

Announcements

Assignments

- HW9 (online)
 - Due Thu 4/16, 11:59 pm

TA Applications:

- Please apply to TA with us! Link for MLD applications will be in piazza.

Participation points

- Starting now, we're capping the denominator (57 polls) in the participation points calculation

Introduction to Machine Learning

Clustering GMM and EM

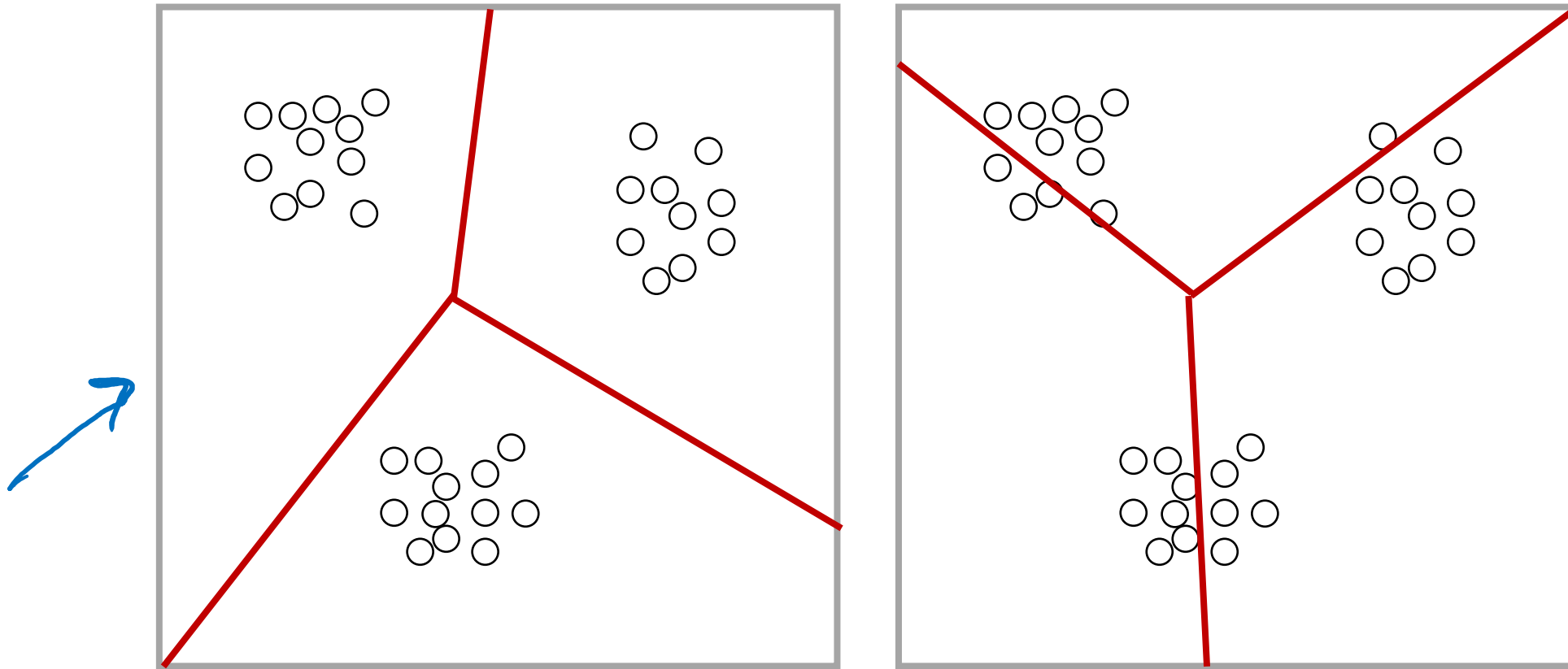
Instructor: Pat Virtue

Slide credits: Aarti Singh, Eric Xing, Carlos Guestrin

K-means Optimization

Question: Which of these partitions is “better”?

min



K-means Optimization

Input: $\vec{x}^{(1)}, \dots, \vec{x}^{(N)}$ K $\vec{x}^{(i)} \in \mathbb{R}^M$

Output: $\vec{z}^{(1)}, \dots, \vec{z}^{(N)}$ $\vec{C} = \{\vec{C}_1, \dots, \vec{C}_K\}$ $\vec{C}_k \in \mathbb{R}^M$

$$\vec{C} = \operatorname{argmin}_{\vec{C}} \sum_{i=1}^N \min_{j \in \{1..K\}} \|\vec{x}^{(i)} - \vec{C}_j\|_2^2$$

$$\vec{C}, \vec{z} = \operatorname{argmin}_{\vec{C}} \sum_{i=1}^N \min_{z^{(i)} \in \{1..K\}} \|\vec{x}^{(i)} - \vec{C}_{z^{(i)}}\|_2^2$$

$$= \operatorname{argmin}_{\vec{C}, \vec{z}} \sum_{i=1}^N \|\vec{x}^{(i)} - \vec{C}_{z^{(i)}}\|_2^2$$

K-means Optimization

Alternating minimization

$$a) \vec{z} = \operatorname{argmin}_{\vec{z}} \sum_{i=1}^N \|x^i - \underline{c}_z\|_2^2$$

$$b) C = \operatorname{argmin}_C \sum_{i=1}^N \|x^i - c_z\|_2^2$$

$$\begin{array}{l|l} a) z^{(1)} = \operatorname{argmin}_k \|x^{(1)} - c_k\|_2^2 & b) \vec{c}_1 = \operatorname{argmin}_{c_1} \sum_{i=z^{(1)}=1} \|x^{(i)} - c_1\|_2^2 \\ \vdots & \vdots \\ z^{(N)} = " & \vec{c}_k = \operatorname{argmin}_{c_k} \sum_{i=z^{(i)}=k} \|x^{(i)} - c_k\|_2^2 \end{array}$$

Piazza Poll 1

[True/False] The alternating minimization algorithm will find the global minimum of the k-means objective.

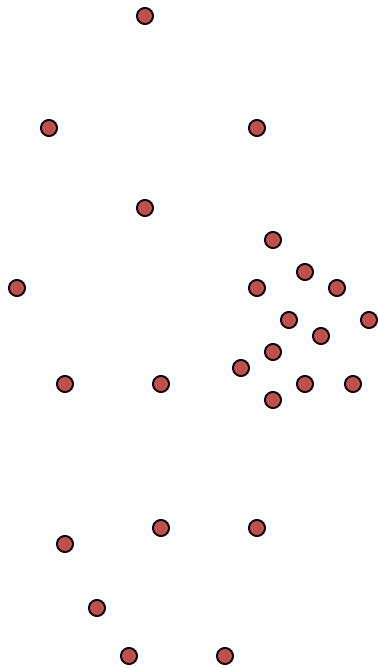
$$\mathbf{C}, \mathbf{z} = \operatorname{argmin}_{\mathbf{C}, \mathbf{z}} \sum_{i=1}^N \|\mathbf{x}^{(i)} - \mathbf{c}_{z^{(i)}}\|_2^2$$

A.

B.

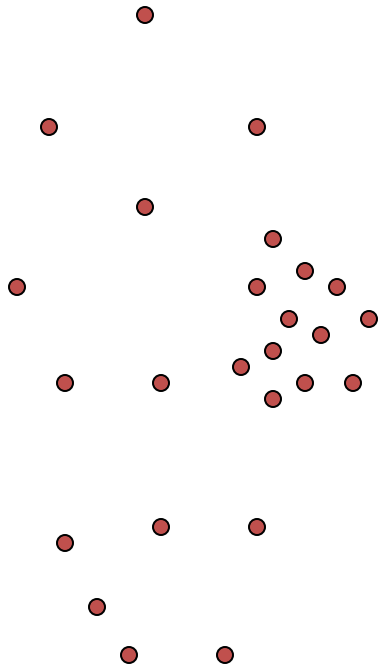
C.

(One) bad case for K-means



- Clusters may overlap
- Some clusters may be “wider” than others
- Clusters may not be linearly separable

(One) bad case for K-means



- Clusters may overlap
- Some clusters may be “wider” than others
- Clusters may not be linearly separable

Partitioning Algorithms

- K-means
 - **hard assignment**: each object belongs to only one cluster
- Mixture modeling
 - **soft assignment**: probability that an object belongs to a cluster

Generative approach

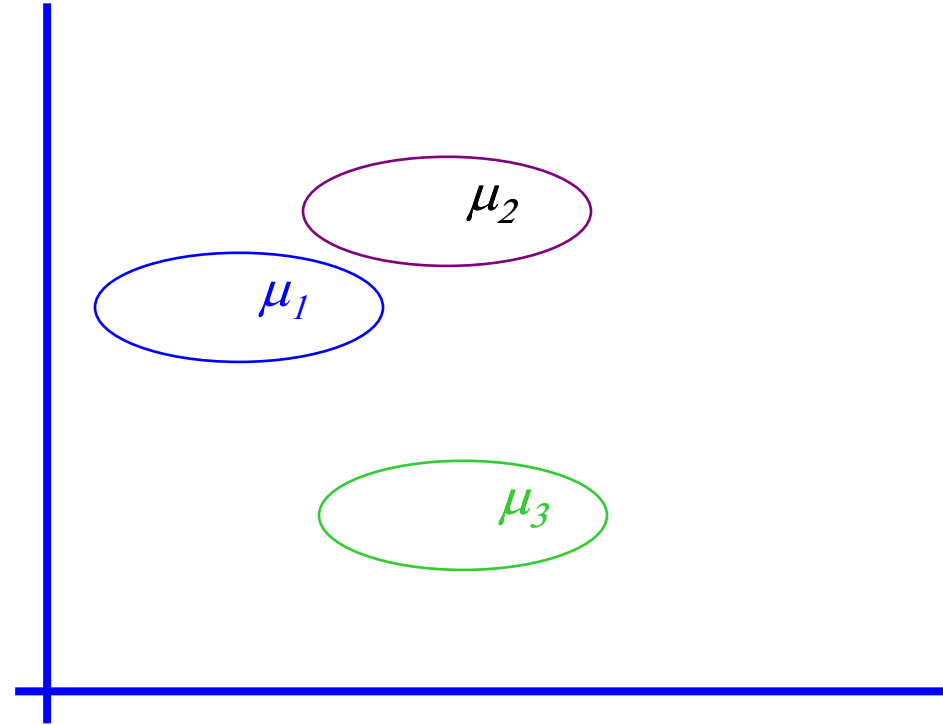
Gaussian Mixture Model

Mixture of K Gaussian distributions: (Multi-modal distribution)

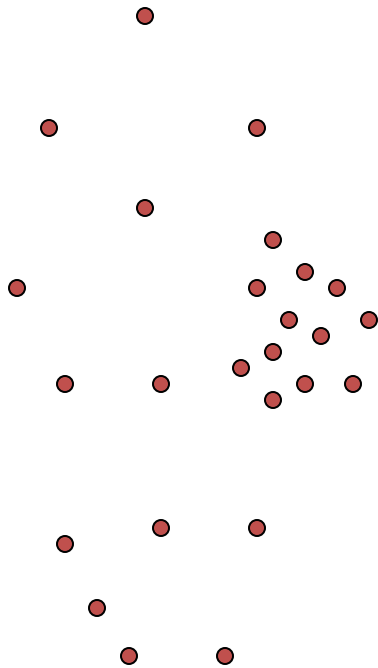
$$p(x/y=i) \sim N(\mu_i, \sigma^2 I)$$

$$p(x) = \sum_i p(x/y=i) P(y=i)$$

↓ ↓
Mixture **Mixture**
component **proportion**



(One) bad case for K-means



- Clusters may overlap
- Some clusters may be “wider” than others
- Clusters may not be linearly separable

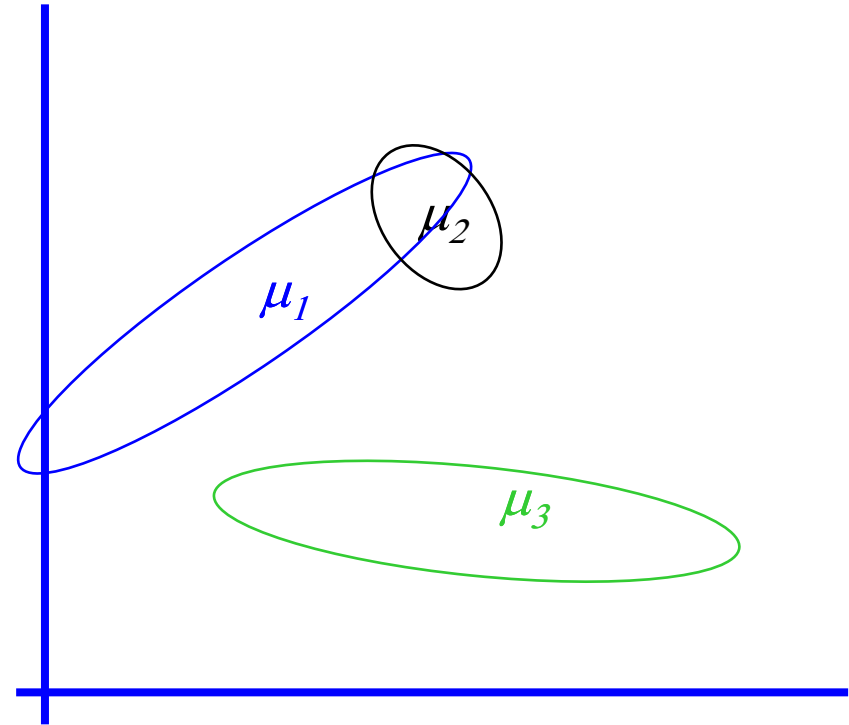
General GMM

GMM – Gaussian Mixture Model (Multi-modal distribution)

$$p(x/y=i) \sim N(\mu_i, \Sigma_i)$$

$$p(x) = \sum_i p(x/y=i) P(y=i)$$

↓ ↓
Mixture **Mixture**
component **proportion**



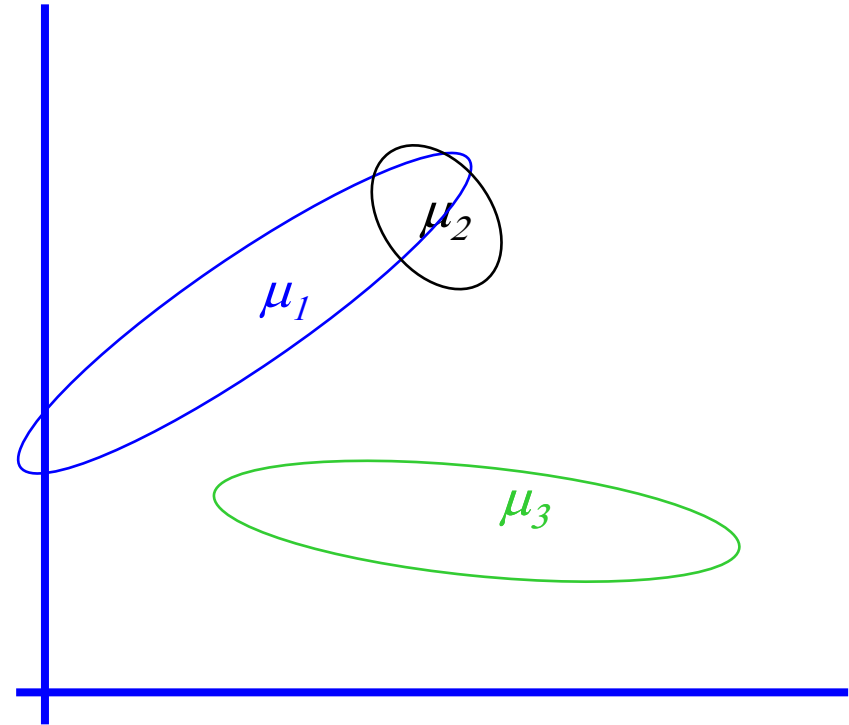
General GMM

GMM – Gaussian Mixture Model (Multi-modal distribution)

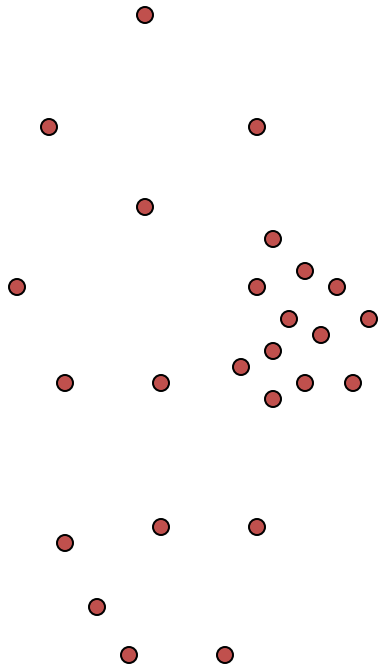
- There are k components
- Component i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix Σ_i

Each data point is generated according to the following recipe:

- 1) Pick a component at random:
Choose component i with probability $P(y=i)$
- 2) Datapoint $x \sim N(\mu_i, \Sigma_i)$



(One) bad case for K-means



- Clusters may overlap
- Some clusters may be “wider” than others
- Clusters may not be linearly separable

General GMM

GMM – Gaussian Mixture Model (Multi-modal distribution)

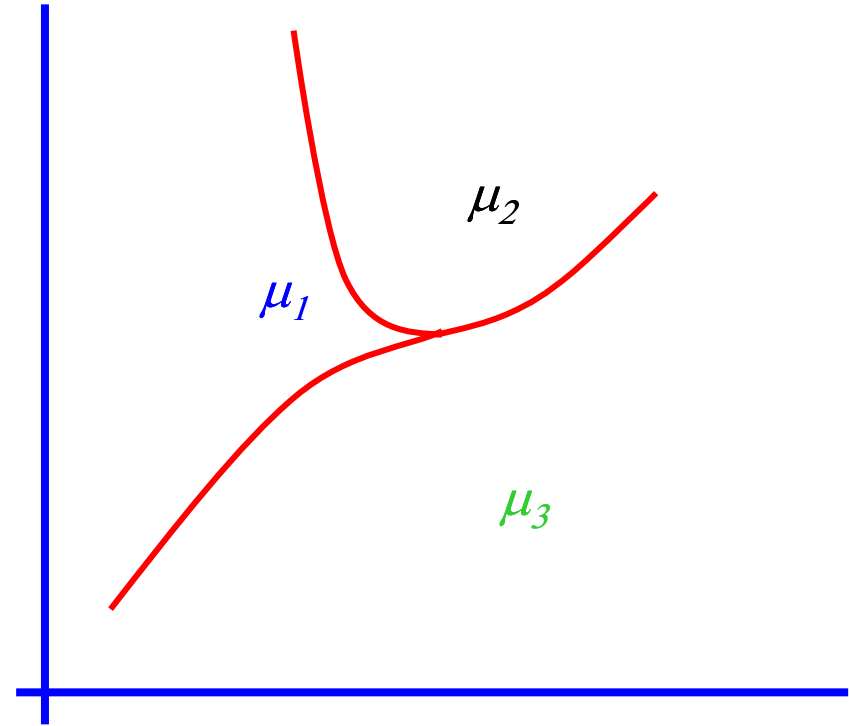
$$p(x|y=i) \sim N(\mu_i, \Sigma_i)$$

Decision boundary when probabilities are equal:

$$\log \frac{P(y=i|x)}{P(y=j|x)}$$

$$= \log \frac{p(x|y=i)P(y=i)}{p(x|y=j)P(y=j)}$$

$$= x^T \underbrace{W}_{\text{Depend on } \mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K, P(y=1), \dots, P(y=K)} x + \underbrace{w}_{\text{Depend on } \mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K, P(y=1), \dots, P(y=K)}$$



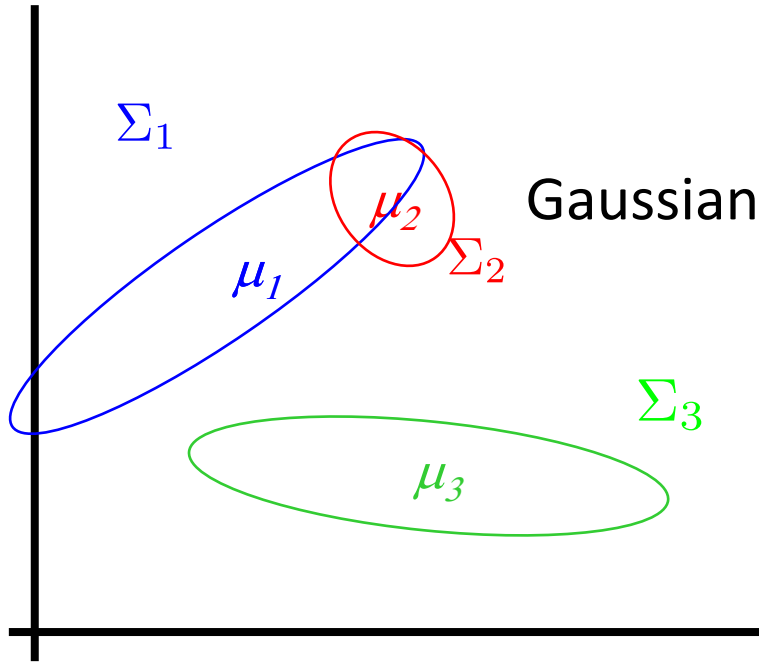
“Quadratic Decision boundary” – second-order terms don’t cancel out

Learning General GMM

$$x_1, \dots, x_m \sim p(x) = \sum_{i=1}^k p(x|Y = i) P(Y = i)$$

↓
**Mixture
component**

↓
**Mixture
proportion, p_i**



Gaussian mixture model

$$p(x|Y = i) \sim \mathcal{N}(\mu_i, \Sigma_i)$$

Parameters: $\{p_i, \mu_i, \Sigma_i\}_{i=1}^K$

- How to estimate parameters? Max Likelihood
But don't know labels Y

Learning General GMM

Maximize marginal likelihood:

$$\begin{aligned}\operatorname{argmax} \prod_j P(x_j) &= \operatorname{argmax} \prod_j \sum_{i=1}^K P(y_j=i, x_j) \\ &= \operatorname{argmax} \prod_j \sum_{i=1}^K P(y_j=i) p(x_j | y_j=i)\end{aligned}$$

$P(y_j=i) = P(y=i)$ Mixture component i is chosen with prob $P(y = i)$

$$= \operatorname{argmax} \prod_{j=1}^m \sum_{i=1}^k P(y = i) \frac{1}{\sqrt{\det(\Sigma_i)}} \exp\left[-\frac{1}{2} (x_j - \mu_i)^T \Sigma_i^{-1} (x_j - \mu_i)\right]$$

How do we find the μ_i, Σ_i s and $P(y=i)$ s which give max. marginal likelihood?

* Set $\frac{\partial}{\partial \mu_i} \log \text{Prob} (\dots) = 0$ and solve for μ_i 's. Non-linear not-analytically solvable

* Use gradient descent: Doable, but often slow

MLE Optimization

MLE Optimization

GMM vs. k-means

Maximize marginal likelihood:

$$\begin{aligned}\operatorname{argmax} \prod_j P(x_j) &= \operatorname{argmax} \prod_j \sum_{i=1}^K P(y_j=i, x_j) \\ &= \operatorname{argmax} \prod_j \sum_{i=1}^K P(y_j=i) p(x_j | y_j=i)\end{aligned}$$

- What happens if we assume **Hard assignment**?

$$\begin{aligned}P(y_j = i) &= 1 \text{ if } i = C(j) \\ &= 0 \text{ otherwise}\end{aligned}$$

$$\operatorname{argmax} \prod_j P(x_j) = \operatorname{argmax} \prod_j p(x_j | y_j=C(j))$$

Same as
k-means!

$$= \operatorname{argmax} \prod_{j=1}^n \exp\left(\frac{-1}{2\sigma^2} \|x_j - \mu_{C(j)}\|^2\right)$$

$$= \operatorname{argmin} \sum_{j=1}^n \|x_j - \mu_{C(j)}\|^2 = \operatorname{argmin}_{\mu, C} F(\mu, C)$$

Expectation-Maximization (EM)

A general algorithm to deal with hidden data, but we will study it in the context of unsupervised learning (hidden labels) first

- No need to choose step size as in Gradient methods.
- EM is an Iterative algorithm with two linked steps:
 - E-step: fill-in hidden data (Y) using inference
 - M-step: apply standard MLE/MAP method to estimate parameters $\{\mu_i, \Sigma_i\}_{i=1}^k$
- We will see that this procedure monotonically improves the likelihood (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.

EM for spherical, same variance GMMs

E-step

Compute “expected” classes of all datapoints for each class

M-step

Compute Max. like μ given our data’s class membership distributions (weights)

Iterate.

EM for spherical, same variance GMMs

E-step

Compute “expected” classes of all datapoints for each class

$$P(y = i | x_j, \mu_1 \dots \mu_k) \propto \exp\left(-\frac{1}{2\sigma^2} \|x_j - \mu_i\|^2\right) P(y = i)$$

In K-means “E-step”
we do hard assignment

EM does soft assignment

M-step

Compute Max. like μ given our data’s class membership distributions (weights)

$$\mu_i = \frac{\sum_{j=1}^m P(y = i | x_j) x_j}{\sum_{j=1}^m P(y = i | x_j)}$$

Exactly same as MLE with
weighted data

Iterate.

EM for general GMMs

Iterate. On iteration t let our estimates be

$$\lambda_t = \{ \mu_1^{(t)}, \mu_2^{(t)} \dots \mu_k^{(t)}, \Sigma_1^{(t)}, \Sigma_2^{(t)} \dots \Sigma_k^{(t)}, p_1^{(t)}, p_2^{(t)} \dots p_k^{(t)} \}$$

$p_i^{(t)}$ is shorthand for
estimate of $P(y=i)$ on
 t 'th iteration

E-step

Compute “expected” classes of all datapoints for each class

$$P(y = i | x_j, \lambda_t) \propto p_i^{(t)} P(x_j | \mu_i^{(t)}, \Sigma_i^{(t)})$$

*Just evaluate a
Gaussian at x_j*

M-step

Compute MLEs given our data's class membership distributions (weights)

$$\mu_i^{(t+1)} = \frac{\sum_j P(y = i | x_j, \lambda_t) x_j}{\sum_j P(y = i | x_j, \lambda_t)} \quad \Sigma_i^{(t+1)} = \frac{\sum_j P(y = i | x_j, \lambda_t) (x_j - \mu_i^{(t+1)})(x_j - \mu_i^{(t+1)})^T}{\sum_j P(y = i | x_j, \lambda_t)}$$

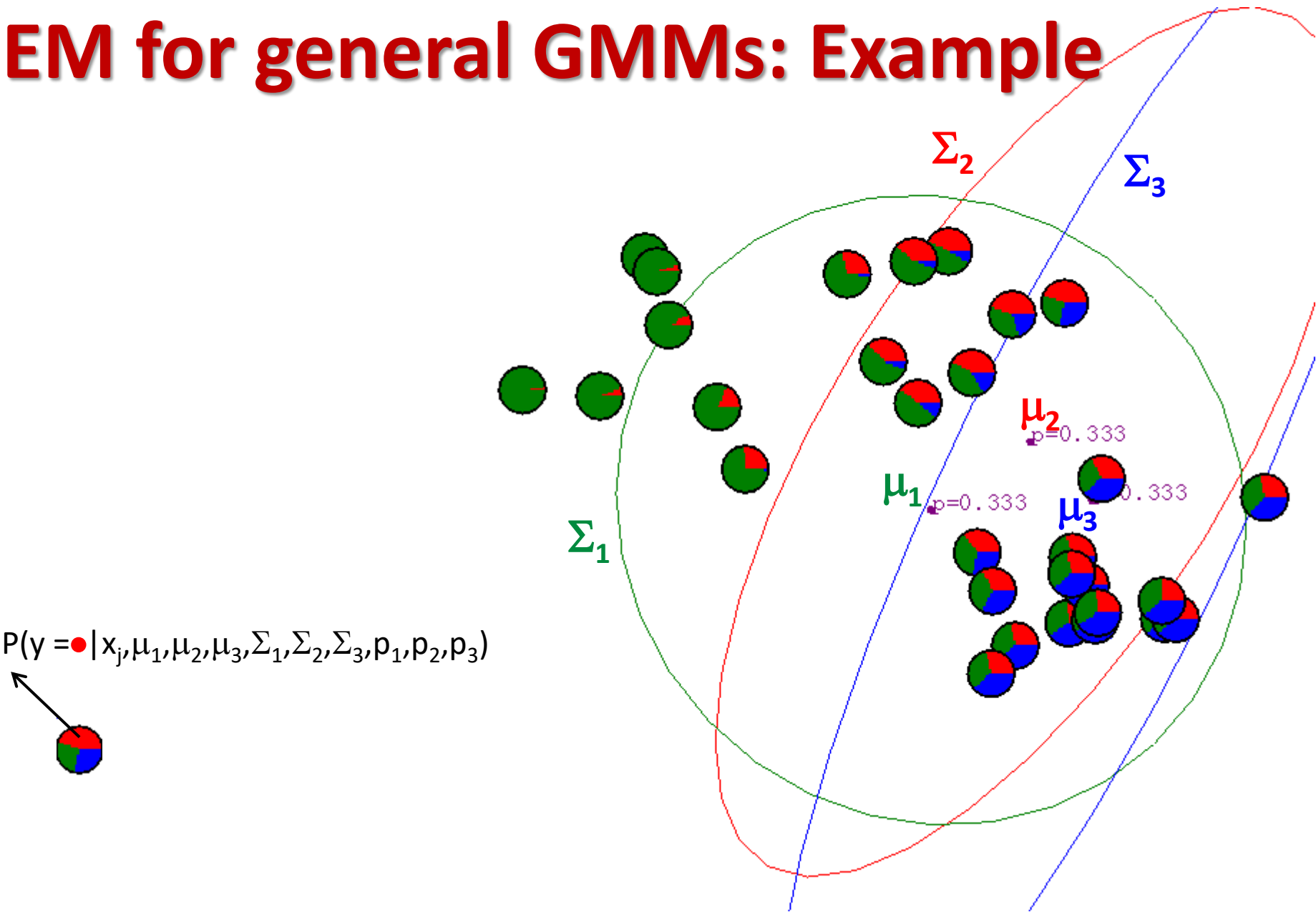
$$p_i^{(t+1)} = \frac{\sum_j P(y = i | x_j, \lambda_t)}{m}$$

$m = \text{\#data points}$

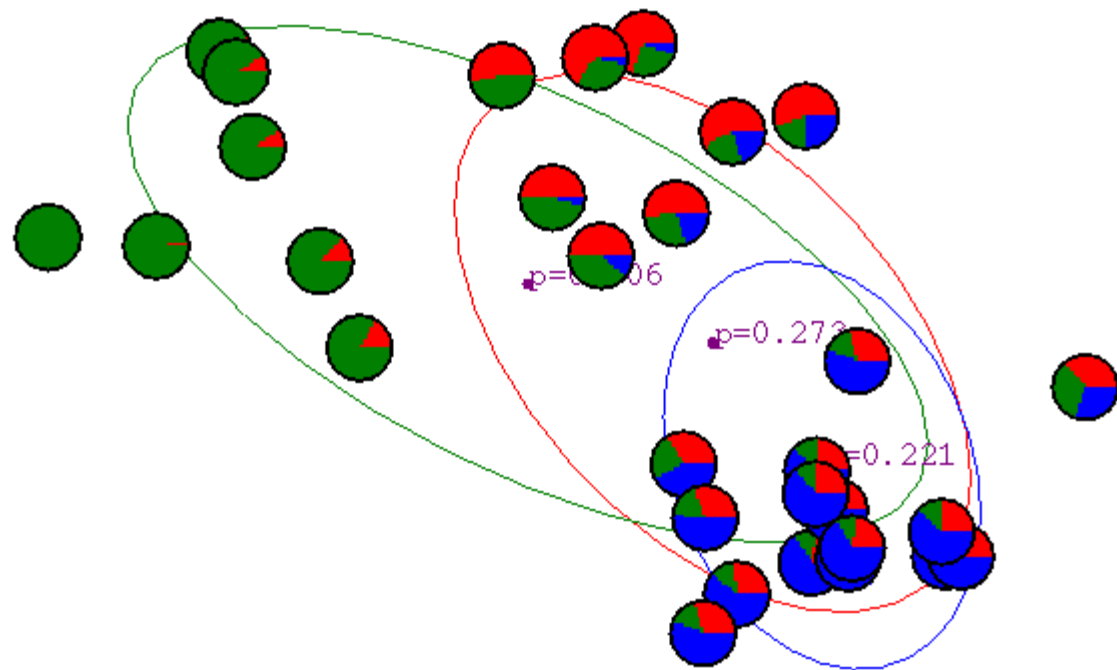
EM Convergence

EM for general GMMs: Example

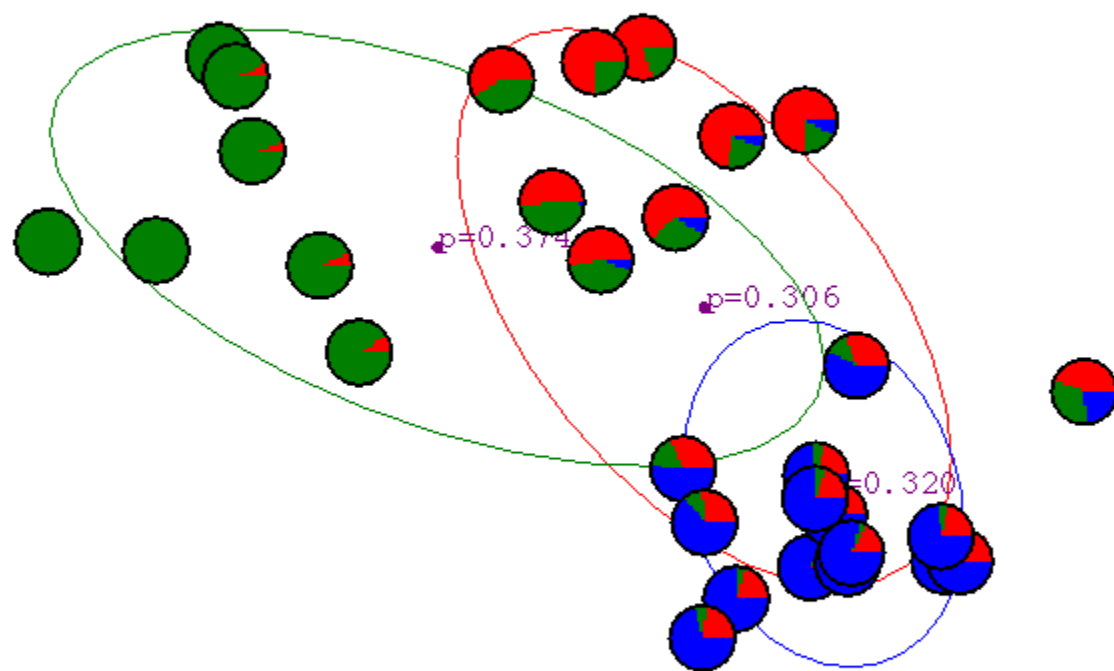
$$P(y = \bullet | x_j, \mu_1, \mu_2, \mu_3, \Sigma_1, \Sigma_2, \Sigma_3, p_1, p_2, p_3)$$



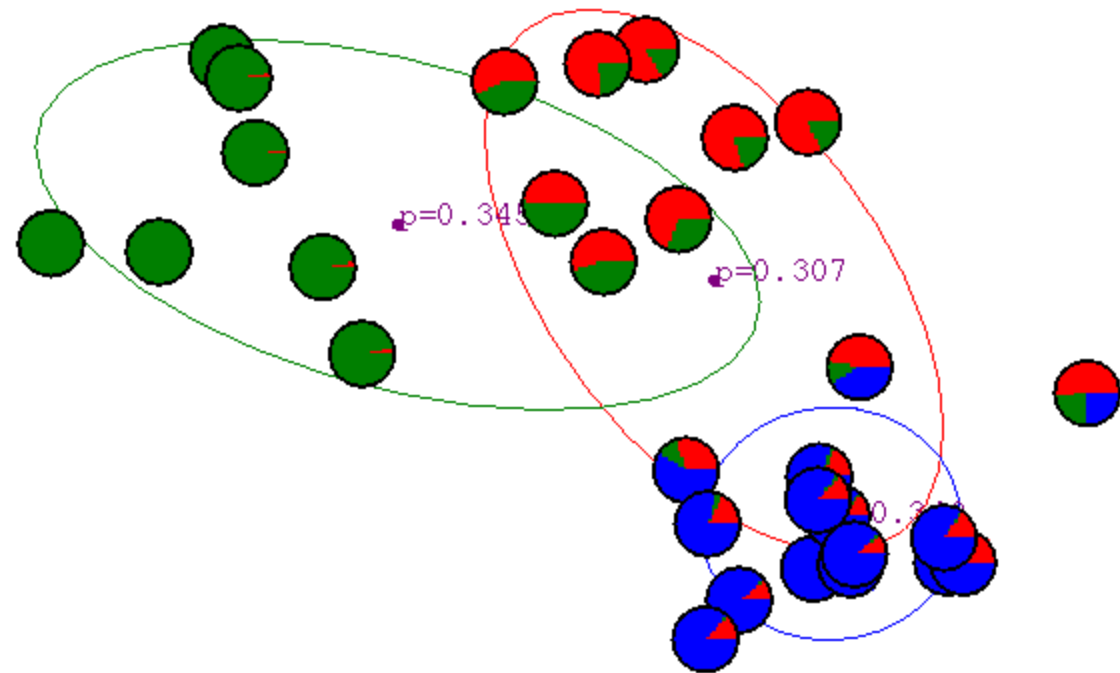
After 1st iteration



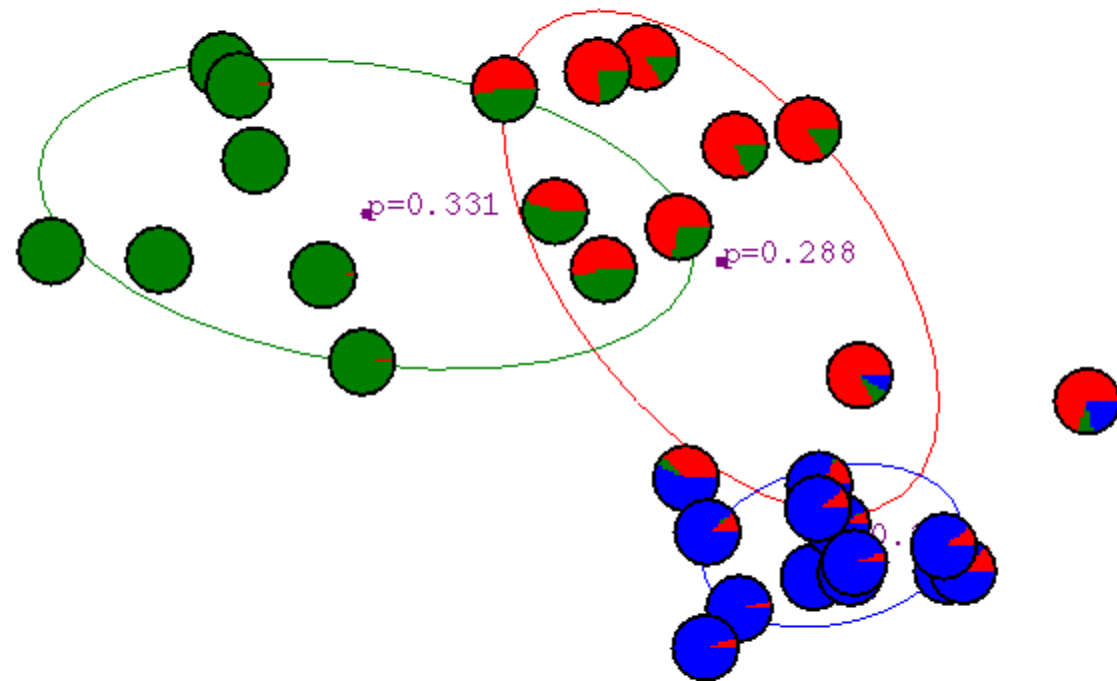
After 2nd iteration



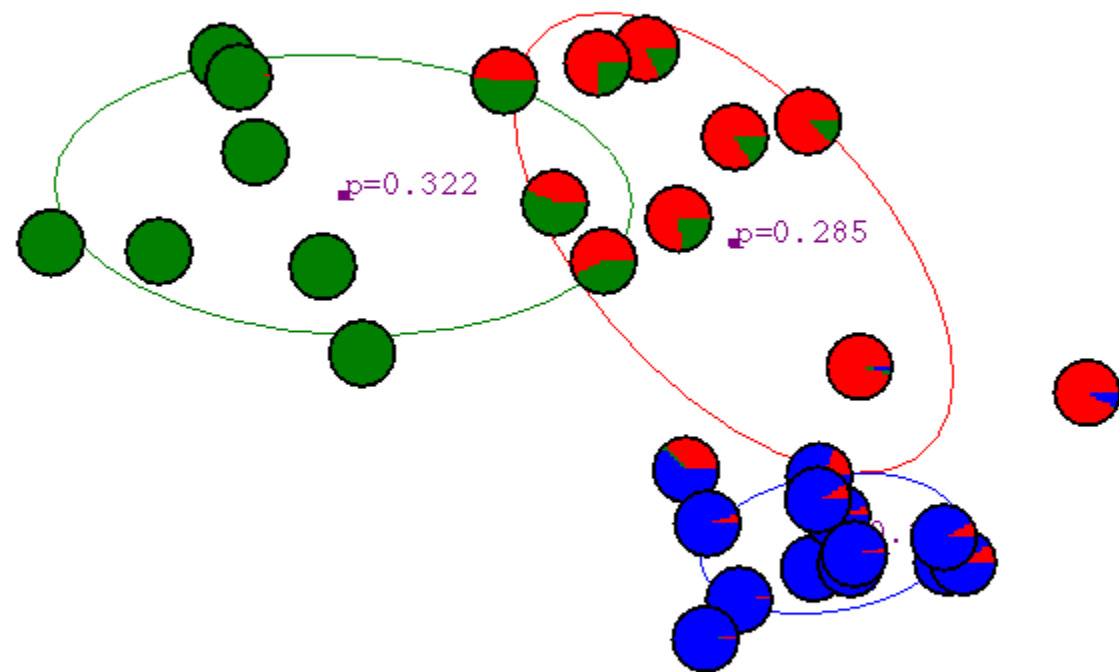
After 3rd iteration



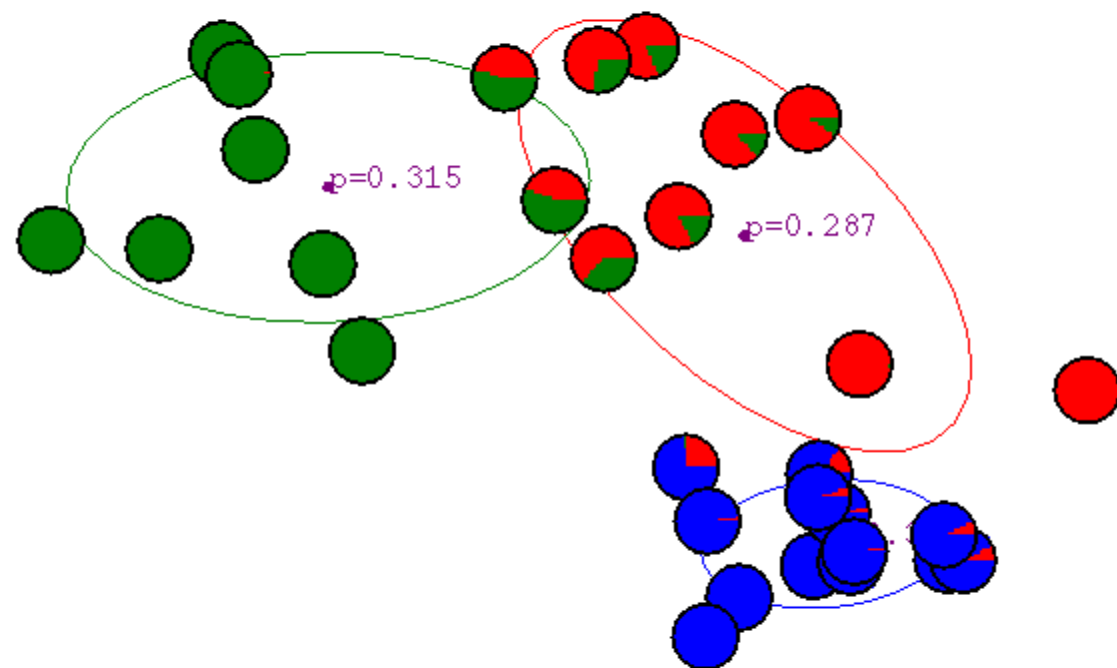
After 4th iteration



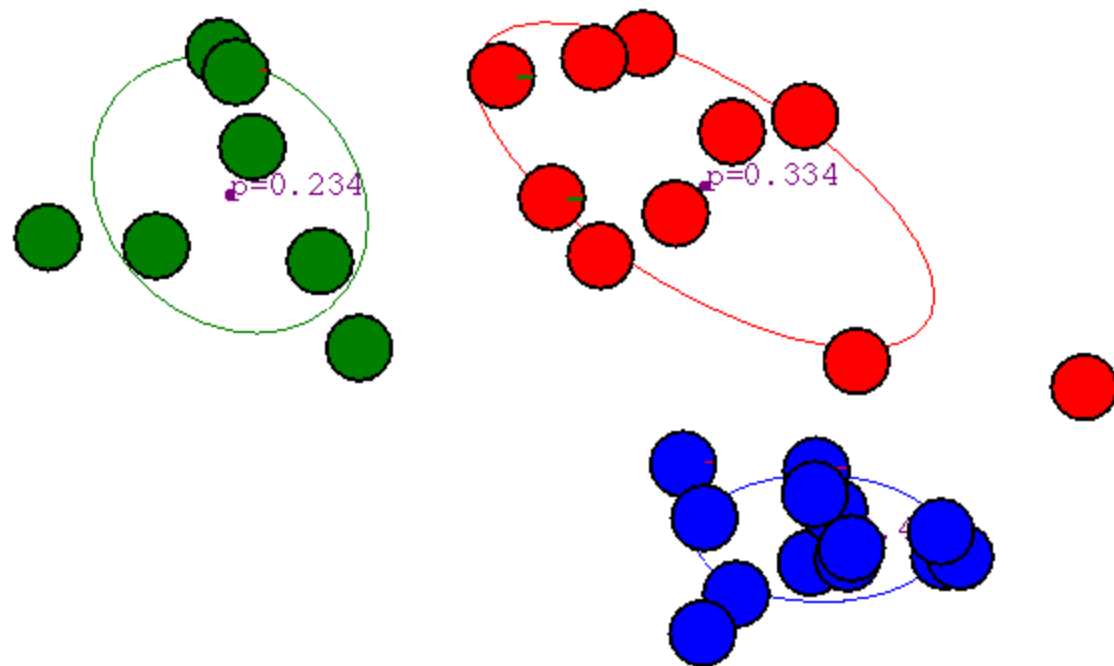
After 5th iteration



After 6th iteration



After 20th iteration



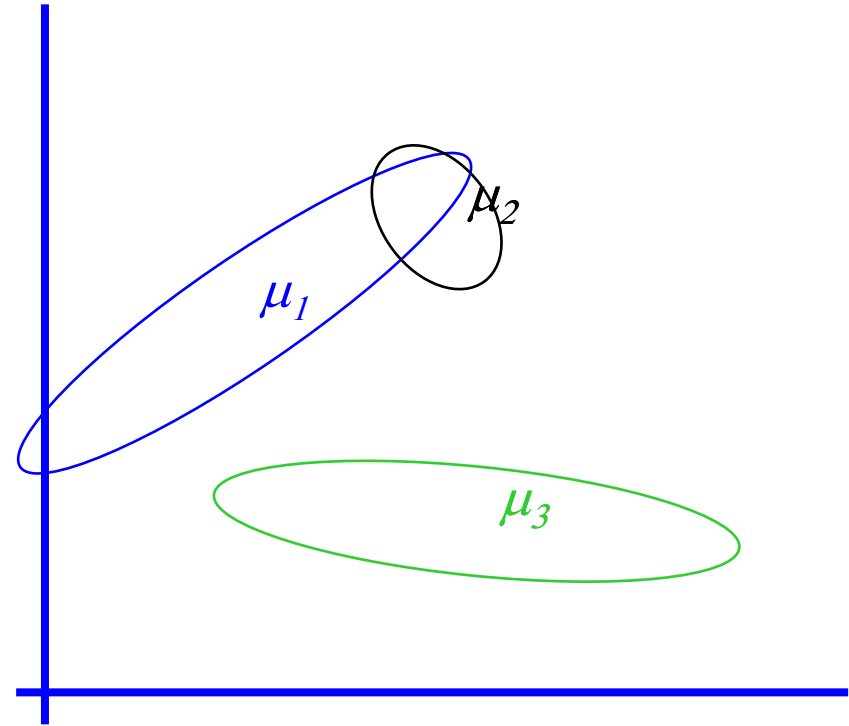
General GMM

GMM – Gaussian Mixture Model (Multi-modal distribution)

$$p(x) = \sum_i p(x|y=i) P(y=i)$$

↓ ↓
Mixture **Mixture**
component **proportion**

$$p(x|y=i) \sim N(\mu_i, \Sigma_i)$$



What you need to know...

- Hierarchical clustering algorithms
 - Single-linkage
 - Complete-linkage
 - Centroid-linkage
 - Average-linkage
- Partition based clustering algorithms
 - K-means
 - Coordinate descent
 - Seeding
 - Choosing K
 - Mixture models
 - EM algorithm

General EM algorithm

Marginal likelihood – $\mathbf{x}$ is observed, $\mathbf{z}$ is missing:

$$\begin{aligned}\log P(\mathbf{D}; \theta) &= \log \prod_{j=1}^m P(\mathbf{x}_j \mid \theta) \\ &= \sum_{j=1}^m \log P(\mathbf{x}_j \mid \theta) \\ &= \sum_{j=1}^m \log \sum_{\mathbf{z}} P(\mathbf{x}_j, \mathbf{z} \mid \theta)\end{aligned}$$

$$\mathbf{D} = \{\mathbf{x}_j\}_{j=1}^m$$

θ - model parameter(s)

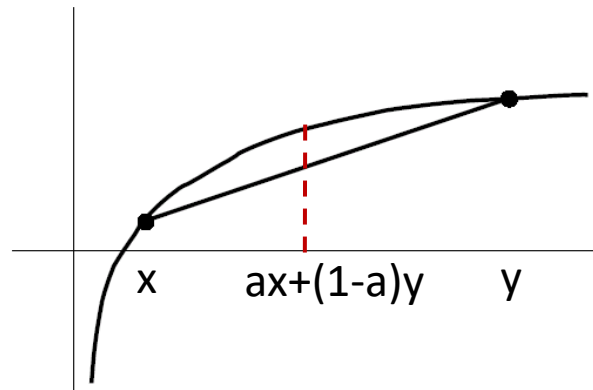
How to maximize marginal likelihood using EM?

Lower-bound on marginal likelihood

$$\begin{aligned}\log P(D; \theta) &= \sum_{j=1}^m \log \sum_{\mathbf{z}} P(\mathbf{x}_j, \mathbf{z} \mid \theta) \\ &= \sum_{j=1}^m \log \sum_{\mathbf{z}} \underbrace{Q(\mathbf{z} \mid \mathbf{x}_j)}_{P(\mathbf{z})} \underbrace{\frac{P(\mathbf{z}, \mathbf{x}_j \mid \theta)}{Q(\mathbf{z} \mid \mathbf{x}_j)}}_{f(\mathbf{z})}\end{aligned}$$

Variational
approach

Jensen's inequality: $\log \sum_{\mathbf{z}} P(\mathbf{z}) f(\mathbf{z}) \geq \sum_{\mathbf{z}} P(\mathbf{z}) \log f(\mathbf{z})$



$\log$: concave function

$$\log(ax+(1-a)y) \geq a \log(x) + (1-a) \log(y)$$

Lower-bound on marginal likelihood

$$\begin{aligned}\log P(D; \theta) &= \sum_{j=1}^m \log \sum_{\mathbf{z}} P(\mathbf{x}_j, \mathbf{z} \mid \theta) \\ &= \sum_{j=1}^m \log \sum_{\mathbf{z}} \underbrace{Q(\mathbf{z} \mid \mathbf{x}_j)}_{P(\mathbf{z})} \underbrace{\frac{P(\mathbf{z}, \mathbf{x}_j \mid \theta)}{Q(\mathbf{z} \mid \mathbf{x}_j)}}_{f(\mathbf{z})}\end{aligned}$$

Jensen's inequality: $\log \sum_{\mathbf{z}} P(\mathbf{z}) f(\mathbf{z}) \geq \sum_{\mathbf{z}} P(\mathbf{z}) \log f(\mathbf{z})$

$$\geq \sum_{j=1}^m \sum_{\mathbf{z}} Q(\mathbf{z} \mid \mathbf{x}_j) \log \frac{P(\mathbf{z}, \mathbf{x}_j \mid \theta)}{Q(\mathbf{z} \mid \mathbf{x}_j)} =: F(\theta, Q)$$

EM as Coordinate Ascent

$$\log P(D; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$Q^{t+1} = \arg \max_Q F(\theta^t, Q)$$

M-step: Fix Q , maximize F over θ

$$\theta^{t+1} = \arg \max_{\theta} F(\theta, Q^{t+1})$$

Convergence of EM

$$\log P(D; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$Q^{t+1} = \arg \max_Q F(\theta^t, Q)$$

E-step maximizes lower bound F on marginal likelihood => doesn't decrease the marginal likelihood

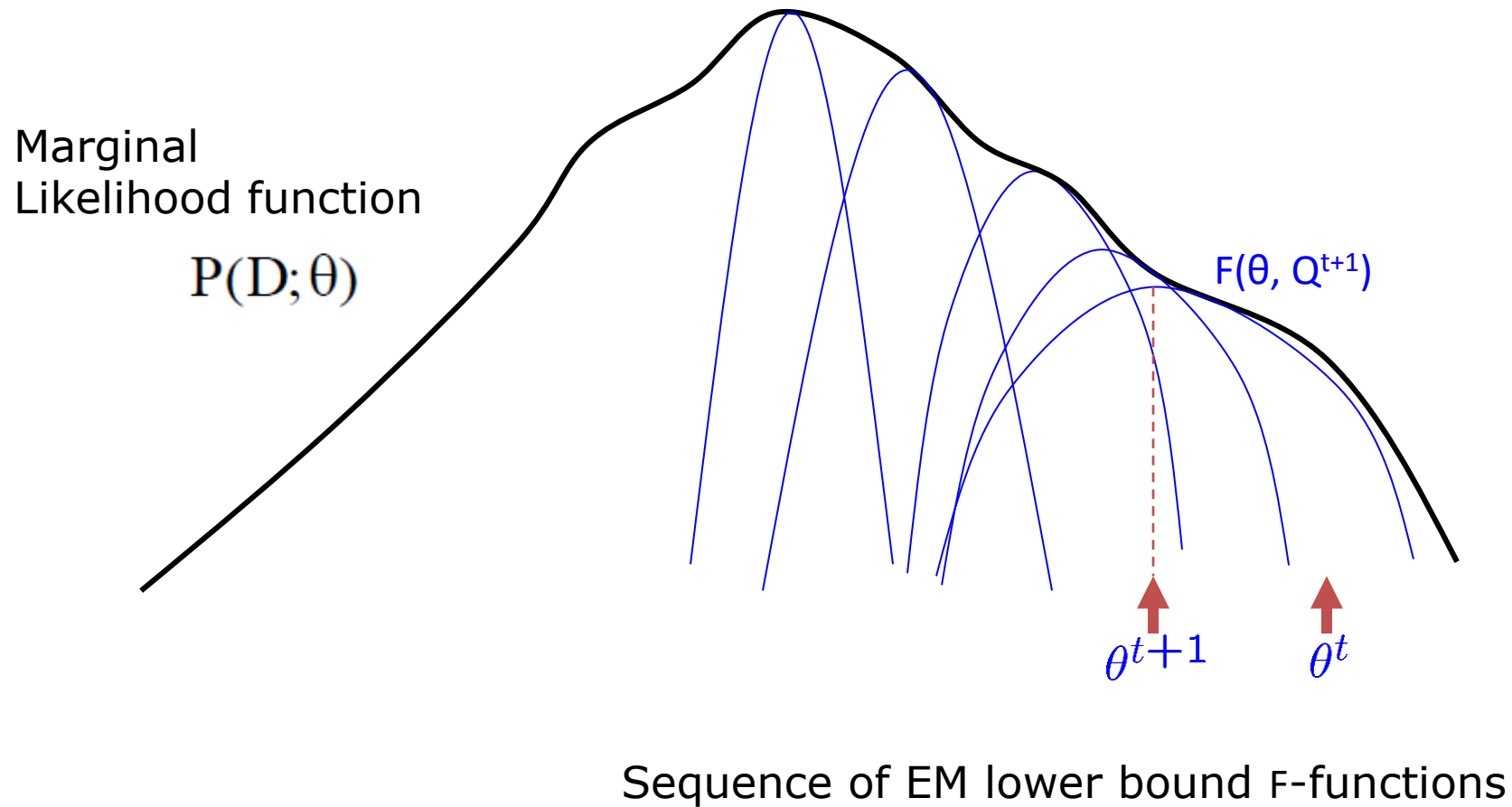
M-step: Fix Q , maximize F over θ

$$\theta^{t+1} = \arg \max_{\theta} F(\theta, Q^{t+1})$$

M-step maximizes lower bound F on marginal likelihood => doesn't decrease the marginal likelihood

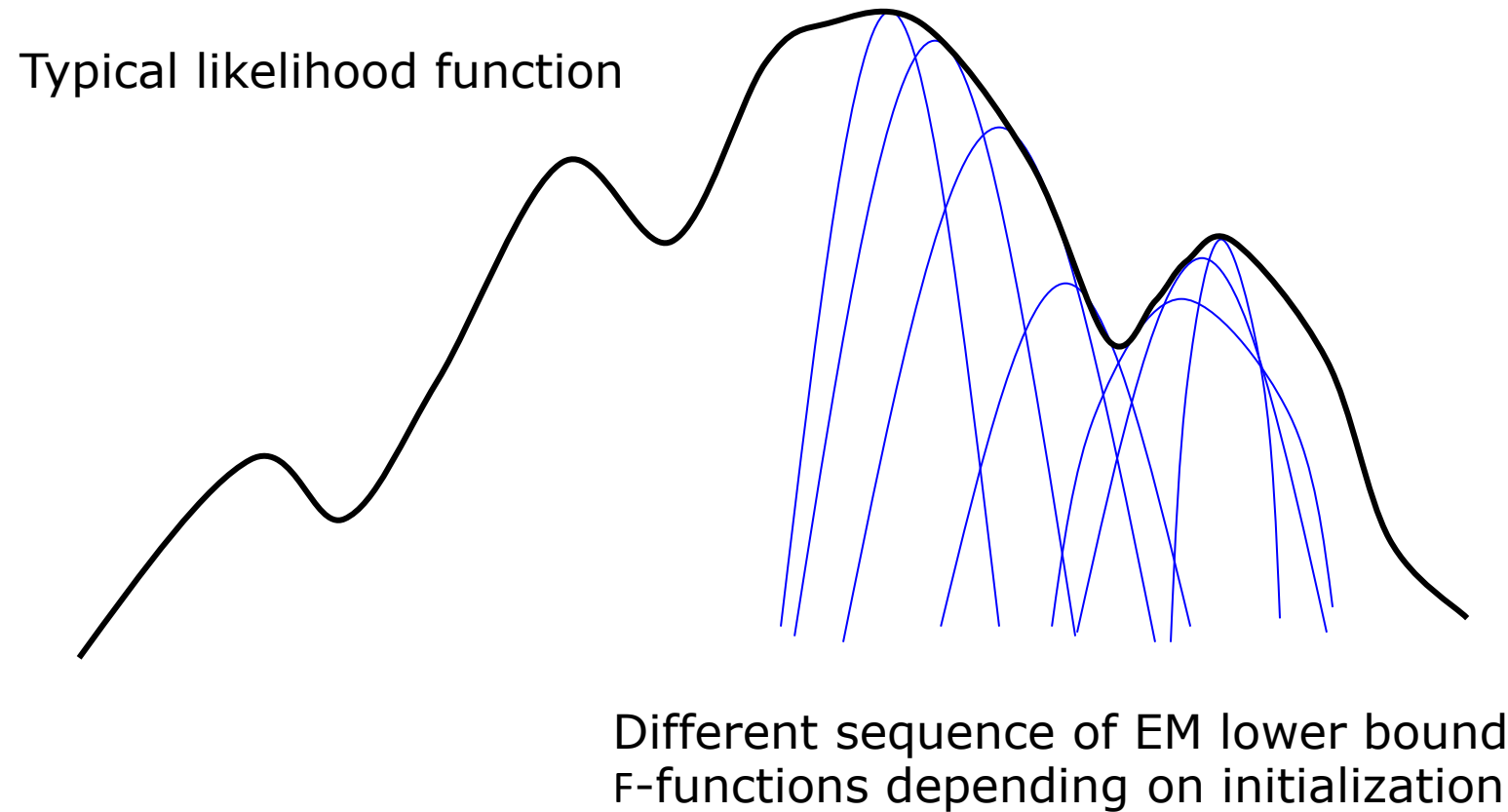
Since marginal likelihood is bounded, convergence follows!

Convergence of EM



EM monotonically converges to a local maximum of likelihood !

EM & Local Maxima



Use multiple, randomized initializations in practice

EM as Coordinate Ascent

$$\log P(D; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

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M-step: Fix Q , maximize F over θ

$$\theta^{t+1} = \arg \max_{\theta} F(\theta, Q^{t+1})$$

E step

$$\log P(\mathbf{D}; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$\begin{aligned} \log P(\mathbf{D}; \theta^{(t)}) &\geq F(\theta^{(t)}, Q) = \sum_{j=1}^m \sum_{\mathbf{z}} Q(\mathbf{z} | \mathbf{x}_j) \log \frac{P(\mathbf{z}, \mathbf{x}_j | \theta^{(t)})}{Q(\mathbf{z} | \mathbf{x}_j)} \\ &= \sum_{j=1}^m \sum_{\mathbf{z}} Q(\mathbf{z} | \mathbf{x}_j) \log \frac{P(\mathbf{z} | \mathbf{x}_j, \theta^{(t)}) P(\mathbf{x}_j | \theta^{(t)})}{Q(\mathbf{z} | \mathbf{x}_j)} \\ &= \underbrace{\sum_{j=1}^m \sum_{\mathbf{z}} Q(\mathbf{z} | \mathbf{x}_j) \log \frac{P(\mathbf{z} | \mathbf{x}_j, \theta^{(t)})}{Q(\mathbf{z} | \mathbf{x}_j)}}_{-KL(Q(\mathbf{z}|\mathbf{x}_j), P(\mathbf{z}|\mathbf{x}_j, \theta^{(t)}))} + \underbrace{\sum_{j=1}^m \sum_{\mathbf{z}} \cancel{Q(\mathbf{z}|\mathbf{x}_j)} \log P(\mathbf{x}_j | \theta^{(t)})}_{\log P(\mathbf{D}; \theta^{(t)})} \end{aligned}$$

KL divergence between two distributions

E step

$$\log P(\mathbf{D}; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$\begin{aligned} \log P(\mathbf{D}; \theta^{(t)}) &\geq F(\theta^{(t)}, Q) = \sum_{j=1}^m \sum_{\mathbf{z}} Q(\mathbf{z} | \mathbf{x}_j) \log \frac{P(\mathbf{z}, \mathbf{x}_j | \theta^{(t)})}{Q(\mathbf{z} | \mathbf{x}_j)} \\ &= \sum_{j=1}^m -KL(Q(\mathbf{z} | \mathbf{x}_j), P(\mathbf{z} | \mathbf{x}_j, \theta^{(t)})) + \log P(\mathbf{D}; \theta^{(t)}) \end{aligned}$$

KL ≥ 0 , above expression is maximized if KL divergence = 0

KL(Q,P) = 0 iff Q = P

Therefore,

$$\textbf{E step: } Q^{(t+1)}(\mathbf{z} | \mathbf{x}_j) = P(\mathbf{z} | \mathbf{x}_j, \theta^{(t)})$$

E step

$$\log \mathbf{P}(\mathbf{D}; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$\log \mathbf{P}(\mathbf{D}; \theta^{(t)}) \geq F(\theta^{(t)}, Q) = \sum_{j=1}^m -KL(Q(\mathbf{z}|\mathbf{x}_j), P(\mathbf{z}|\mathbf{x}_j, \theta^{(t)})) + \log \mathbf{P}(\mathbf{D}; \theta^{(t)})$$

$$\rightarrow Q^{(t+1)}(\mathbf{z} | \mathbf{x}_j) = P(\mathbf{z} | \mathbf{x}_j, \theta^{(t)})$$

Compute probability of missing data $\mathbf{z}$ given current choice of θ

Re-aligns F with marginal likelihood !!

$$F(\theta^{(t)}, Q^{(t+1)}) = \log \mathbf{P}(\mathbf{D}; \theta^{(t)})$$

M step

$$\log P(D; \theta) \geq F(\theta, Q)$$

M-step: Fix Q , maximize F over θ

$$\log P(D; \theta) \geq F(\theta, Q^{(t+1)}) = \sum_{j=1}^m \sum_{\mathbf{z}} Q^{(t+1)}(\mathbf{z} \mid \mathbf{x}_j) \log \frac{P(\mathbf{z}, \mathbf{x}_j \mid \theta)}{Q^{(t+1)}(\mathbf{z} \mid \mathbf{x}_j)}$$

$$= \sum_{j=1}^m \sum_{\mathbf{z}} Q^{(t+1)}(\mathbf{z} \mid \mathbf{x}_j) \log P(\mathbf{z}, \mathbf{x}_j \mid \theta) + \sum_{j=1}^m \underbrace{H(Q^{(t+1)}(\mathbf{z} \mid \mathbf{x}_j))}_{\text{Fixed (Independent of } \theta \text{)}}$$

$$\underbrace{\sum_{\mathbf{z}} \sum_{j=1}^m \log P(\mathbf{z}, \mathbf{x}_j \mid \theta) Q^{(t+1)}(\mathbf{z} \mid \mathbf{x}_j)}_{\text{Expected log likelihood wrt } Q}$$

||

Log likelihood if $\mathbf{z}$ was known

M step

$$\log P(\mathbf{D}; \theta) \geq F(\theta, Q)$$

M-step: Fix Q , maximize F over θ

$$\log P(\mathbf{D}; \theta) \geq F(\theta, Q^{(t+1)}) = \sum_{\mathbf{z}} \sum_{j=1}^m \log P(\mathbf{z}, \mathbf{x}_j | \theta) Q^{(t+1)}(\mathbf{z} | \mathbf{x}_j) + \sum_{j=1}^m \underbrace{H(Q^{(t+1)}(\mathbf{z} | \mathbf{x}_j))}_{\text{Fixed (Independent of } \theta \text{)}}$$

$$\theta^{(t+1)} \leftarrow \arg \max_{\theta} \underbrace{\sum_{\mathbf{z}} \sum_{j=1}^m \log P(\mathbf{z}, \mathbf{x}_j | \theta) Q^{(t+1)}(\mathbf{z} | \mathbf{x}_j)}_{\text{Expected log likelihood wrt } Q^{(t+1)}}$$

Use expected counts instead of counts when computing MLE:

If learning requires $\text{Count}(\mathbf{x}, \mathbf{z})$, Use $E_{Q^{(t+1)}}[\text{Count}(\mathbf{x}, \mathbf{z})]$

EM as Coordinate Ascent

$$\log P(D; \theta) \geq F(\theta, Q)$$

E-step: Fix θ , maximize F over Q

$$Q^{t+1} = \arg \max_Q F(\theta^t, Q)$$

$$Q^{(t+1)}(z | \mathbf{x}_j) = P(z | \mathbf{x}_j, \theta^{(t)}) \quad \text{E.g., } P(y = i | x_j, m)$$

Compute probability of missing data given current choice of θ

M-step: Fix Q , maximize F over θ

$$\theta^{t+1} = \arg \max_{\theta} F(\theta, Q^{t+1})$$

$$\theta^{(t+1)} \leftarrow \arg \max_{\theta} \sum_z \sum_{j=1}^m \log P(z, \mathbf{x}_j | \theta) Q^{(t+1)}(z | \mathbf{x}_j)$$

Compute estimate of θ by maximizing marginal likelihood using $Q^{(t+1)}(z | \mathbf{x}_j)$

Summary: EM Algorithm

- A way of maximizing likelihood function for hidden 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:
 1. E-step: $Q^{t+1} = \arg \max_Q F(\theta^t, Q)$
 2. M-step: $\theta^{t+1} = \arg \max_{\theta} F(\theta, Q^{t+1})$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.
- EM performs coordinate ascent on F , can get stuck in local minima.
- BUT Extremely popular in practice.