Unsupervised clustering

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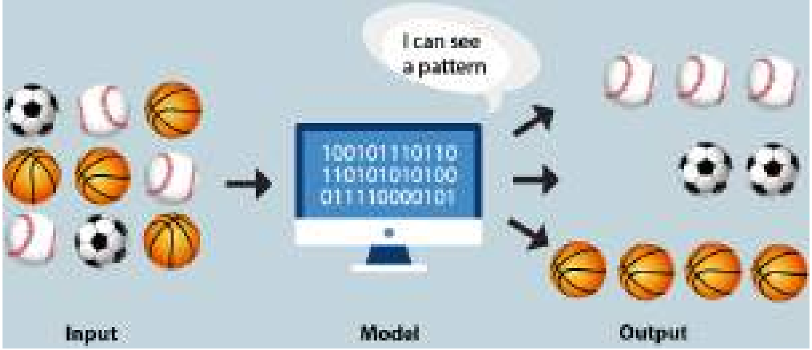
Why do we care?

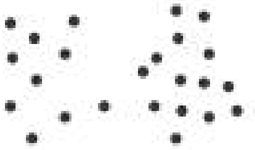
Clustering: Group the input data into clusters that share some characteristics.
(yup, that's a vague definition)

→ Find general patterns in the data (data mining problem)
→ Visualize the data (in a simpler way)
→ Infer some properties of a given data point based on how it relates to other data points (statistical learning)



Why is it tricky?

→ Clustering belongs to unsupervised learning ⇒ no ground truth available to learn/evaluate the quality of a clustering algorithm.



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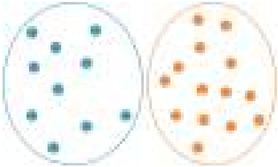

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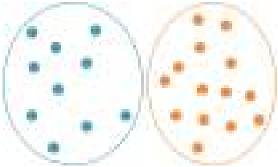

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- ⇒ Which criteria (features) are the more relevant for our problem?
- ⇒ Which metric makes the most sense?

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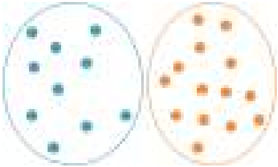

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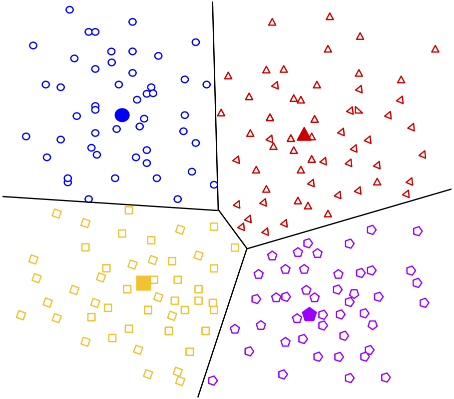
→ How to assess the soundness of the created clusters? Is that even a relevant question?

One can try to divide existing clustering approaches into several categories:

Centroid-based clustering Clusters are summarized using a single representative point, and points are assigned to clusters based on their distance to this *centroid* (k-means and its direct variants).



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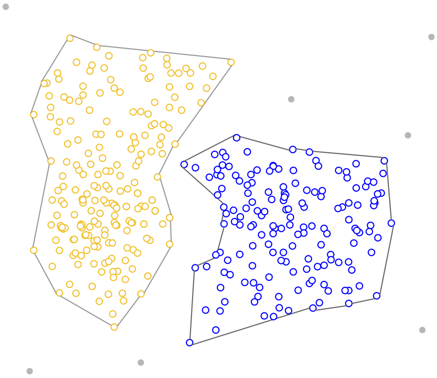

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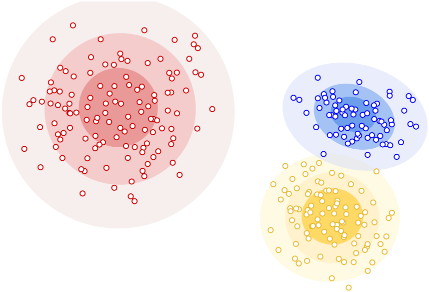

Families of clustering approaches

Clusteringception

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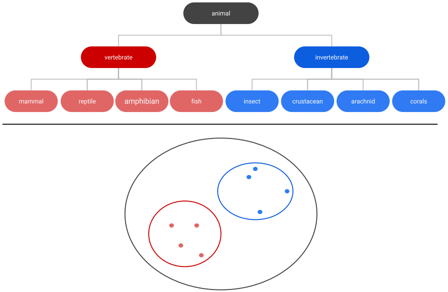

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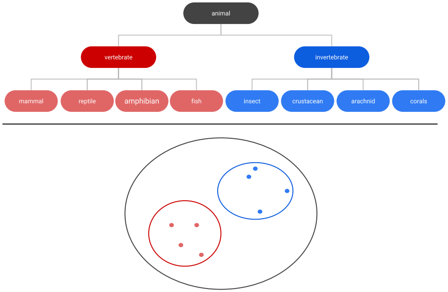
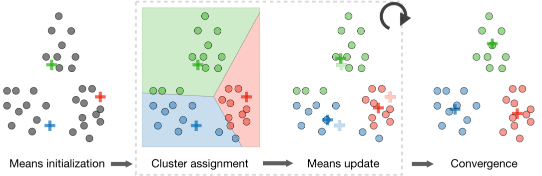


Partition n observations $\mathbf{x}_1, \dots, \mathbf{x}_n$ into k clusters $\mathbf{C} = \{C_1, \dots C_k\}$ where each observation $\mathbf{x}_i$ belongs to the clusters $C_{j^\star}$ whose mean $\boldsymbol{\mu}_{j^\star}$ is the closest: $\mathbf{x}_i \in S_{j^\star}$ with $j^\star = \arg\min_j \|\mathbf{x}_i - \boldsymbol{\mu}_j\|_2$.

Algorithm Basic K-means algorithm.

1: Select K points as initial centroids.
2: **repeat**
3: Form K clusters by assigning each point to its closest centroid.
4: Recompute the centroid of each cluster.
5: **until** Centroids do not change.



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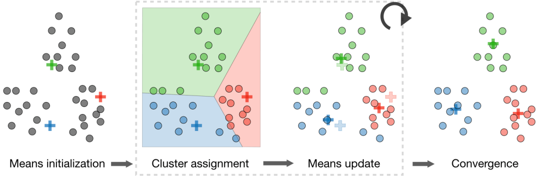
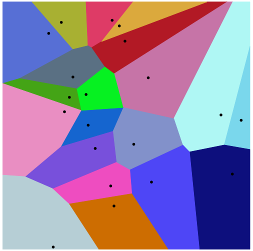


- $\rightarrow$ Minimizes within-cluster sum of squares (variance)
- $\rightarrow$ Overall optimization problem: $$\underset{\mathbf{C}=\{C_1,\ldots C_k\}}{\arg\min} \sum_{i=1}^{k} \sum_{\mathbf{x}\in C_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$
- $\rightarrow$ NP-hard problem, no guarantee to find the global optimum
- $\rightarrow$ Stochastic and very sensitive to initial conditions
- $\rightarrow$ Sensitive to outliers (thank you, L_2 norm...)
- $\rightarrow$ Yet it's probably the most used clustering algorithm out there

k-means and Voronoi tesselation



Voronoi tesselation: partition of the Euclidean space relatively to discrete points/seeds. Each region/Voronoi cell is composed of all the points in the space that are closer to the cell seed than to any other seed

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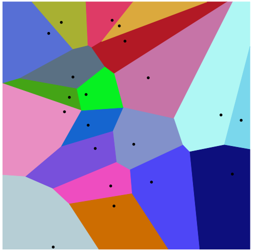

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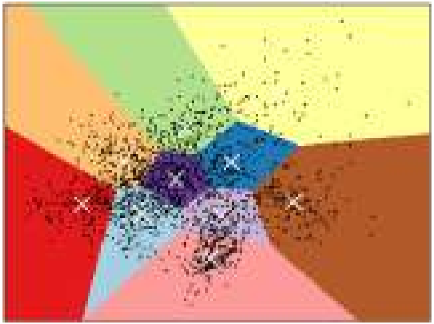
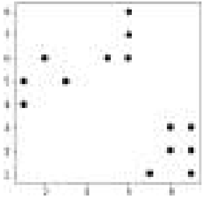
→ k-means provides a way to obtain a Voronoi tesselation of the input space, where seeds are the final cluster means.

→ Alternatively, one can use some pre-computed Voronoi tesselation seeds as initial clusters for k-means



How many clusters for this data set?



Determining the optimal number of clusters with the elbow method

Empirical af, but still better than nothing...

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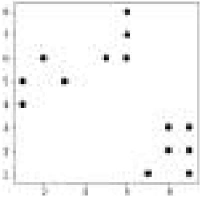

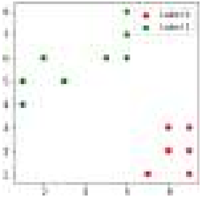

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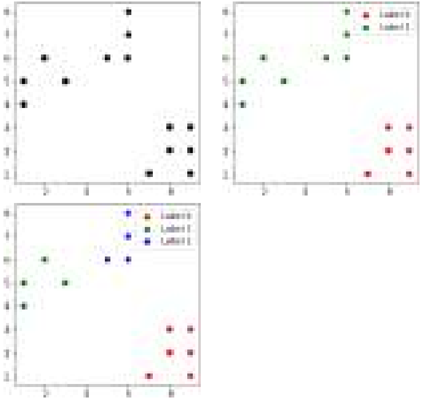

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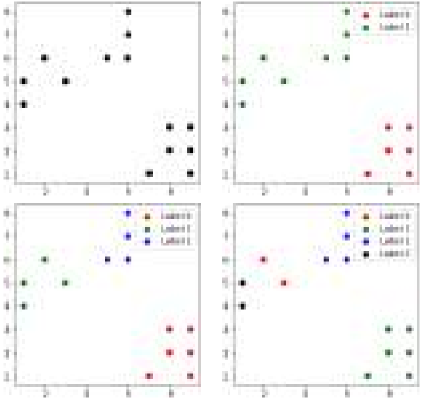

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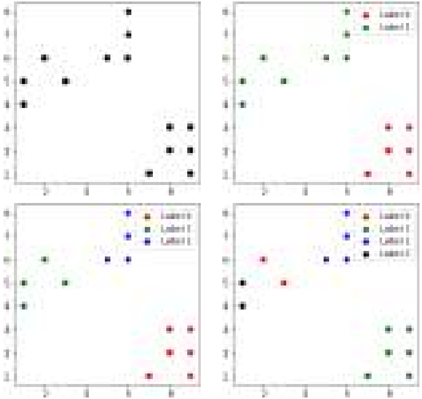
How many clusters for this data set?

→ Compute explained variance for an increasing number of clusters k

$$\mathrm{Var}(\mathbf{C} = \{C_1, \dots C_k\}) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

→ Plot and find the bend of the elbow



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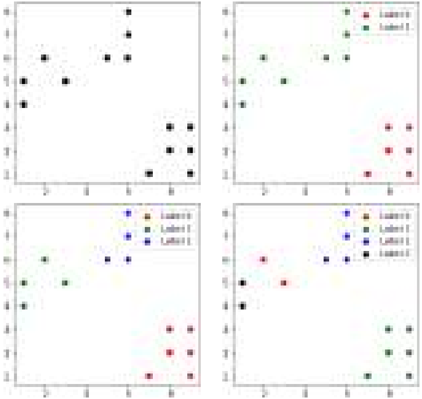

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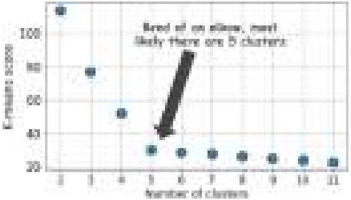

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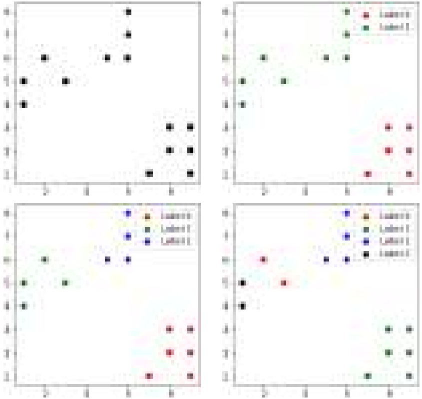
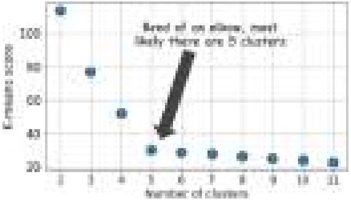
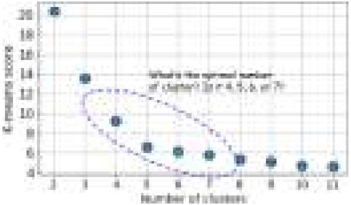
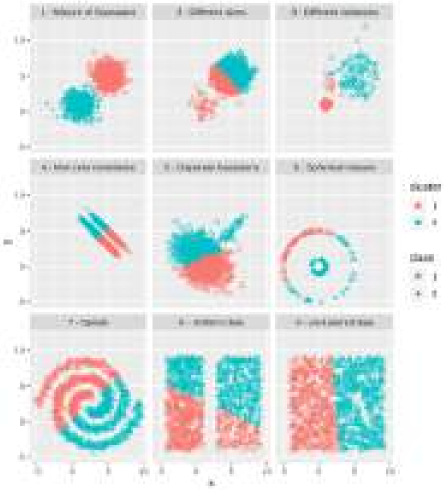






But most of the time, not as expected. And it is probably because of the L_2 norm that k-means tries to minimize:



→ Sensible to curse of dimensonality

→ Form "normalized Gaussian" clusters (spherical)

→ Does not adapt to manifold geometry

→ Sensible to class imbalance

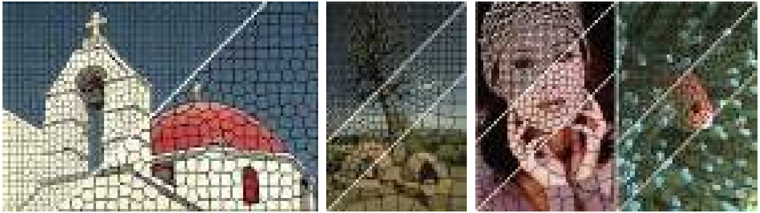
→ Sensible to outliers

SLIC superpixels uses a modified k-means clustering in the *Labxy* space to produce *k* clusters regularly sampled and perceptually coherent from a color point of view.

Algorithm SLIC superpixel segmentation

Initialize cluster centers $C_k = [l_k, a_k, b_k, x_k, y_k]^T$ by sampling pixels at regular grid steps S.
Perturb cluster centers in an $n \times n$ neighborhood, to the lowest gradient position.
repeat
  for each cluster center C_k **do**
    Assign the best matching pixels from a $2S \times 2S$ square neighborhood around the cluster center according to the distance measure (Eq. 1).
  end for
  Compute new cluster centers and residual error E {L1 distance between previous centers and recomputed centers}
until $E \le$ threshold
Enforce connectivity.

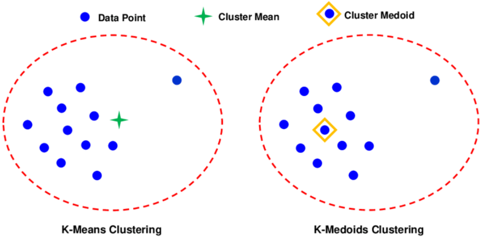
$$d_{lab} = \sqrt{(l_k - l_i)^2 + (a_k - a_i)^2 + (b_k - b_i)^2}$$
$$d_{xy} = \sqrt{(x_k - x_i)^2 + (y_k - y_i)^2} \quad (1)$$
$$D_s = d_{lab} + \frac{m}{S} d_{xy},$$



k-medoids clustering

A possible extension to k-means

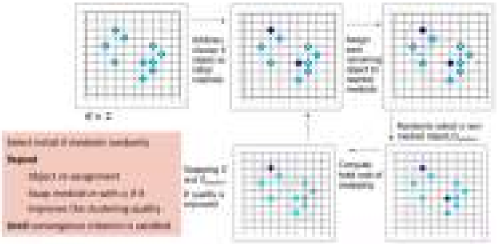
Clusters centroids are not initial data points $\rightarrow$ can be problematic



$\Rightarrow$ Replace centroid by medoid (point with the smallest distance to all other points in the cluster)

$$\mathbf{m}_{\mathcal{C}} = \arg\min_{\mathbf{x} \in \mathcal{C}} \sum_{\mathbf{x}_i \in \mathcal{C}} d(\mathbf{x}, \mathbf{x}_i)$$

$\Rightarrow$ k-medoids algorithm



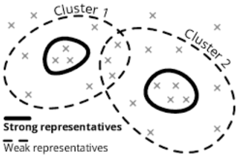
Overall objective: find k medoids $\mathbf{m}_1, \ldots, \mathbf{m}_k$ that minimize the partitioning cost

$$\sum_{i=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_i} d(\mathbf{x}, \mathbf{m}_i)$$

Fuzzy c-means clustering
Let it fuzz

k-means is a *hard* clustering method → each data point 100% belongs to its cluster.

Soft (aka *fuzzy*) clustering methods allow each data point to belong to several clusters with various degrees of membership.



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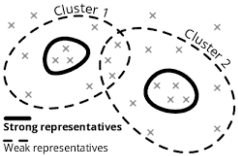
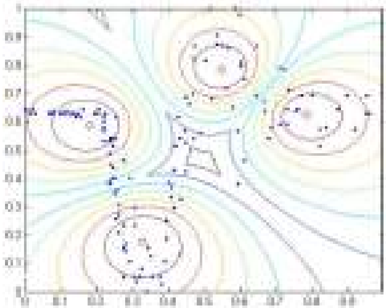


FCM clustering: outputs clusters $\mathcal{C}_1, \ldots, \mathcal{C}_k$ and membership matrix $\mathbf{W}_{n \times k}$ ($w_{ij} = \%(\mathbf{x}_i \in \mathcal{C}_j)$)

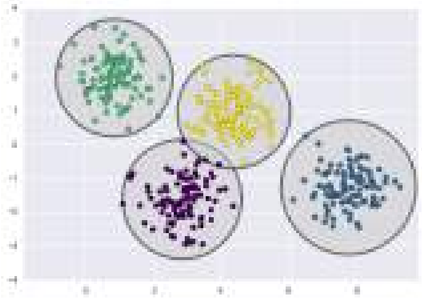
$\Rightarrow \arg\min_{\mathbf{C}=\{C_1,\ldots C_k\}} \sum_{i=1}^{n} \sum_{j=1}^{k} w_{ij}^{m} \left\|\mathbf{x}_i - \boldsymbol{\mu}_j\right\|^2$

$\Rightarrow$ Alternatively update $\boldsymbol{\mu}_j = \frac{\sum_{\mathbf{x}_i} w_{ij}^m \mathbf{x}_i}{\sum_{\mathbf{x}_i} {w_{ij}}^m}$ and

$$w_{ij} = \frac{1}{\sum_{l=1}^{k} \left(\frac{\left\|\mathbf{x}_i - \boldsymbol{\mu}_j\right\|}{\left\|\mathbf{x}_i - \boldsymbol{\mu}_l\right\|} \right)^{\frac{2}{m-1}}}$$



k-means works for spherical clusters, but fails in any other case $\Rightarrow$ try harder
Model probability density function f of data as a mixture of multivariate Gaussian



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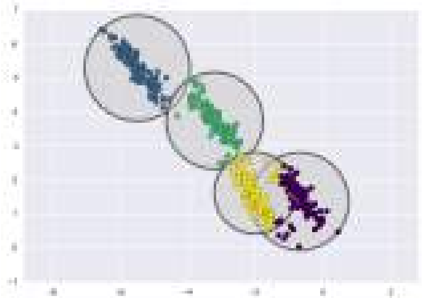

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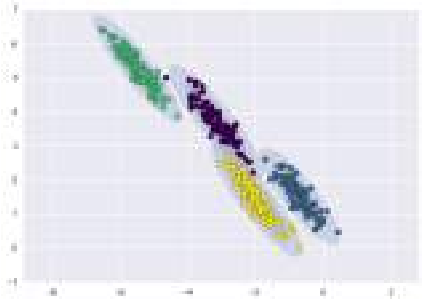

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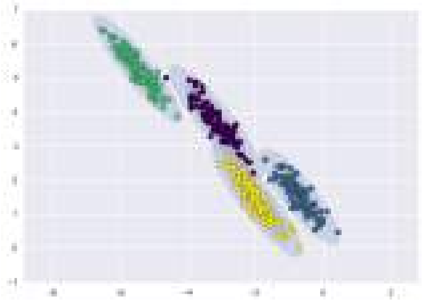

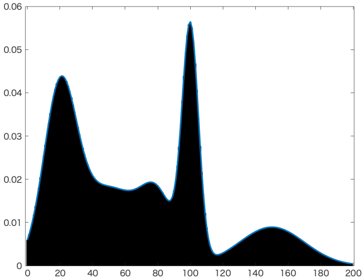

Gaussian mixture models

k-means on steroids

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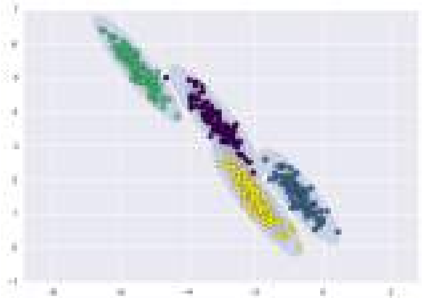

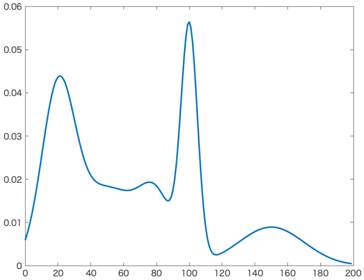

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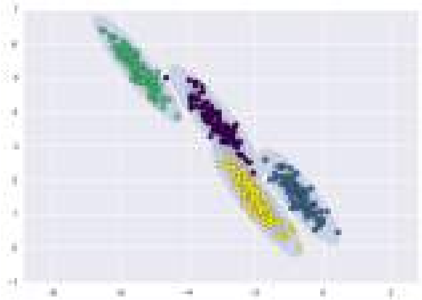

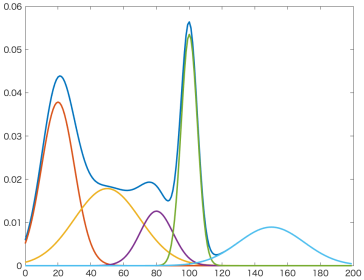

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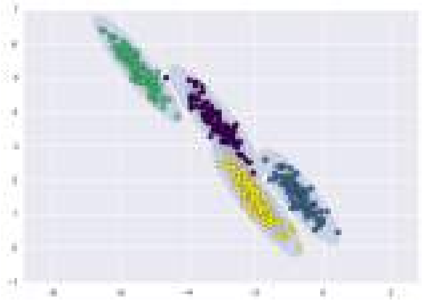

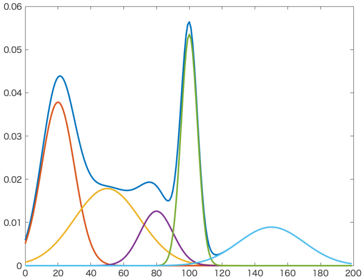

Gaussian mixture model: $f(\mathbf{x}) = \sum_{i=1}^{k} \phi_i \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_i, \Sigma_i)$

recall that $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^N \det(\Sigma)}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})\right)$ for $\mathbf{x} \in \mathbb{R}^N$

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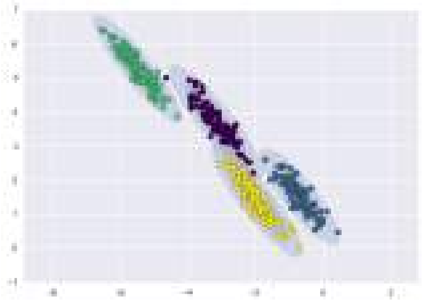
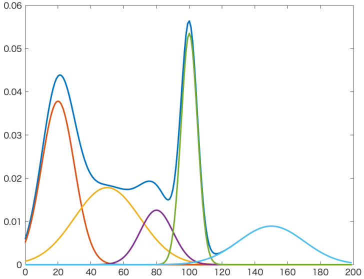
Model probability density function f of data as a mixture of multivariate Gaussian





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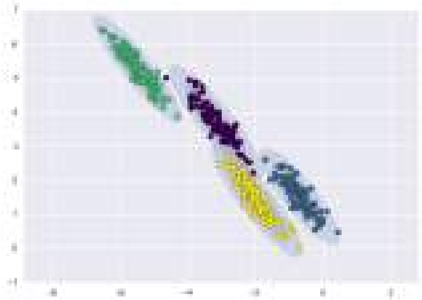

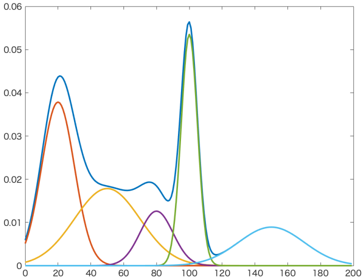

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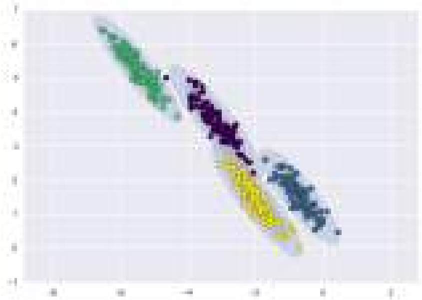

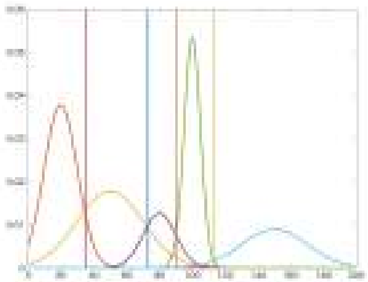

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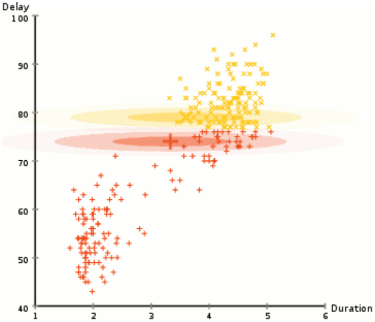

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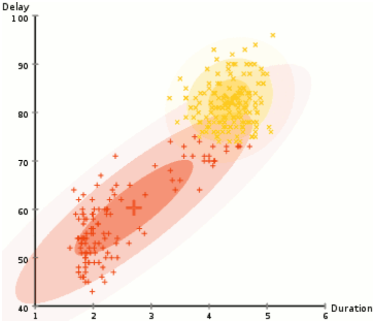

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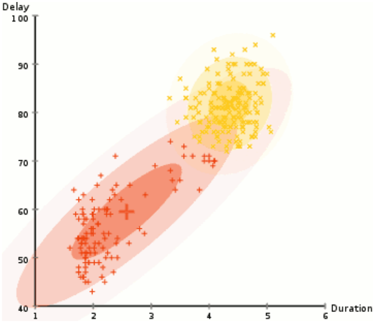

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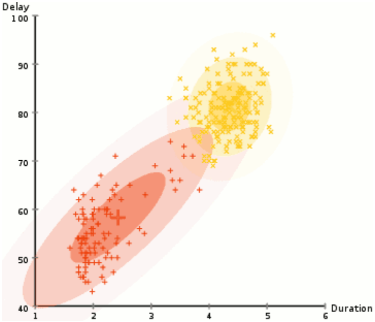

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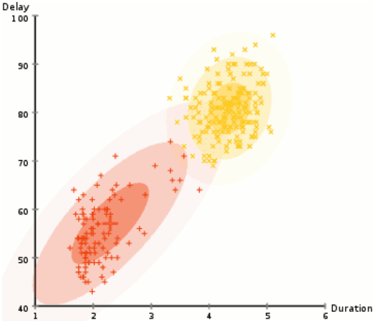

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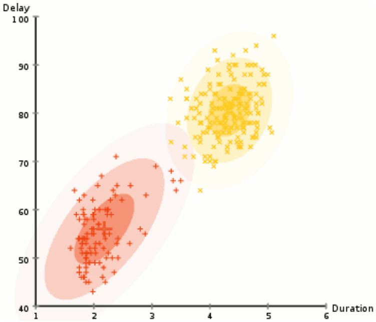

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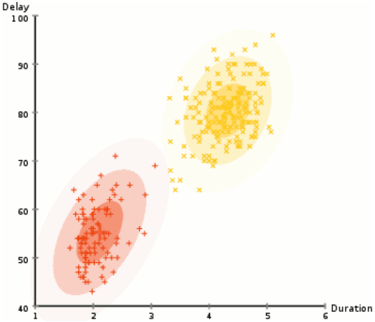

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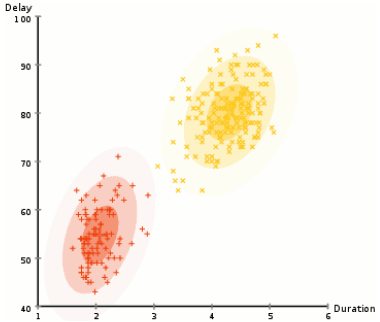

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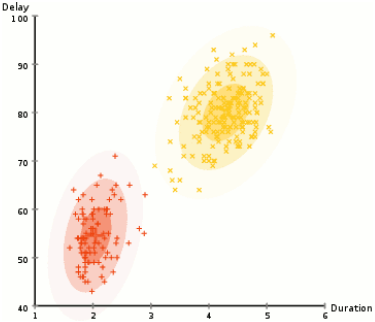

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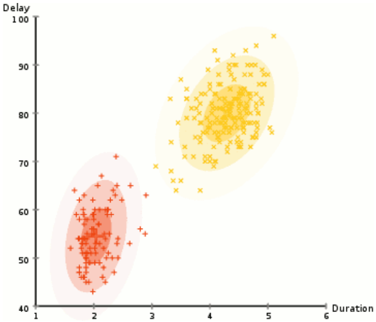

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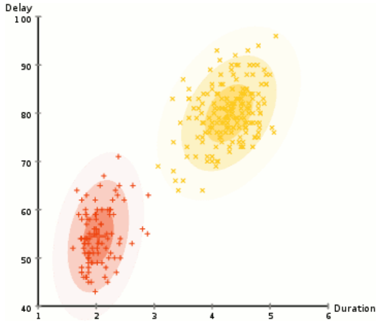

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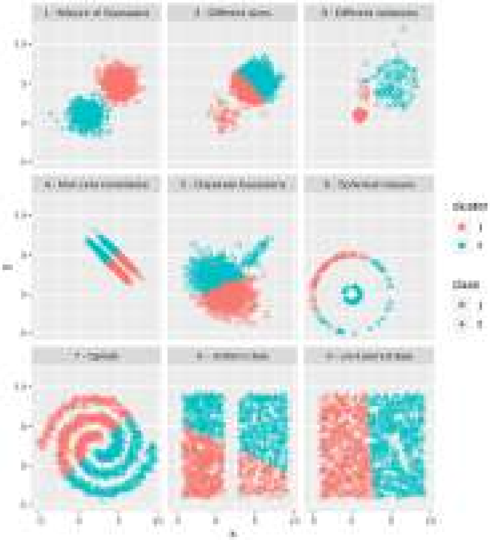
k-means vs GMM

Let the fight begin

k-means



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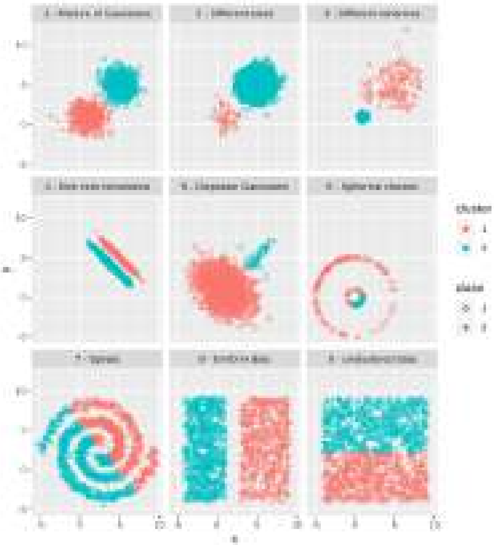

Worth the pain, right?

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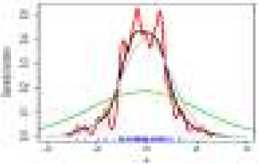
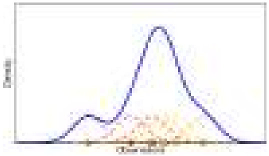
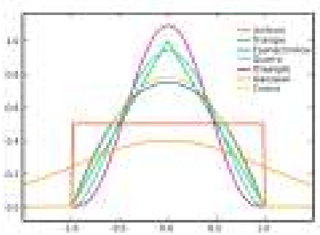




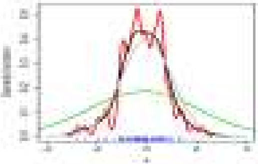


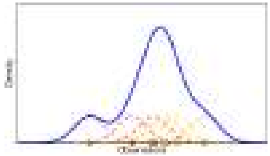
The kernel density estimator with bandwidth h at a given point x is given by

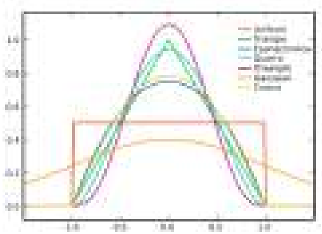
$$\widehat{f}_h(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i) = \frac{1}{nh}\sum_{i=1}^{n} K\Big(\frac{x - x_i}{h}\Big),$$

Kernel density estimation
Nonparametric estimation

Goal: Estimate probability density function f based on observation $x_1 \dots, x_n$ only, assumed to derive from f (otherwise wtf are we doing here?)







The kernel density estimator with bandwidth h at a given point x is given by

$$\widehat{f_h}(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right),$$