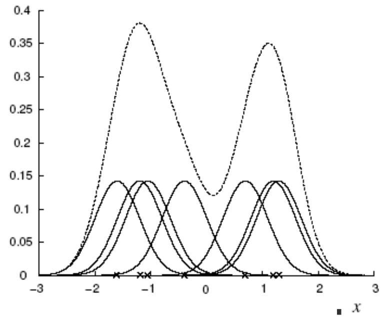
Gaussian Mixture Models (GMMs)

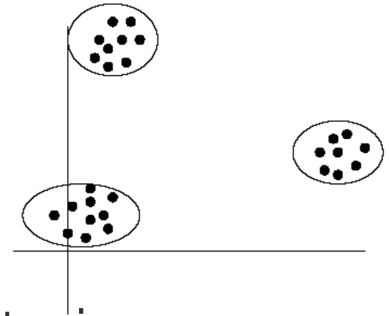
- Consider a mixture of K Gaussian components:

$$p(x_n|\mu,\Sigma)=\sum_k \pi_k N(x,|\,\mu_k,\Sigma_k)$$

mixture proportion   mixture component





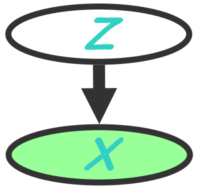


- This model can be used for unsupervised clustering.
  - This model (fit by AutoClass) has been used to discover new kinds of stars in astronomical data, etc.

GGM Likelihood

- Consider a mixture of K Gaussian components:
  - Z is a latent class indicator vector:

$$p(z_n) = \mathrm{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$



  - X is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n \mid z_n^k = 1, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{ -\tfrac{1}{2} (x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) \right\}$$

  - The likelihood of a sample:

mixture component

mixture proportion

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z^k = 1 \mid \pi) p(x, \mid z^k = 1, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k) \end{aligned}$$

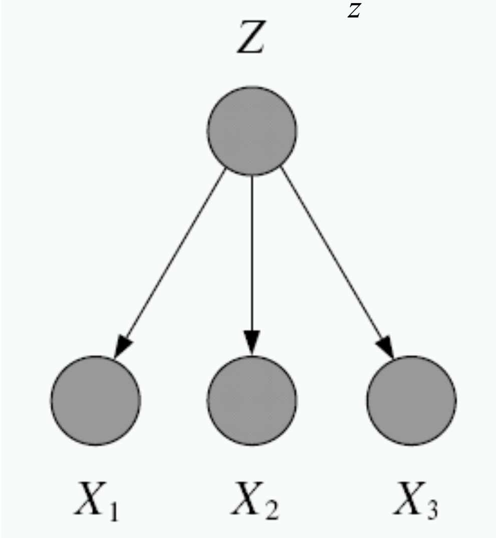
Why is Learning Harder?

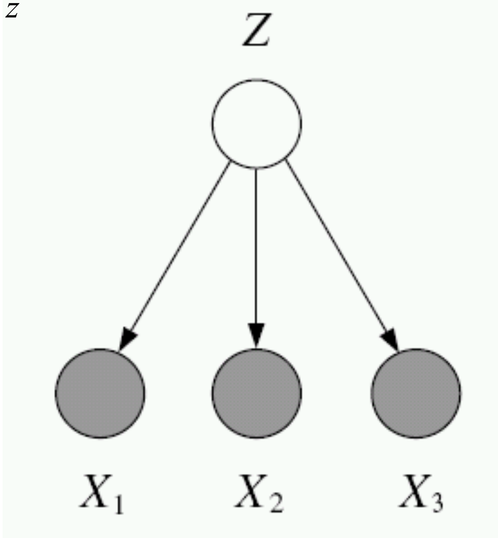
- In fully observed iid settings, the log likelihood decomposes into a sum of local terms.

$$\ell_c(\theta; D) = \log p(x, z \mid \theta) = \log p(z \mid \theta_z) + \log p(x \mid z, \theta_x)$$

- With latent variables, all the parameters become coupled together via *marginalization*

$$\ell_c(\theta; D) = \log \sum_z p(x, z \mid \theta) = \log \sum_z p(z \mid \theta_z) p(x \mid z, \theta_x)$$





Gradient Learning for mixture models

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

$$\ell(\theta) = \log p(\mathrm{x} \mid \theta) = \log \sum_k \pi_k p_k(\mathrm{x} | \theta_k)$$

$$\begin{aligned}
\frac{\partial \ell}{\partial \theta} &= \frac{1}{p(\mathrm{x} \mid \theta)} \sum_k \pi_k \frac{\partial p_k(\mathrm{x} | \theta_k)}{\partial \theta} \\
&= \sum_k \frac{\pi_k}{p(\mathrm{x} \mid \theta)} p_k(\mathrm{x} | \theta_k) \frac{\partial \log p_k(\mathrm{x} | \theta_k)}{\partial \theta} \\
&= \sum_k \pi_k \frac{p_k(\mathrm{x} | \theta_k)}{p(\mathrm{x} \mid \theta)} \frac{\partial \log p_k(\mathrm{x} | \theta_k)}{\partial \theta_k} = \sum_k r_k \frac{\partial \ell_k}{\partial \theta_k}
\end{aligned}$$

- 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. $\Sigma_k \pi_k = 1$, Σ being symmetric positive definite (hence $\Sigma_{ii} > 0$).
- We can use constrained optimization, or we can reparameterize in terms of unconstrained values.
  - For normalized weights, use the softmax transform:
  - For covariance matrices, use the Cholesky decomposition:

$$\Sigma^{-1} = \mathbf{A}^T \mathbf{A}$$

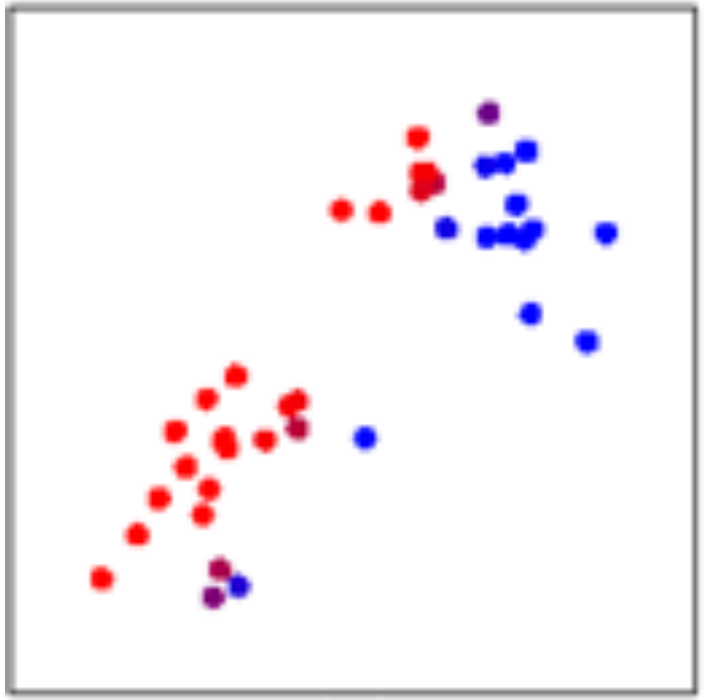
where A is upper diagonal with positive diagonal:

$$\mathbf{A}_{ii} = \exp(\lambda_i) > 0 \quad \mathbf{A}_{ij} = \eta_{ij} \ \ (j > i) \quad \mathbf{A}_{ij} = 0 \ \ (j < i)$$

the parameters γ_i, λ_i, $\eta_{ij} \in \mathrm{R}$ are unconstrained.

  - Use chain rule to compute $\dfrac{\partial \ell}{\partial \pi}, \dfrac{\partial \ell}{\partial \mathbf{A}}$.

The Expectation-Maximization (EM) Algorithm



GGM Likelihood
-- a close look

- E.g., mixture of K Gaussians:
  - Z is a latent class indicator vector

$$p(z_n) = \text{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$

Recap: MLE of conditional Gaussian

- Data log-likelihood

$$\ell(\boldsymbol{\theta}; D) = \log \prod_n p(x_n, y_n) = \log \prod_n p(y_n \mid \pi) p(x_n \mid y_n, \mu, \sigma)$$

- MLE

$$\hat{\pi}_{k,MLE} = \arg\max_{\pi} \ell(\boldsymbol{\theta}; D), \qquad \hat{\pi}_{k,MLE} = \sum_n y_{n,k} \Big/ N = n_k \big/ N$$

the fraction of samples of class m

$$\hat{\mu}_{k,MLE} = \arg\max \ell(\boldsymbol{\theta}; D), \qquad \hat{\mu}_{k,MLE} = \frac{\sum_n y_{n,k} x_n}{\sum_n y_{n,k}} = \frac{\sum_n y_{n,k} x_n}{n_k}$$

the average of samples of class m

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- X is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n \mid z_n^k = 1, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{-\tfrac{1}{2}(x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k)\right\}$$

- The likelihood of a sample:

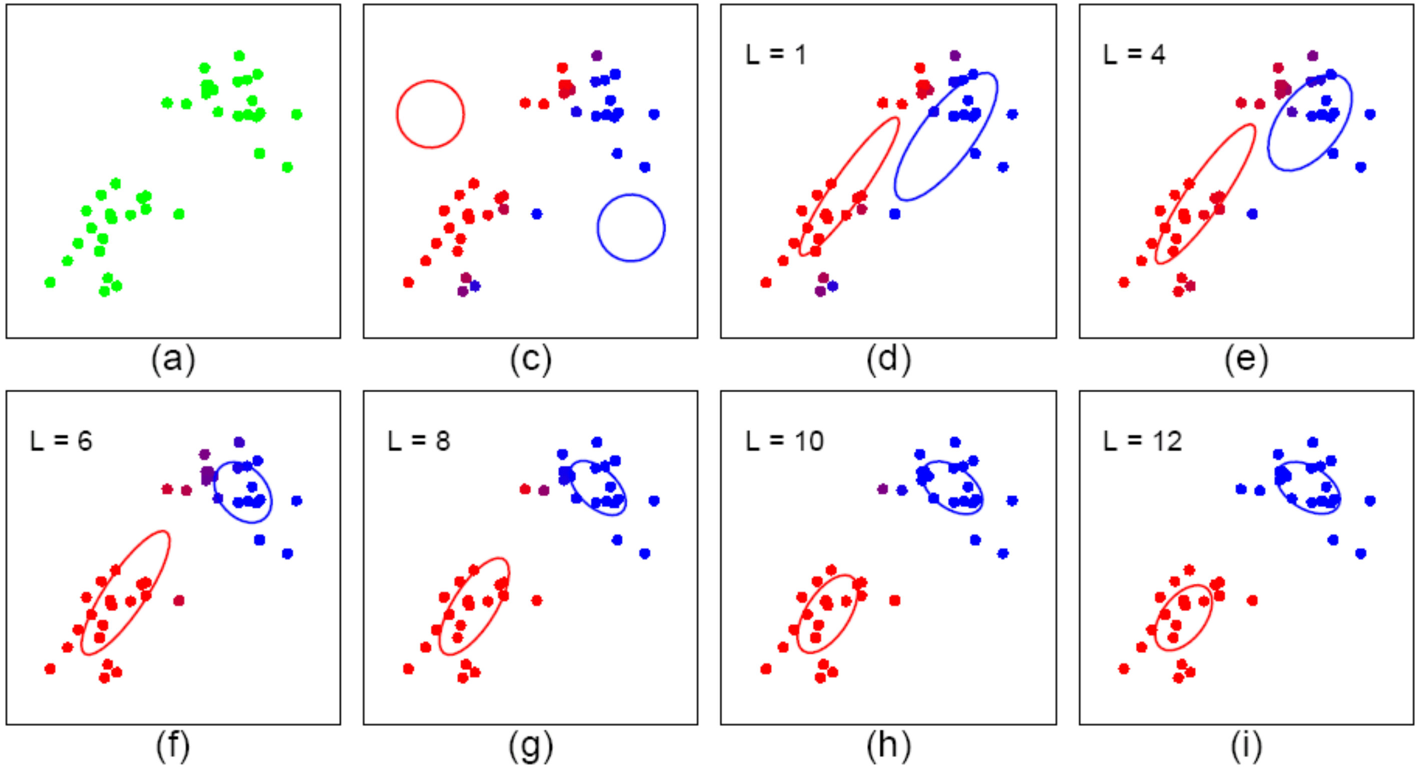
$$p(x_n | \mu, \Sigma) = \sum_k p(z^k = 1 \mid \pi) p(x, | z^k = 1, \mu, \Sigma)$$
$$= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, | \mu_k, \Sigma_k)$$

- ***If we do not know z_n***

$$z_n \rightarrow p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)})$$

An EM heuristic for GMM

- Start:
  - "Guess" the centroid μ_k and coveriance Σ_k of each of the K clusters
- Loop



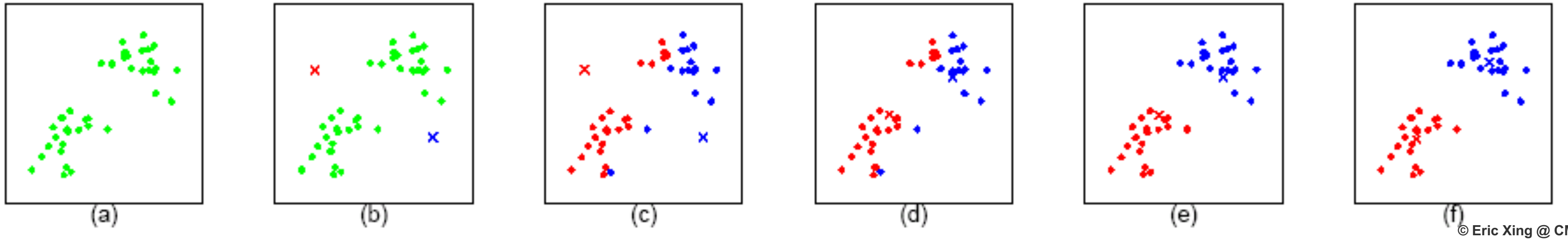
Recall K-means

- Start:
  - "Guess" the centroid μ_k and coveriance Σ_k of each of the K clusters
- Loop
  - For each point n=1 to N,
    compute its cluster label:

$$z_n^{(t)} = \arg\max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

  - For each cluster k=1:K

$$\mu_k^{(t+1)} = \frac{\sum_n \delta(z_n^{(t)}, k) x_n}{\sum_n \delta(z_n^{(t)}, k)} \qquad \Sigma_k^{(t+1)} = \ldots$$

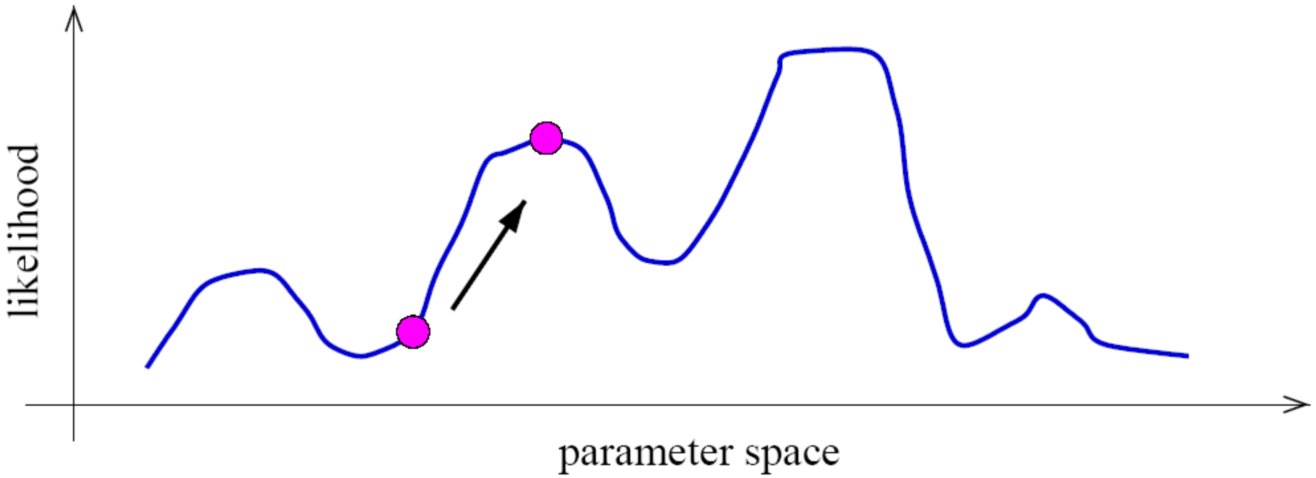


Notes on EM

- 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, $p(z|x, \theta^t)$.
  - M-step: update parameters t+1 using standard MLE/MAP method applied to completed data
- We will prove that this procedure monotonically improves (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.

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.



How is EM derived?

- A mixture of K Gaussians:
  - Z is a latent class indicator vector

$$p(z_n) = \mathrm{multi}(z_n : \pi) = \prod_k (\pi_k)^{z_n^k}$$

  - X is a conditional Gaussian variable with a class-specific mean/covariance

$$p(x_n \mid z_n^k = 1, \mu, \Sigma) = \frac{1}{(2\pi)^{m/2} |\Sigma_k|^{1/2}} \exp\left\{-\tfrac{1}{2}(x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k)\right\}$$

  - The likelihood of a sample:

$$\begin{aligned} p(x_n | \mu, \Sigma) &= \sum_k p(z_n^k = 1 \mid \pi) p(x, \mid z_n^k = 1, \mu, \Sigma) \\ &= \sum_{z_n} \prod_k \left((\pi_k)^{z_n^k} N(x_n : \mu_k, \Sigma_k)^{z_n^k} \right) = \sum_k \pi_k N(x, \mid \mu_k, \Sigma_k) \end{aligned}$$

- The "complete" likelihood

$$p(x_n, z_n^k = 1 | \mu, \Sigma) = p(z_n^k = 1 \mid \pi) p(x, \mid z_n^k = 1, \mu, \Sigma) = \pi_k N(x, \mid \mu_k, \Sigma_k)$$

$$p(x_n, z_n | \mu, \Sigma) = \prod_k \left[\pi_k N(x, \mid \mu_k, \Sigma_k) \right]^{z_n^k}$$

But this is itself a random variable! Not good as objective function

How is EM derived?

- The complete log likelihood:

$$\ell(\boldsymbol{\theta}; D) = \log \prod_n p(z_n, x_n) = \log \prod_n p(z_n \mid \pi) p(x_n \mid z_n, \mu, \sigma)$$

$$= \sum_n \log \prod_k \pi_k^{z_n^k} + \sum_n \log \prod_k N(x_n; \mu_k, \sigma)^{z_n^k}$$

$$= \sum_n \sum_k z_n^k \log \pi_k - \sum_n \sum_k z_n^k \frac{1}{2\sigma^2} (x_n - \mu_k)^2 + C$$

- The expected complete log likelihood

$$\langle \ell_c(\boldsymbol{\theta}; x, z) \rangle = \sum_n \langle \log p(z_n \mid \pi) \rangle_{p(z|x)} + \sum_n \langle \log p(x_n \mid z_n, \mu, \Sigma) \rangle_{p(z|x)}$$

$$= \sum_n \sum_k \langle z_n^k \rangle \log \pi_k - \frac{1}{2} \sum_n \sum_k \langle z_n^k \rangle \left((x_n - \mu_k)^T \Sigma_k^{-1} (x_n - \mu_k) + \log |\Sigma_k| + C \right)$$

E-step

- We maximize $\langle l_c(\theta) \rangle$ iteratively using the following iterative procedure:

  – Expectation step: computing the expected value of the sufficient statistics of the hidden variables (i.e., z) given current est. of the parameters (i.e., π and μ).

$$\tau_n^{k(t)} = \langle z_n^k \rangle_{q^{(t)}} = p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} N(x_n, \mid \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} N(x_n, \mid \mu_i^{(t)}, \Sigma_i^{(t)})}$$

  - Here we are essentially doing inference

M-step

- We maximize $\langle l_c(\boldsymbol{\theta}) \rangle$ iteratively using the following iterative procedure:

  – Maximization step: compute the parameters under current results of the expected value of the hidden variables

$$\pi_k^* = \arg\max \langle l_c(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \frac{\partial}{\partial \pi_k} \langle l_c(\boldsymbol{\theta}) \rangle = 0, \forall k, \quad \text{s.t.} \sum_{\mathrm{k}} \pi_k = 1$$

$$\Rightarrow \pi_k^* = \sum_n \langle z_n^k \rangle_{q^{(t)}} \Big/ N = \sum_n \tau_n^{k(t)} \Big/ N = \langle n_k \rangle \Big/ N$$

$$\mu_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \mu_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} x_n}{\sum_n \tau_n^{k(t)}}$$

$$\Sigma_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \qquad \Rightarrow \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

Fact:

$$\frac{\partial \log |\mathrm{A}^{-1}|}{\partial \mathrm{A}^{-1}} = \mathrm{A}^T$$

$$\frac{\partial \mathbf{x}^T \mathrm{A} \mathbf{x}}{\partial \mathrm{A}} = \mathbf{x}\mathbf{x}^T$$

  - This is isomorphic to MLE except that the variables that are hidden are replaced by their expectations (in general they will by replaced by their corresponding "sufficient statistics")

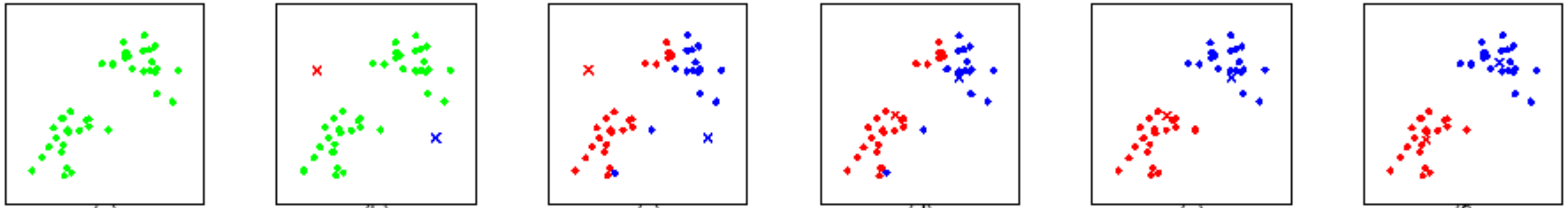
Compare: K-means

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

$$z_n^{(t)} = \arg\max_k (x_n - \mu_k^{(t)})^T \Sigma_k^{-1(t)} (x_n - \mu_k^{(t)})$$

- 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:

$$\mu_k^{(t+1)} = \frac{\sum_n \delta(z_n^{(t)}, k) x_n}{\sum_n \delta(z_n^{(t)}, k)}$$



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

Theory underlying EM

- What are we doing?
- Recall that according to MLE, we intend to learn the model parameter that would have maximize the likelihood of the data.
- But we do not observe z, so computing

  is difficult! $$\ell_c(\theta; D) = \log \sum_z p(x, z \mid \theta) = \log \sum_z p(z \mid \theta_z) p(x \mid z, \theta_x)$$

- What shall we do?

Complete & Incomplete Log Likelihoods

- Complete log likelihood

  Let X denote the observable variable(s), and Z denote the latent variable(s). If Z could be observed, then

$$\ell_c(\theta; x, z) \stackrel{\text{def}}{=} \log p(x, z \mid \theta)$$

  - Usually, optimizing $l_c()$ given both z and x is straightforward (c.f. MLE for fully observed models).
  - Recalled that in this case the objective for, e.g., MLE, decomposes into a sum of factors, the parameter for each factor can be estimated separately.
  - **But given that Z is not observed, $l_c()$ is a random quantity, cannot be maximized directly.**

- Incomplete log likelihood

  With z unobserved, our objective becomes the log of a marginal probability:

$$\ell_c(\theta; x) = \log p(x \mid \theta) = \log \sum_z p(x, z \mid \theta)$$

  - **This objective won't decouple**

Expected Complete Log Likelihood

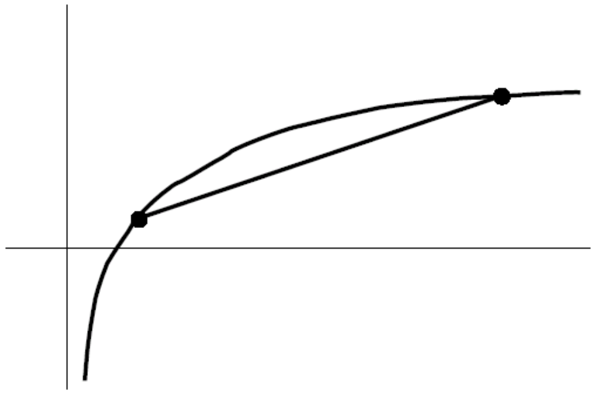
- For *any* distribution $q(z)$, define *expected complete log likelihood*:

$$\langle \ell_c(\theta; x, z) \rangle_q \stackrel{\text{def}}{=} \sum_z q(z \mid x, \theta) \log p(x, z \mid \theta)$$

  - A deterministic function of θ
  - Linear in $l_c()$ --- inherit its factorizabiility
  - Does maximizing this surrogate yield a maximizer of the likelihood?

- Jensen's inequality

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



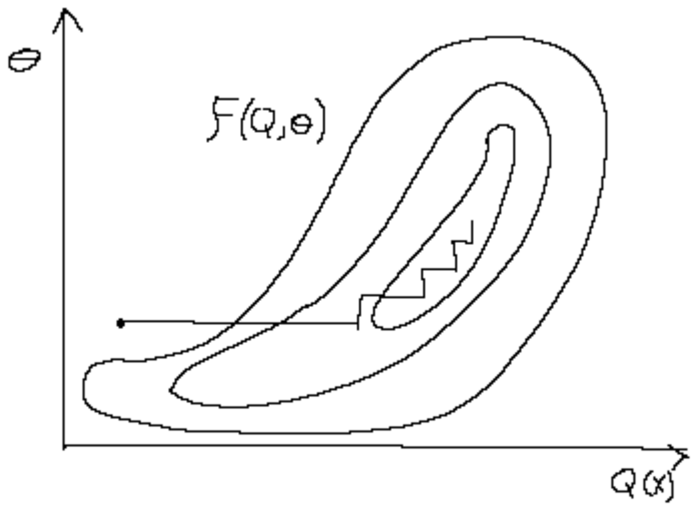
$$\Rightarrow \quad \ell(\theta; x) \geq \langle \ell_c(\theta; x, z) \rangle_q + H_q$$

Lower Bounds and Free Energy

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

$$F(q,\theta) \stackrel{\text{def}}{=} \sum_z q(z \mid x) \log \frac{p(x,z \mid \theta)}{q(z \mid x)} \leq \ell(\theta; x)$$

- The EM algorithm is coordinate-ascent on F:
  - E-step: $q^{t+1} = \arg\max_q F(q, \theta^t)$
  - M-step: $\theta^{t+1} = \arg\max_\theta F(q^{t+1}, \theta^t)$



E-step: maximization of expected l_c w.r.t. q

- Claim:

$$q^{t+1} = \arg\max_q F(q, \theta^t) = p(z \mid x, \theta^t)$$

  - 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 attains the bound $l(\theta;x) \geq F(q, \theta)$

$$\begin{aligned} F(p(z|x,\theta^t),\theta^t) &= \sum_z p(z|x,\theta^t) \log \frac{p(x,z \mid \theta^t)}{p(z|x,\theta^t)} \\ &= \sum_z p(z|x,\theta^t) \log p(x \mid \theta^t) \\ &= \log p(x \mid \theta^t) = \ell(\theta^t; x) \end{aligned}$$

- Can also show this result using variational calculus or the fact that

$$\ell(\theta; x) - F(q, \theta) = \mathrm{KL}\big(q \,\|\, p(z \mid x, \theta)\big)$$

E-step ≡ plug in posterior expectation of latent variables

- Without loss of generality: assume that $p(x,z|\theta)$ is a generalized exponential family distribution:

$$p(x,z|\theta)=\frac{1}{Z(\theta)}h(x,z)\exp\left\{\sum_i \theta_i f_i(x,z)\right\}$$

  - Special cases: if $p(X|Z)$ are GLIMs, then $f_i(x,z)=\eta_i^T(z)\xi_i(x)$

- The expected complete log likelihood under $q^{t+1}=p(z|x,\theta^t)$ is

$$\begin{aligned}
\left\langle \ell_c(\theta^t;x,z)\right\rangle_{q^{t+1}} &= \sum_z q(z|x,\theta^t)\log p(x,z|\theta^t)-A(\theta) \\
&= \sum_i \theta_i^t \left\langle f_i(x,z)\right\rangle_{q(z|x,\theta^t)} - A(\theta) \\
&\overset{p\sim\text{GLIM}}{=} \sum_i \theta_i^t \left\langle \eta_i(z)\right\rangle_{q(z|x,\theta^t)} \xi_i(x) - A(\theta)
\end{aligned}$$

M-step: maximization of expected l_c w.r.t. θ

- Note that the free energy breaks into two terms:

$$
\begin{aligned}
F(q,\theta) &= \sum_z q(z|x) \log \frac{p(x,z|\theta)}{q(z|x)} \\
&= \sum_z q(z|x) \log p(x,z|\theta) - \sum_z q(z|x) \log q(z|x) \\
&= \langle \ell_c(\theta; x, z) \rangle_q + H_q
\end{aligned}
$$

  - 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:

$$
\theta^{t+1} = \arg\max_\theta \langle \ell_c(\theta; x, z) \rangle_{q^{t+1}} = \arg\max_\theta \sum_z q(z|x) \log p(x,z|\theta)
$$

  - Under optimal q^{t+1}, this is equivalent to solving a standard MLE of fully observed model $p(x,z|\theta)$, with the sufficient statistics involving z replaced by their expectations w.r.t. $p(z|x,\theta)$.

Summary: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of 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 the best guess (posterior) and updating the parameters based on this guess:

  - E-step: $q^{t+1} = \arg\max_q F(q, \theta^t)$
  - M-step: $\theta^{t+1} = \arg\max_\theta F(q^{t+1}, \theta^t)$

- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

EM Variants

- Sparse EM:

  Do not re-compute 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). Recall the IRLS step in the mixture of experts model.

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

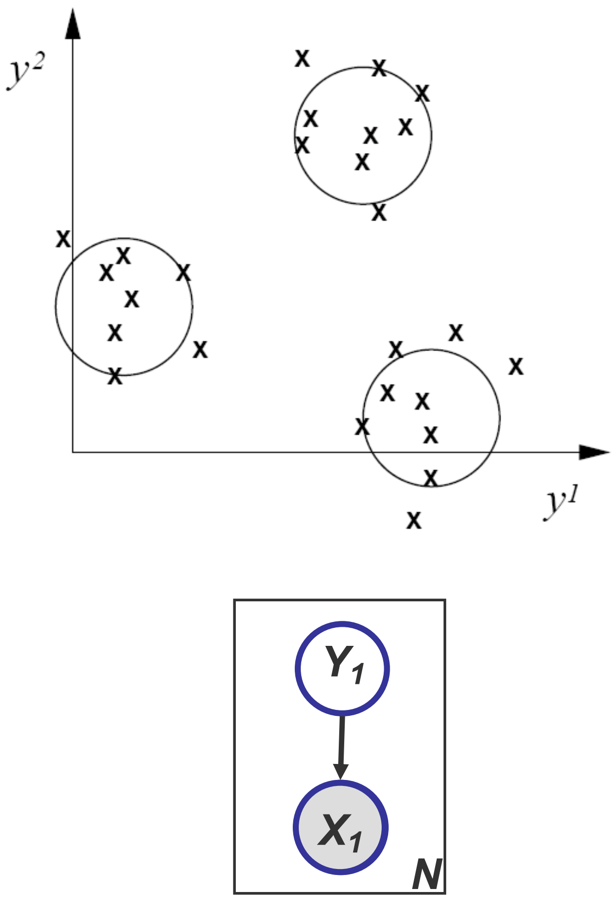
- Some bad things about EM:
  - can get stuck in local minima
  - can be slower than conjugate gradient (especially near convergence)
  - requires expensive inference step
  - is a maximum likelihood/MAP method

Supplementary

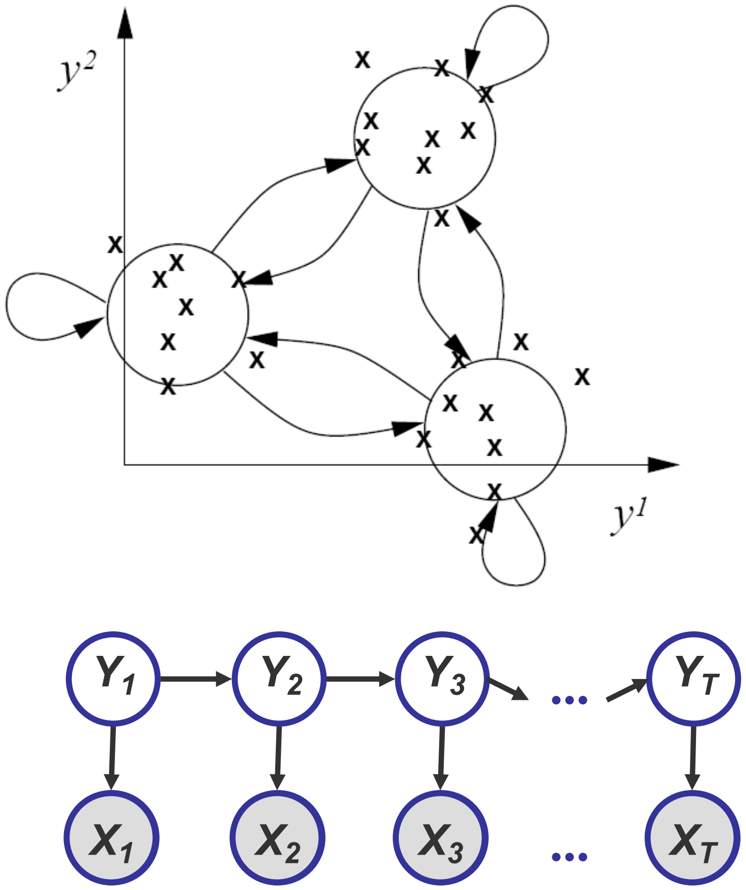
EM for Hidden Markov Modles

From static to dynamic mixture models

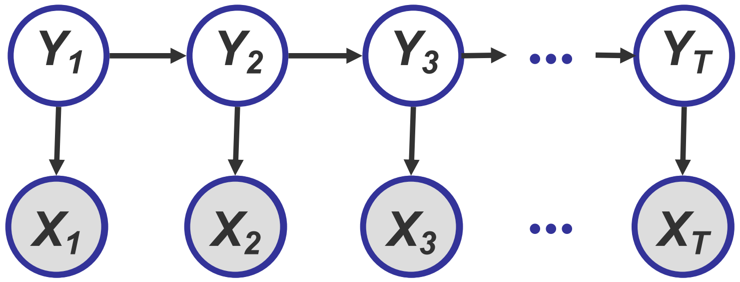
Static mixture



Dynamic mixture



Hidden Markov Models



The underlying source:

genomic entities,

dice,

The sequence:

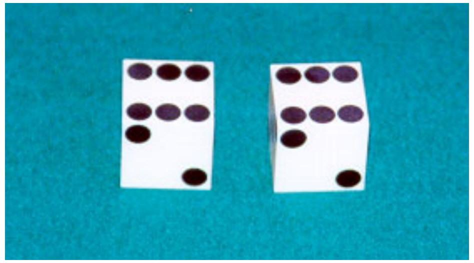
CGH signal,

sequence of rolls,

Markov property:

This problem in IMPORTANT!!! -☺

An experience in a casino



<u>Game:</u>

1. You bet $1
2. You roll (always with a fair die)
3. Casino player rolls (maybe with fair die, maybe with loaded die)
4. Highest number wins $2

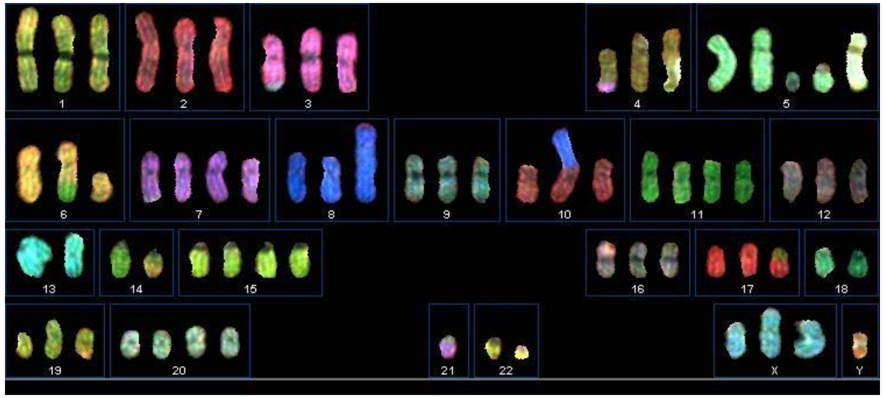
Question:

124552646214614613613666166466163 6
61636616361651561511514612356234 4

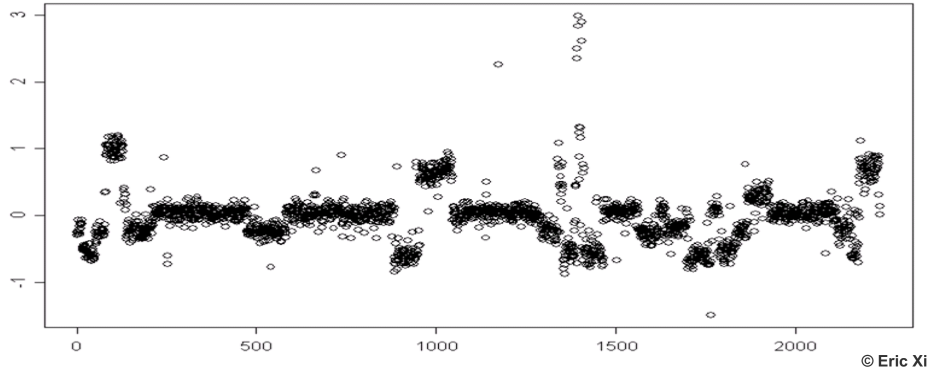
Which die is being used in each play?

A more serious question …
☹

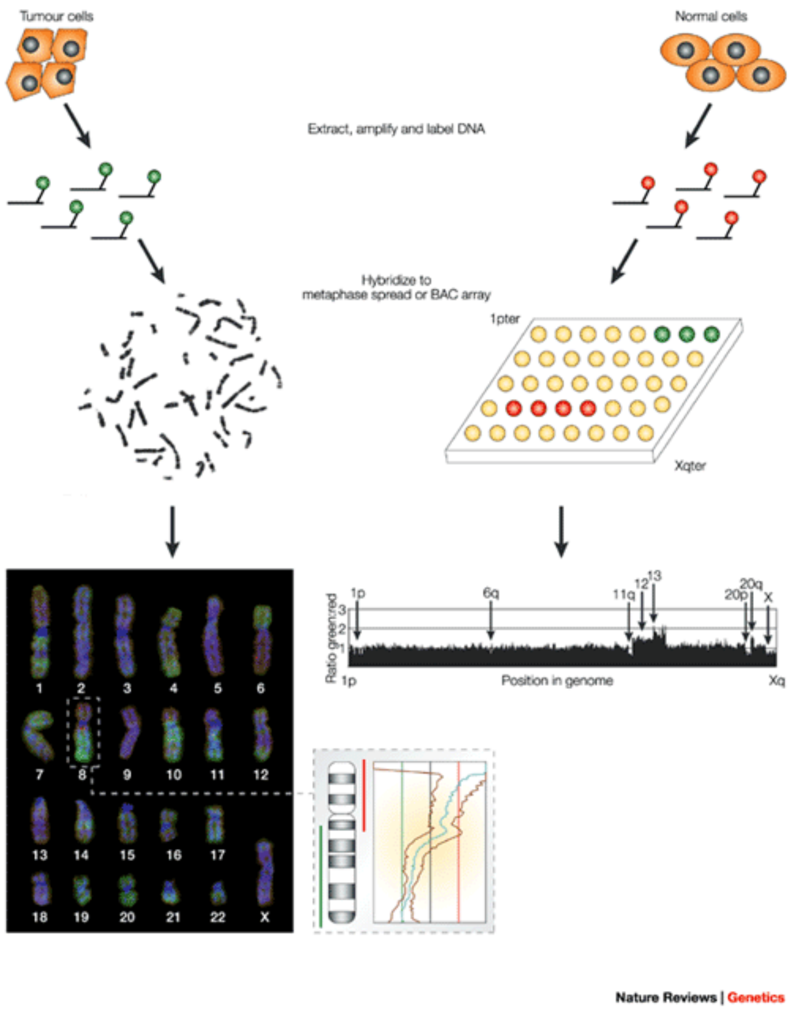
- Naturally, data points arrive one at a time
  - Does the ordering index carry (additional) clustering information besides the data value itself ?
  - Example:
    Chromosomes of tumor cell:



Copy number measurements (known as CGH)



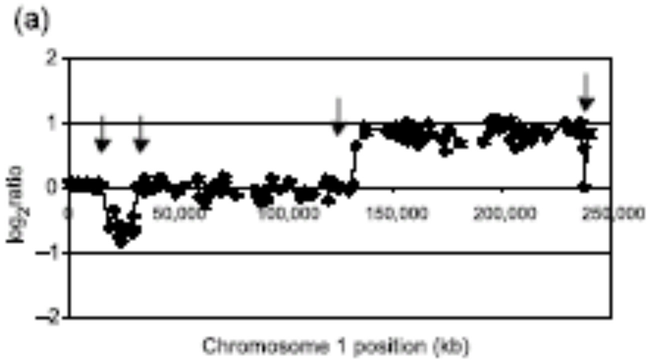
Array CGH (comparative genomic hybridization)



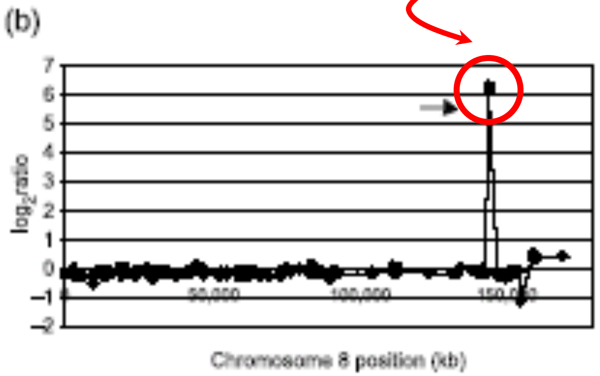
- The basic assumption of a CGH experiment is that the ratio of the binding of test and control DNA is proportional to the ratio of the copy numbers of sequences in the two samples.
- But various kinds of noises make the true observations less easy to interpret …

DNA Copy number aberration types in breast cancer

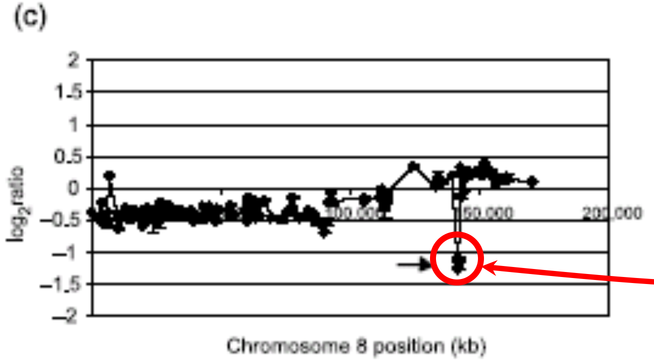
60-70 fold amplification of CMYC region



Copy number profile for chromosome 1 from 600 MPE cell line



Copy number profile for chromosome 8 from COLO320 cell line

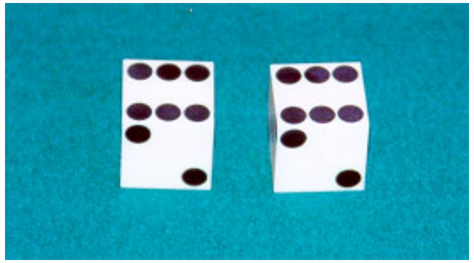


Copy number profile for chromosome 8 in MDA-MB-231 cell line

deletion

Suppose you were told about the following story before heading to Vegas…

The Dishonest Casino !!!



A casino has two dice:

- Fair die

  P(1) = P(2) = P(3) = P(5) = P(6) = 1/6
- Loaded die

  P(1) = P(2) = P(3) = P(5) = 1/10

  P(6) = 1/2

Casino player switches back-&-forth between fair and loaded die once every 20 turns

Puzzles Regarding the Dishonest Casino

GIVEN: A sequence of rolls by the casino player

1245526462146146136136661664661636616366163616515615115146123562344

QUESTION

- How likely is this sequence, given our model of how the casino works?
  - This is the EVALUATION problem
- What portion of the sequence was generated with the fair die, and what portion with the loaded die?
  - This is the DECODING question
- How "loaded" is the loaded die? How "fair" is the fair die? How often does the casino player change from fair to loaded, and back?
  - This is the LEARNING question

Three Main Questions on HMMs

1. Evaluation

GIVEN an HMM $\boldsymbol{M}$, and a sequence $\boldsymbol{x}$,
FIND Prob ($\boldsymbol{x} \mid \boldsymbol{M}$)
ALGO. Forward

2. Decoding

GIVEN an HMM $\boldsymbol{M}$, and a sequence $\boldsymbol{x}$,
FIND the sequence $\mathbf{y}$ of states that maximizes, e.g., P($\boldsymbol{y} \mid \boldsymbol{x}$, $\boldsymbol{M}$), or the most probable subsequence of states
ALGO. Viterbi, Forward-backward

3. Learning

GIVEN an HMM M, with unspecified transition/emission probs., and a sequence $\boldsymbol{x}$,
FIND parameters $\theta = (\pi_i, a_{ij}, \eta_{ik})$ that maximize $P(\boldsymbol{x} \mid \theta)$
ALGO. Baum-Welch (EM)

Definition (of HMM)

- Observation space

  Alphabetic set: $\mathrm{C} = \{c_1, c_2, \cdots, c_K\}$

  Euclidean space: R^d

- Index set of hidden states

  $$\mathrm{I} = \{1, 2, \cdots, M\}$$

- Transition probabilities between any two states

  $$p(y_t^j = 1 \mid y_{t-1}^i = 1) = a_{i,j},$$

  or
  $$p(y_t \mid y_{t-1}^i = 1) \sim \mathrm{Multinomial}(a_{i,1}, a_{i,2}, \ldots, a_{i,M}), \forall i \in \mathrm{I}.$$

- Start probabilities

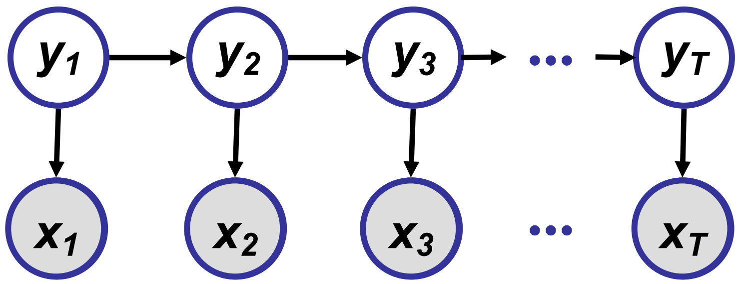
  $$p(y_1) \sim \mathrm{Multinomial}(\pi_1, \pi_2, \ldots, \pi_M).$$

- Emission probabilities associated with each state

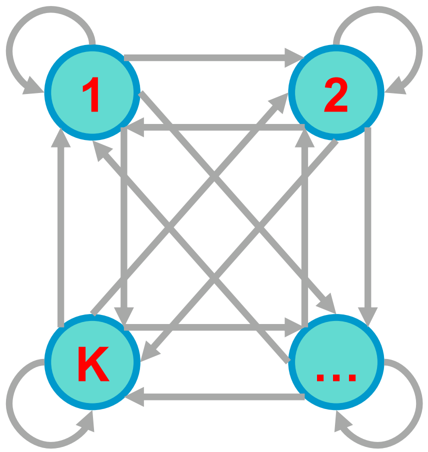
  $$p(x_t \mid y_t^i = 1) \sim \mathrm{Multinomial}(b_{i,1}, b_{i,2}, \ldots, b_{i,K}), \forall i \in \mathrm{I}.$$

  or in general:

  $$p(x_t \mid y_t^i = 1) \sim \mathrm{f}(\cdot \mid \theta_i), \forall i \in \mathrm{I}.$$



Graphical model



State automata

Learning HMM: two scenarios

- Supervised learning: estimation when the “right answer” is known
  - Examples:

    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands

    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls

- Unsupervised learning: estimation when the “right answer” is unknown
  - Examples:

    GIVEN: the porcupine genome; we don’t know how frequent are the CpG islands there, neither do we know their composition

    GIVEN: 10,000 rolls of the casino player, but we don’t see when he changes dice

- QUESTION: Update the parameters θ of the model to maximize $P(x|\theta)$ --- Maximal likelihood (ML) estimation

Supervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is known,
  - Define:

    A_{ij} = # times state transition $i \rightarrow j$ occurs in y

    B_{ik} = # times state i in y emits k in x

  - We can show that the maximum likelihood parameters θ are:

$$a_{ij}^{ML} = \frac{\#(i \rightarrow j)}{\#(i \rightarrow \bullet)} = \frac{\sum_n \sum_{t=2}^T y_{n,t-1}^i y_{n,t}^j}{\sum_n \sum_{t=2}^T y_{n,t-1}^i} = \frac{A_{ij}}{\sum_{j'} A_{ij'}}$$

$$b_{ik}^{ML} = \frac{\#(i \rightarrow k)}{\#(i \rightarrow \bullet)} = \frac{\sum_n \sum_{t=1}^T y_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^T y_{n,t}^i} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

  - What if x is continuous? We can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as $N \times T$ observations of, e.g., a Gaussian, and apply learning rules for Gaussian …

Unsupervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is unknown,

  - EXPECTATION MAXIMIZATION

0. Starting with our best guess of a model M, parameters θ:
1. Estimate A_{ij} , B_{ik} in the training data
   - How? , ,
   - Update θ according to A_{ij} , B_{ik}
   - Now a "supervised learning" problem

$$A_{ij} = \sum_{n,t} \left\langle y_{n,t-1}^{i} y_{n,t}^{j} \right\rangle \qquad B_{ik} = \sum_{n,t} \left\langle y_{n,t}^{i} \right\rangle x_{n,t}^{k}$$

2. Repeat 1 & 2, until convergence

This is called the Baum-Welch Algorithm

We can get to a provably more (or equally) likely parameter set θ each iteration

The Baum Welch algorithm – an EM algorithm

- The complete log likelihood

$$\ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) = \log p(\mathbf{x},\mathbf{y}) = \log \prod_n \left(p(y_{n,1}) \prod_{t=2}^{T} p(y_{n,t} \mid y_{n,t-1}) \prod_{t=1}^{T} p(x_{n,t} \mid x_{n,t}) \right)$$

- The expected complete log likelihood

$$\left\langle \ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) \right\rangle = \sum_n \left(\left\langle y_{n,1}^i \right\rangle_{p(y_{n,1}|\mathbf{x}_n)} \log \pi_i \right) + \sum_n \sum_{t=2}^{T} \left(\left\langle y_{n,t-1}^i y_{n,t}^j \right\rangle_{p(y_{n,t-1},y_{n,t}|\mathbf{x}_n)} \log a_{i,j} \right) + \sum_n \sum_{t=1}^{T} \left(x_{n,t}^k \left\langle y_{n,t}^i \right\rangle_{p(y_{n,t}|\mathbf{x}_n)} \log b_{i,k} \right)$$

- EM
  - The **E** step

$$\gamma_{n,t}^i = \left\langle y_{n,t}^i \right\rangle = p(y_{n,t}^i = 1 \mid \mathbf{x}_n)$$

$$\xi_{n,t}^{i,j} = \left\langle y_{n,t-1}^i y_{n,t}^j \right\rangle = p(y_{n,t-1}^i = 1, y_{n,t}^j = 1 \mid \mathbf{x}_n)$$

  - The **M** step ("symbolically" identical to MLE)

$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N} \qquad a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i} \qquad b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^{T} \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$