Unsupervised learning. $\{X_i\}_{i=1}^n$ — dimensionality reduction : PCA; Clustering

Clustering with k-means

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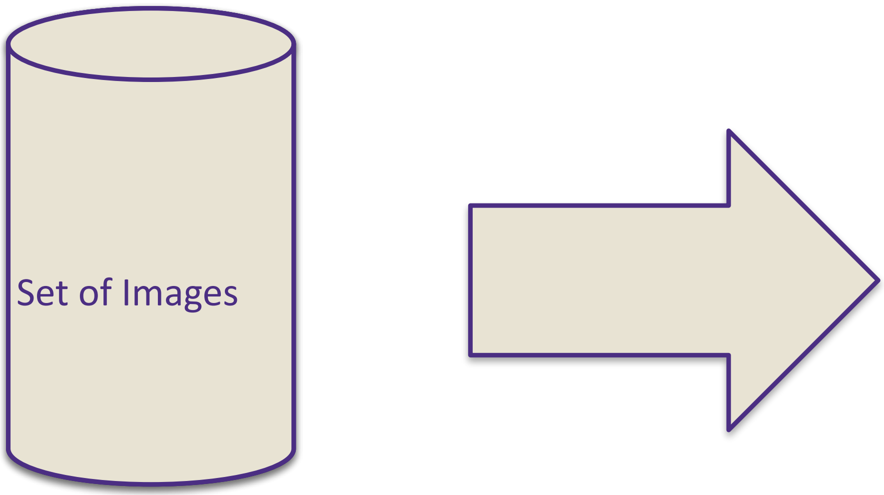
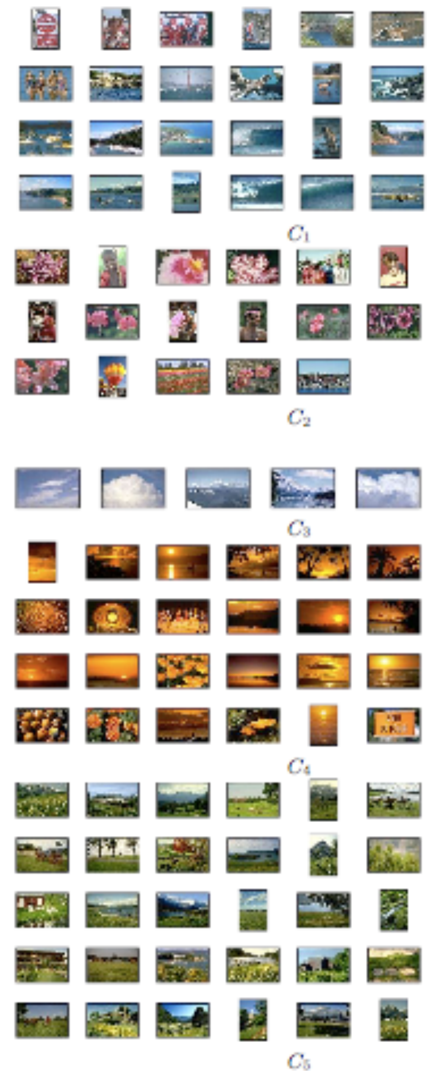
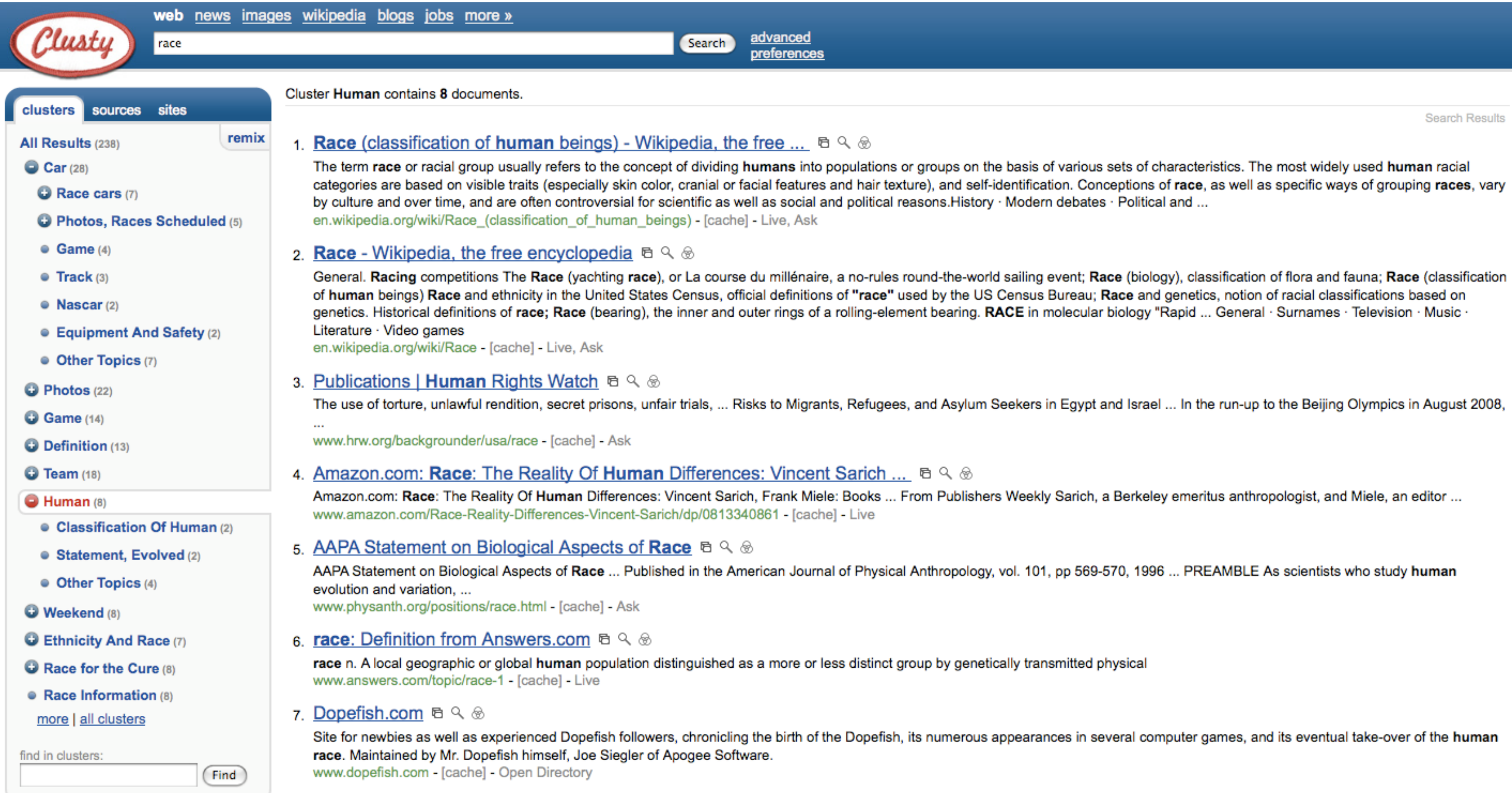
Clustering images



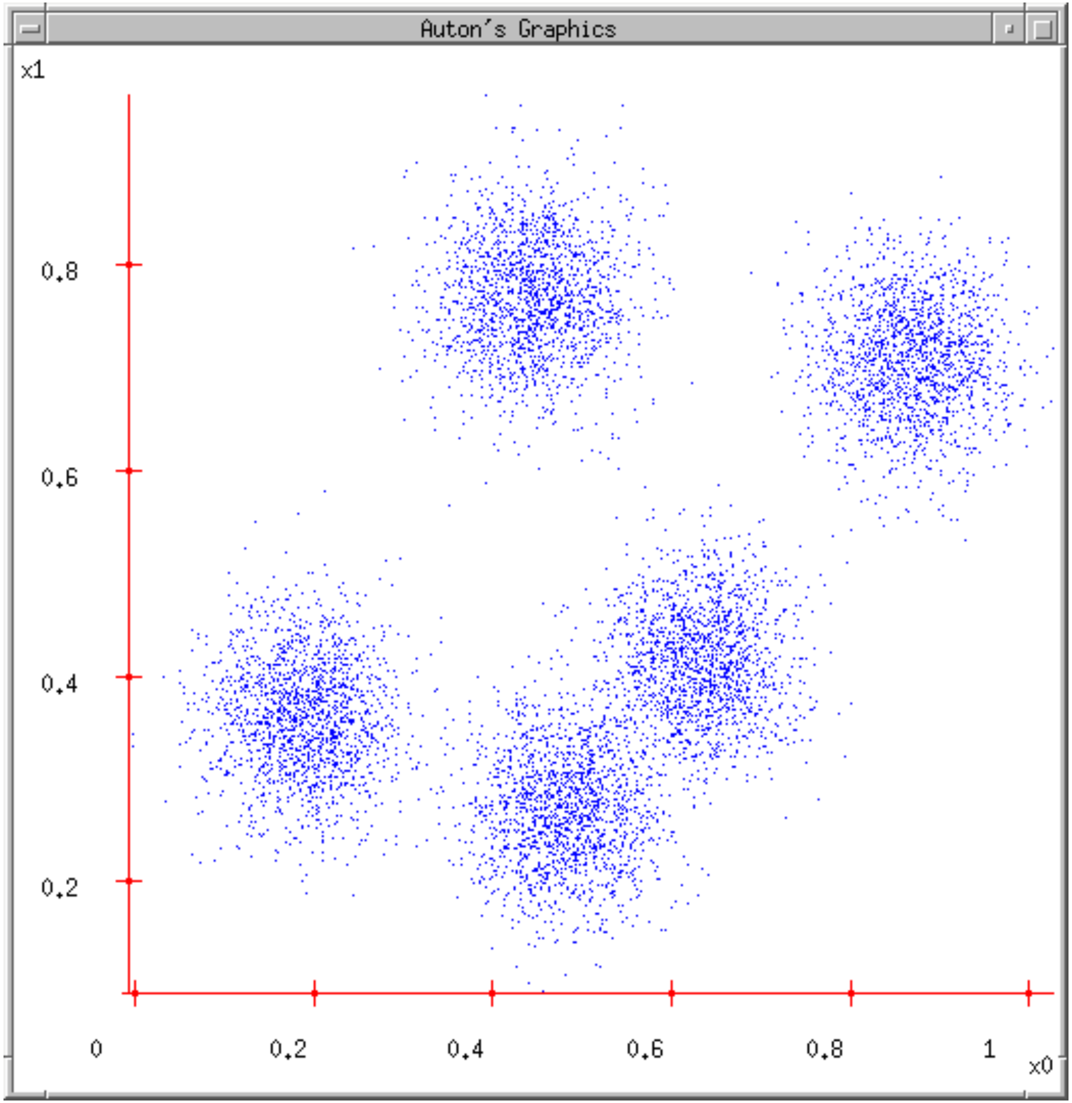


[Goldberger et al.]

Clustering web search results

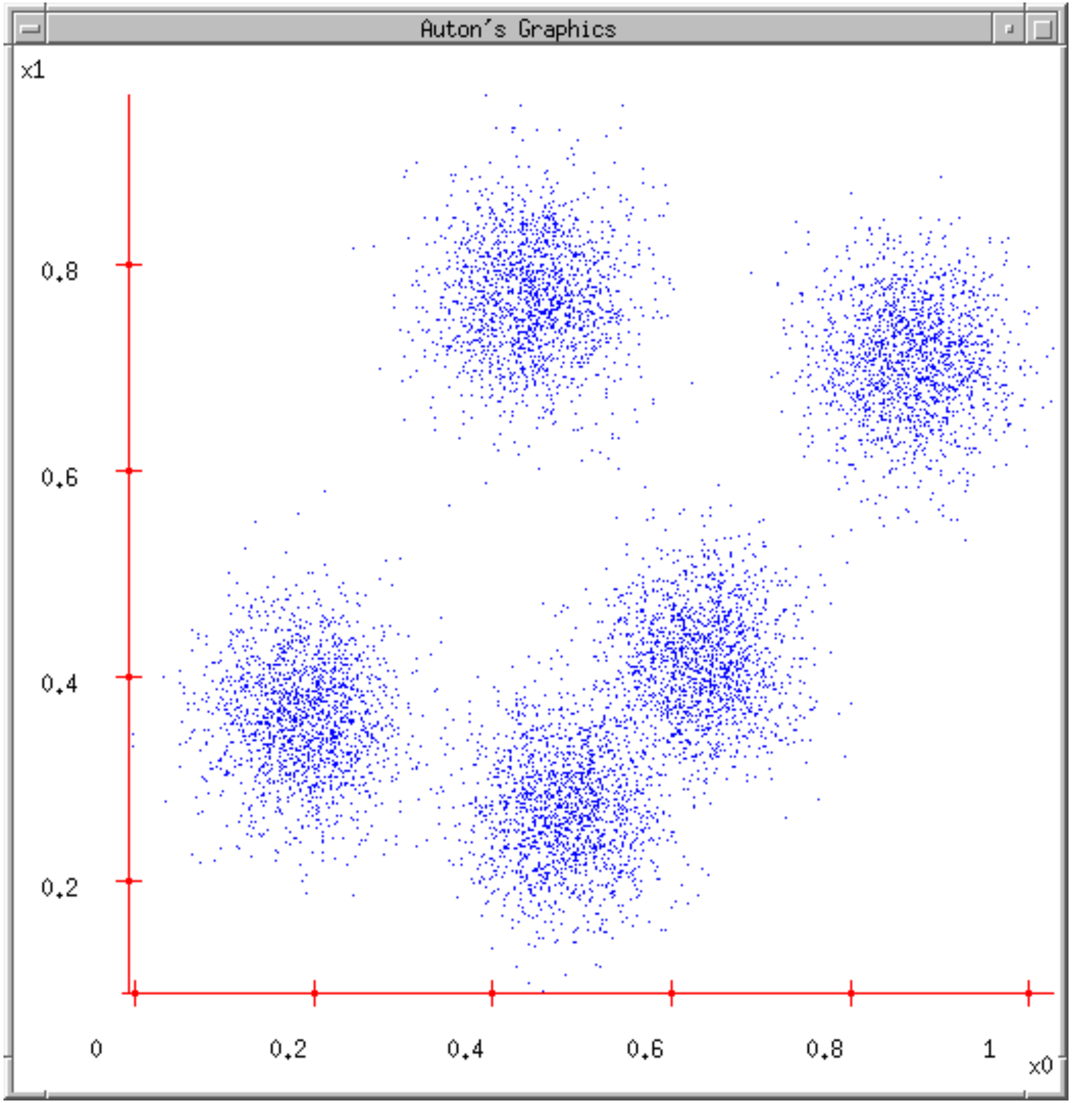


Some Data



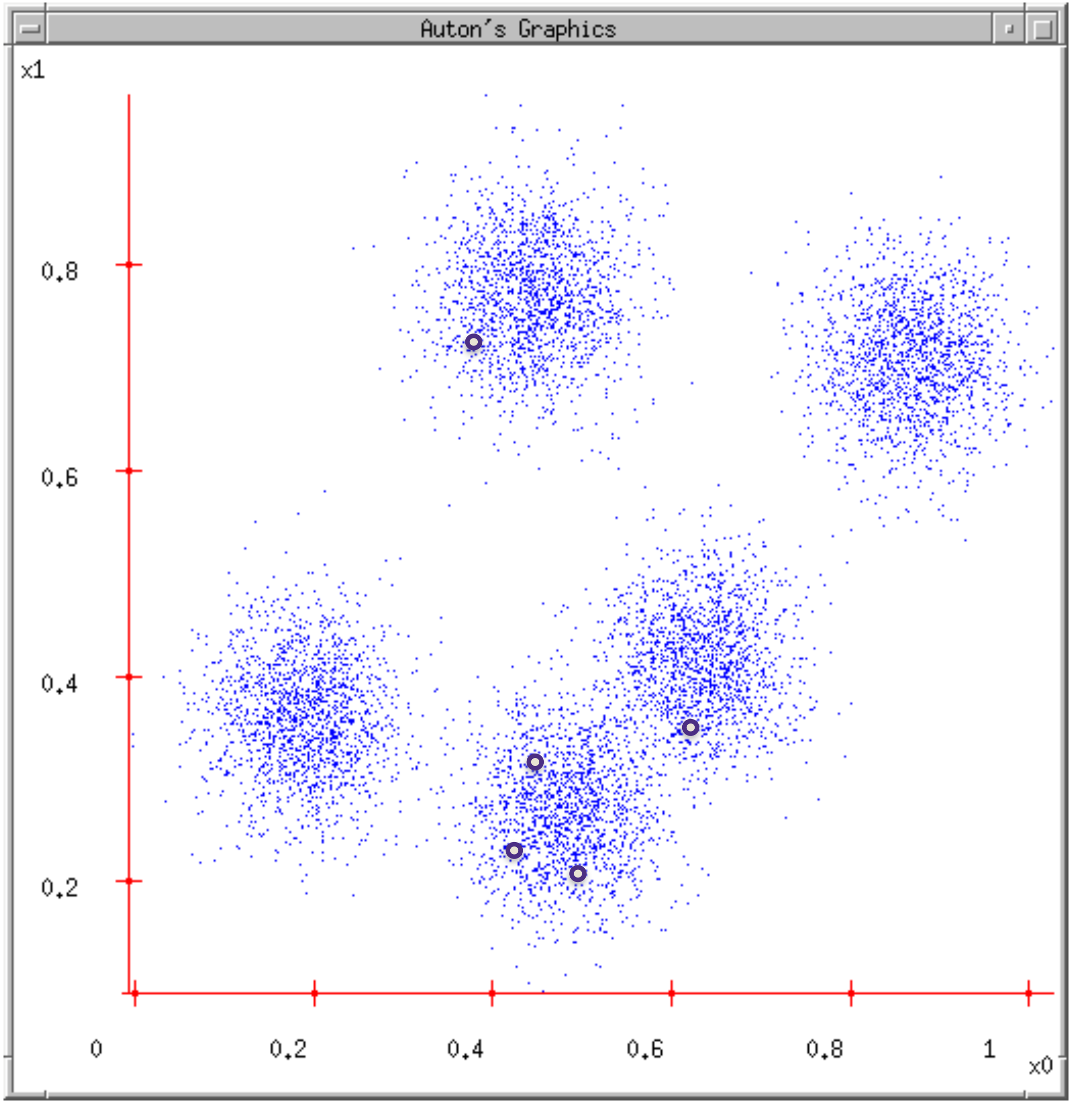
k-means

1. Ask user how many clusters they'd like. (e.g. k=5)



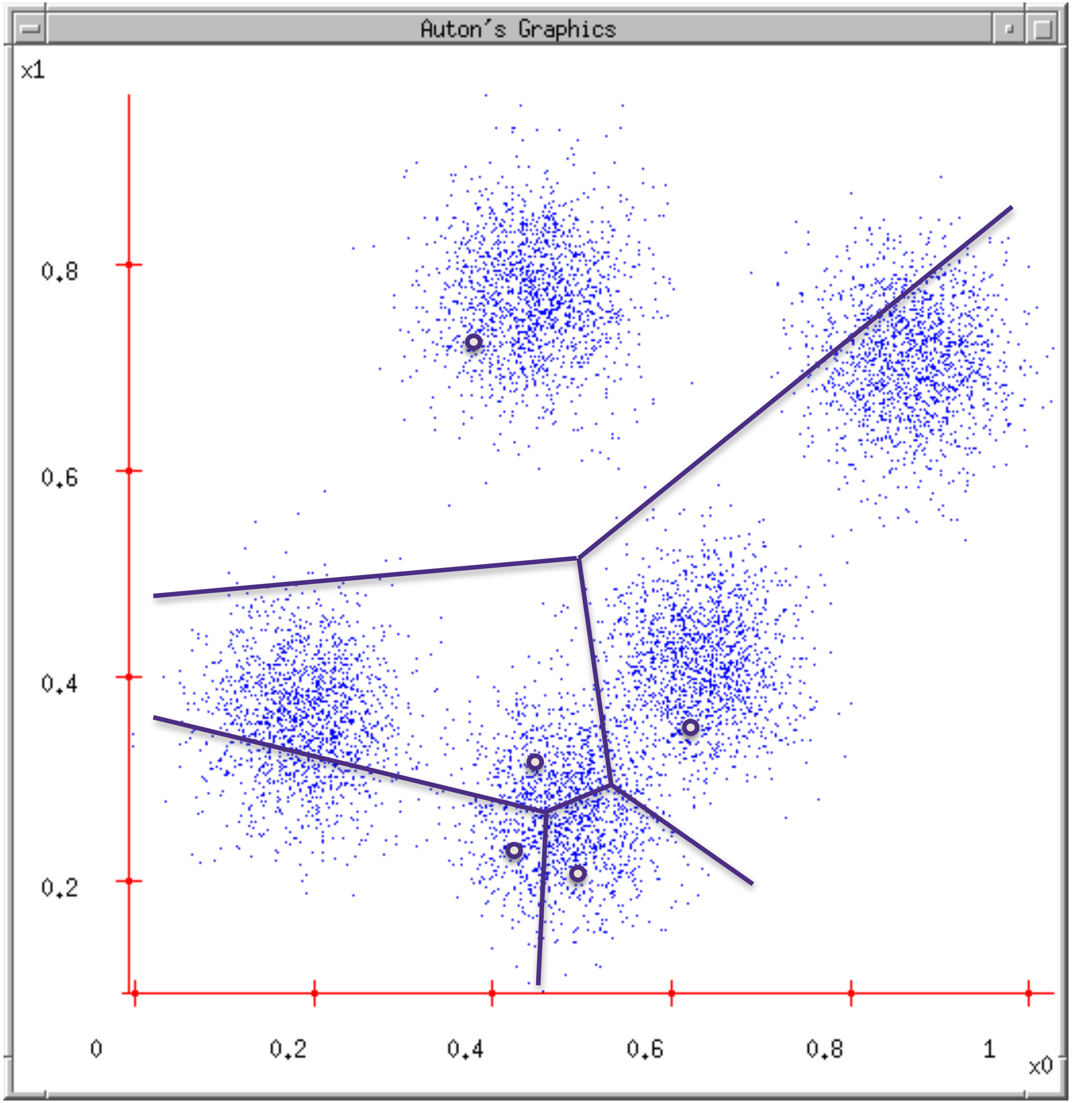
k-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Initialize: Randomly guess k cluster Center locations



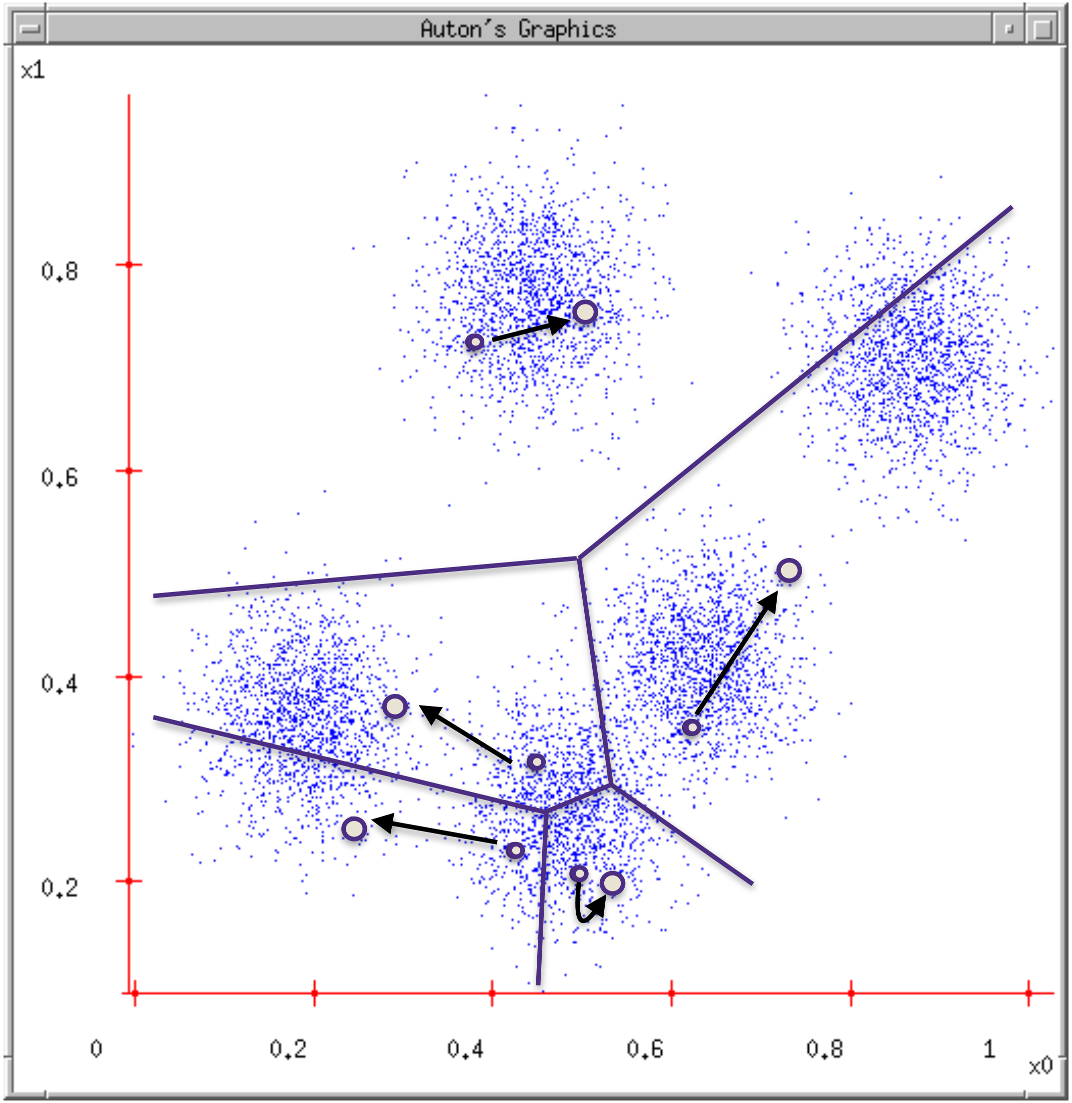
k-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Initialize: Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to. (Thus each Center "owns" a set of datapoints)



k-means

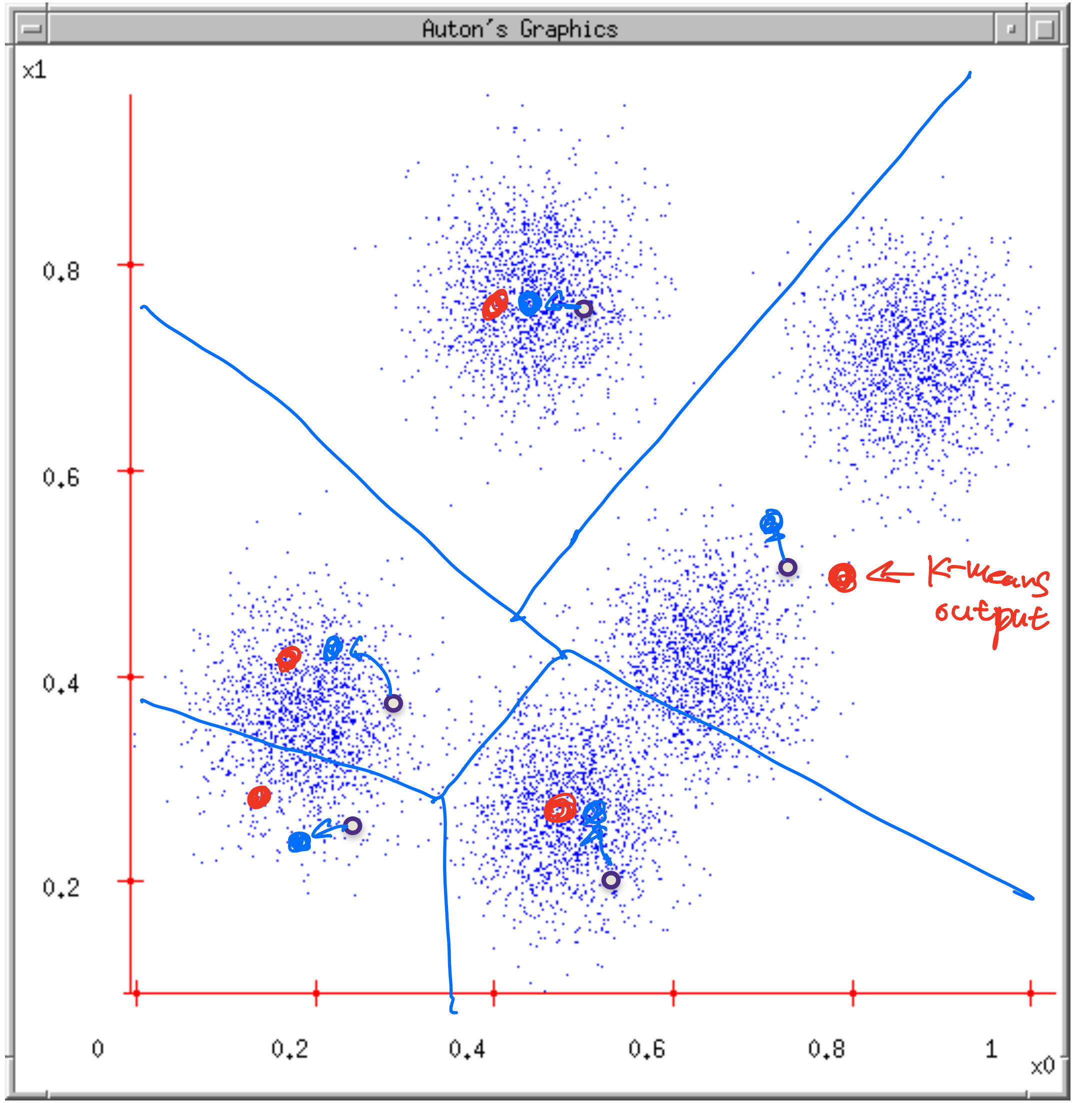
1. Ask user how many clusters they'd like. (e.g. k=5)
2. Initialize: Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the **centroid** of the points it owns



k-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Initialize: Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the **centroid** of the points it owns…
5. …and jumps there
6. …Repeat until terminated!

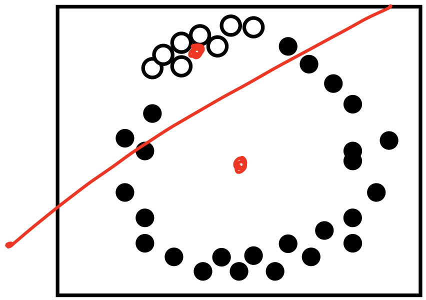
Average of all data points in that region



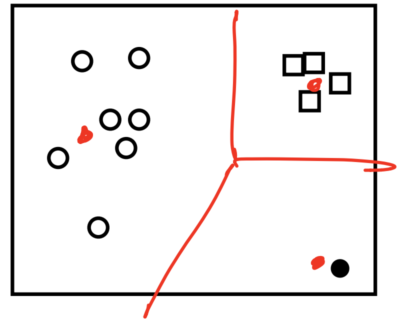
Which one is a snapshot of a converged k-means

Can this be output of terminated k-means

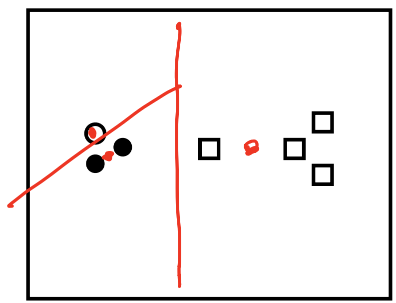
Example (a) No



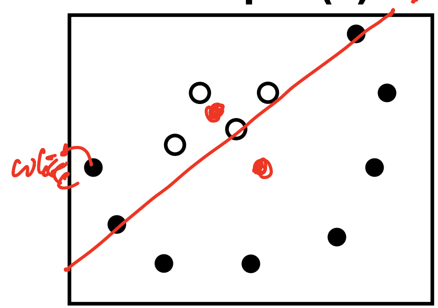
Example (b) (o)



Example (c) Yes



Example (d) ? No.



k-means

> **Initialize** k centers (as random data points)

- $\mu^{(0)} = (\mu_1^{(0)}, \ldots, \mu_k^{(0)})$

> **Classify:** assign each point j∈{1,…n} to nearest center:

- For each $j \in \{1,\ldots,n\}$, $C^{(t)}(j) \leftarrow \arg\min_{i \in \{1,\ldots,k\}} \|\mu_i^{(t)} - x_j\|_2^2$

$\{1, \ldots, k\}$

distance

> **Recenter:** μ_i **becomes centroid of its point:**

- For each $i \in \{1,\ldots,k\}$, $\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C^{(t)}(j)=i} \|\mu - x_j\|_2^2$

- Equivalent to $\mu_i \leftarrow$ average of its points!

$\mu^* = \frac{1}{|C^{(t)}(j)|} \sum_{j: C^{(t)}(j)=i} x_j$

↑ size of cluster

↑ no longer true for other distance.

k-means

- **Initialize** k centers (as random data points)
  - $\mu^{(0)} = (\mu_1^{(0)}, \dots , \mu_k^{(0)})$

- **Classify:** assign each point j∈{1,…n} to nearest center:
  - For each $j \in \{1,\ldots,n\}$, $\quad C^{(t)}(j) \leftarrow \arg \min_{i \in \{1,\ldots,k\}} \|\mu_i^{(t)} - x_j\|_2^2$

- **Recenter:** μ_i **becomes centroid of its point:**
  - For each $i \in \{1,\ldots,k\}$, $\quad \mu_i^{(t+1)} \leftarrow \arg \min_{\mu} \sum_{j:C^{(t)}(j)=i} \|\mu - x_j\|_2^2$
  - Equivalent to $\mu_i \leftarrow$ average of its points!

What does k-means do? Coordinate descent on

$$F(\mu, C) = \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

$C(1) \cdots C(n)$

$\mu_1 \cdots \mu_k$

Does k-means converge??

- k-means is trying to minimize the following objective

$$\min_{\mu_1 \cdots \mu_k} \min_{C(1) \cdots C(n)} F(\mu, C) = \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

- Via coordinate descent:
  - Fix μ, optimize C

$$\min_{C(1) \cdots C(n)} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

→ decomposed into n separate problems.

$$\forall j \quad \min_{C(j) \in \{1 \cdots k\}} \|\mu_{C(j)} - x_j\|_2^2$$

Does k-means converge??

- k-means is trying to minimize the following objective

$$F(\mu, C) = \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

- Via coordinate descent:
  - Fix μ, optimize C

$$\min_{C} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

    by solving n separate problems:

$$\min_{C(j)} \|\mu_{C(j)} - x_j\|_2^2$$

    whose solution is

$$C(j) \leftarrow \arg \min_{i \in \{1,\ldots,k\}} \|\mu_{C(j)} - x_j\|_2^2$$

Does k-means converge??

- k-means is trying to minimize the following objective

$$F(\mu, C) = \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

- Via coordinate descent:
  - Fix C, optimize μ

$$\min_{\mu} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|_2^2$$

by solving k separate problems

$$\min_{\mu_i} \sum_{j:C(j)=i} \|\mu_i - x_j\|_2^2$$

whose solution is

$$\mu_i \leftarrow \frac{1}{|\{j : C(j) = i\}|} \sum_{j:C(j)=i} x_j$$

Does k-means converge??

- there is only a finite set of values that $\{C(j)\}_{j=1}^n$ can take (k^n is large but finite)
- so there is only finite, k^n at most, values for μ also
- each time we update them, we will never increase the objective function $\sum_{i=1}^{k} \sum_{j:C(j)=i} \|x_j - \mu_i\|_2^2$
- the objective is lower bounded by zero
- after at most k^n steps, the algorithm must converge (as the assignments $\{C(j)\}_{j=1}^n$ cannot return to previous assignments in the course of k-means iterations)

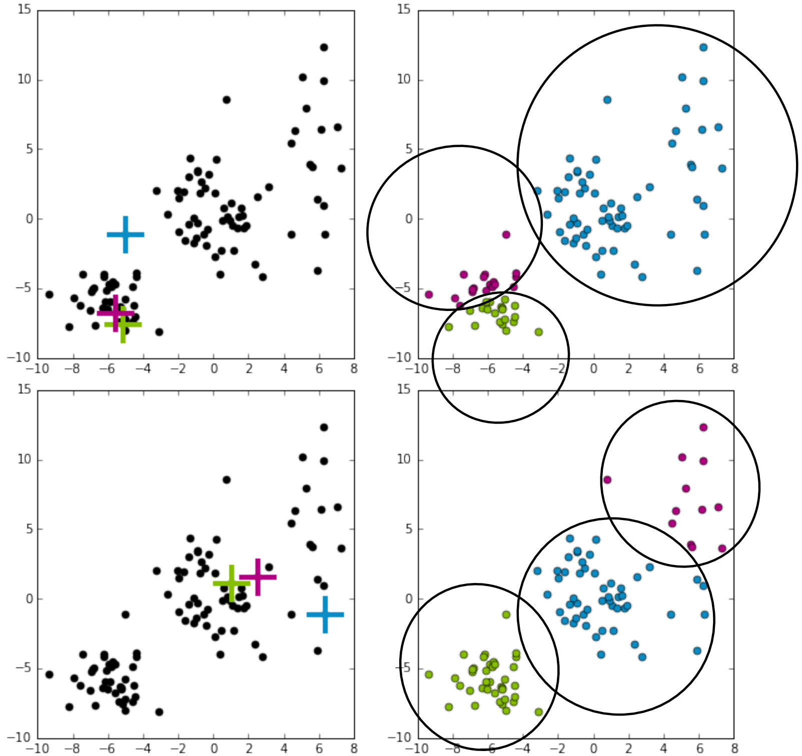
Downside of k-means

- the final solution depends on the initialization
  (as it is a coordinate descent on a non-convex problem)

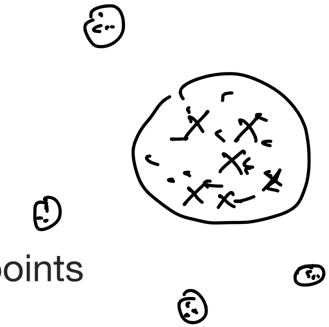
Initial position of centers final converged assignment

Trial 1

Trial 2



k-means ++: a smart initialization



Smart initialization:

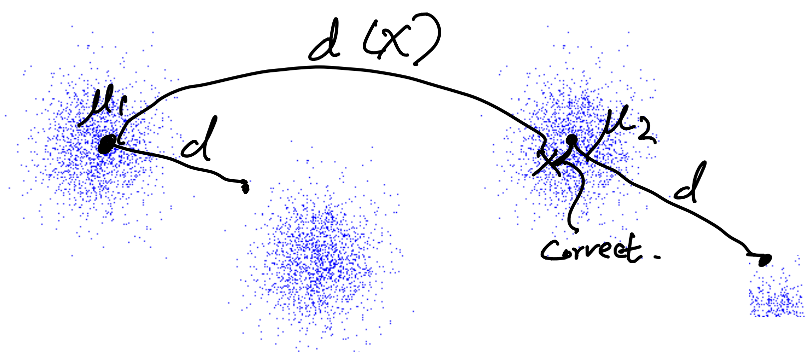
1. Choose first cluster center uniformly at random from data points

2. Repeat $k - 1$ times

   3. For each data point x_j, compute distance d_j to the nearest cluster center

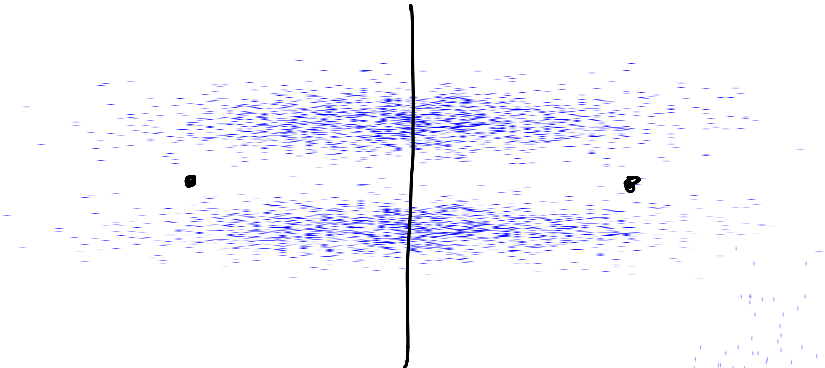
   4. Choose new cluster center from amongst data points, with probability of x_j being chosen proportional to $(d_j)^2$

- apply standard K-means after the initialization
- k-means++ achieves k-means error at most a factor of $\log k$ worse than the optimal [Arther,Vassilvitskii,2007]

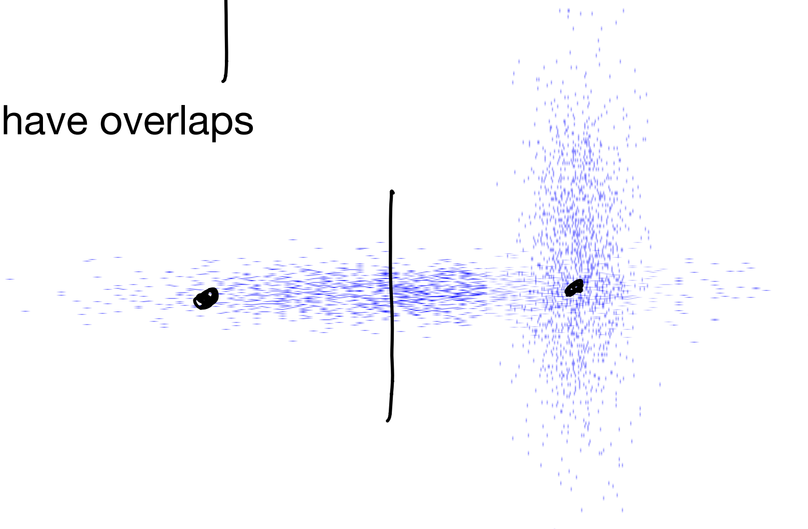


Downside of k-means

- Cluster shapes can be different

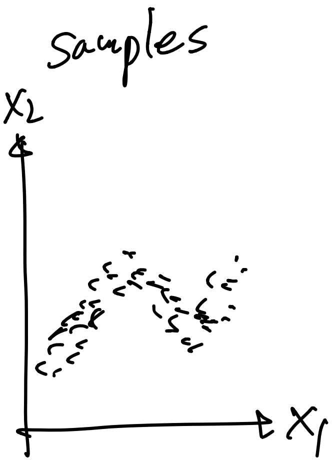


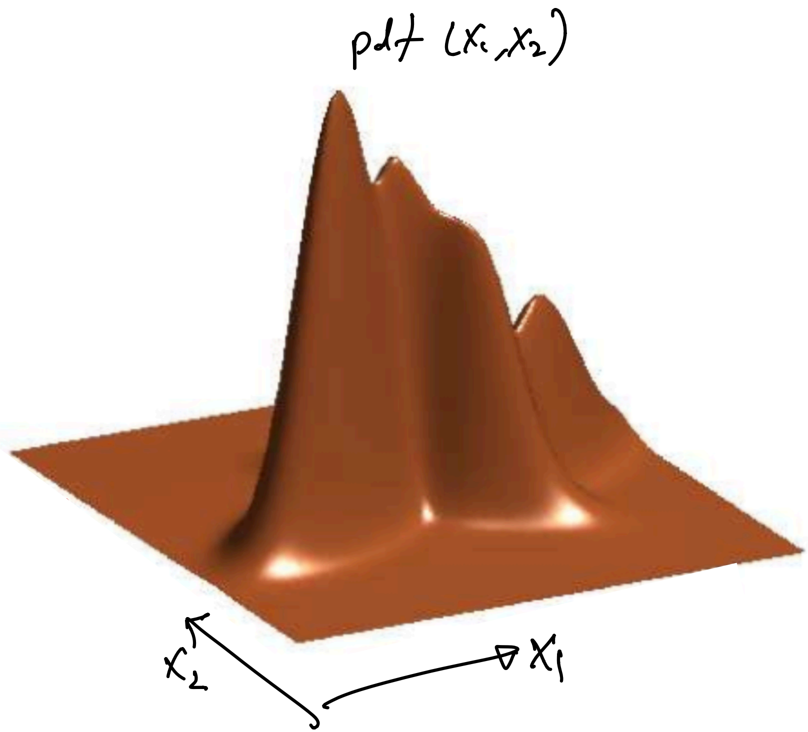
- Or clusters can have overlaps



Solution: density estimation

> Estimate probability density function from n i.i.d. samples $x_1, x_2, \ldots, x_n$

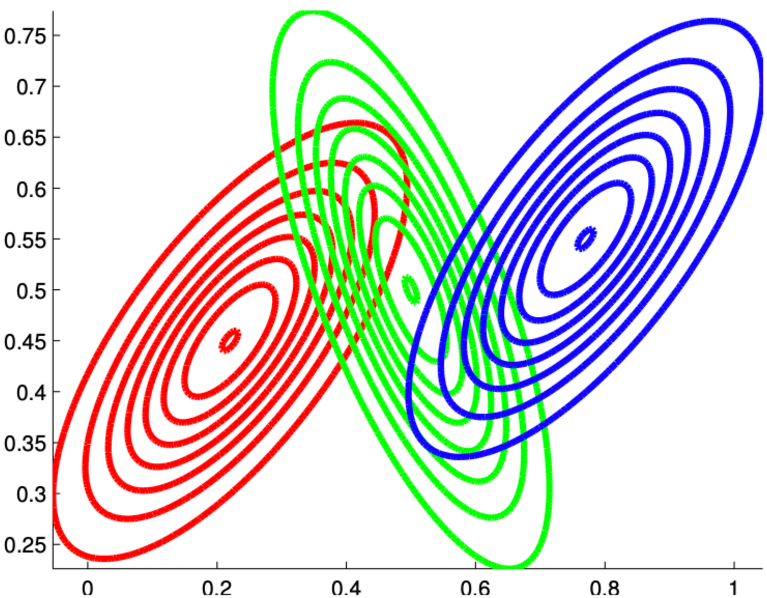




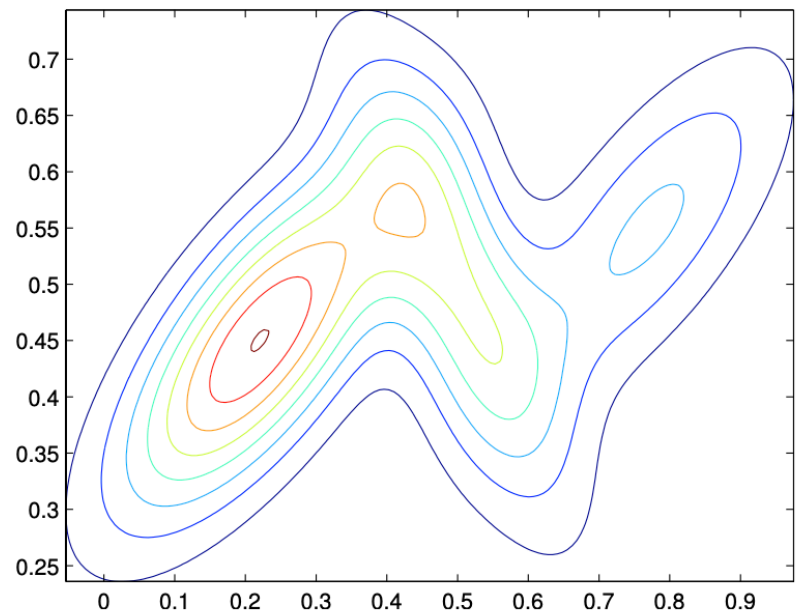
Density as mixture of Gaussians

> Approximate unknown density with a mixture of Gaussians

Mixture of 3 Gaussians



Contour Plot of Joint Density



Mixture of Gaussians

$$P(x;\mu,\Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}}\exp\left\{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right\}$$

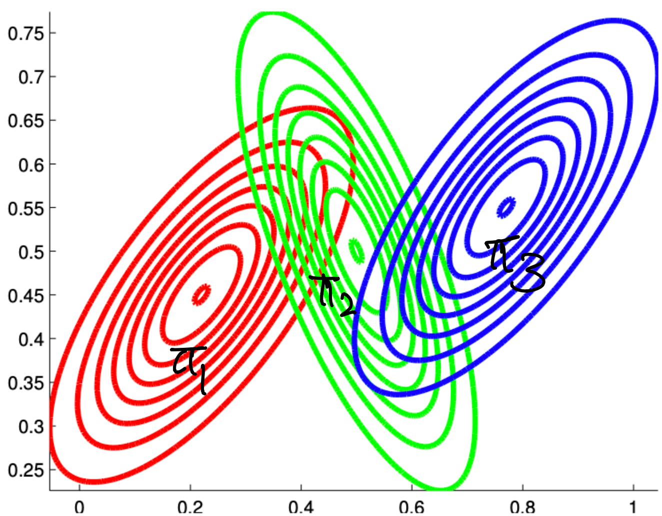
> Approximate unknown density with a mixture of Gaussians

$$P(x_j;\pi,\mu,\Sigma) =$$

(π_1, π_2, π_3) (μ_1, μ_2, μ_3) $(\Sigma_1, \Sigma_2, \Sigma_3)$

$$\pi_1 \, \mathbb{P}(x_j;\mu_1,\Sigma_1) + \pi_2 \, \mathbb{P}(x_j;\mu_2,\Sigma_2) + \pi_3 \, \mathbb{P}(x_j;\mu_3,\Sigma_3)$$

Mixture of 3 Gaussians



$$\sum_{i=1}^{k}\pi_i = 1$$

$$\pi_i \geq 0$$

Maximum likelihood solves clustering

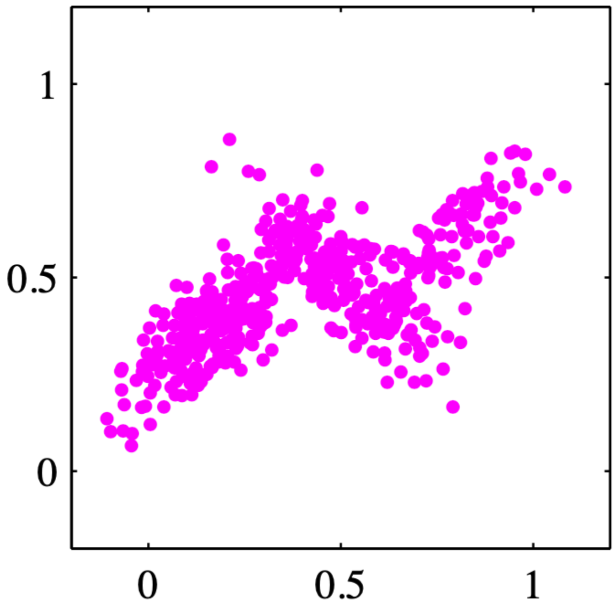
$$\max_{\pi,\mu,\Sigma} \sum_{j=1}^{n} \log P(x_j; (\pi, \mu, \Sigma))$$

→ π^*, μ^*, Σ^*

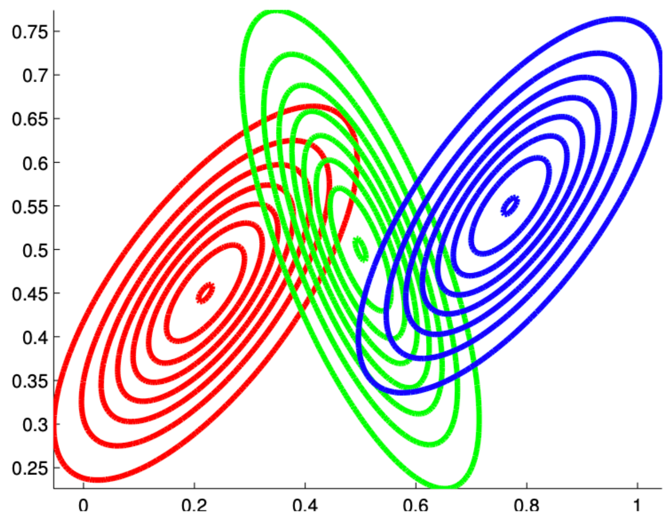
Algorithm

E-M (Expectation Maximization)

Our actual observations



Mixture of 3 Gaussians



Maximum likelihood solves clustering

$\mathbb{P}(z_j, x_j ; \pi, \mu, \Sigma)$

π, μ, Σ = parameters → $z_j \sim \pi$, $x_j \sim N(\mu_{z_j}, \Sigma_{z_j})$

To assign clusters, we define latent cluster indicator $z_j \in \{1, \ldots, k\}$

Suppose for just now that we have z_j (true cluster indicator), $\in \{1, 2, 3\}$

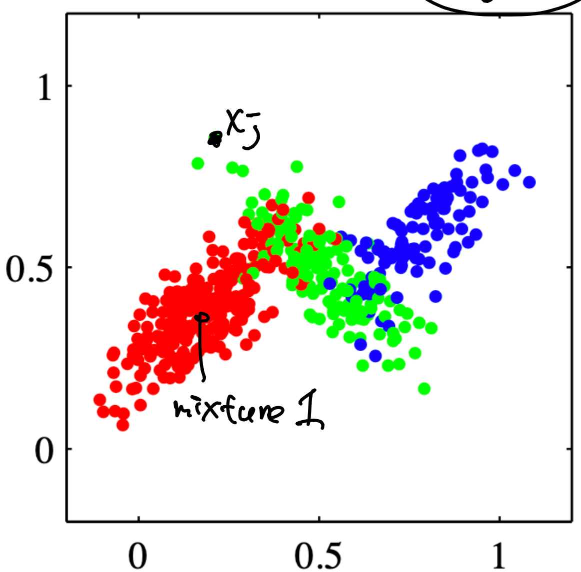
then we have $P(x_j; z_j, \pi^*, \mu^*, \Sigma^*) =$

$\pi_{z_j} \cdot \mathbb{P}(x_j ; \mu_{z_j}, \Sigma_{z_j})$

$z_j = 1$

$= \pi_1 \cdot \mathbb{P}(x_j ; \mu_1, \Sigma_1)$

$= \mathbb{P}(x_j, z_j = 1 ; \pi, \mu, \Sigma)$



Complete data labeled by true cluster assignments

We can now infer the clusters for each sample using this formula

$\mathbb{P}(x_j \mid z_j = 1 ; \pi, \mu, \Sigma)$

$= \mathbb{P}(x_j ; \mu_1, \Sigma_1)$

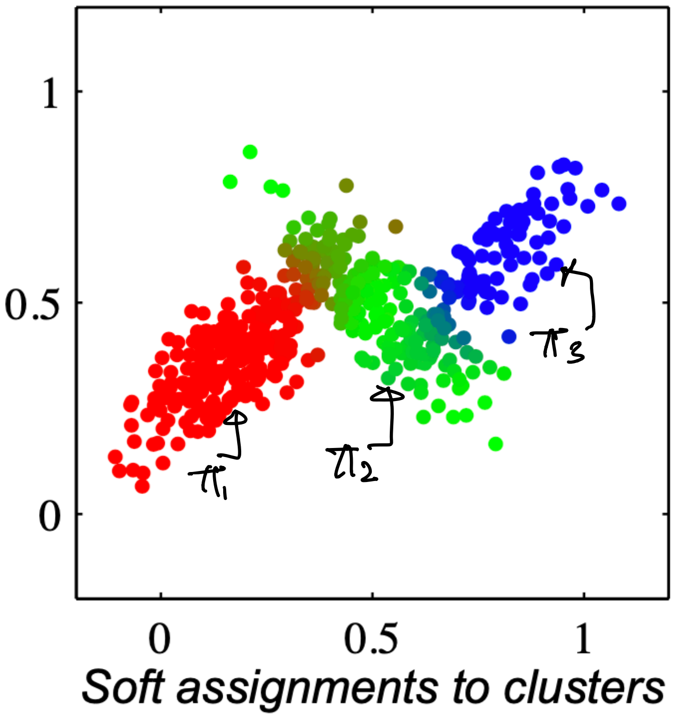
Maximum likelihood solves clustering

But in practice we do not know z_j's

but we can now infer the clusters, by computing the posterior probability on z_j's

① pick a cluster with prob. $(\pi_1, \pi_2, \pi_3) \to z_j$

② sample x_j from Gaussian from z_j-cluster.



$$r_{ji} = P(\text{sample j belongs to cluster i})$$

$$= P(z_j = i \,|\, x_j; \pi, \mu, \Sigma)$$

$$= \frac{\pi_i P(x_j; \mu_i, \Sigma_i)}{\sum_{i'} \pi_{i'} P(x_j; \mu_{i'}, \Sigma_{i'})}$$

find π^*, μ^*, Σ^* depends on initialization

Recap: Mixture of Gaussians for clustering

Given a set of samples

1. Fit a mixture of Gaussian model with maximum likelihood
2. Use posterior assignment probability for soft clustering

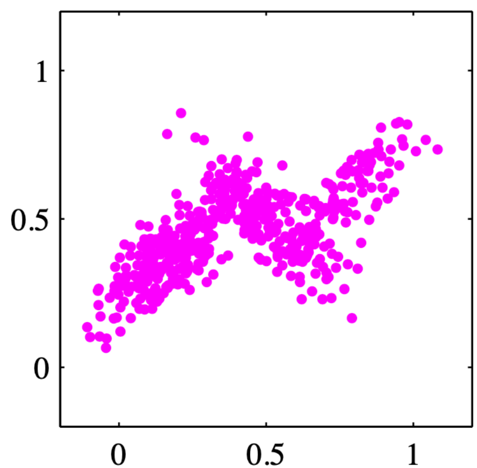
k-means → hard clustering $r_i = [1, 0, 0]$ → cluster 1

G.M. → soft clustering → $r_i = [1/3, 1/2, 1/6]$

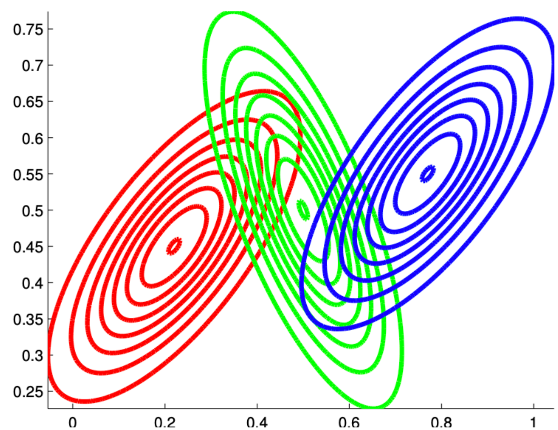
Thresholding → hard

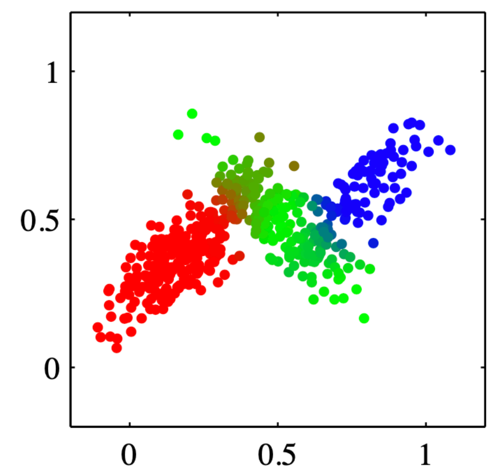
this can handle overlapping clusters, and clusters of various (oval) shapes and not just circles

Our actual observations



Mixture of 3 Gaussians





Soft assignments to clusters

Questions?