CS 189/289

Today's lecture outline

1. Clustering (k-means, mixture of Gaussians)

Recall, Unsupervised learning

- Seen *supervised learning*, $\{(x_i, y_i)\}$ for $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$ or $y \in \mathbb{Z}$.
- Much ML is focused on modeling $\{x_i\}$, *unsupervised learning*, which includes:

i. Dimensionality reduction, $z \in \mathbb{R}^m = f_\theta(x)$, $m \ll d$.

ii. Clustering, $z \in \mathbb{Z} = f_\theta(x)$.

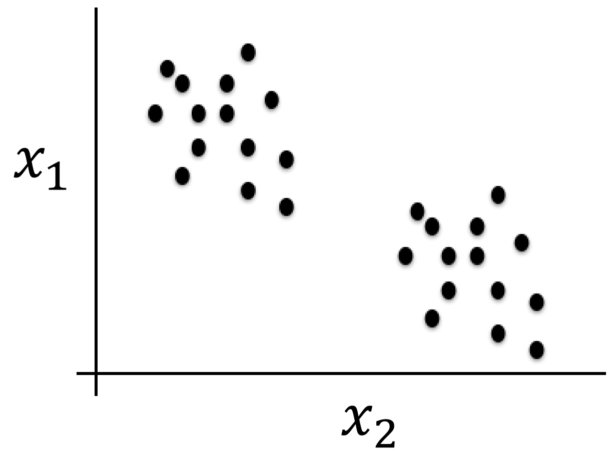
iii. Representation learning, $z \in \mathbb{R}^m$, $z = f_\theta(x)$, or $z \sim p_\theta(x)$.

iv. Density estimation, evaluate $p_\theta(x)$.

v. "Generative" modeling, $x \sim p_\theta(x)$

The main idea of *clustering* $\{x_i\}$

Suppose we had only input features, and no class labels:



We may want to infer/assign discrete "class labels" from the data, based on the structure in the input space.

https://www.quora.com/What-is-the-difference-between-Clustering-and-Classification-in-Machine-Learning

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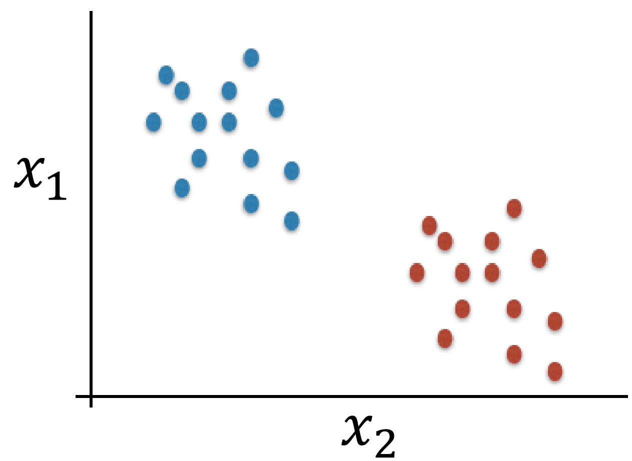

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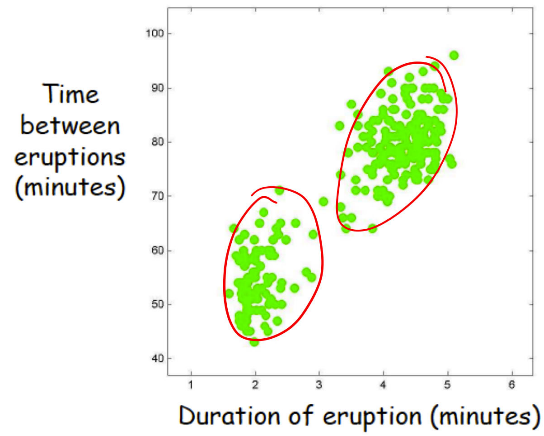
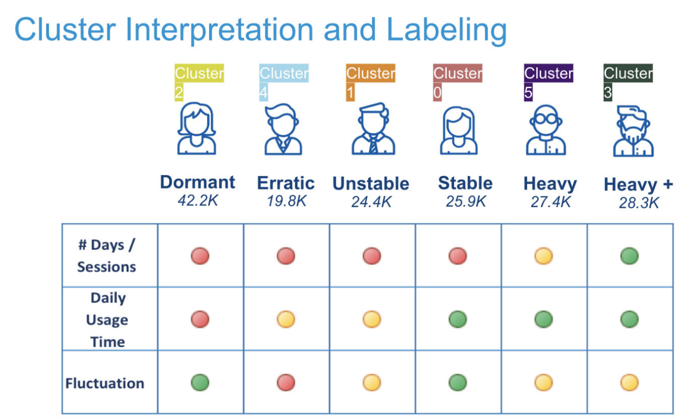
Clustering for data exploration

e.g. find hidden subgroups:

- Types of customers in a database from customer activities.
- Subtypes of disease for therapeutics.
- Types of cells in a tissue from single cell data.
- Ancestry groups from genetic data.
- Finding topics in on-line documents.
- etc.

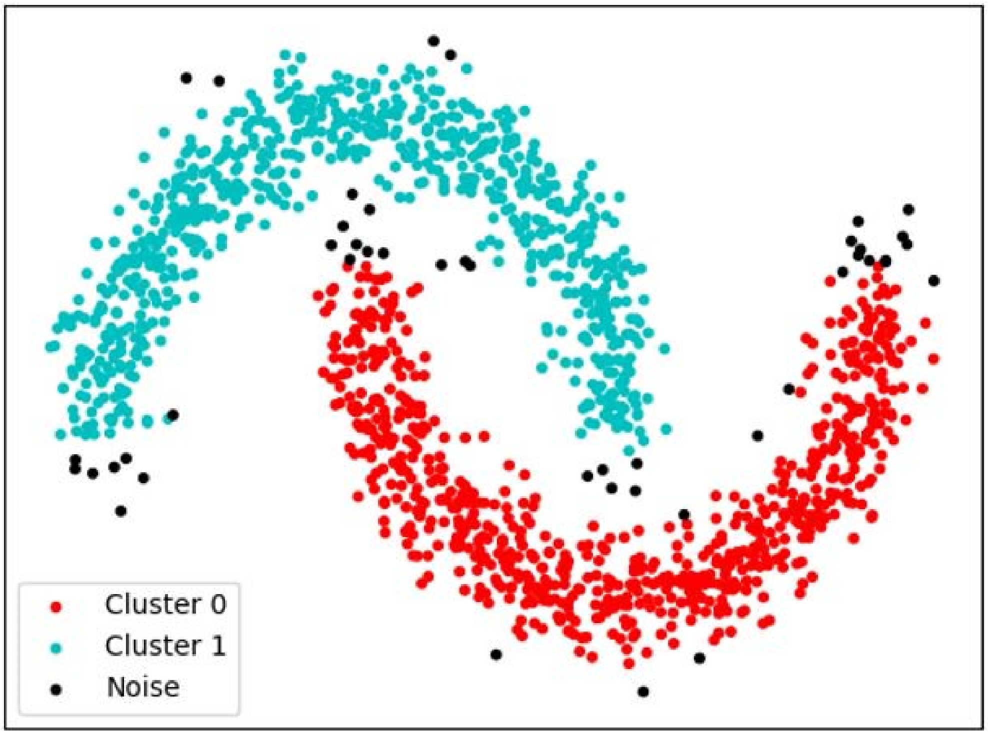




https://medium.com/@sygong/k-means-clustering-for-customer-segmentations-a-practical-real-world-example-196a10323b9f

Bishop book on Pattern recognition

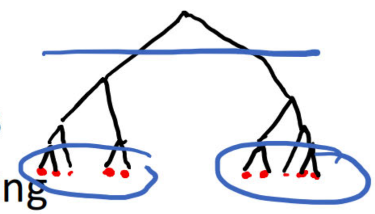
Clustering for outlier detection



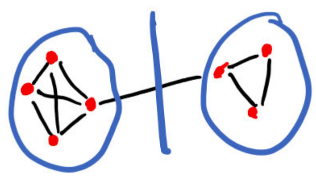
https://www.imperva.com/blog/2017/07/clustering-and-dimensionality-reduction-understanding-the-magic-behind-machine-learning/

Three broad approaches to clustering

- Hierarchical clustering
  - Build a tree (bottom-up or top-down), representing distances among data points
  - **Example**: single-, average- linkage clustering



- Partitional approaches
  - Define and optimize a notion of "cost" defined over partitions
  - **Example**: Spectral clustering, graph-cut based approaches

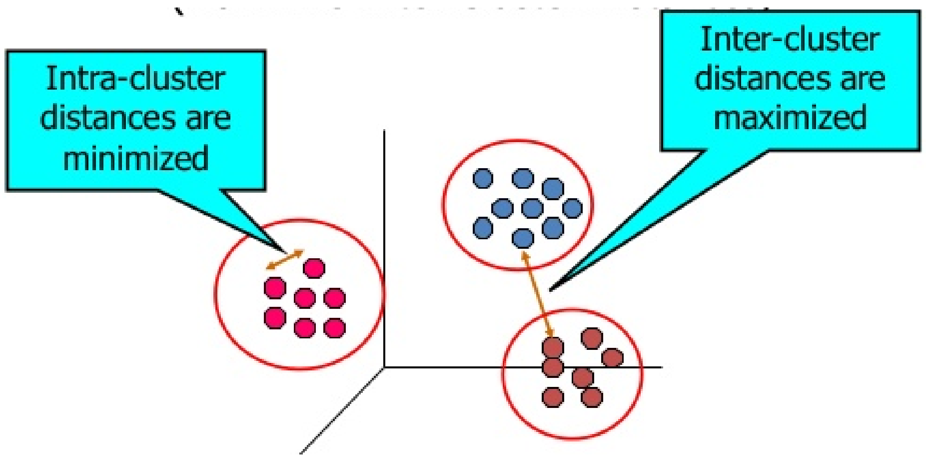


- Model-based approaches
  - Maintain cluster "models" and infer cluster membership (e.g., assign each point to closest center)
  - **Example**: k-means, Gaussian mixture models, …

[slide from Andrea Krause]

Main desiderata of clustering

1. Want high intra-cluster similarity.
2. Want low inter-cluster similarity.



3. Similarity/distance is in the eye of the beholder!

https://www.slideshare.net/NontawatB/08-clustering

Aside: distances, metrics and similarities.

- “want points to be similar/dissimilar”
- “want distance to be minimized/maximized”.

Properties of a distance function (metric):

Aside: distances, metrics and similarities.

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Properties of a distance function (metric):

1. $j = k$ iff $d(j, k) = 0$.
2. $j \neq k$ iff $d(j, k) > 0$.
3. *symmetry,* $d(j, k) = d(k, j)$ *(why KL-divergence is not a distance)*
4. *triangle inequality,* $d(i, j) + d(i, k) \geq d(j, k)$

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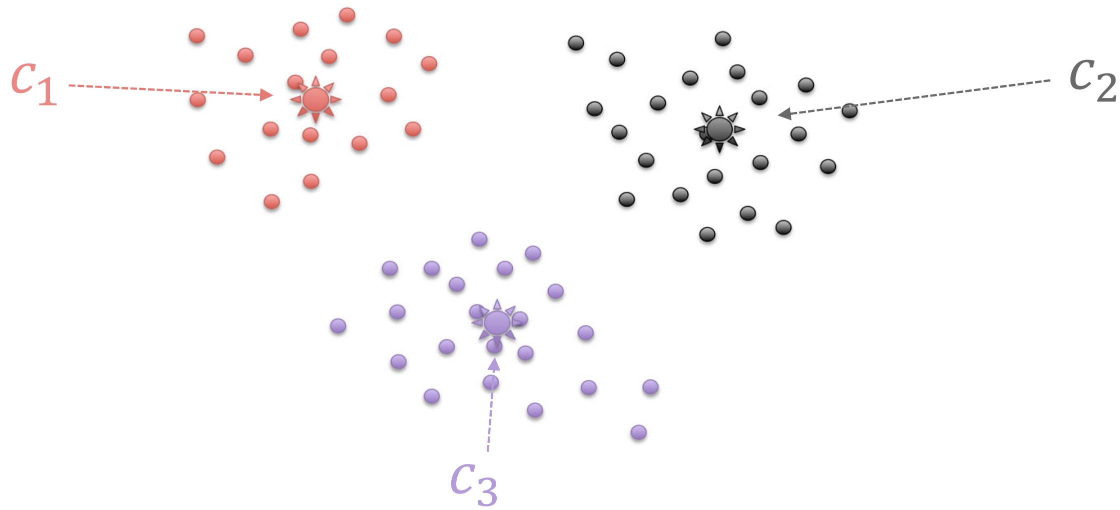
dissimilarity: *satisfies at least 1,2, and 3 above*

similarity: *complement of dissimilarity:*

$$similarity(j,k) = 1 - dissimilarity(j,k)$$

Centroid-based clustering

- Each cluster is represented by a point in the input space--a centroid--though not necessarily in the training data), $c_k \in R^d$ (for $X \in R^d$).

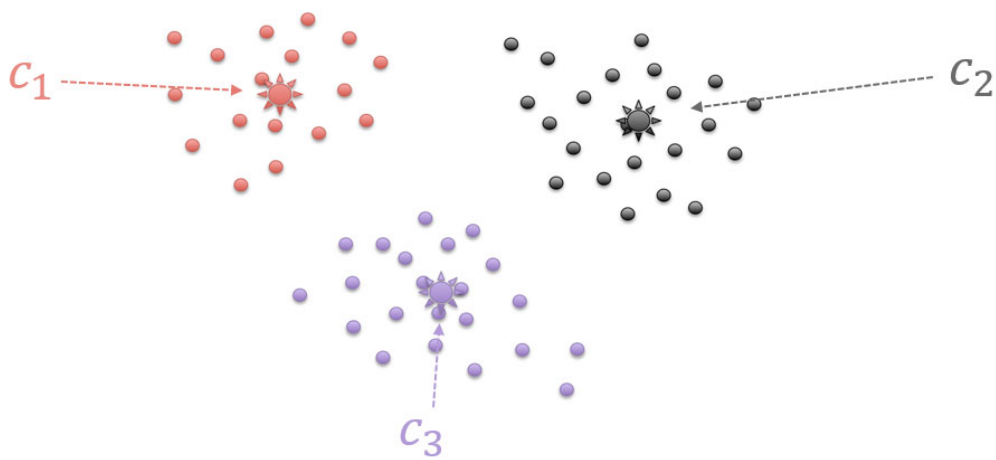


- "K-means" is the most common centroid-based approach.

Portions of some slides courtesy of Yisong Yue at Caltech.

K-means clustering

- Parameters are $\{c_k\}$.
- Chosen such that:
  - the distance of each point, x_i, to its assigned centroid, is minimized.



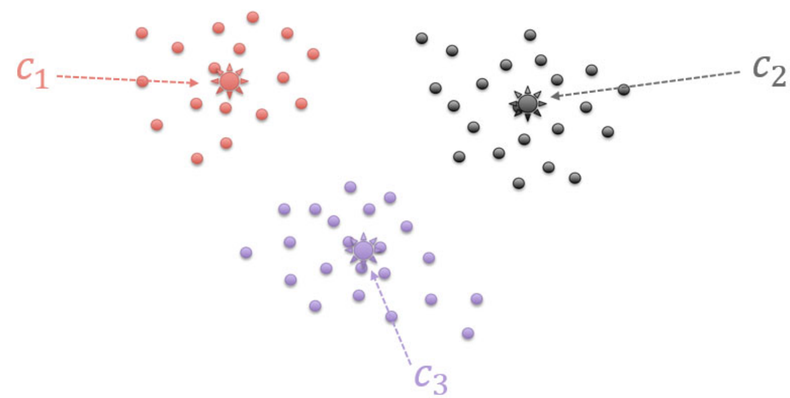
Formally: K-means clustering

- Training data, $X = \{x_i\}_{i=1}^{n}, x_i \in R^d$.
- Parameters are $\{c_k \in R^d\}$.
- A cluster partition, $C_1 \cup C_2 \cup \cdots C_K$, wherein every $\boldsymbol{x_i}$ is assigned to one (and only one) of the K clusters.
- Optimization problem:

$$\underset{S=C_1\cup\ldots\cup C_K,\ \{c_1,\ldots,c_K\}}{\operatorname{argmin}} \sum_{k} \sum_{x\in C_k} \left\| x - c_k \right\|^2$$

cluster partition

cluster centroids



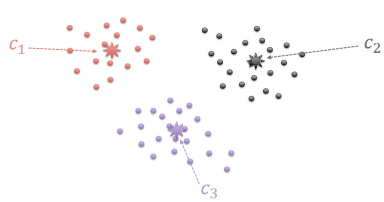
Parameter learning in K-means

- Suppose we knew $C_1 \cup C_2 \cup \cdots C_K$ how could we find $\{c_k\}$?
- The optimization problem would reduce to:

$$\hat{c}_k = \underset{c_k}{\operatorname{argmin}} \sum_{x \in C_k} \|x - c_k\|^2$$

- For which one can show that the answer is $\hat{c}_k = \frac{1}{N} \sum_{x \in C_k} x$

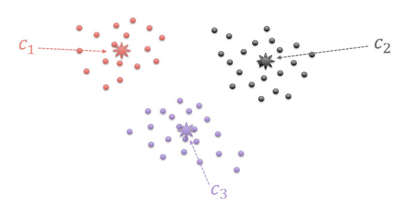
$$\underset{S = C_1 \cup \ldots \cup C_K,\ \{c_1, \ldots, c_K\}}{\operatorname{argmin}} \sum_k \sum_{x \in C_k} \|x - c_k\|^2$$



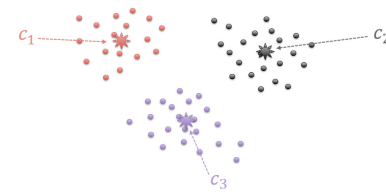
Other way around (parameter learning)

- Suppose we knew $\{c_k\}$, how could we find $C_1 \cup C_2 \cup \cdots C_K$?
- Answer: choose the cluster which is closest to each point, $z_i \equiv \underset{k}{\operatorname{argmin}} \|x_i - c_k\|^2$, and then $\hat{C}_k = \{x_i | z_i = k\}$.

$$\underset{S=C_1\cup\ldots\cup C_K,\ \{c_1,\ldots,c_K\}}{\operatorname{argmin}} \sum_k \sum_{x\in C_k} \|x - c_k\|^2$$



The K-Means algorithm



$$\underset{S=C_1\cup\ldots\cup C_K,\ \{c_1,\ldots,c_K\}}{\operatorname{argmin}} \sum_{k} \sum_{x\in C_k} \left\|x-c_k\right\|^2$$

1. Initialize the cluster centers, $\{c_k\}$

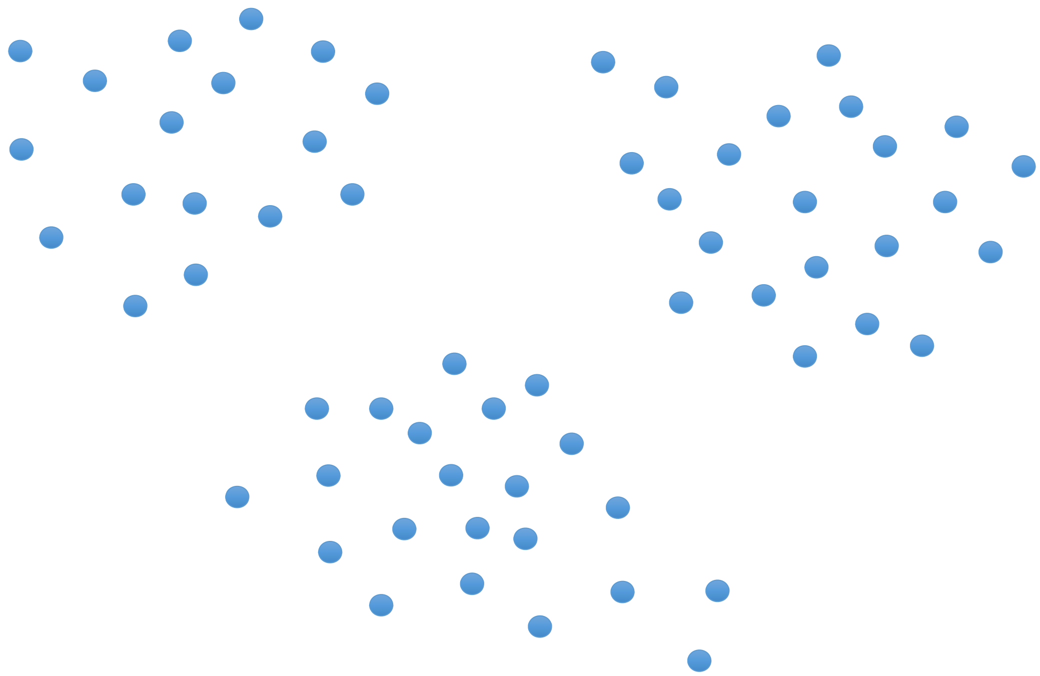
   (e.g., pick k points at random from your training data).

2. Repeat until convergence:
   i. Compute partition $C_1 \cup C_2 \cup \cdots C_K$, given the $\{c_k\}$.
   ii. Compute centers $\{c_k\}$, given $C_1 \cup C_2 \cup \cdots C_K$.

Does this converge?

- Yes: at each step, we are reducing the objective function or have converged.
- If assignments do not change, we have a local min.

The K-Means algorithm



[slide courtesy Yisong Yue]

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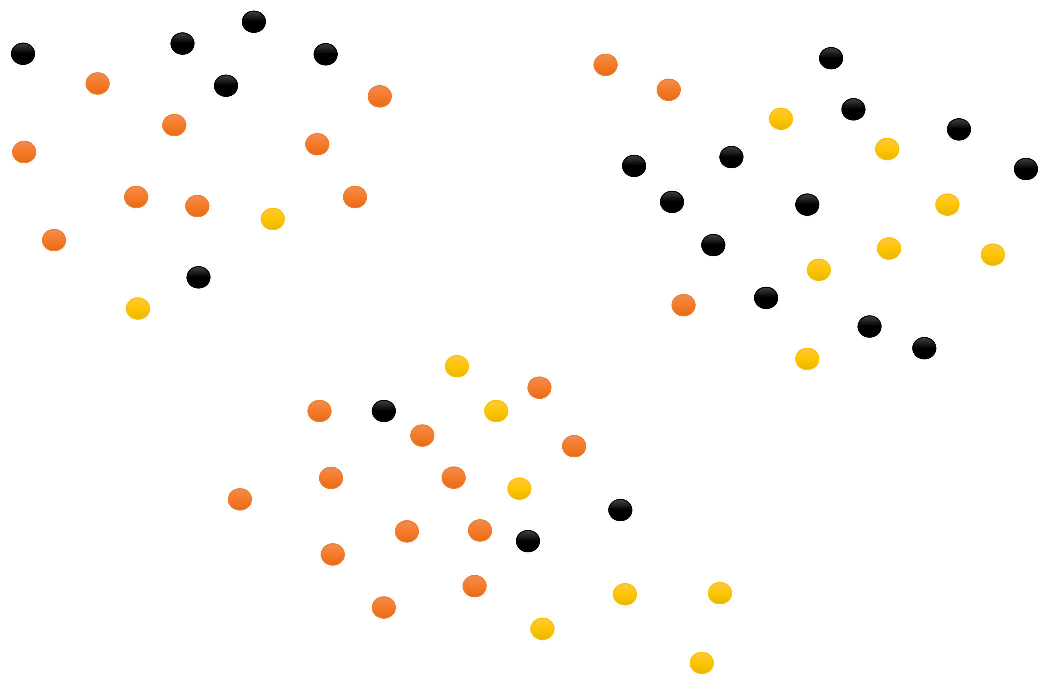

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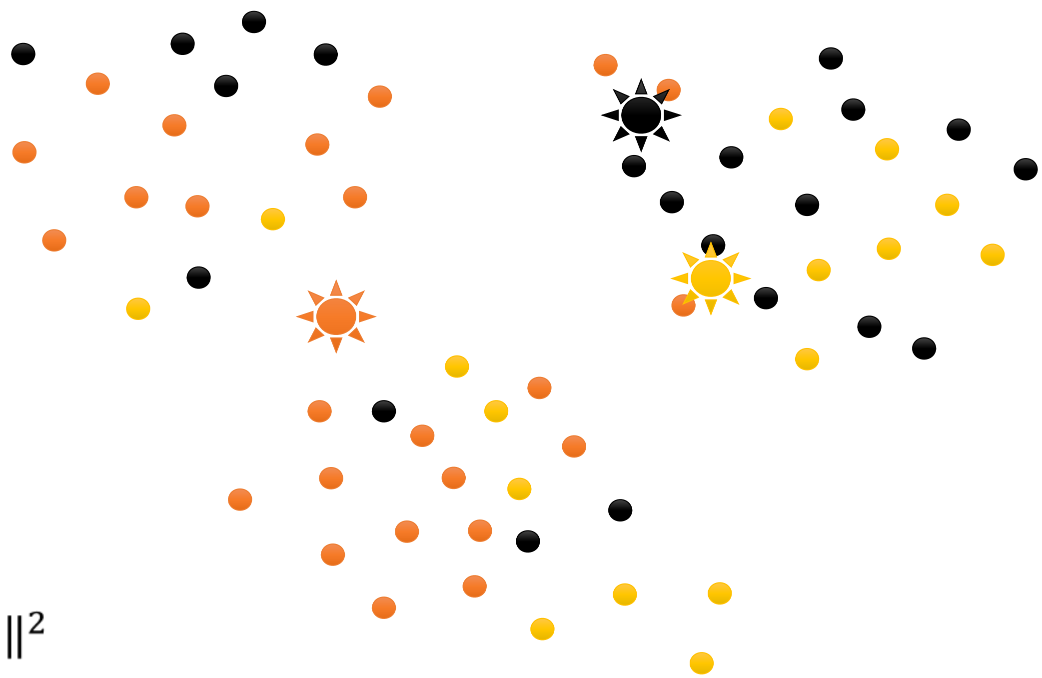

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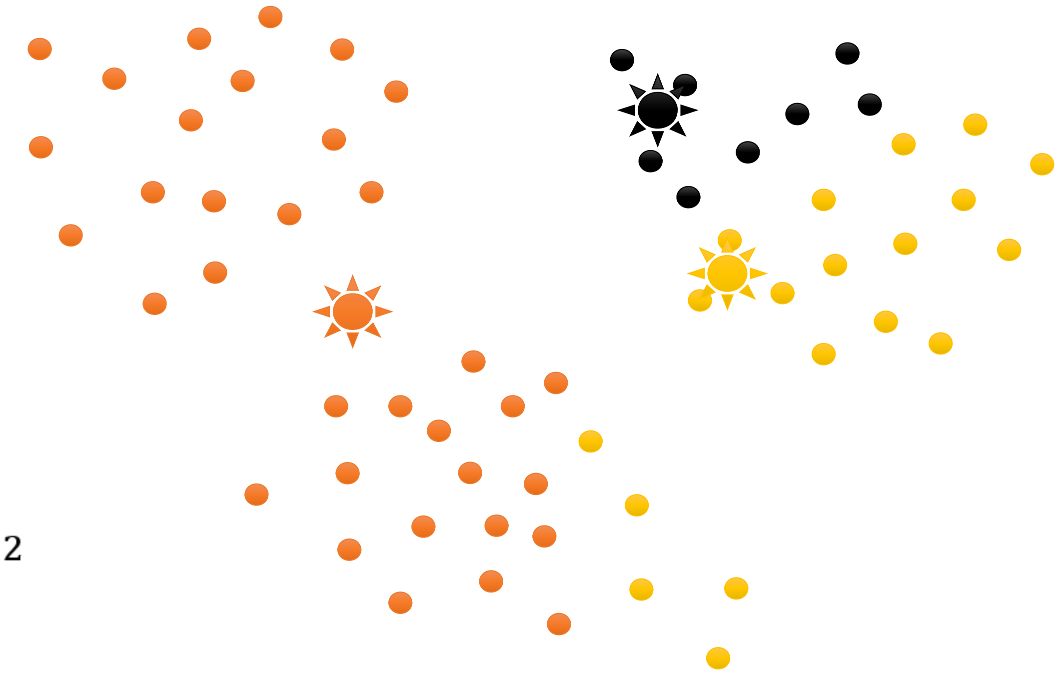

$$z_i \equiv \underset{k}{\operatorname{argmin}} \|x_i - c_k\|^2$$
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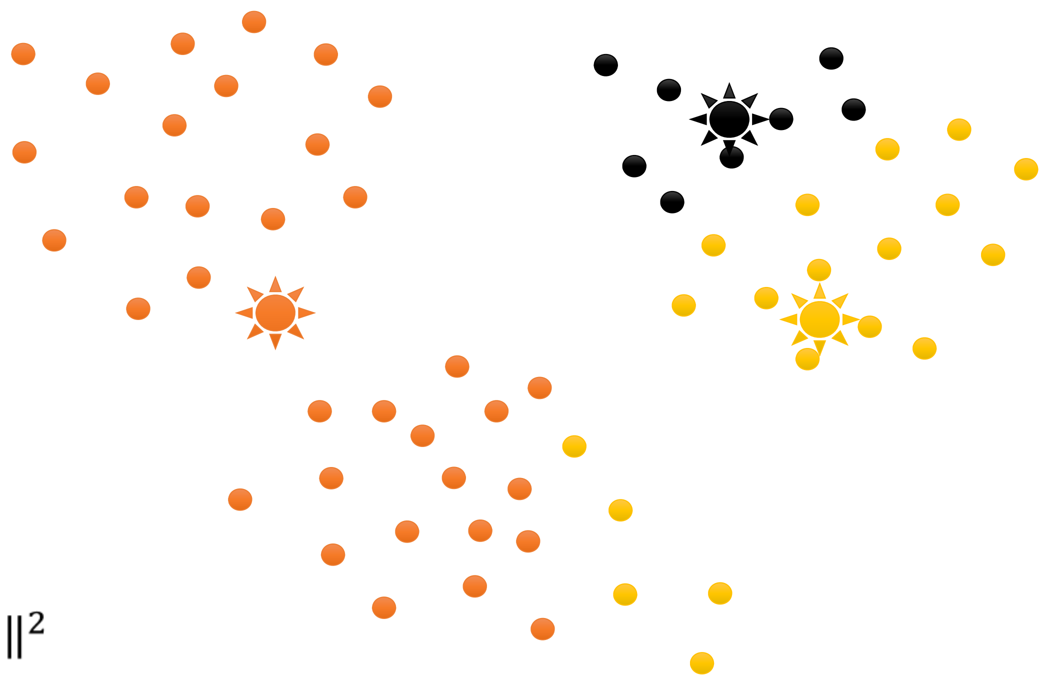

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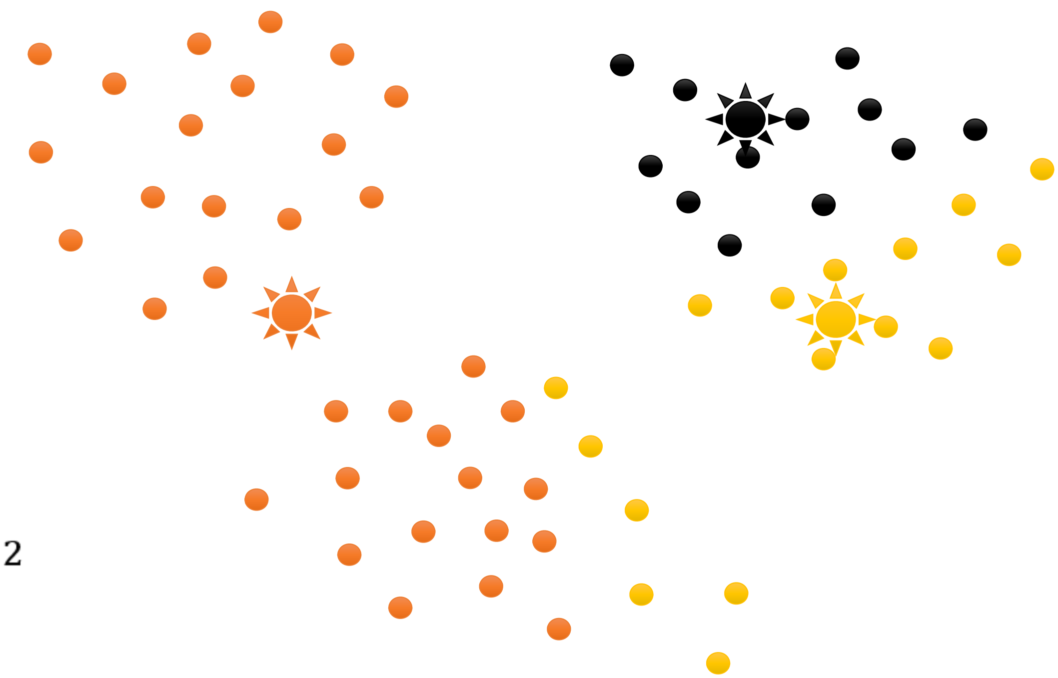

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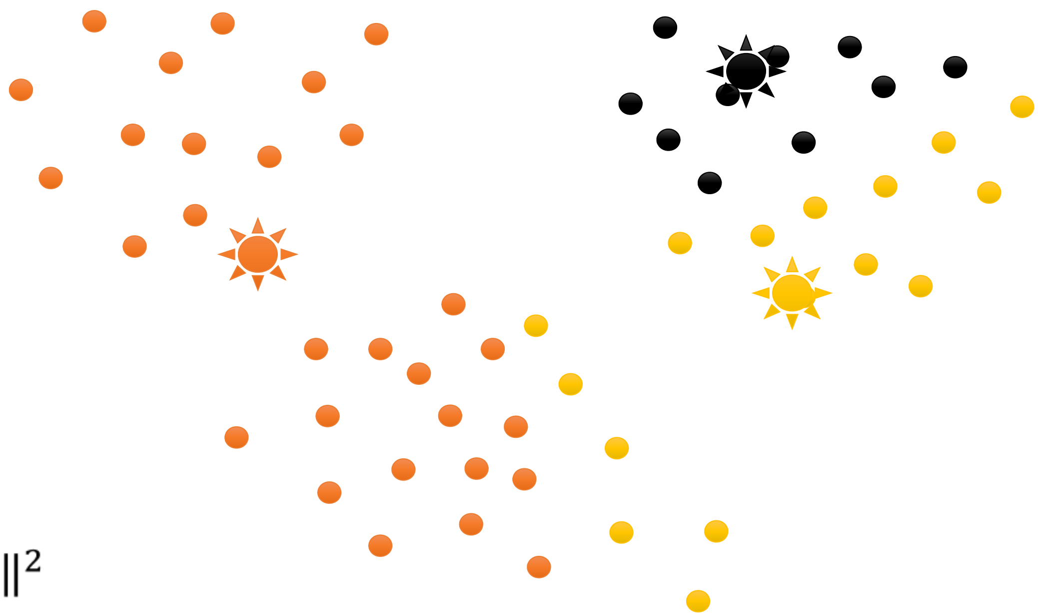

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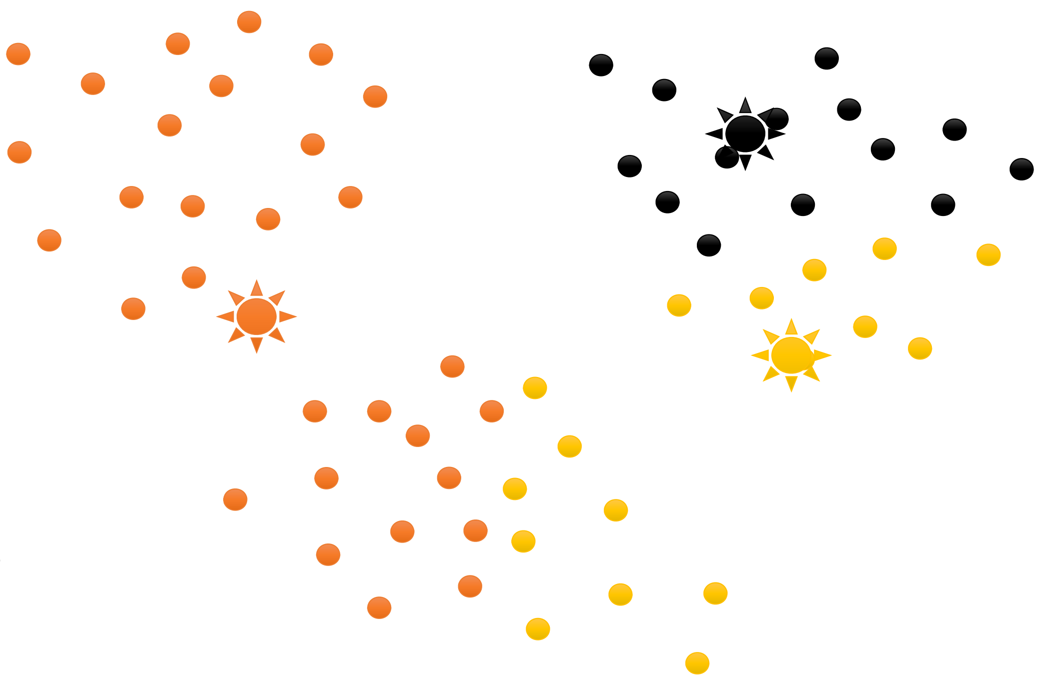

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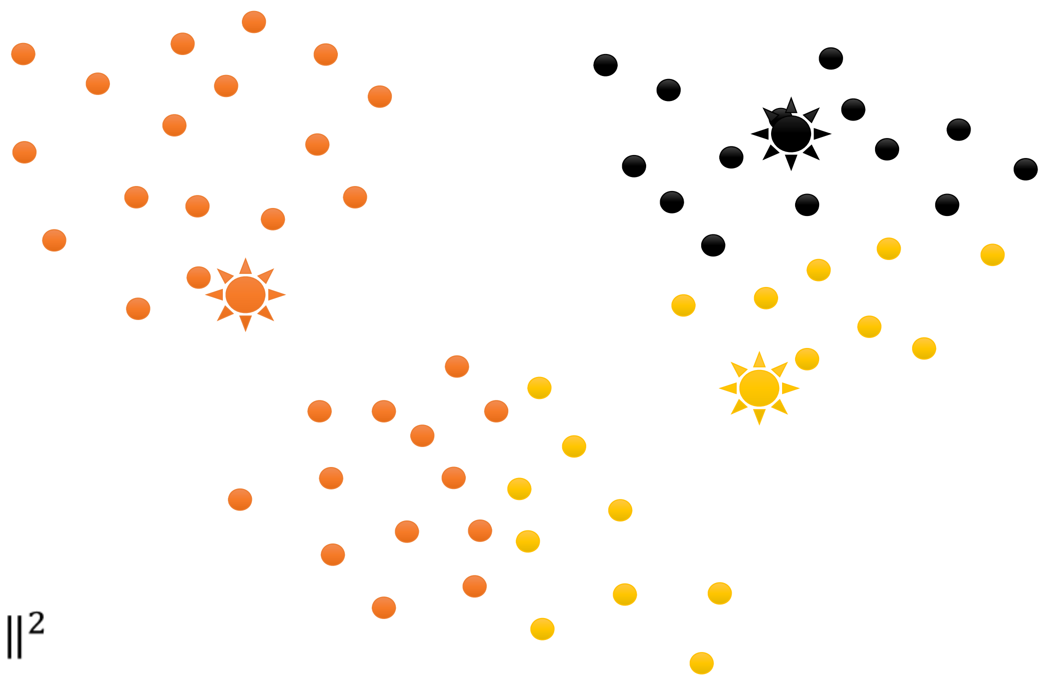

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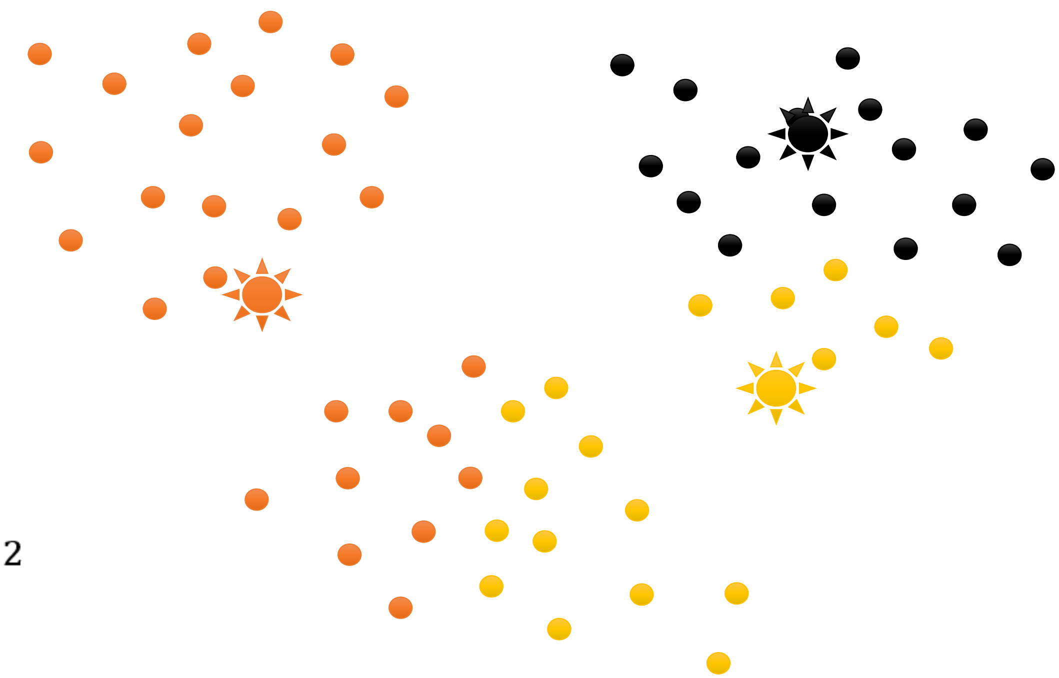

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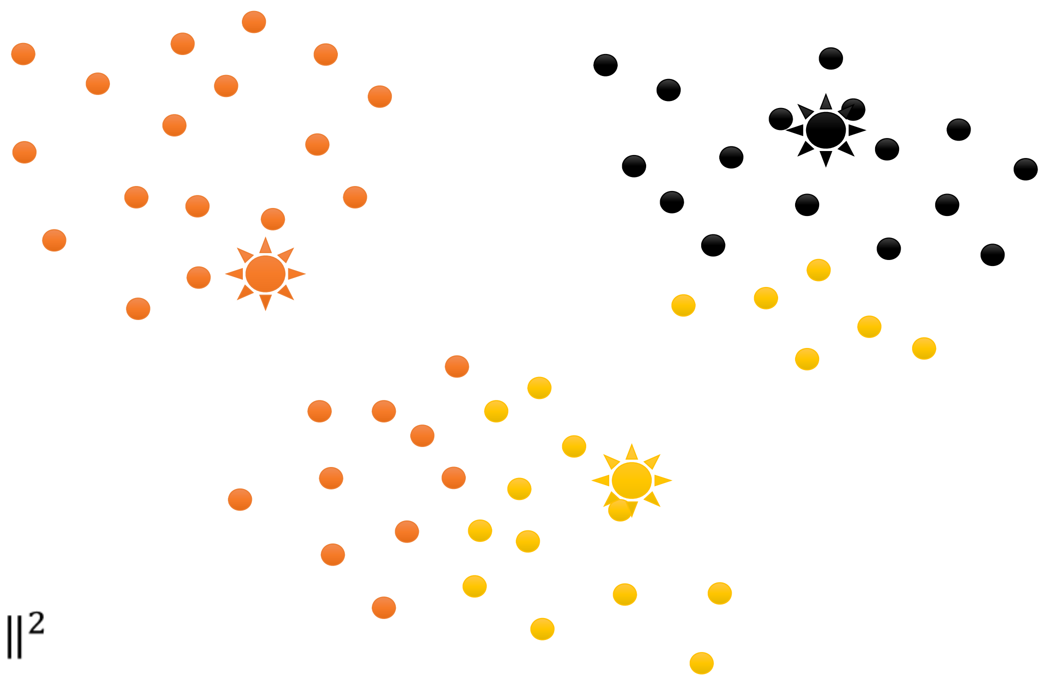

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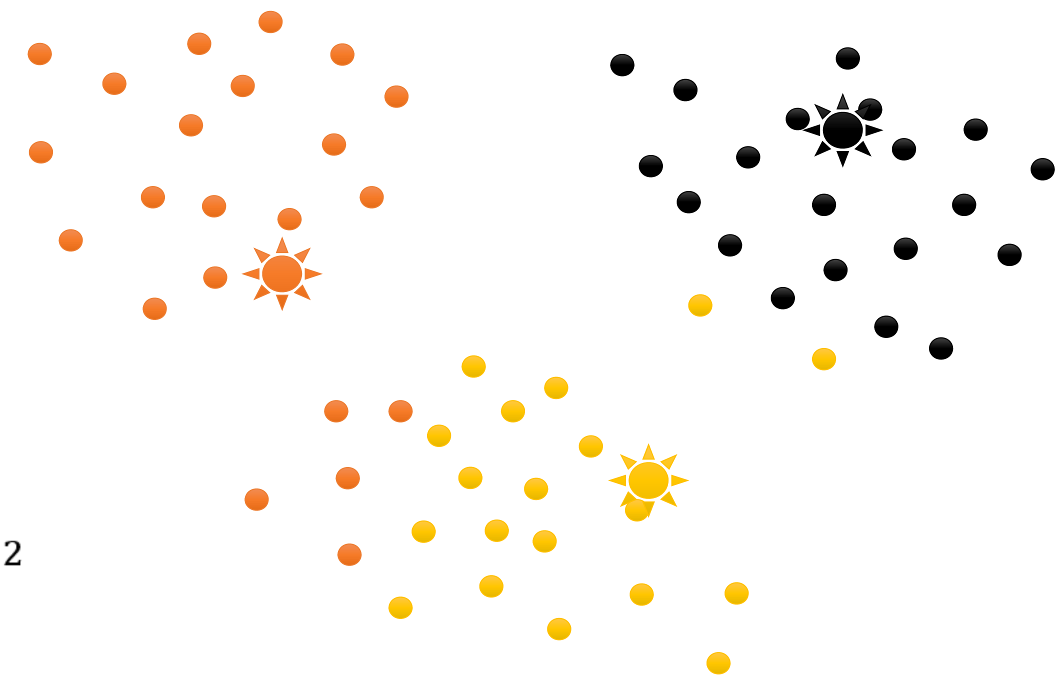

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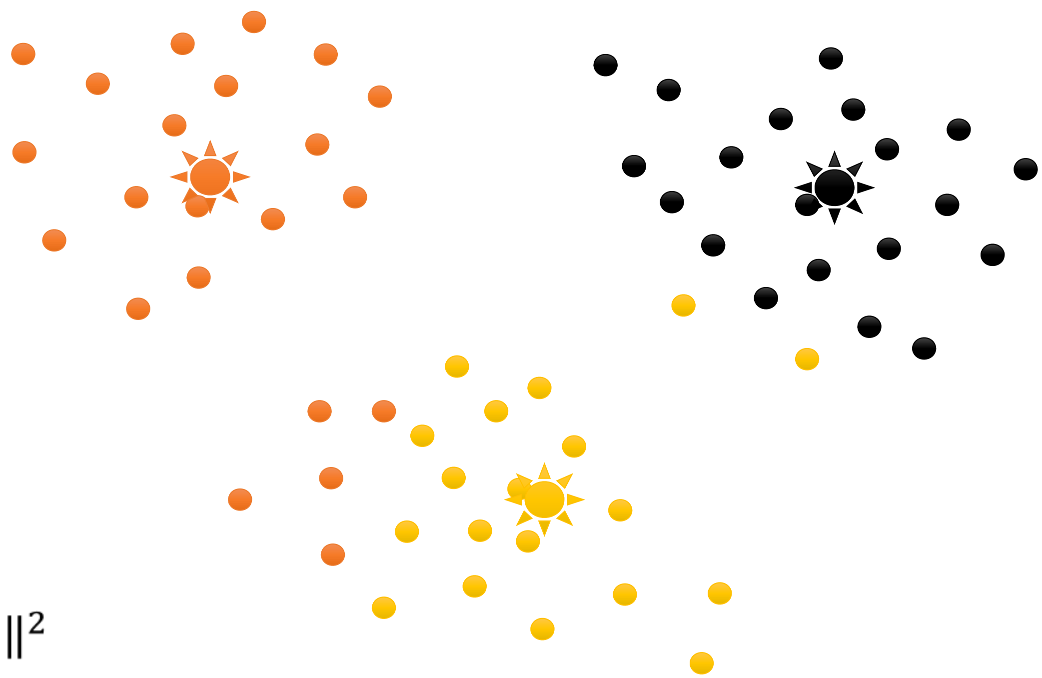

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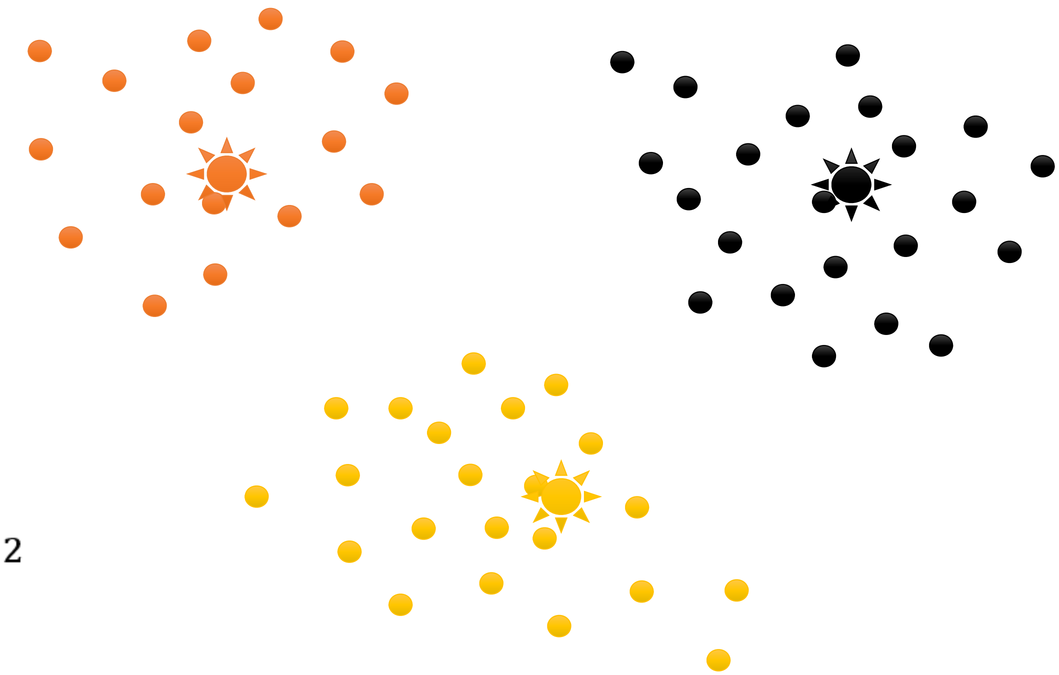

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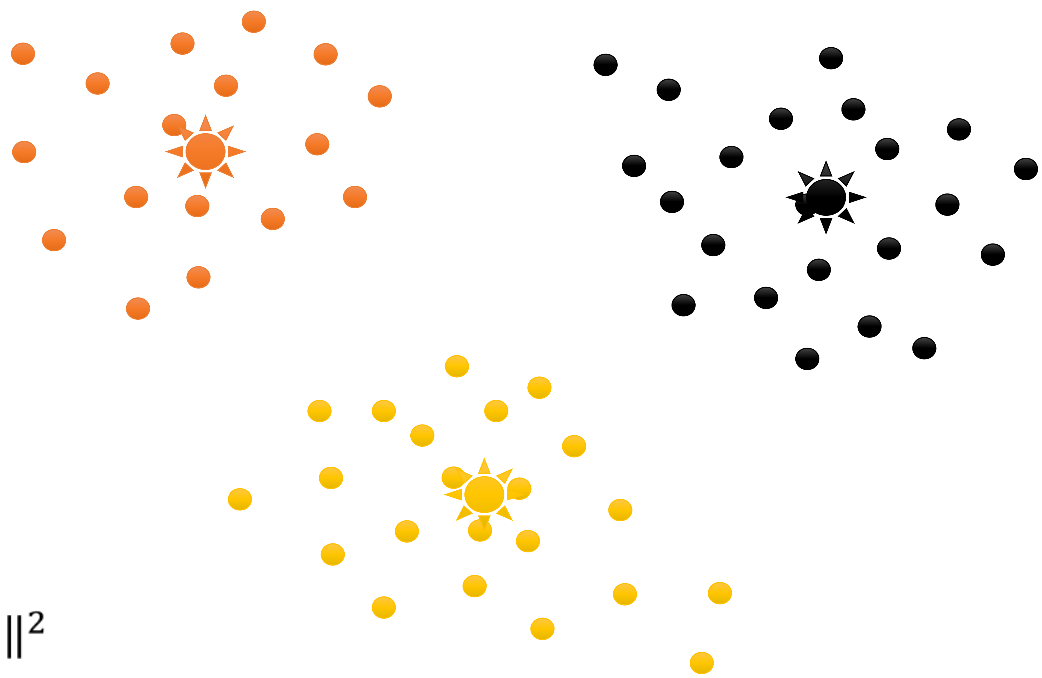


$$\hat{c}_k = \underset{c_k}{\operatorname{argmin}} \sum_{x \in C_k} \|x - c_k\|^2$$

[slide courtesy Yisong Yue]

Could we also use gradient descent?

$$loss = L(\{c_k, C_k\}) = \sum_k \sum_{x \in C_k} \|x - c_k\|^2$$

$$\Rightarrow L(\{c_k\}) = \sum_i \min_k \|x_i - c_k\|^2$$

Let r_i be the closest centroid to x_i.

$$\Rightarrow \nabla_{c_k} L(\{c_k\}) = -2(x_i - c_k)[r_i = k]$$

- No more discrete variables, can use gradient descent!
- Is this a sleight of hand? Where is the discreteness?

[Bottou & Bengio NIPS 1995]

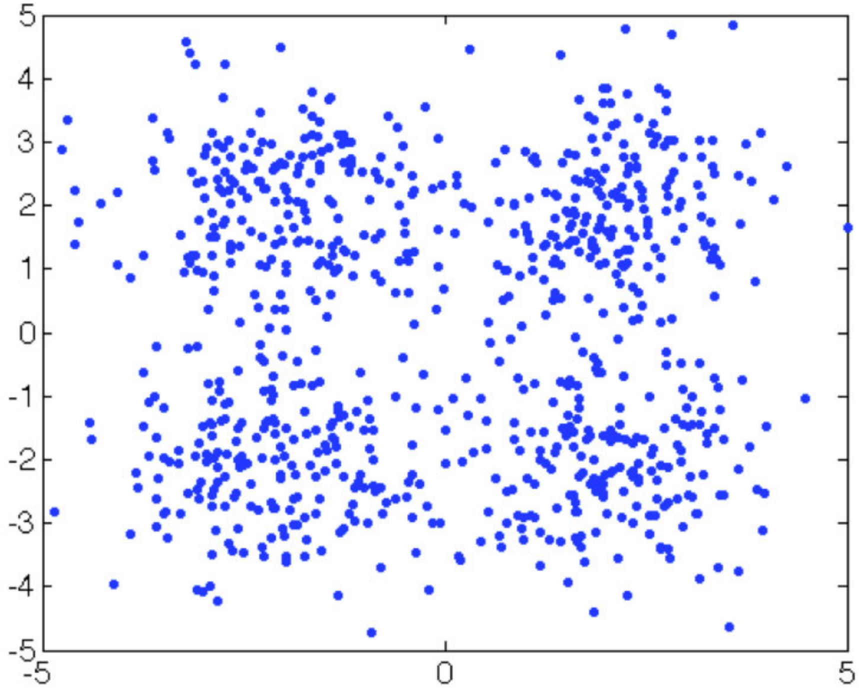
Aside: gradient of min function:

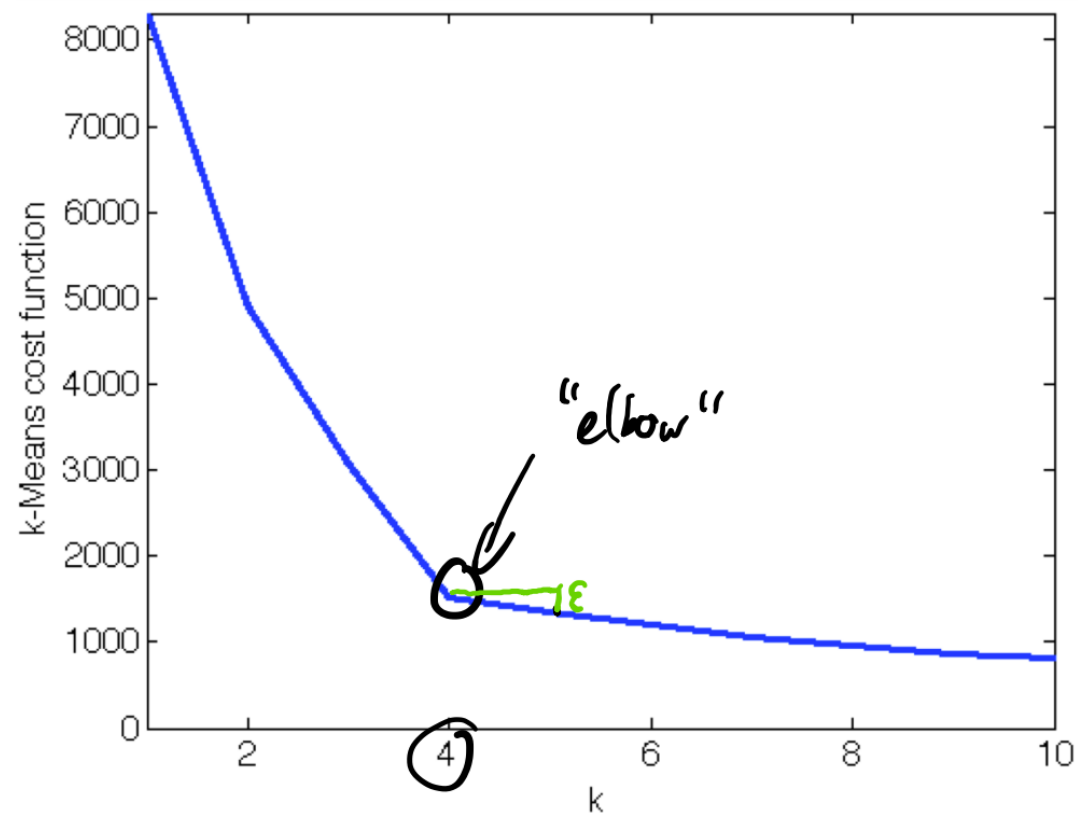
$$f(x, y) = \min(x, y) = \begin{cases} x & \text{if } x \leq y \\ y & \text{if } x > y \end{cases}$$

$$\frac{\partial f(x, y)}{\partial x} = \begin{cases} 1 & \text{if } x < y \\ 0 & \text{if } x > y \end{cases}$$

$$\frac{\partial f(x, y)}{\partial y} = \begin{cases} 0 & \text{if } x < y \\ 1 & \text{if } x > y \end{cases}$$

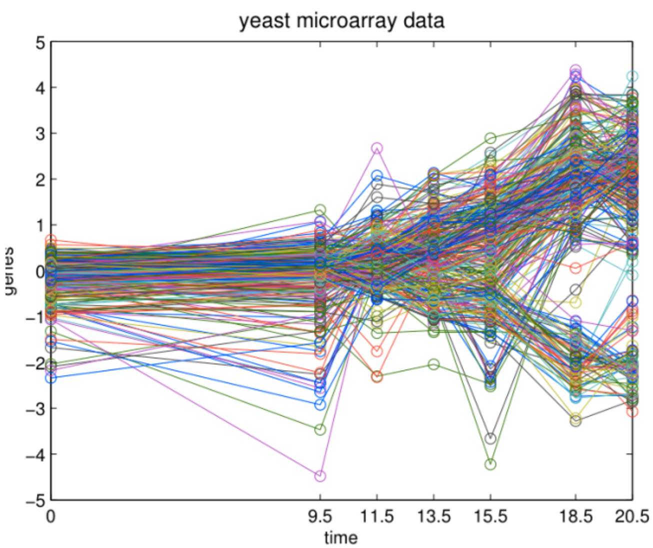
How to find good # of clusters?

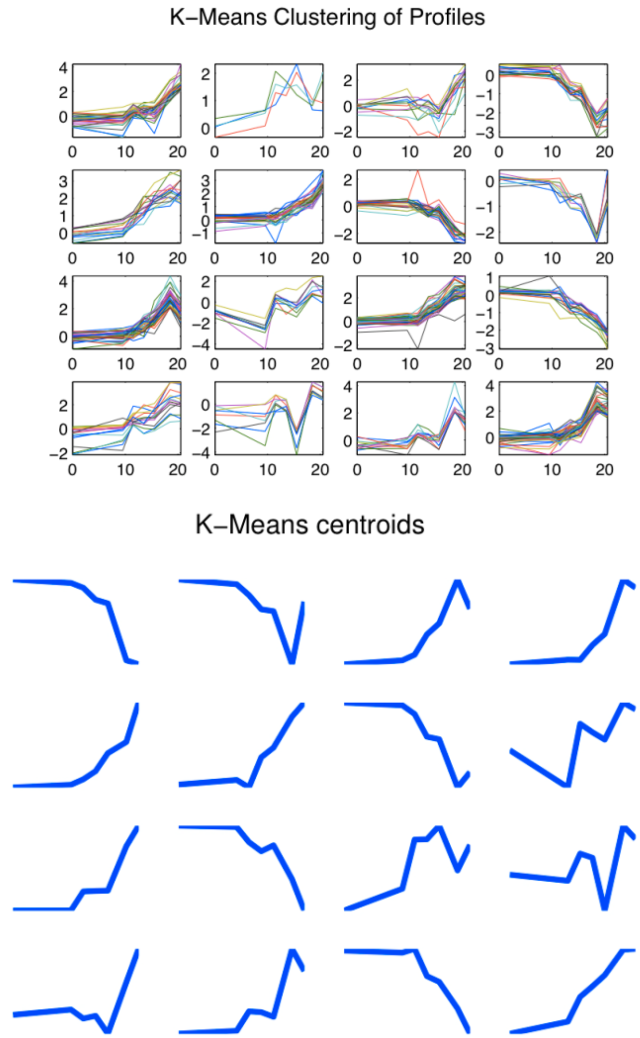




[slide from Andrea Krause]

Application of K-Means Clustering

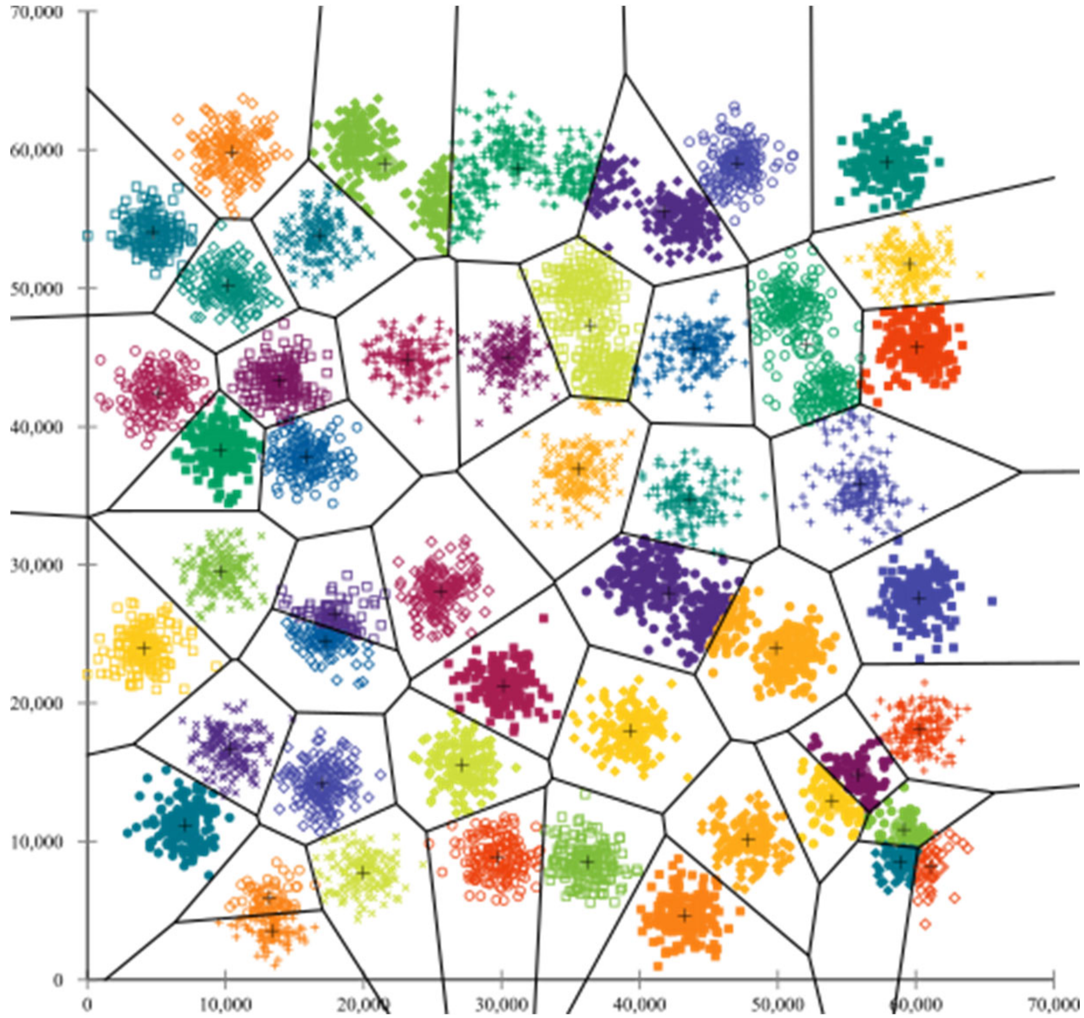




clustering yeast genes by their "gene expression" measurements over time

http://www.cs.toronto.edu/~urtasun/courses/CSC2515/CSC2515_Winter15.html

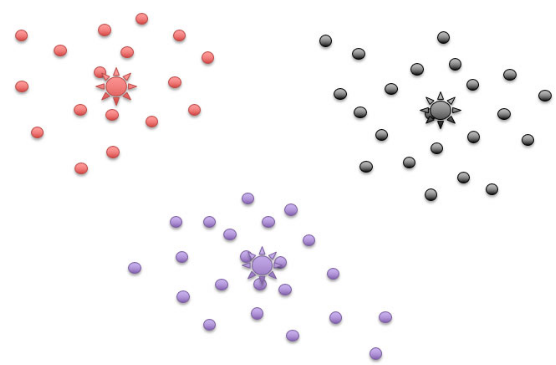
Example of bad local minimum in K-means



https://stats.stackexchange.com/questions/133656/how-to-understand-the-drawbacks-of-k-means

More on clustering desiderata

So far we have mentioned:



1. Want high intra-cluster similarity.
2. Want low inter-cluster similarity.

Can you think of any others?

- May want invariances to rotation and or scaling of $\{x_i\}$.
- If clustering depends only on distance/similarity, then whatever invariances these have, the clustering will also have.

Aside: Kleinberg's Impossibility Theorem for Clustering

Three (more) clustering desiderata of which provably, one **can achieve only two at a time for a given clustering algorithm**:

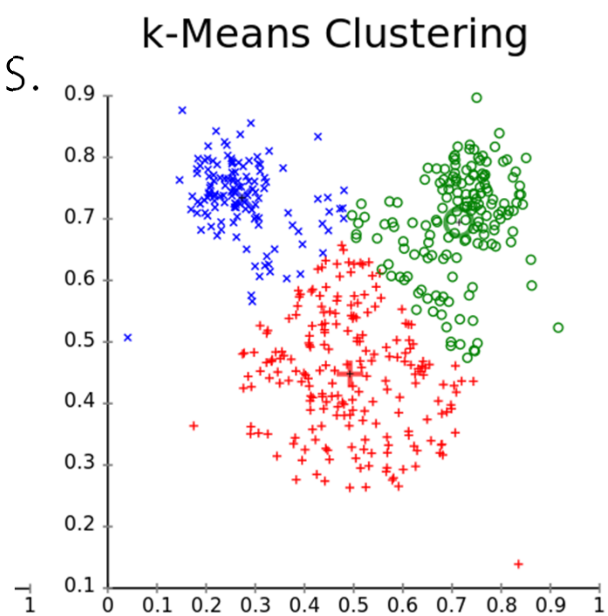
1. **Scale-Invariance** (if stretch the data out ($\tilde{d}(j,k) = c \times d(j,k)$), then clustering should stay the same).
2. **Consistency** (if stretch data such that distance within cluster only gets smaller, and between clusters only gets bigger, then clustering should stay the same).
3. **Richness** (clustering function should be able to produce any arbitrary partition/clustering of data points).

[NIPS 2002]

Lets revisit K-means—any weaknesses?

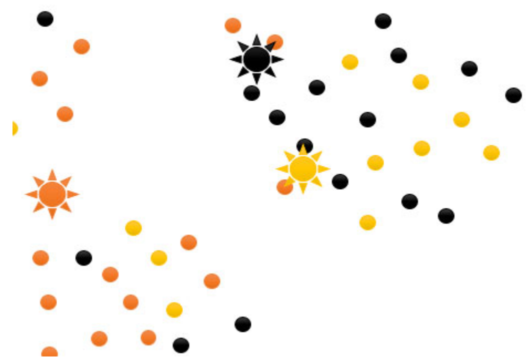
$$\underset{S=C_1\cup\ldots\cup C_K,\ \{c_1,\ldots,c_K\}}{\operatorname{argmin}} \sum_k \sum_{x\in C_k} \left\| x - c_k \right\|^2$$

1. No likelihood, so hard to understand assumptions.
2. e.g. implicitly corresponds to clusters with "spherical" shape because each feature is treated equally.
3. Each step in the optimization has a "hard" assignment which means that can't have any uncertainty as to which point belongs to which cluster.



Lets develop a "soft" K-means algorithm

- Previously: $z_i \equiv \underset{k}{\mathbf{argmin}} \|x_i - c_k\|^2$, and then $\hat{C}_k = \{x_i | z_i = k\}$.
- Convert to max, $z_i = \underset{k}{\mathbf{argmax}}\, \mathbf{exp}(-\|x_i - c_k\|^2)$.
- Let $v_{ik} \equiv \mathbf{exp}\left(-\|x_i - c_k\|^2\right)$ so that $z_i = \underset{k}{\mathbf{argmax}}\ \{v_{ik}\}$.
- Now normalize the $\{v_{ik}\}$ so that $r_{ik} \equiv \frac{v_{ik}}{\sum_k v_{ik}}$
- Use r_{ik} as the soft/probabilistic cluster assignments.
- This is just the familiar softmax:
- $r_{ik} = \frac{\mathbf{exp}[v_{ik}]}{\sum_j \mathbf{exp}[v_{ij}]} = softmax\left(\{v_{ij}\}\right)[k]$
- $r_{ik} \equiv \frac{\mathbf{exp}[\beta v_{ik}]}{\sum_j \mathbf{exp}[\beta v_{ij}]} = softmax\left(\{\beta v_{ij}\}\right)[k]$



Consider a "soft" K-means algorithm

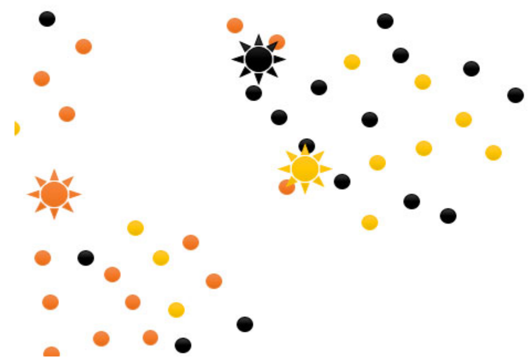
```
In [52]: data=np.array([-5,-3,-7])

In [53]: softmax(data)
Out[53]: array([ 0.11731043,  0.86681333,  0.01587624])

In [54]: softmax(0.00001*data)
Out[54]: array([ 0.33333333,  0.33334    ,  0.33332667])

In [55]: softmax(100*data)
Out[55]: array([  1.38389653e-087,   1.00000000e+000,   1.91516960e-174])
```

- This is just the familiar softmax:
- $r_{ik} = \frac{\exp[v_{ik}]}{\sum_j \exp[v_{ij}]} = softmax(\{v_{ij}\})[k]$
- $r_{ik} = \frac{\exp[\beta v_{ik}]}{\sum_j \exp[\beta v_{ij}]} = softmax(\{\beta v_{ij}\})[k]$



Generalize hard to soft k-means:

Repeat until convergence:

1. Replace $r_i \equiv \underset{k}{\operatorname{argmin}} \|x_i - c_k\|^2$ with

   $r_{ik} = softmax(\{-\beta \|x_i - c_k\|^2\})$ (yields a "soft partition")

2. Replace $\hat{c}_k = \underset{c_k}{\operatorname{argmin}} \sum_{x \in C_k} \|x - c_k\|^2$ with

   $$\hat{c}_k = \underset{c_k}{\operatorname{argmin}} \sum_{i=1}^{N} r_{ik} \|x_i - c_k\|^2$$

   Had, $\hat{c}_k = \frac{1}{N} \sum_{x \in C_k} x$, now have, $\hat{c}_k = \frac{\sum_i r_{ik} x_i}{\sum_i r_{ik}}$.

(Reduces to hard assignment if β is high, which causes $r_{ik} \in \{0,1\}$)

Un-answered issues with “soft” K-means

1. How should we set $\boldsymbol{\beta}$? (not clear)

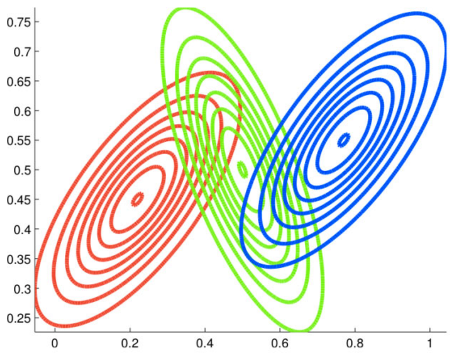
2. We are still treating all the features in $\boldsymbol{x_i}$ equally. Does this make sense? It implies a spherical cluster. But what if cluster would be “better” elongated (non-spherical)? But how?

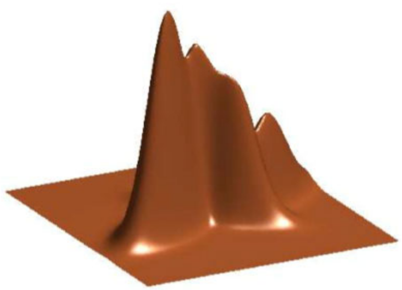
Going “soft” has gotten us some flexibility, but we can do better.

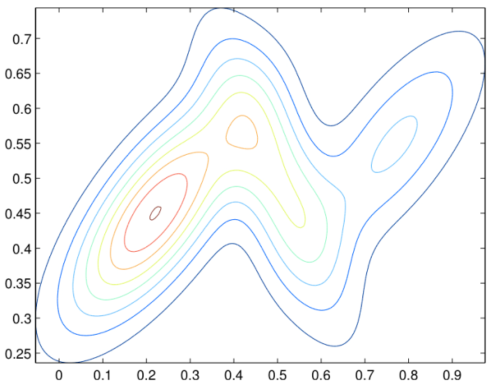
Lets go to a fully probabilistic model! (Mixture of Gaussians)

Mixture of Gaussians (MoG)

- Each cluster is now represented by a Gaussian $N(x_i|u_k, \Sigma_k)$, with two free parameters
- Now we can write down a likelihood and perform MLE!







http://www.cs.toronto.edu/~urtasun/courses/CSC2515/CSC2515_Winter15.html

Mixture of Gaussians (MoG) likelihood for one $\boldsymbol{x_i}$

- Let z_i be a hard (but hidden/unobserved) assignment to cluster—z_i is a latent variable—we don't know it's value, so have to marginalize it (sum it out):

$$\mathrm{L_i} = p(x_i) = \sum_{k=1}^{K} p(x_i, z_i = k)$$

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$$
\begin{aligned}
\mathrm{L_i} &= p(x_i) = \sum_{k=1}^{K} p(x_i, z_i = k) \\
&= \sum_{k=1}^{K} p(x_i | z_i = k) p(z_i = k) \\
&= \sum_{k=1}^{K} N(x_i | \mu_k, \Sigma_k) p(z_i = k)
\end{aligned}
$$

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where $\alpha_k \equiv p(z_i = k)$ and $\sum_k \alpha_k = 1$

- The parameters we want to learn are $\theta \equiv \{\mu_k, \Sigma_k, \alpha_k\}$.
- α_k are called the "mixing weights".
- Now we can use MLE on $LL = log \prod_i L_i = \sum_i log L_i$.

Alternative uses of MoG beyond clustering

Once we have estimated the values of $\theta = \{\mu_k, \Sigma_k, \alpha_k\}$ from the training data, we can make calls to $p(x|\theta)$, for any data point in the training data or otherwise.

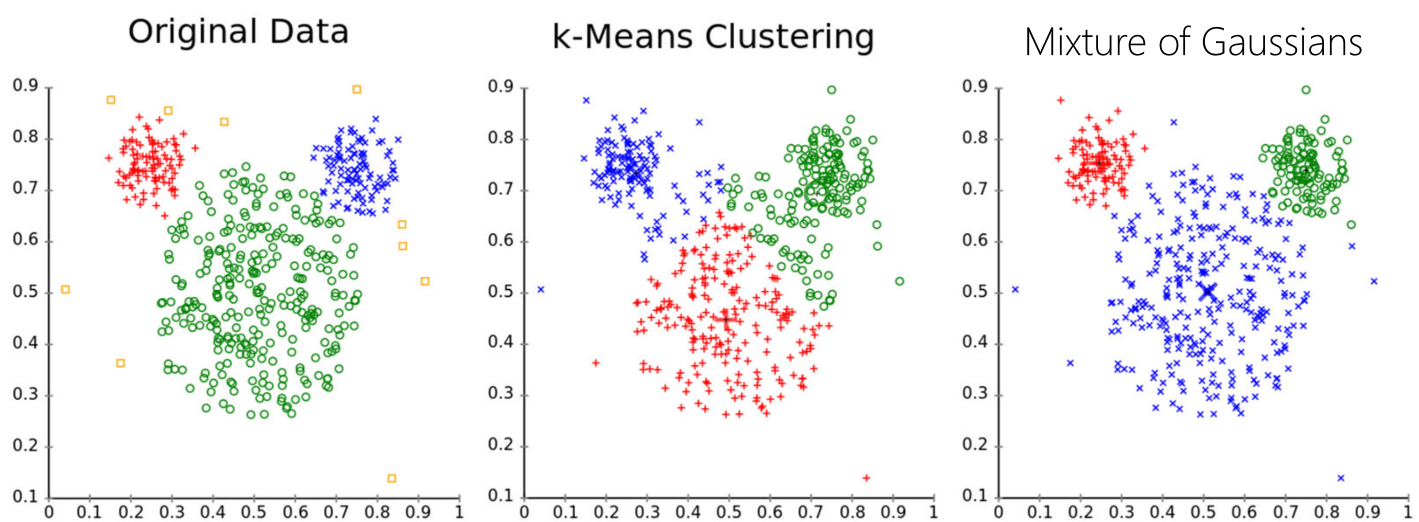
- So we have also performed *density estimation*.

We can also use it to generate data, $x \sim p(x|\theta)$.

- So we have a *generative model*:
  1. For each point, j, sample cluster $c_j \sim multinomial(\{\alpha_k\})$.
  2. Then sample from the corresponding Gaussian.

K-means vs. Mixture of Gaussians

- If we take the zero noise limit in Mixture of Gaussians (zero variance in the Gaussians), we get K-means.
- MoG allows non-spherical clusters (via the covariance matrix).
- And different covariance per cluster, which is helpful here:

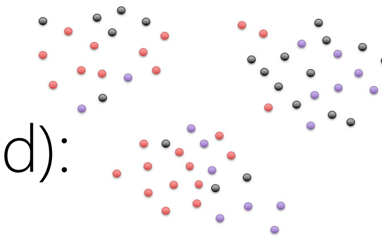


https://en.wikipedia.org/wiki/K-means_clustering

K-means vs. Mixture of Gaussians

- MoG: explicit assumptions in the form of statistical distributions.
- Thus easier to generalize, while understanding assumptions.
- Can derive principled objective in the form of a likelihood, which involves marginalizing over the hidden/latent variable (cluster assignment).
- There is a special form of MLE for these latent variables called Expectation-Maximization.

EM for Mixture of Gaussians $\theta \equiv \{\mu_k, \Sigma_k, \alpha_k\}$.



Intuitive Description of EM (EM is exact maximum likelihood):

Initialize with random cluster assignments

i. use current parameter estimates to (probabilistically) estimate $\{p(z_i|x_i,\theta)\}$(i.e. “fill in the missing data”: E-step)

ii. do MLE on “fully observed” data (where z^n are probabilistically filled in: M-step).

- This is a lot like the K-means algorithm, only now with a principled loss function and parameter estimation principle.
- This procedure yields the MLE solution for MoG (and generally for latent variable models).

EM for Mixture of Gaussians

$\theta \equiv \{\mu_k, \Sigma_k, \alpha_k\}.$