Expectation-Maximization (EM)

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Some slides courtesy of Eric Xing, Carlos Guestrin

Mixture models (Gaussian)

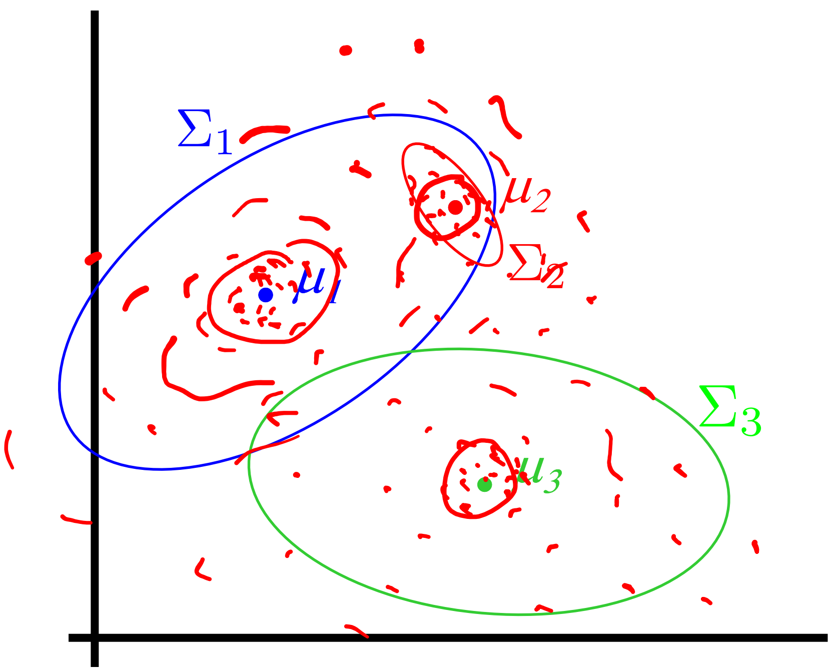
$\sim \mathcal{N}(\mu_i, \Sigma_i)$

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

$x_i \in \mathbb{R}^d$

Mixture component — $p(x|Y=i)$

Mixture proportion, p_i — $P(Y=i)$



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 Marginal Likelihood $p(x)$
  But don't know labels Y (recall Gaussian Bayes classifier)

Expectation-Maximization (EM)

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

- No need to choose step size as in Gradient methods.

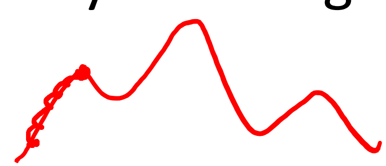
- EM is an Iterative algorithm with two linked steps:

  E-step: fill-in hidden data (Y) using inference

  M-step: apply standard MLE/MAP method to estimate parameters

  $$\{p_i, \mu_i, \Sigma_i\}_{i=1}^{k}$$

- This procedure monotonically improves the marginal likelihood (or leaves it unchanged). Thus it always converges to a local optimum of the likelihood.



EM for spherical, same variance GMMs same mixture proportions

$\to \Sigma_i$

$\to p_i = P(y=i)$

Initialize: $\mu_1, \mu_2, \ldots, \mu_K$ randomly

E-step

Compute "expected" classes of all datapoints for each class

$\forall i, j$

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

In K-means "E-step" we do hard assignment

EM does soft assignment

$$p(y=i|x) \propto \underbrace{p(x|y=i)}_{\sim N(\mu_i;\Sigma_i)}\, p(y=i)$$

$$\Sigma_i = \sigma^2 I$$

$$p_i = \frac{1}{K}$$

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

$$p(x) = \sum_{i=1}^{K} \underbrace{p(x|y=i)}_{\sim N(\mu_i;\Sigma_i)}\, \underbrace{p(y=i)}_{p_i}$$

Bayes rule

$$p(y|x) = \frac{p(x|y)\,p(y)}{p(x)}$$

EM for spherical, same variance GMMs same mixture proportions

Initialize: $\mu_1, \mu_2, \ldots, \mu_K$ randomly

E-step

Compute "expected" classes of all datapoints for each class

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

In K-means "E-step"
we do hard assignment

EM does soft assignment

M-step

$\mu_1 \ldots \mu_K$

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

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

$\frac{1}{m} \sum_{j=1}^{m} x_j \mathbb{1}_{x_j \in C_i}$ ← K-means

Exactly same as MLE with
weighted data

Iterate.

EM for general GMMs

Iterate. On iteration t let our estimates be

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

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

- Initialize: $\lambda_0 \leftarrow$ random

E-step

Compute "expected" classes of all datapoints for each class

$$\rightarrow \mathrm{P}\left(y=i \mid x_j, \lambda_t\right) \propto p_i^{(t)} \mathrm{p}\left(x_j \mid \mu_i^{(t)}, \Sigma_i^{(t)}\right)$$

$= P(x_j \mid y=i)$

Just evaluate a Gaussian at x_j

M-step

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

$$\mu_i^{(t+1)} = \frac{\sum_j \mathrm{P}\left(y=i \mid x_j, \lambda_t\right) x_j}{\sum_j \mathrm{P}\left(y=i \mid x_j, \lambda_t\right)}$$

$$\Sigma_i^{(t+1)} = \frac{\sum_j \mathrm{P}\left(y=i \mid x_j, \lambda_t\right)\left(x_j - \mu_i^{(t+1)}\right)\left(x_j - \mu_i^{(t+1)}\right)^T}{\sum_j \mathrm{P}\left(y=i \mid x_j, \lambda_t\right)}$$

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

$\sum_j 1_{x_j \in C_i}$

$= \frac{m_i}{m} \leftarrow$ equal wts.

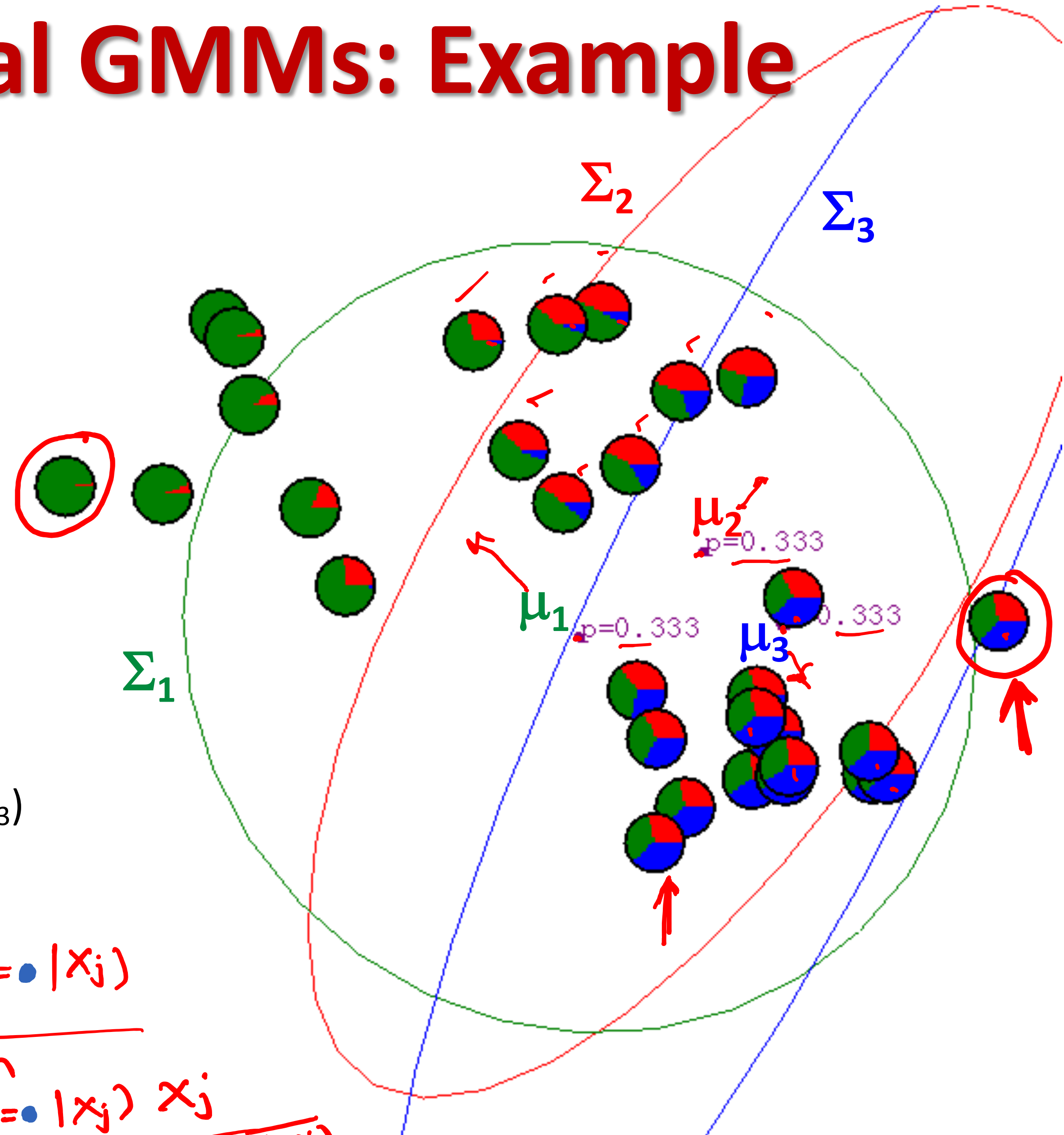
m = #data points

EM for general GMMs: Example

K=3

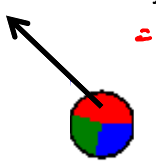
0 Random initialization

$$\left\{ \begin{array}{l} \mu_1, \mu_2, \mu_3 \\ p_1, p_2, p_3 = \frac{1}{3} \leftarrow \\ \Sigma_1, \Sigma_2, \Sigma_3 \end{array} \right.$$



1 E-step

$\rightarrow P(y = \bullet \mid x_j, \mu_1, \mu_2, \mu_3, \Sigma_1, \Sigma_2, \Sigma_3, p_1, p_2, p_3) = \underline{\qquad\qquad}$

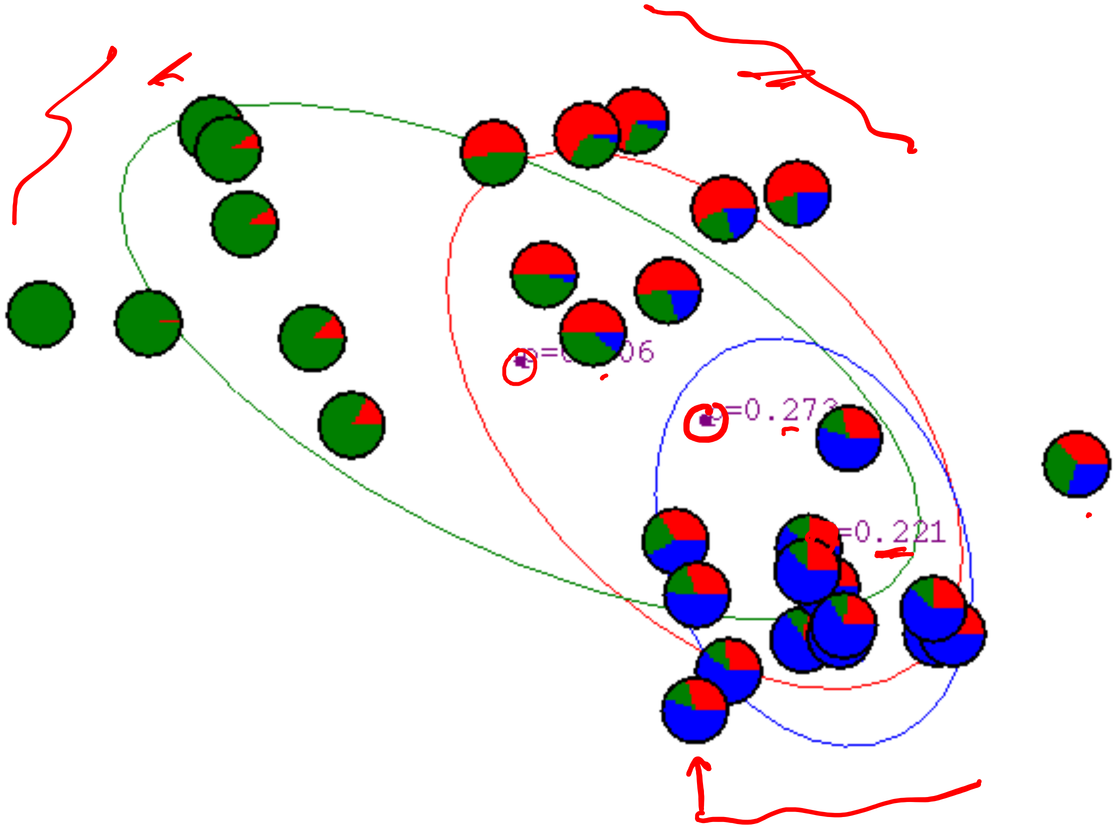


2 M-step

$$p_3 \leftarrow \frac{\sum_{j=1}^{m} p(y=\bullet \mid x_j)}{m}$$

$$\mu_3 \leftarrow \frac{\sum_{j=1}^{m} p(y=\bullet \mid x_j)\, x_j}{\sum_{j=1}^{m} p(y=\bullet \mid x_j)}$$

After 1st iteration



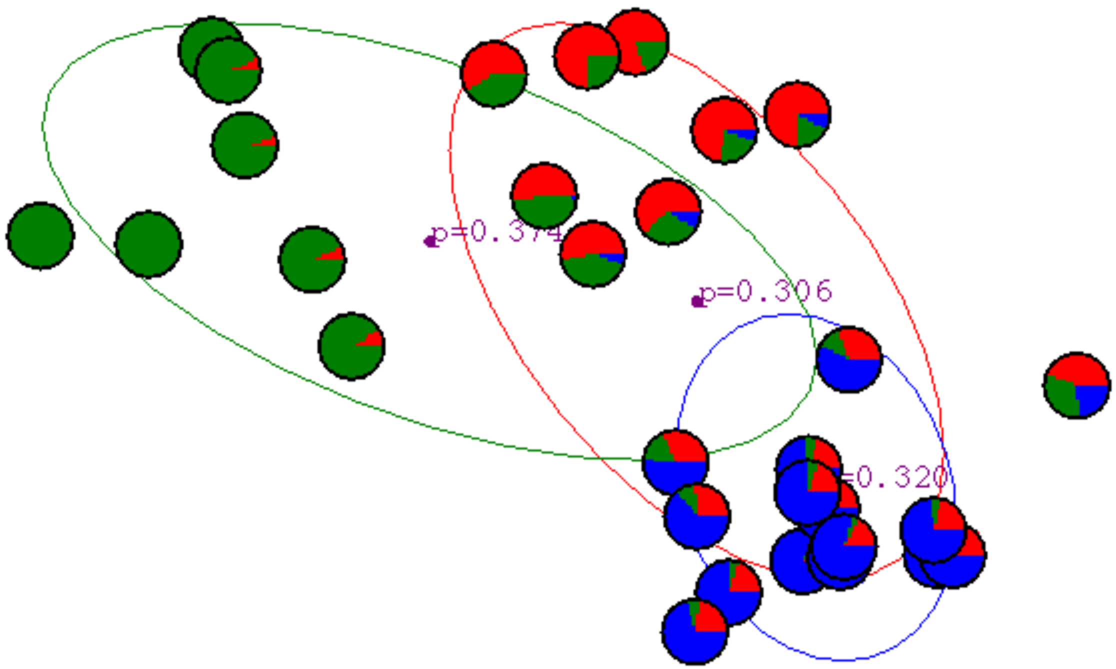
① E-step

$p(y = \square \mid x_j, \ldots)$

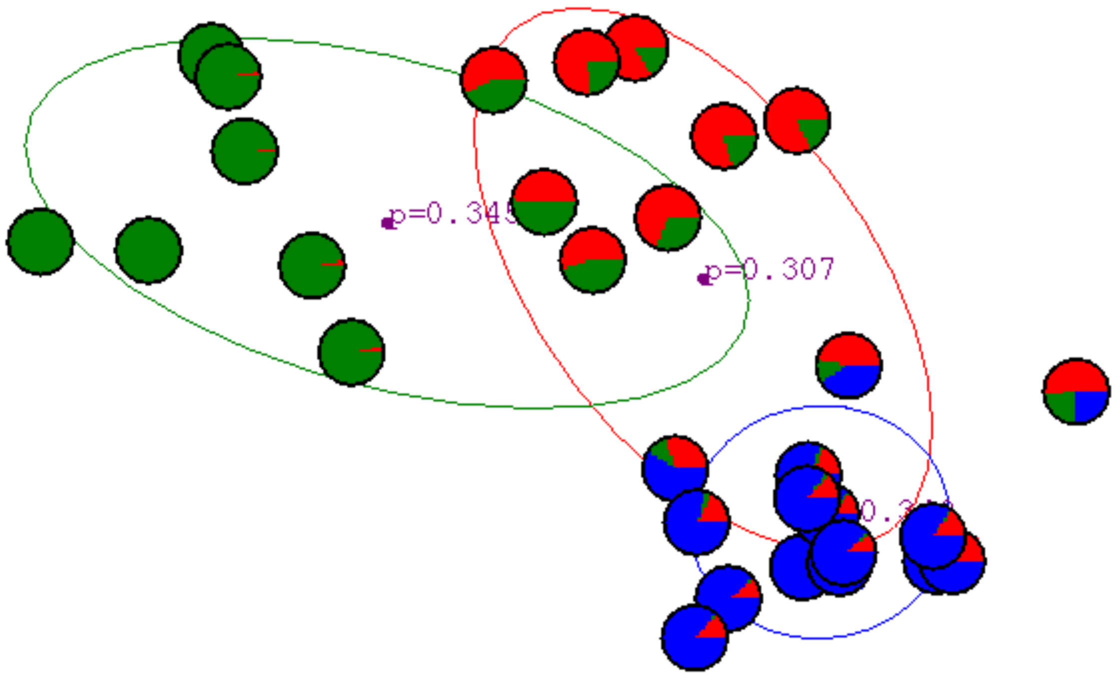
② M-step

μ_i, Σ_i, p_i

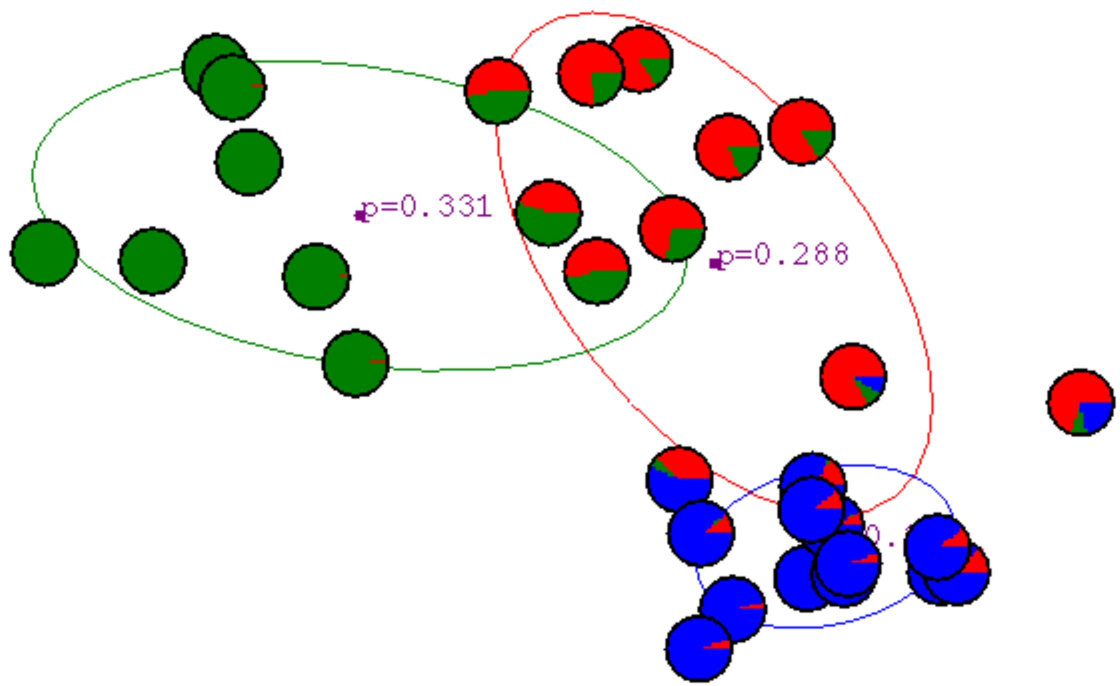
After 2nd iteration



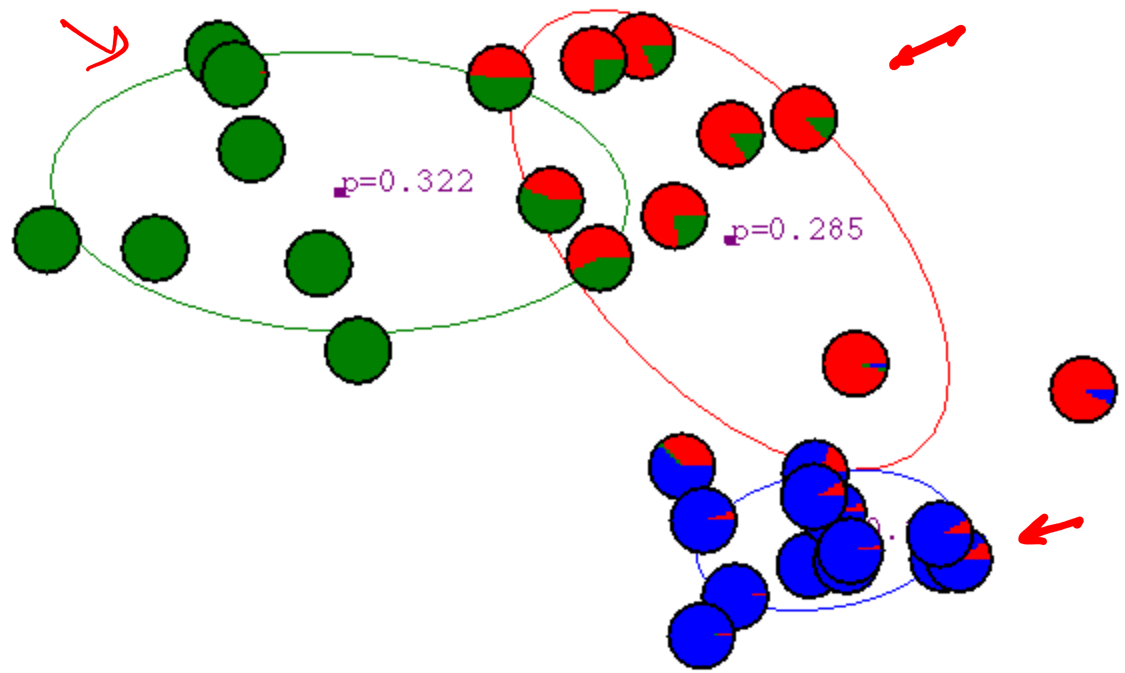
After 3rd iteration



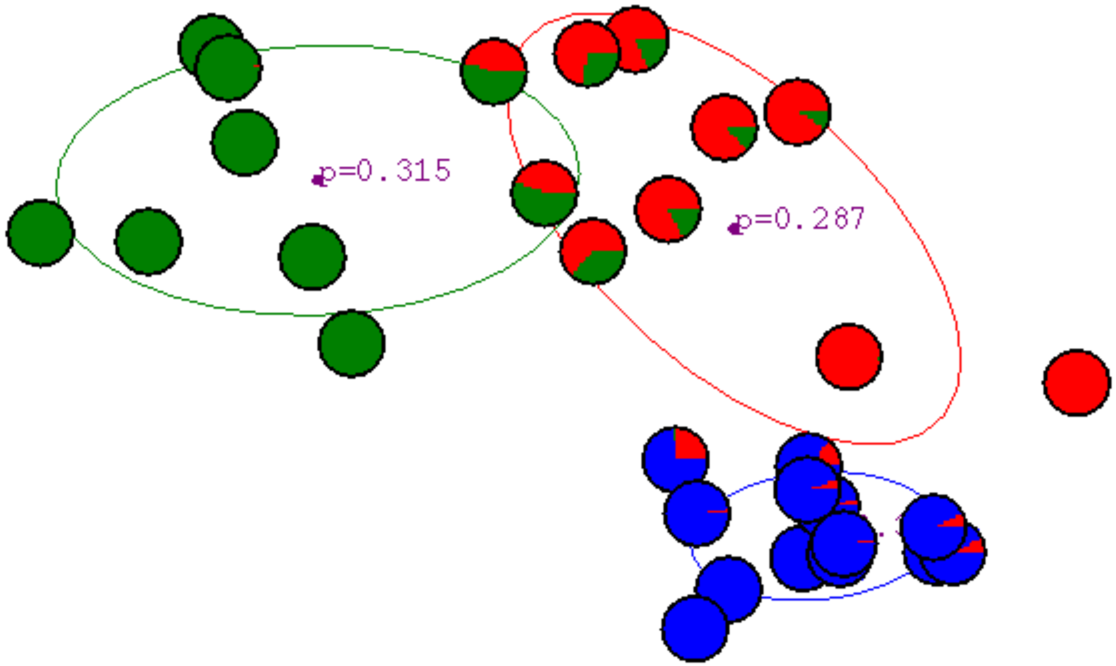
After 4th iteration



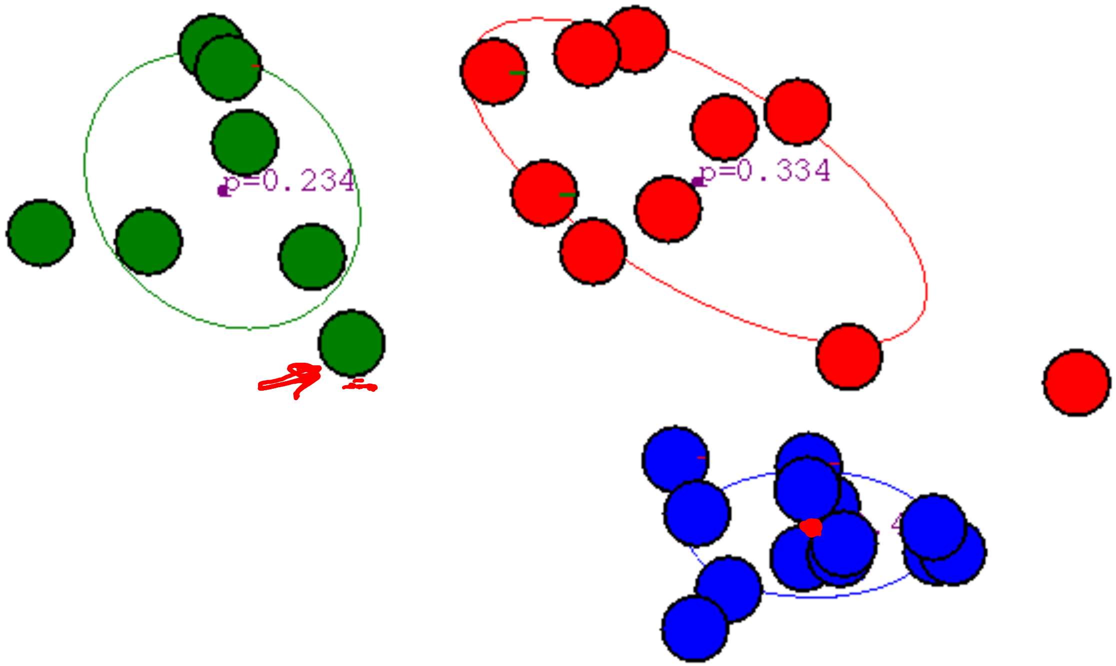
After 5th iteration



After 6th iteration



After 20th iteration

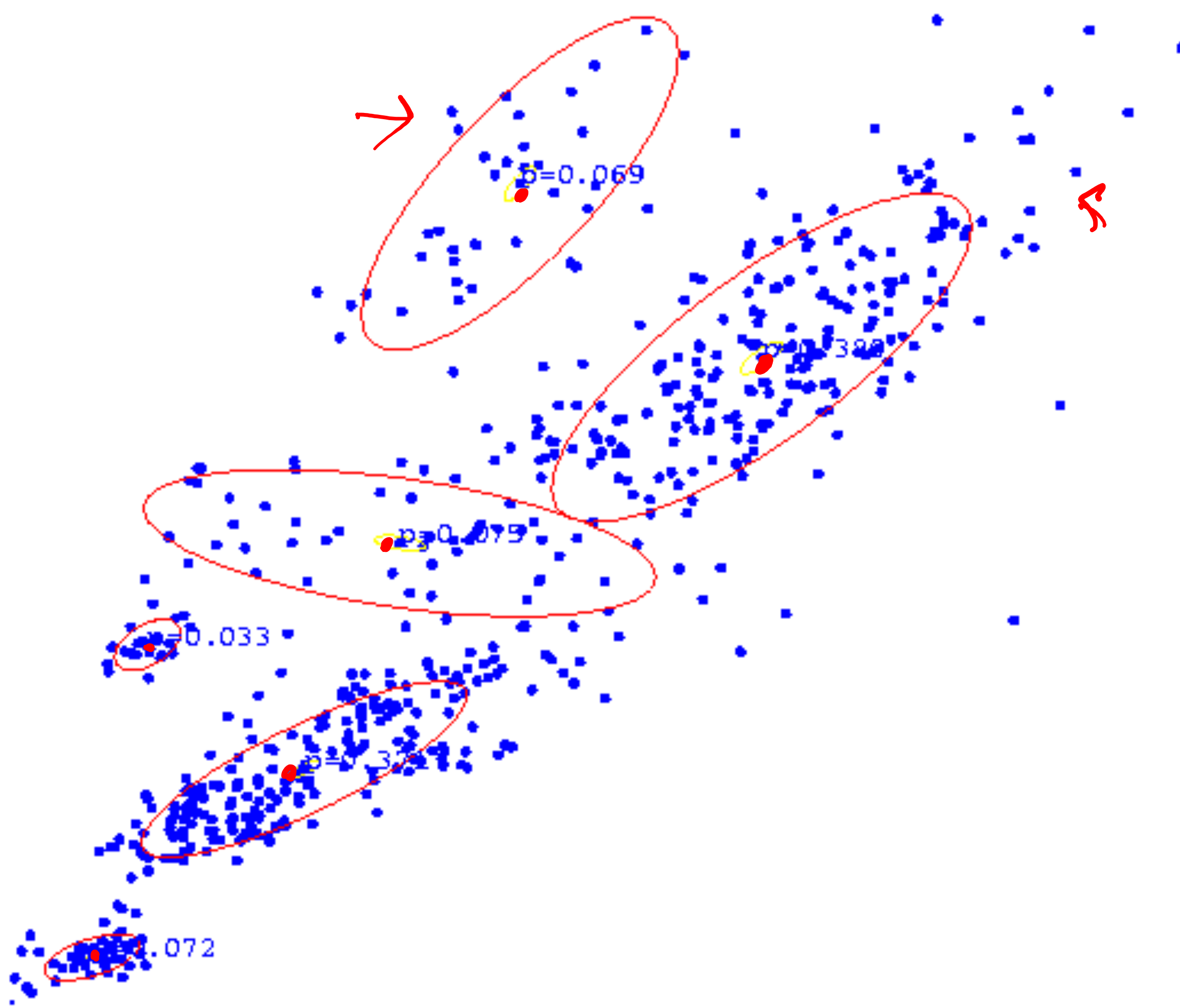


GMM clustering of assay data

p(x)

K choice

" 6



General GMM

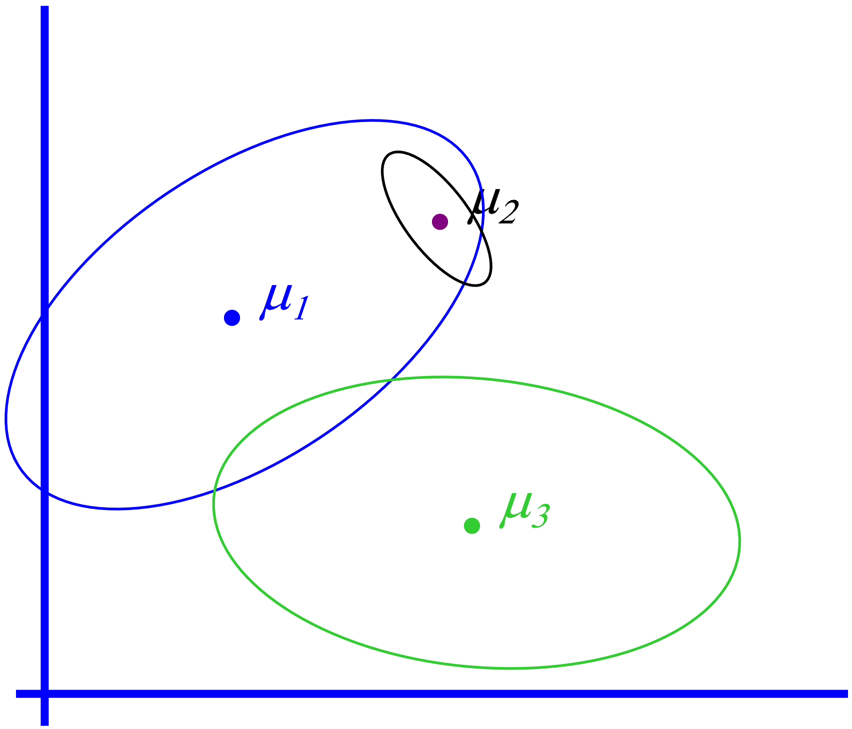
GMM – Gaussian Mixture Model (Multi-modal distribution)

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

$p(x|y=i)$ → **Mixture component**

$P(y=i)$ → **Mixture proportion**

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

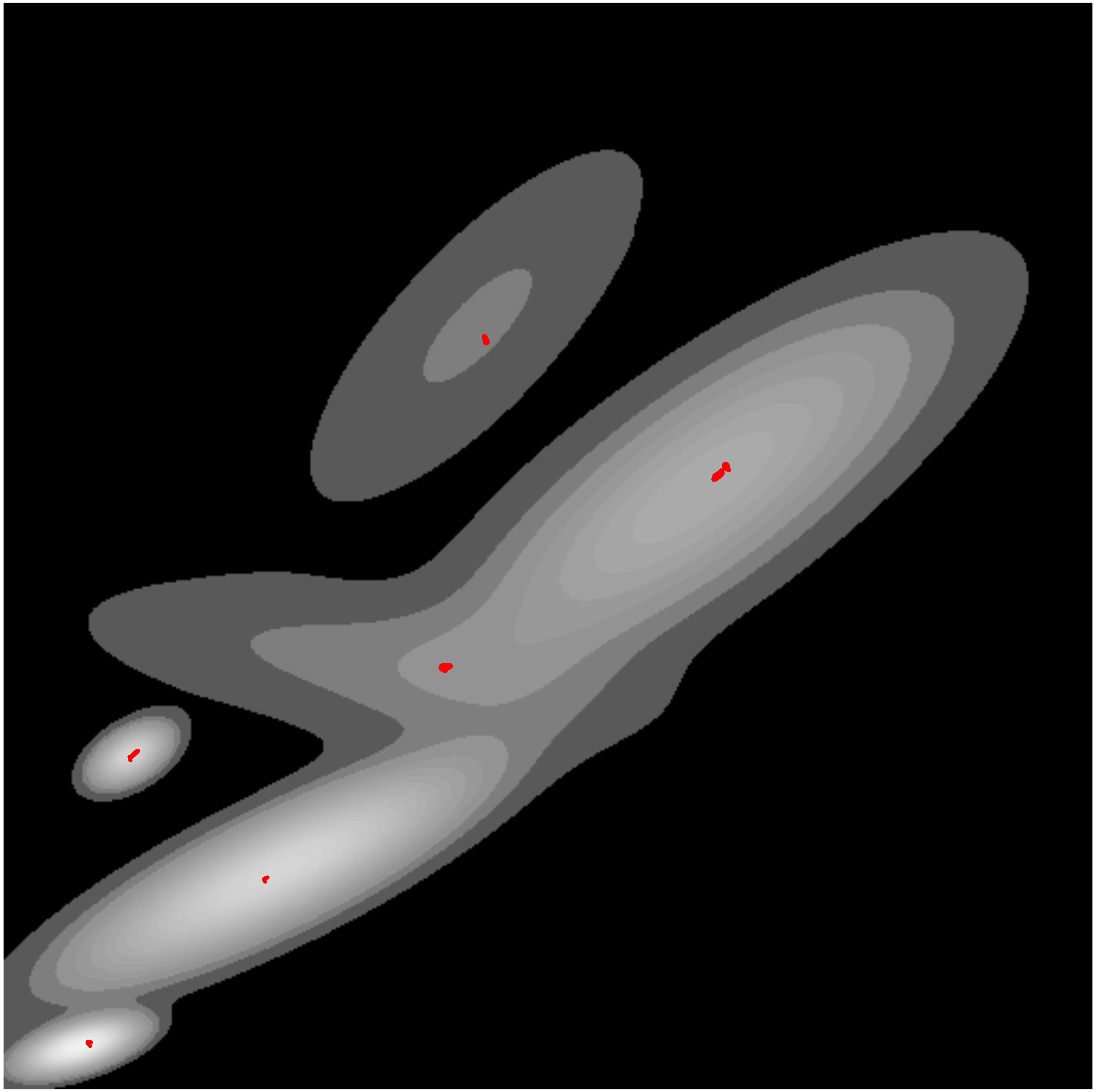


Resulting Density Estimator

Contour plots of $p(x)$

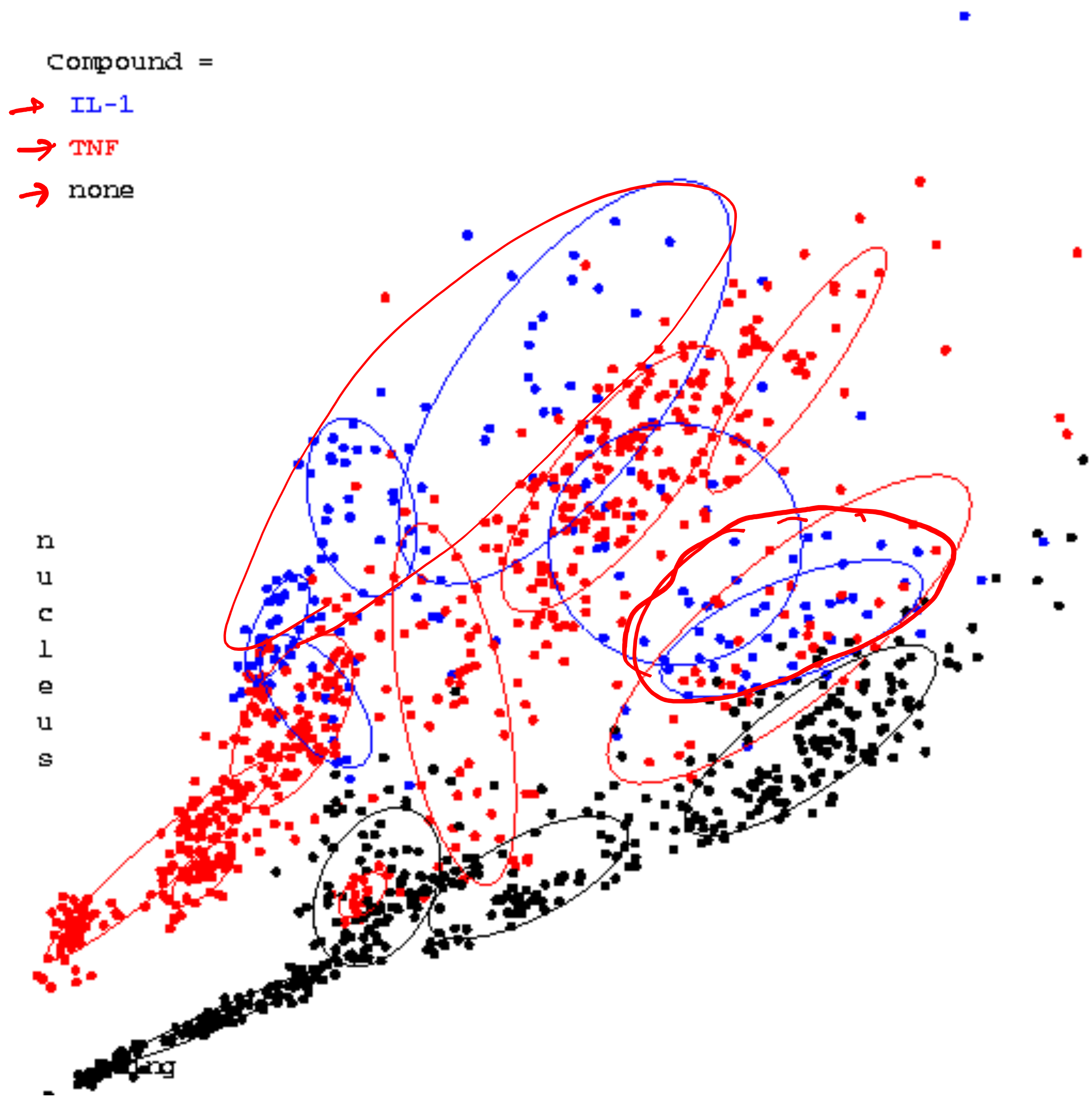
$p(\underline{x} \mid y=0) \sim GMM$

- multimodal

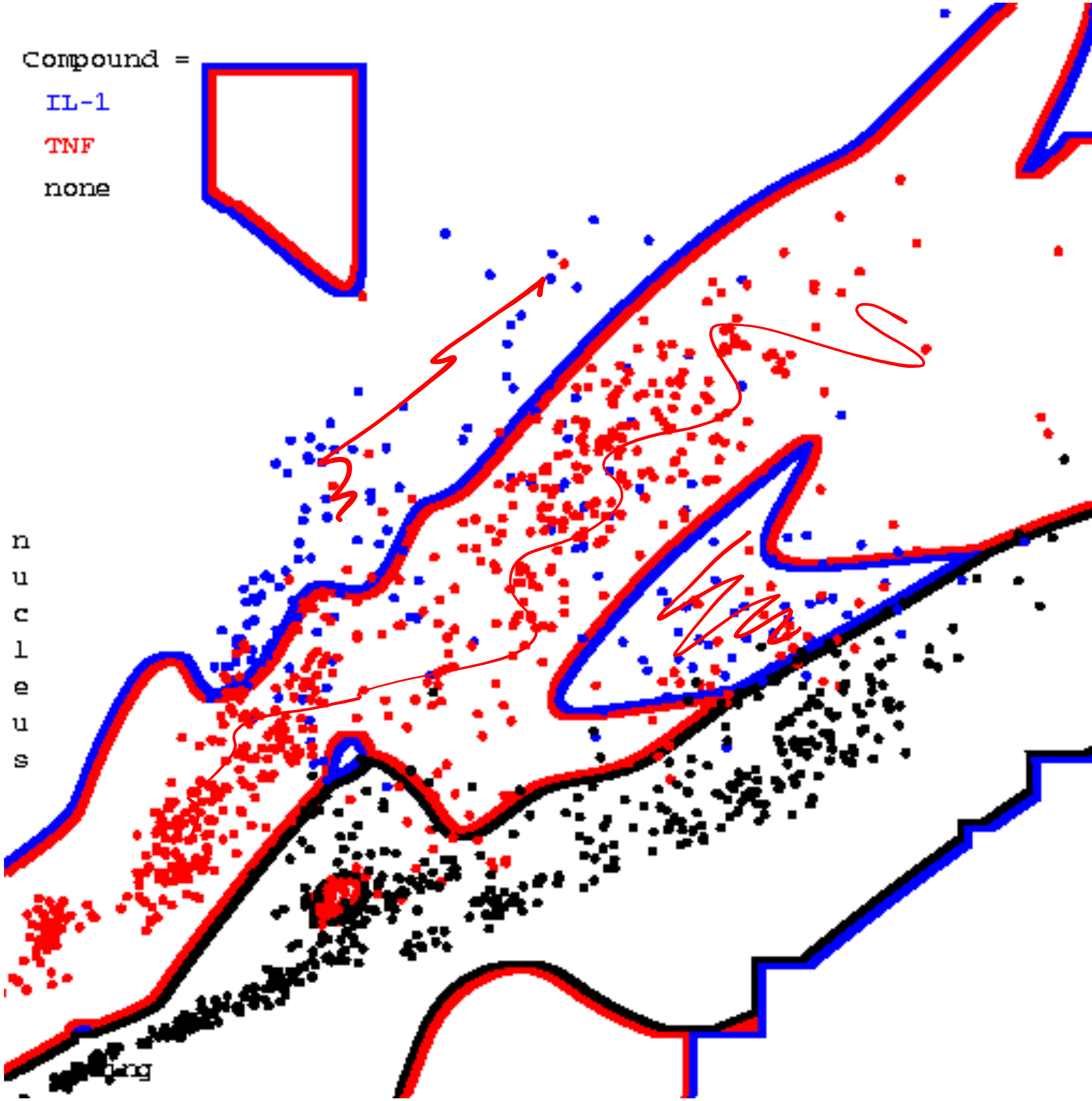


Three classes of assay

(each learned with it's own mixture model)



Resulting Bayes Classifier

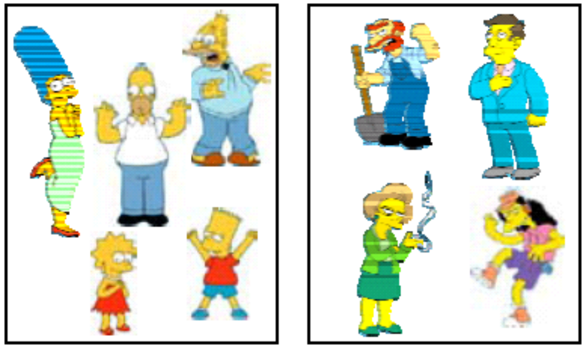


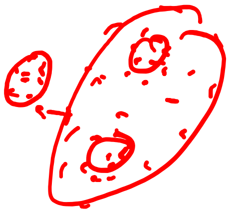
Summary: EM Algorithm

- 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: soft cluster assignment for each data point
  2. M-step: update parameters of each mixture component
- EM can get stuck in local minima. though guaranteed to converge.
- BUT Extremely popular in practice.

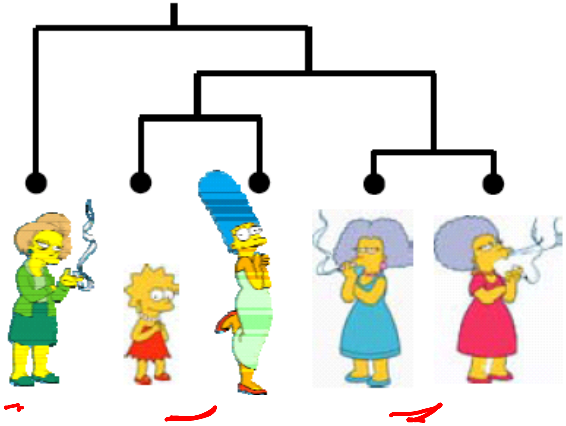
Clustering Algorithms

- Partition algorithms
  - K means clustering
  - Mixture-Model based clustering





- Hierarchical algorithms
  - Single-linkage
  - Average-linkage
  - Complete-linkage
  - Centroid-based



Hierarchical Clustering

- Bottom-Up Agglomerative Clustering

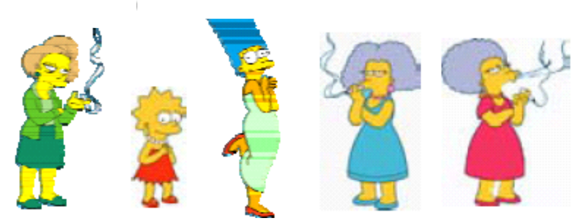
  Starts with each object in a separate cluster, and repeat:

  – Joins the most similar pair of clusters,

  – Update the similarity of the new cluster to others

  until there is only one cluster.

  Greedy – less accurate but simple to implement



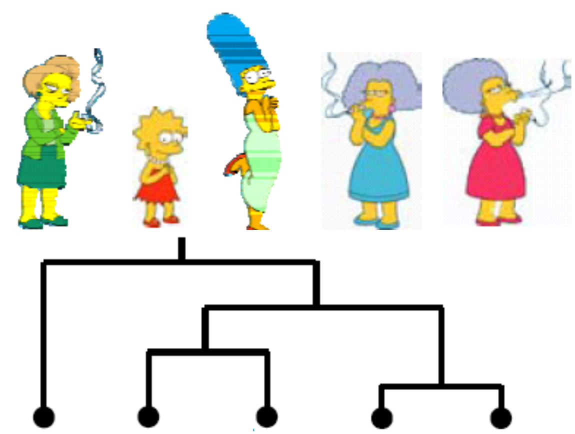
- Top-Down divisive

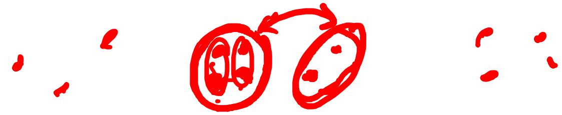
  Starts with all the data in a single cluster, and repeat:

  – Split each cluster into two using a partition algorithm

  Until each object is a separate cluster.

  More accurate but complex to implement

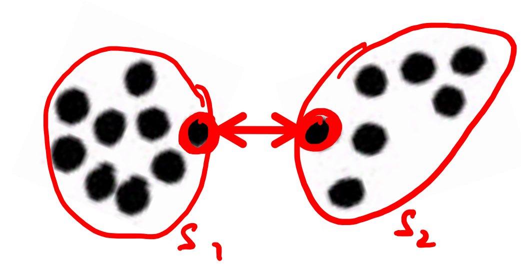




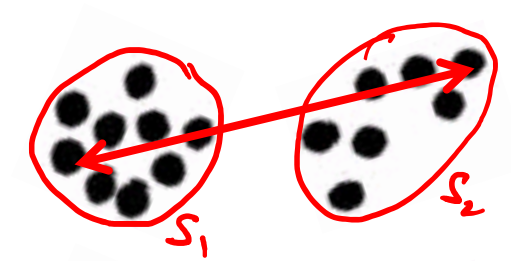
Bottom-up Agglomerative clustering

Different algorithms differ in how the similarities are defined (and hence updated) between two clusters

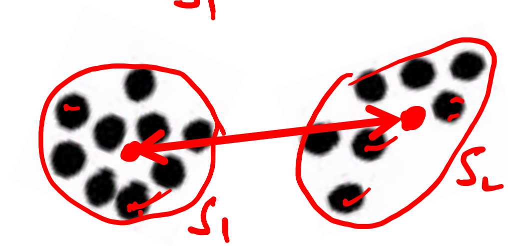
- Single-Linkage
  - Nearest Neighbor: similarity between their closest members.



- Complete-Linkage
  - Furthest Neighbor: similarity between their furthest members.



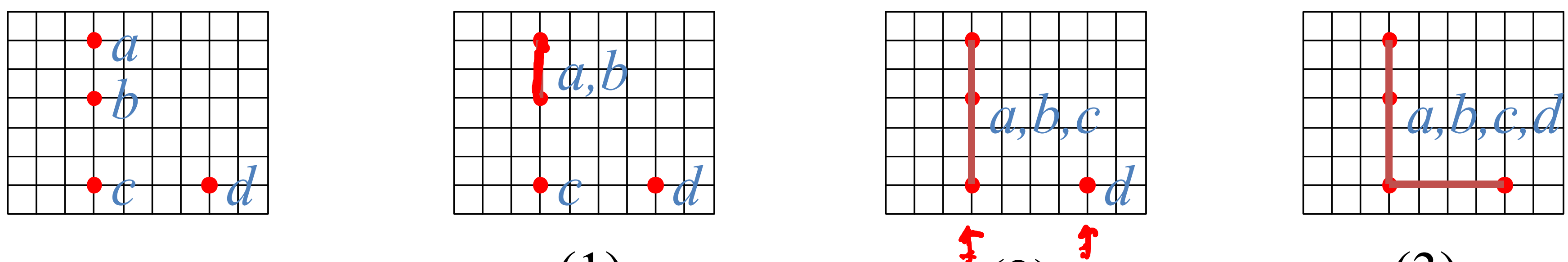
- Centroid
  - Similarity between the centers of gravity



- Average-Linkage
  - Average similarity of all cross-cluster pairs.

Single-Linkage Method

Euclidean Distance



(1) (2) (3)

	b	*c*	*d*
a	2	5	6
b		3	5
c			4

	b	*c*	*d*
a	2	5	6
b		3	5
c			4

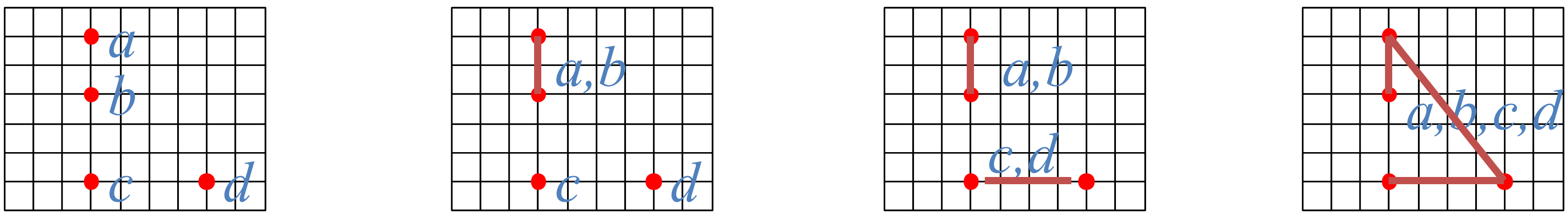
	c	*d*
a,b	3	5
c		4

	d
a,b,c	4

Distance Matrix

Complete-Linkage Method

Euclidean Distance



(1) (2) (3)

	b	c	d
a	2	5	6
b		3	5
c			4

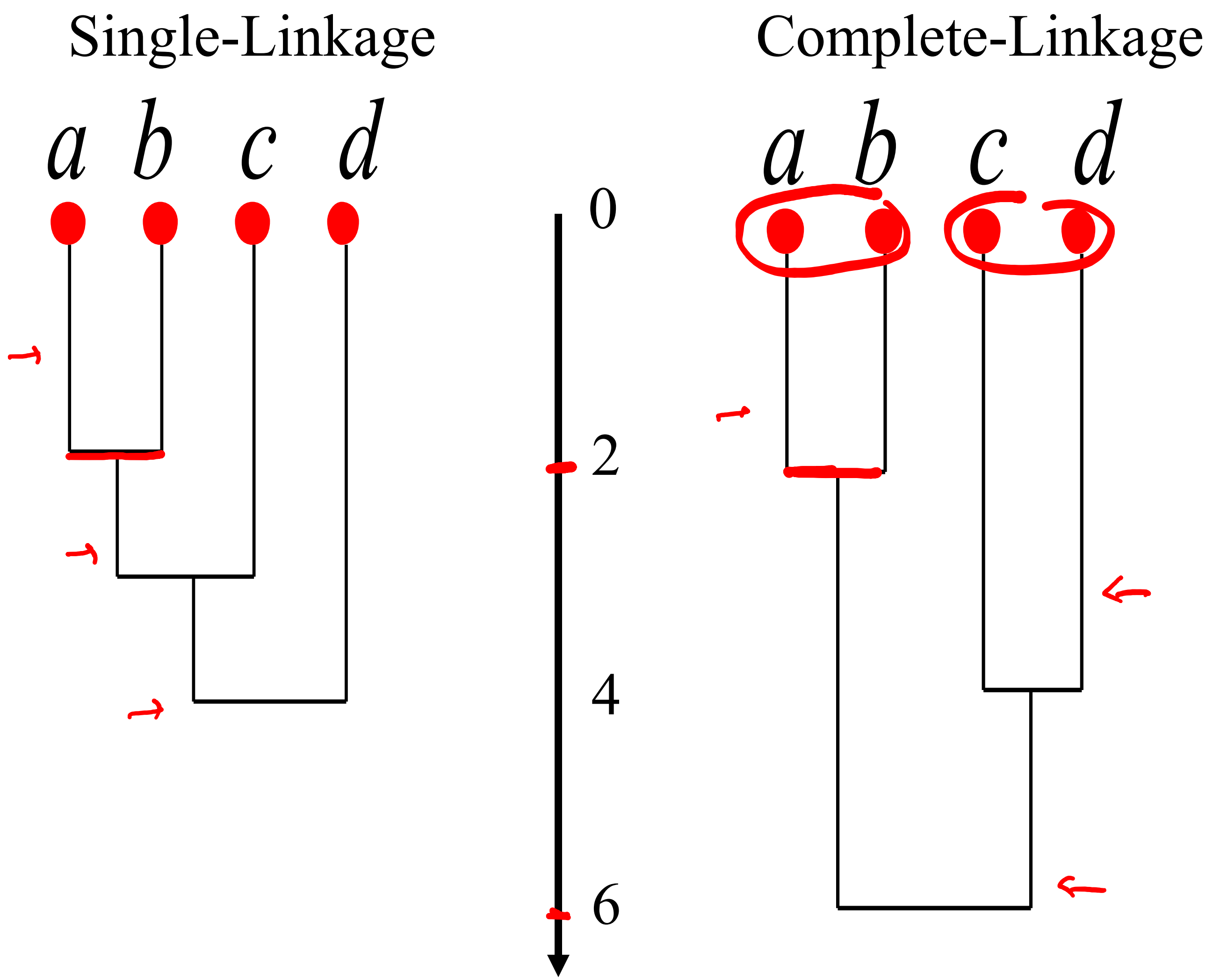
	b	c	d
a	2	5	6
b		3	5
c			4

	c	d
a,b	5	6
c		4

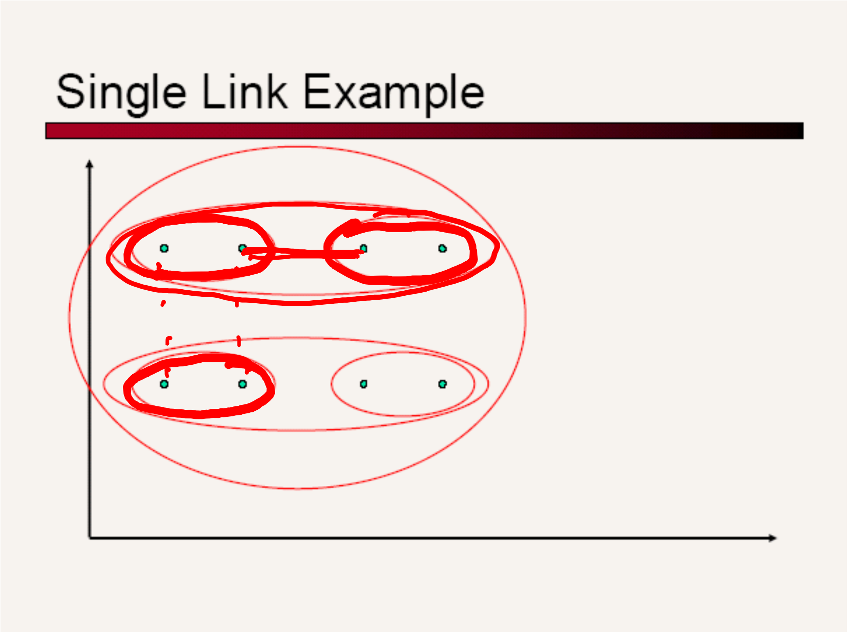
	c,d
a,b	6

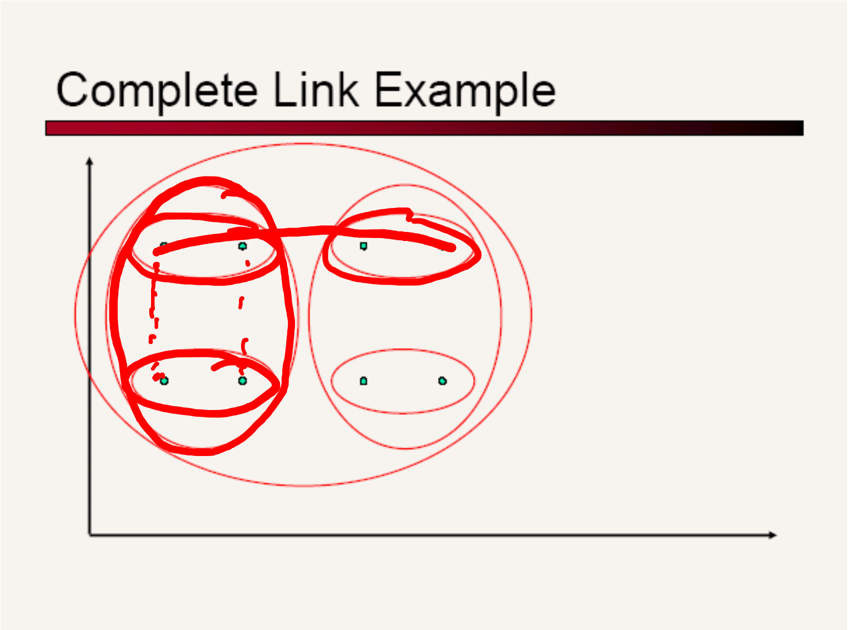
Distance Matrix

Dendrograms



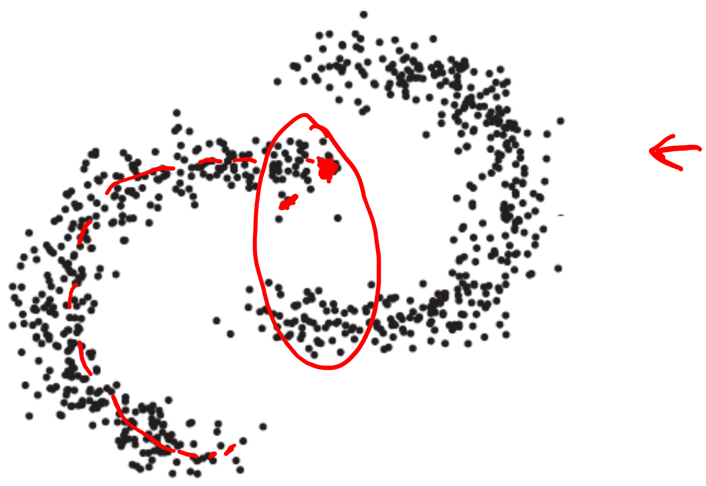
Another Example





Single vs. Complete Linkage

	Shape of clusters
Single-linkage	allows anisotropic and non-convex shapes
Complete-linkage	assumes isotopic, convex shapes



Computational Complexity

bottom-up (linkage)

- All hierarchical clustering methods need to compute similarity of all pairs of *n* individual instances which is $O(n^2)$.

- At each iteration,
  - Sort similarities to find largest one $O(n^2 \log n)$.
  - Update similarity between merged cluster and other clusters.

    Computing similarity to each other cluster can be done in constant time.

- So we get $O(n^2 \log n)$ or $O(n^3)$ (if naïvely implemented)

Computational Complexity (K-means)

- At each iteration,
  - Computing distance between each of the n objects and the K cluster centers is O(Kn).
  - Computing cluster centers: Each object gets added once to some cluster: O(n).

- Assume these two steps are each done once for l iterations: O(lKn).

What you need to know…

- Partition based clustering algorithms
  - K-means
    - Coordinate descent
    - Seeding
    - Choosing K
  - Mixture models
    EM algorithm

- Hierarchical clustering algorithms
  - Single-linkage
  - Complete-linkage
  - Centroid-linkage
  - Average-linkage

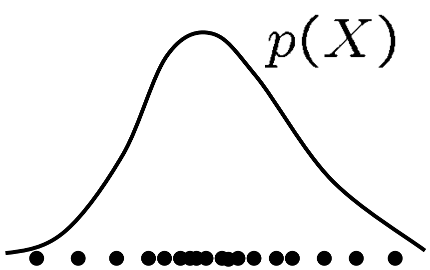
Unsupervised Learning

"Learning from unlabeled/unannotated data" (without supervision)

Training data $\{X_i\}_{i=1}^n$ → **Learning algorithm** → Prediction rule $\widehat{f}_n$

What can we predict from unlabeled data?

- Density estimation



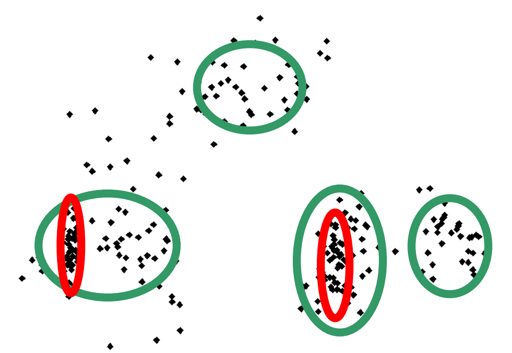
Unsupervised Learning

"Learning from unlabeled/unannotated data" (without supervision)

Training data $\{X_i\}_{i=1}^n$ → **Learning algorithm** → Prediction rule $\widehat{f}_n$

What can we predict from unlabeled data?

- Density estimation
- Groups or clusters in the data



Unsupervised Learning

"Learning from unlabeled/unannotated data" (without supervision)

Training data $\{X_i\}_{i=1}^n$ → **Learning algorithm** → Prediction rule $\widehat{f}_n$

What can we predict from unlabeled data?

- Density estimation
- Groups or clusters in the data
- Dimensionality reduction