CM50264: Machine Learning 1

Unsupervised learning

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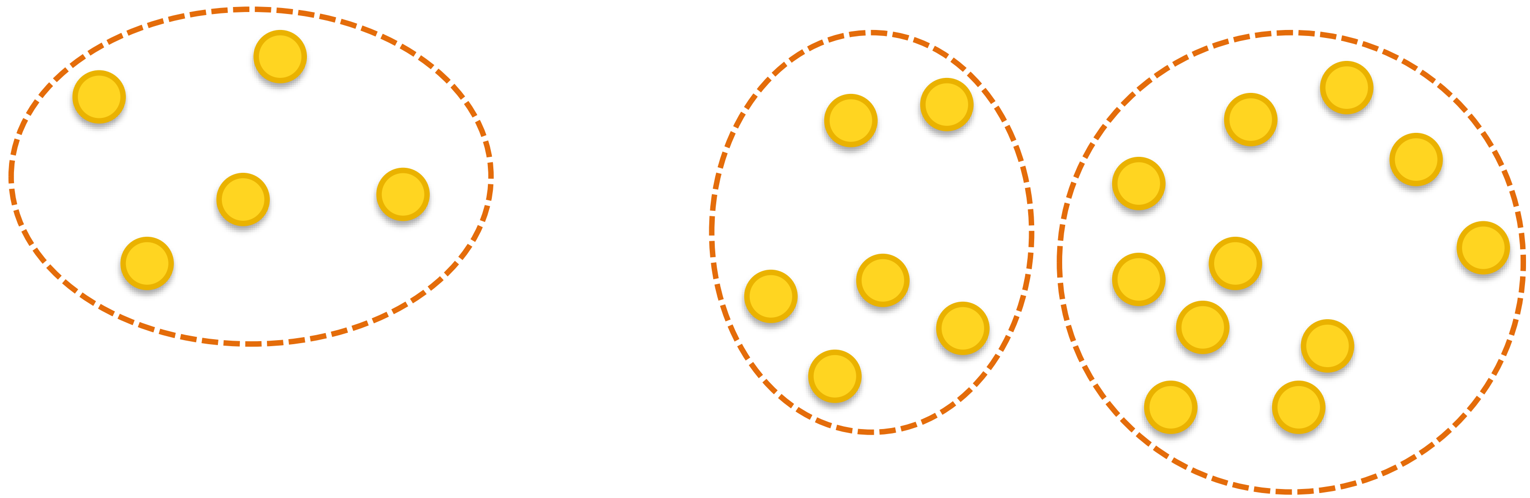
Supervised / unsupervised learning

- Supervised learning
  - learn from labelled examples:
    $$D = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^N, y^N)\}$$
    Pairs of input and the corresponding desired output.
- Unsupervised learning
  - learn from unlabelled examples:
    $$D = \{\mathbf{x}^1, \dots, \mathbf{x}^N\}$$
    Input data only; no desired outputs.
  - Detect underlying structure in data.
  - E.g., clustering and dimensionality reduction.

Clustering

$$D = \{\mathbf{x}^1, \dots, \mathbf{x}^N\} \subset \boldsymbol{X}$$

- Group together similar data instances.
- E.g., $\boldsymbol{X} \subset \mathbf{R}^2$



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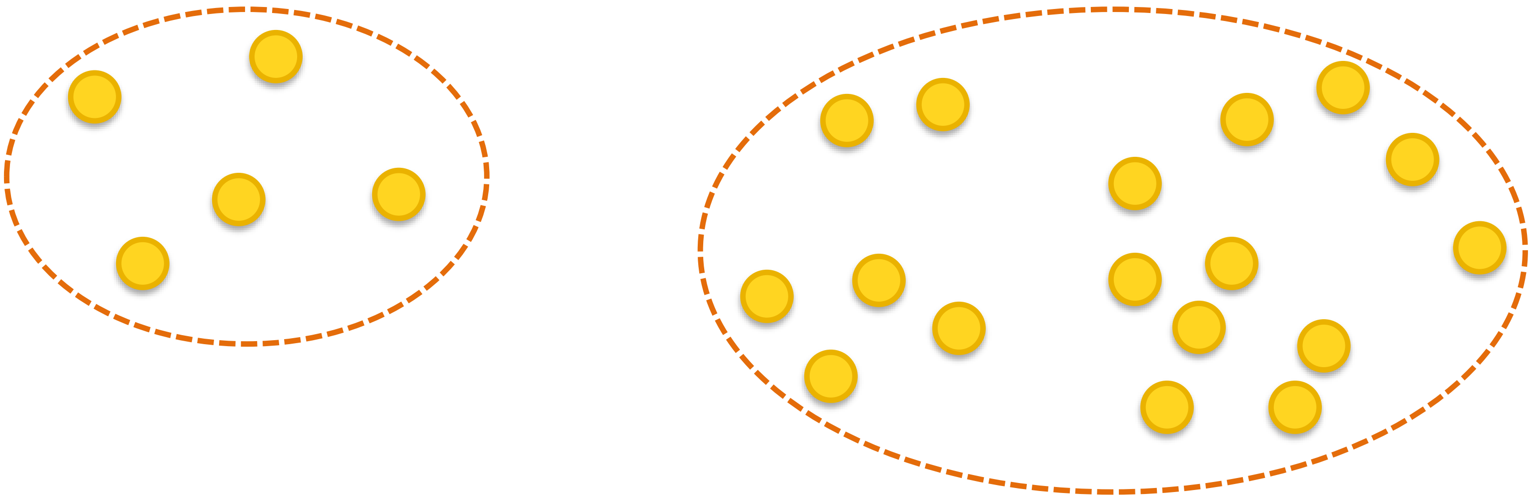

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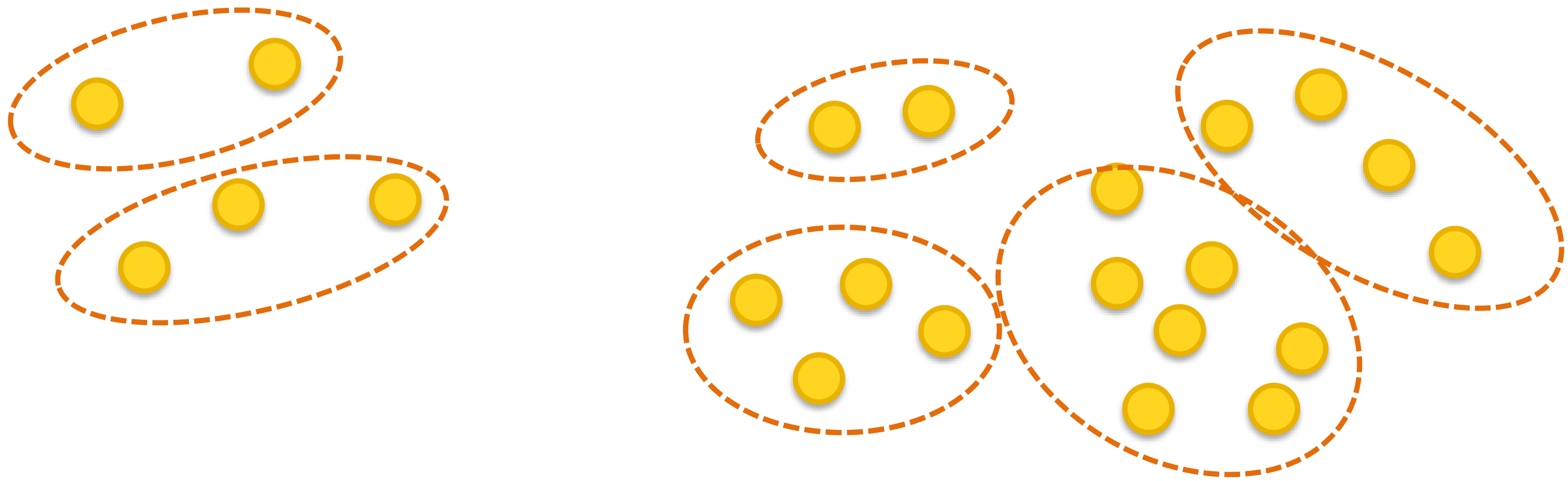


Clustering applications

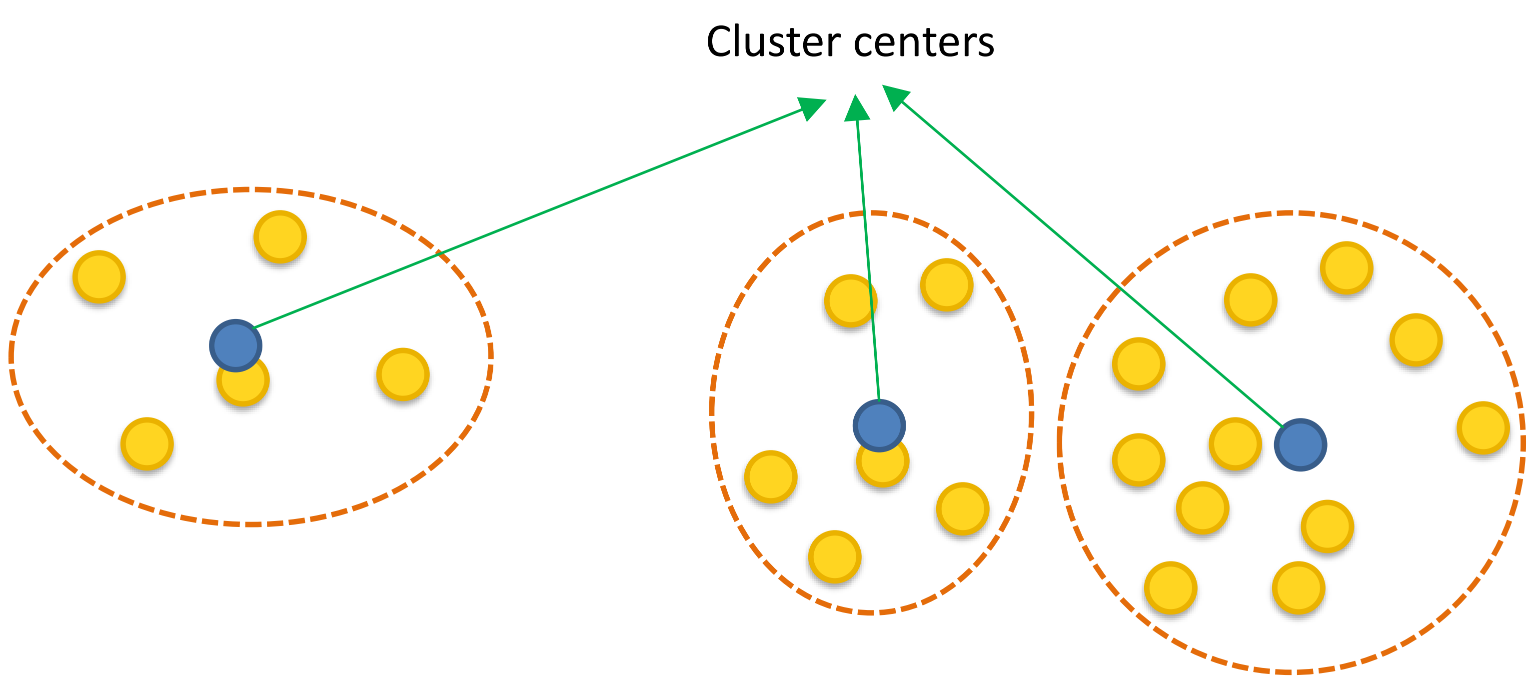
- Marketing: help to discover distinct groups in customer bases, and develop targeted marketing programs.
- Social network analysis: recognize communities within large groups of people.
- Animal ecology: discover and compare communities of organisms.
- Gene sequence analysis: group homologous sequences into gene families.

Image segmentation

- N (# data points): # pixels.
- Feature $\mathbf{x}^i$: color values (R,G,B) + row and column values of i-th pixel.

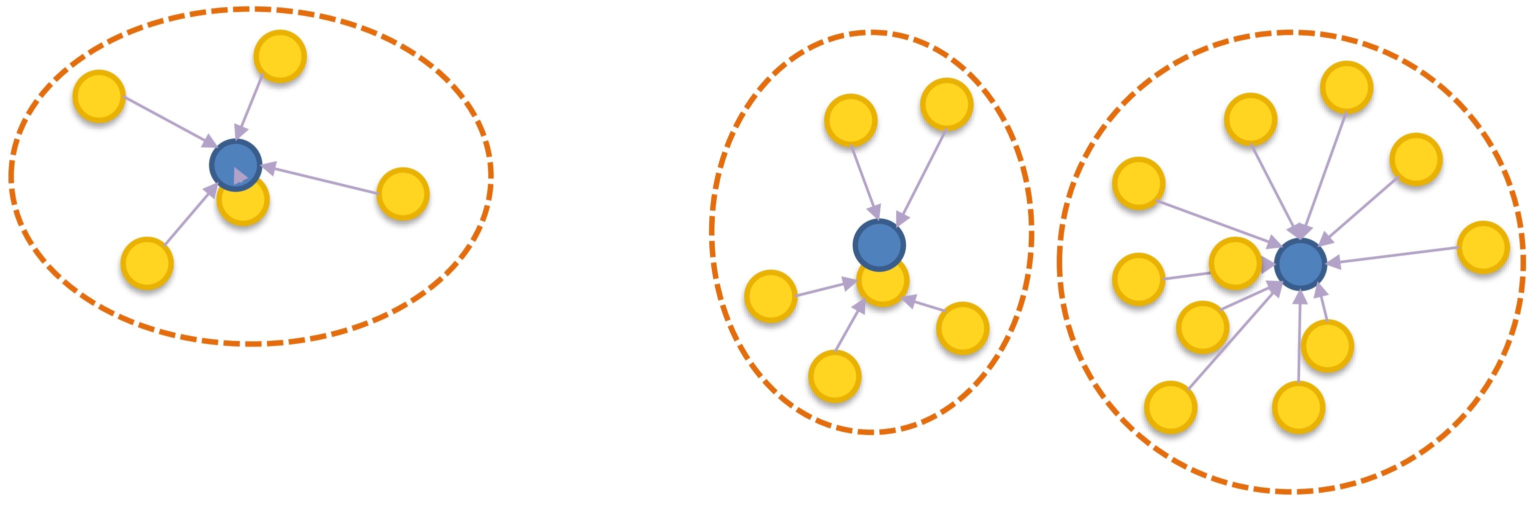

Vector quantization

- Calculate the mean vector (center) for each cluster.



Vector quantization

- Calculate the mean vector (center) for each cluster.
- Replace all elements in each cluster by their respective center.



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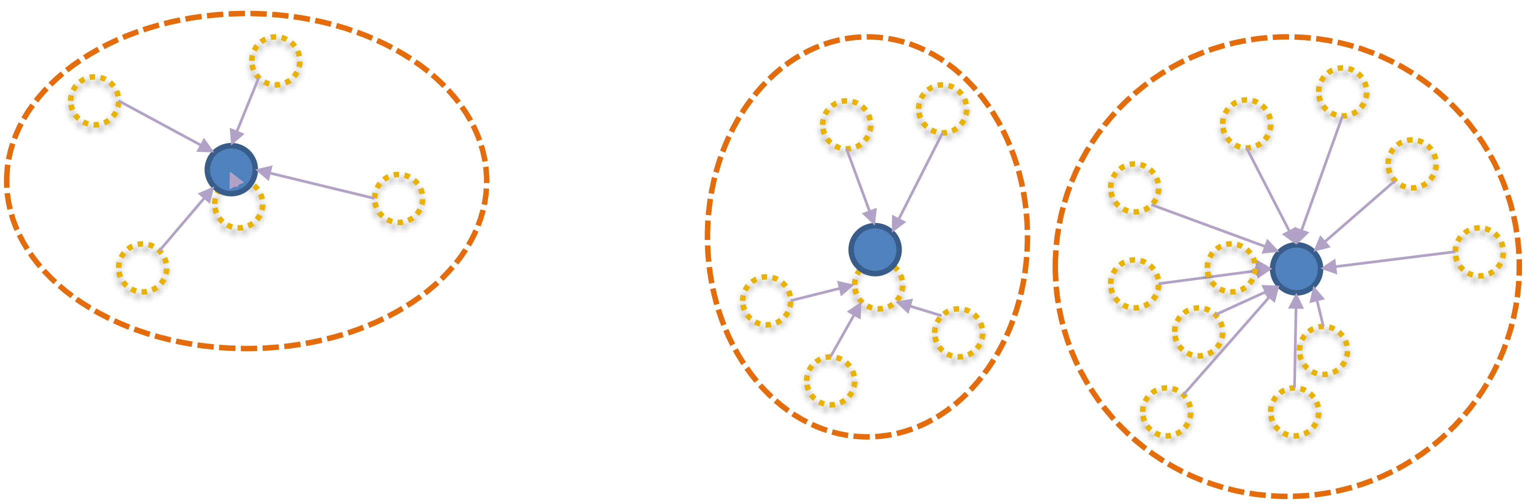
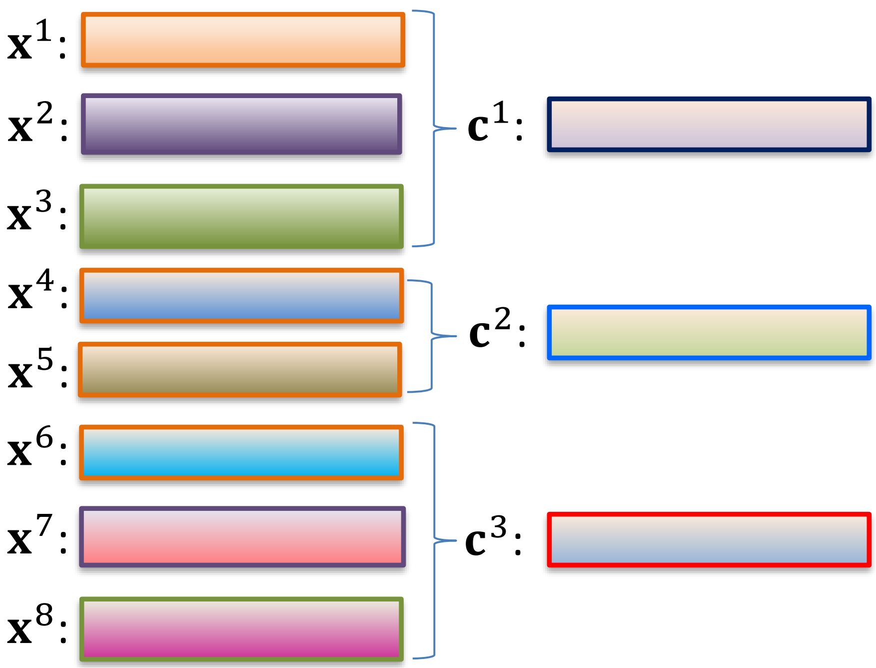


Vector quantization

Data compression: instead of strong all data points, we store the cluster centers plus cluster index for each data entry.



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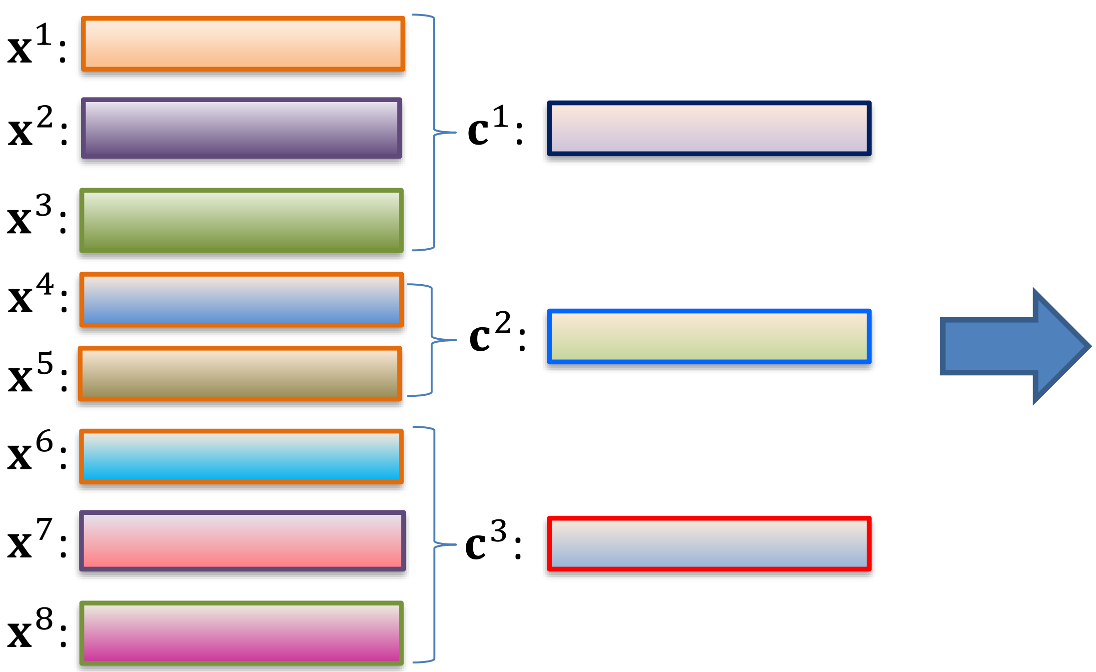


$\mathbf{x}^1$: $I(\mathbf{c}^1)$

$\mathbf{x}^2$: $I(\mathbf{c}^1)$

$\mathbf{x}^3$: $I(\mathbf{c}^1)$

$\mathbf{x}^4$: $I(\mathbf{c}^2)$

$\mathbf{x}^5$: $I(\mathbf{c}^2)$

$\mathbf{x}^6$: $I(\mathbf{c}^3)$

$\mathbf{x}^7$: $I(\mathbf{c}^3)$

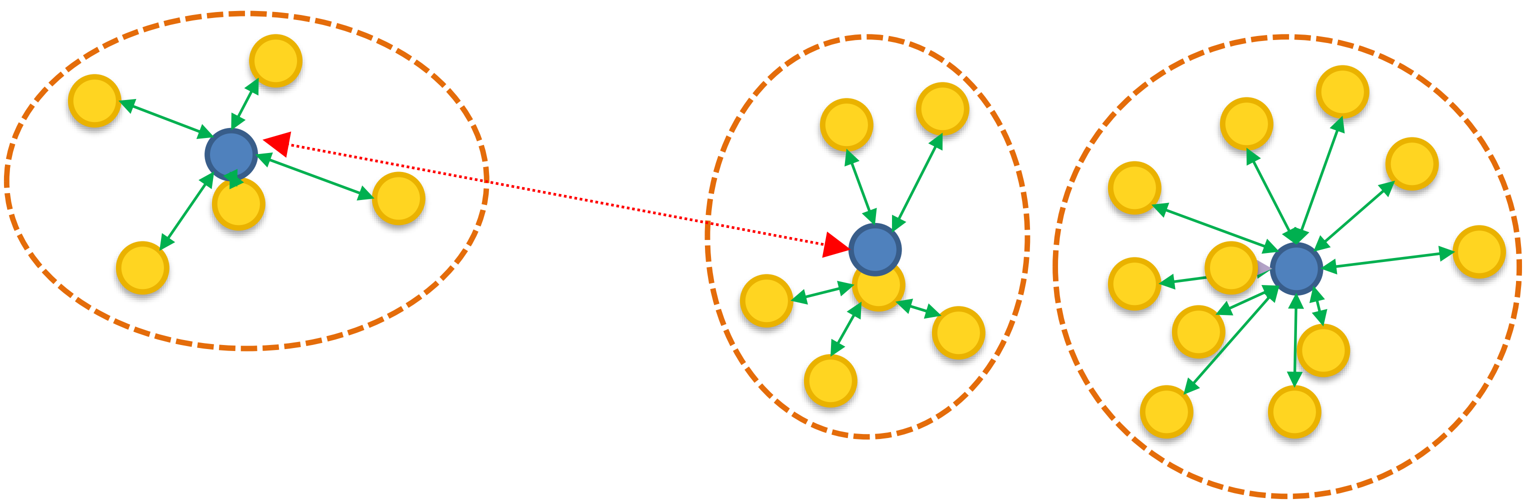
$\mathbf{x}^8$: $I(\mathbf{c}^3)$

What is good clustering?

- A good clustering algorithm will produce
  - Low intra-cluster distances.
  - High inter-cluster distances.
- The quality of a clustering depends on the distance measure, e.g., Euclidean distance.
- Objective evaluation is challenging: done by human / expert inspection.

What is good clustering?

- A good clustering algorithm will produce
  - Low intra-cluster distances.
  - High inter-cluster distances.
- Finding such a clustering is NP-hard.

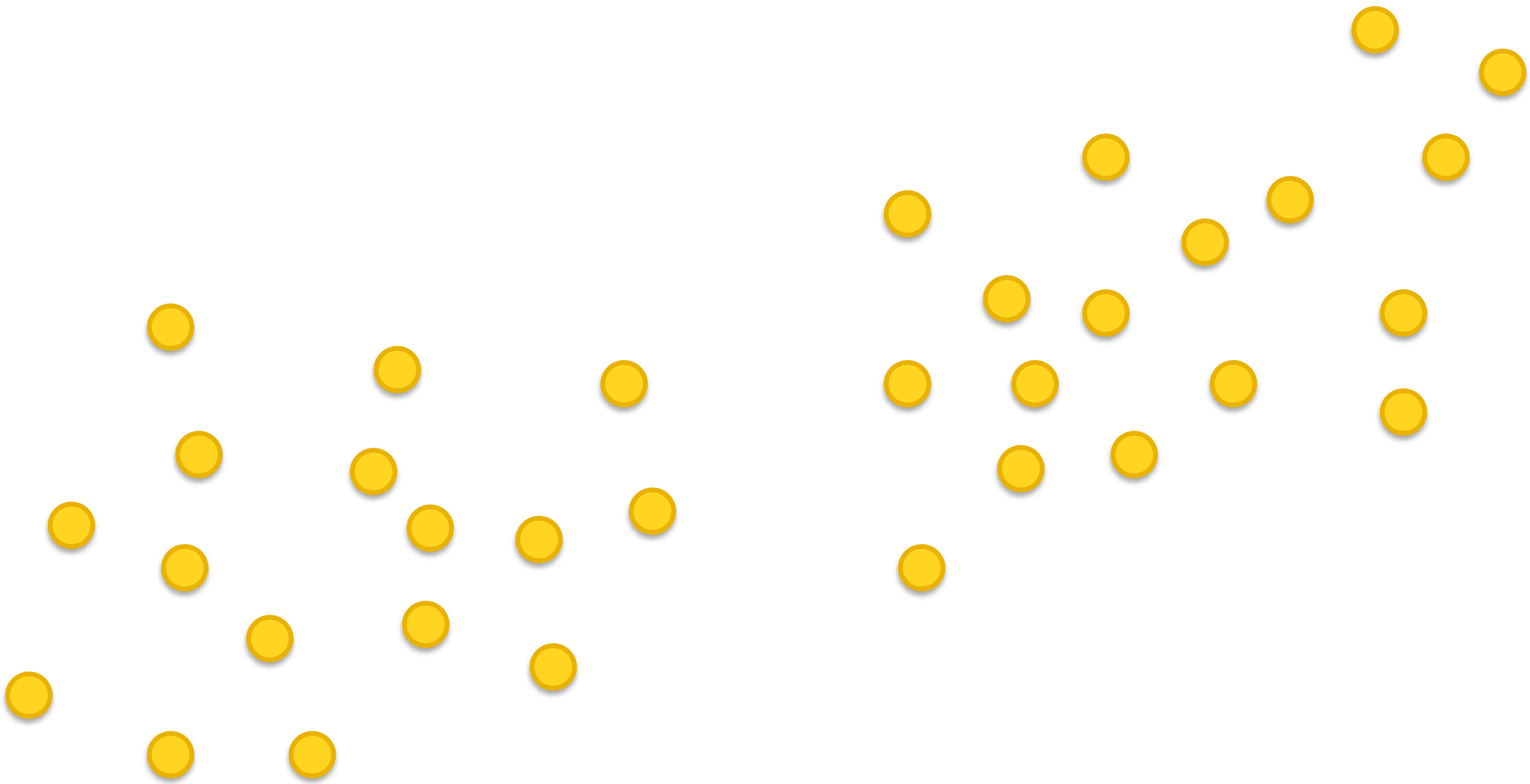


K-means clustering

An iterative clustering algorithm

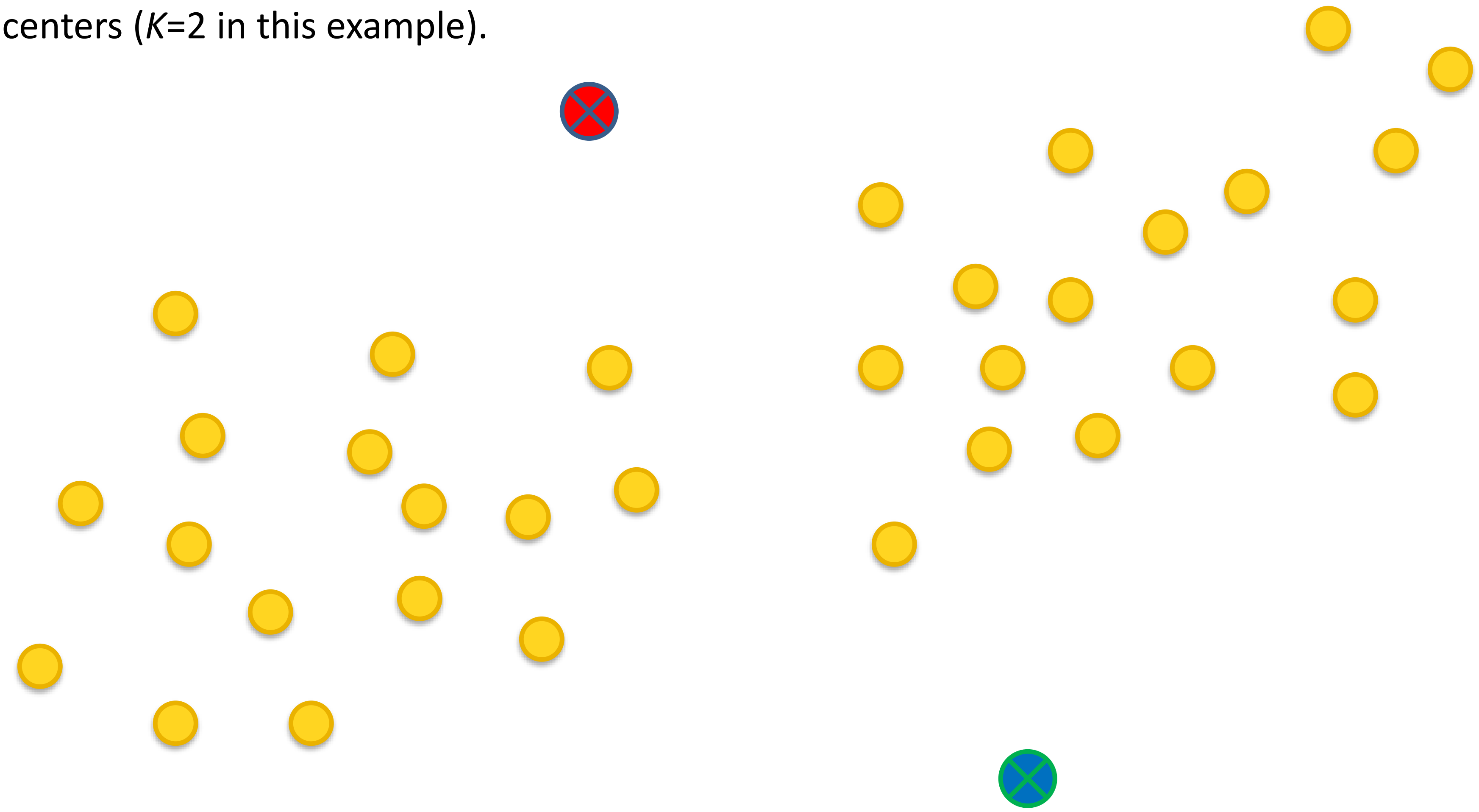
1. Initialize: pick *K* random points as cluster centers.
2. Iterate
   - Assign data points to closest cluster center.
   - Change the cluster center to the average of its assigned points.
3. Stop when no point assignments change.

K-means clustering example



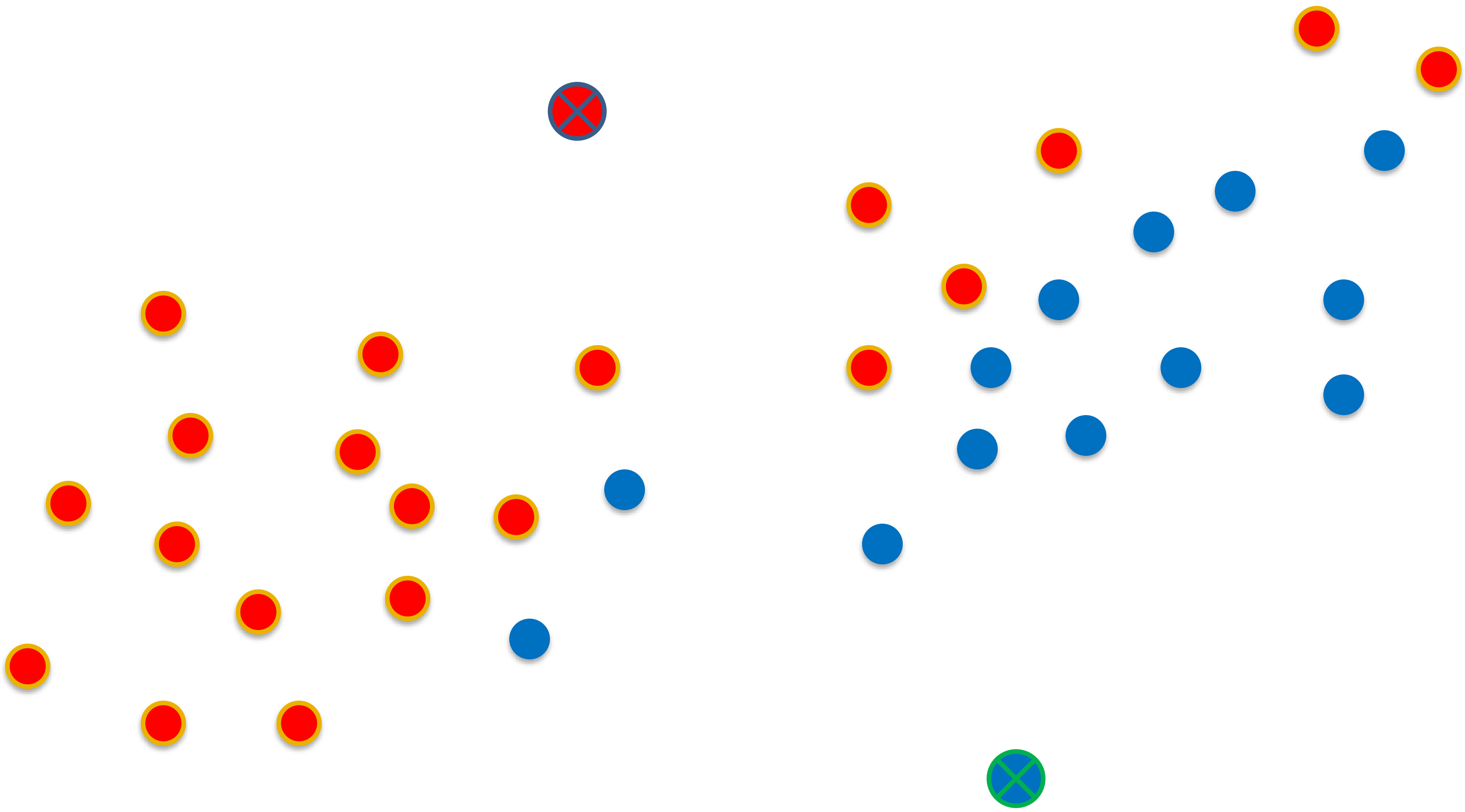
K-means clustering example

Initialize: pick *K* random points as cluster centers (*K*=2 in this example).



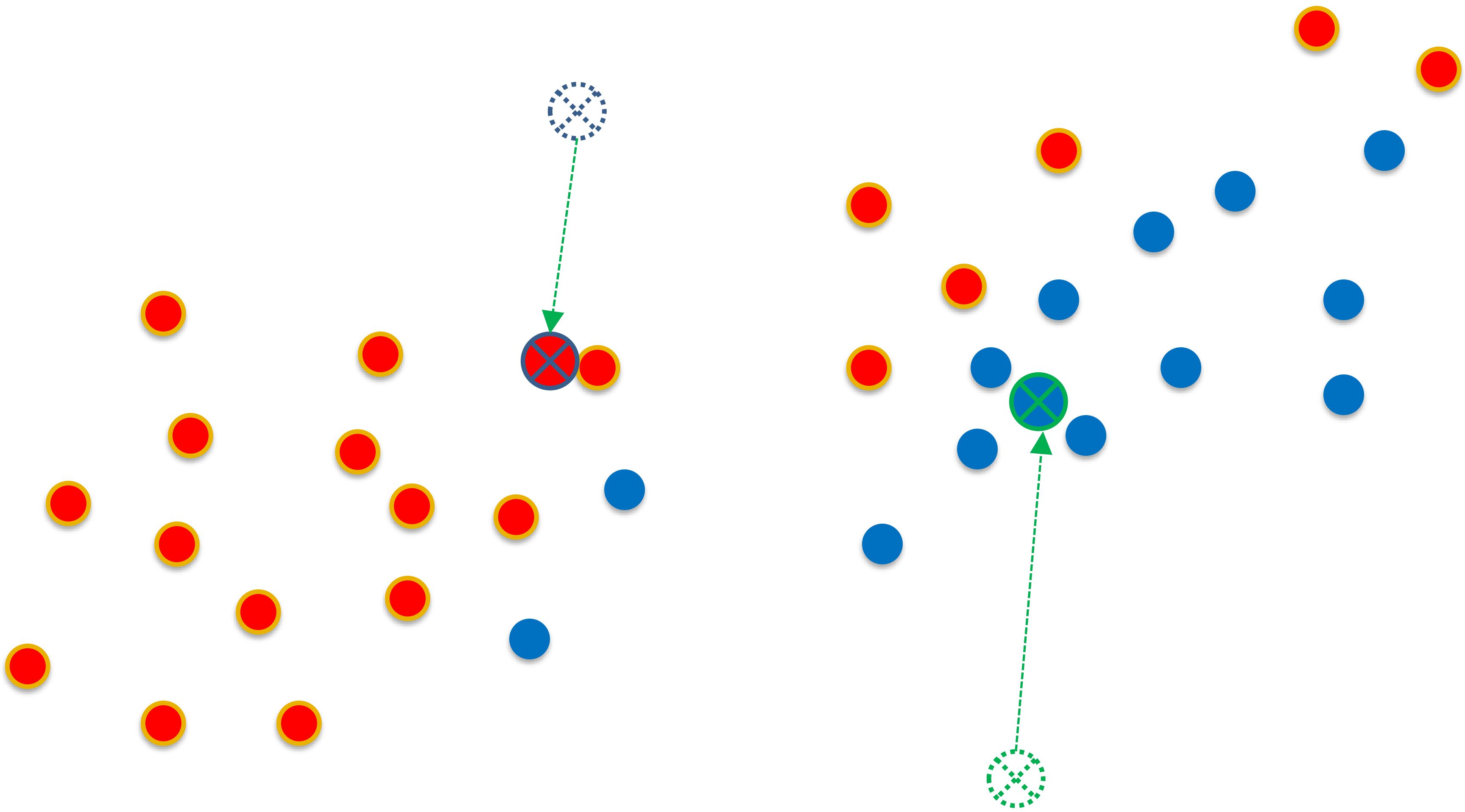
K-means clustering example

Assign data points to closest cluster center.



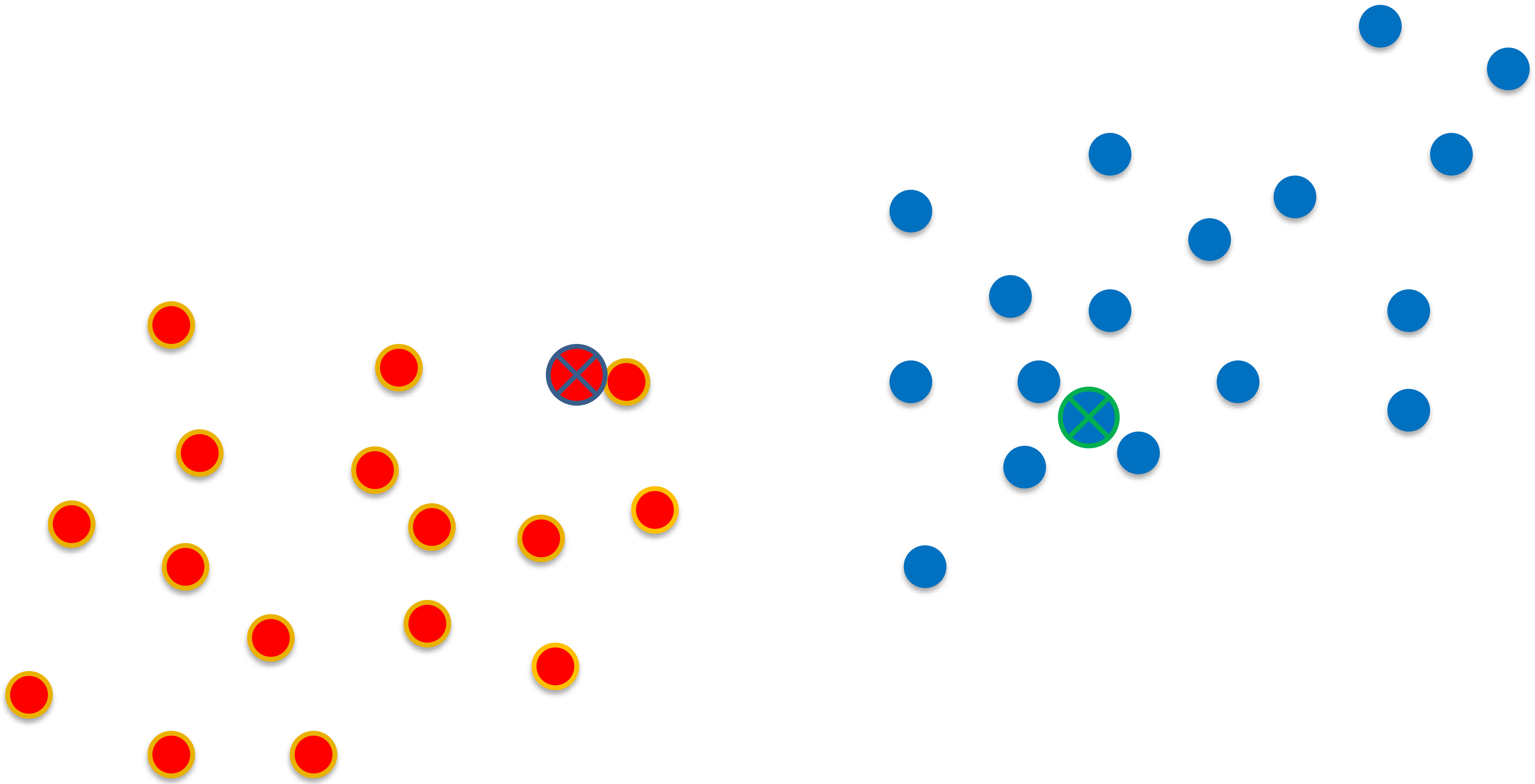
K-means clustering example

Change each cluster center to the average of its assigned points.



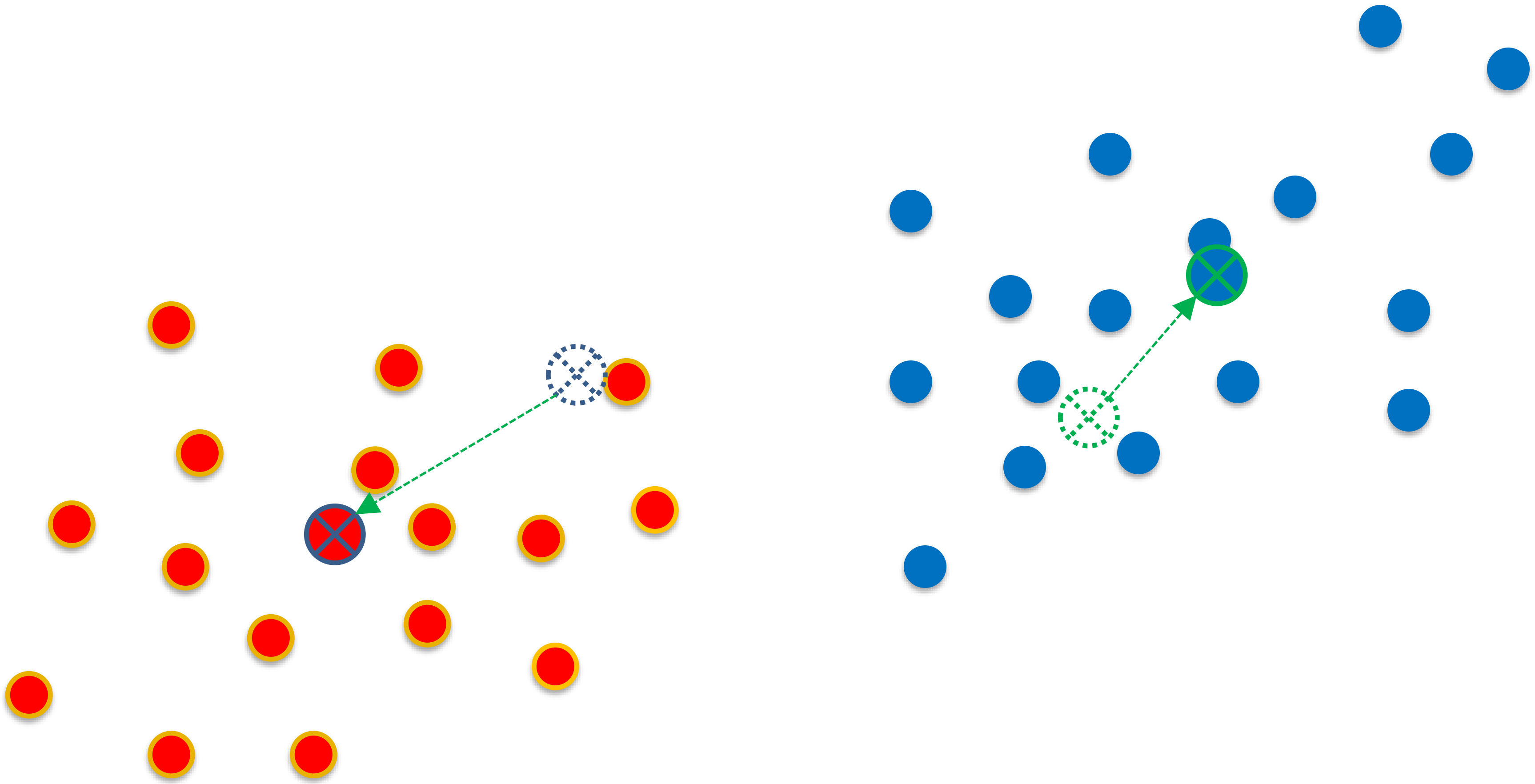
K-means clustering example

Assign data points to closest cluster center.



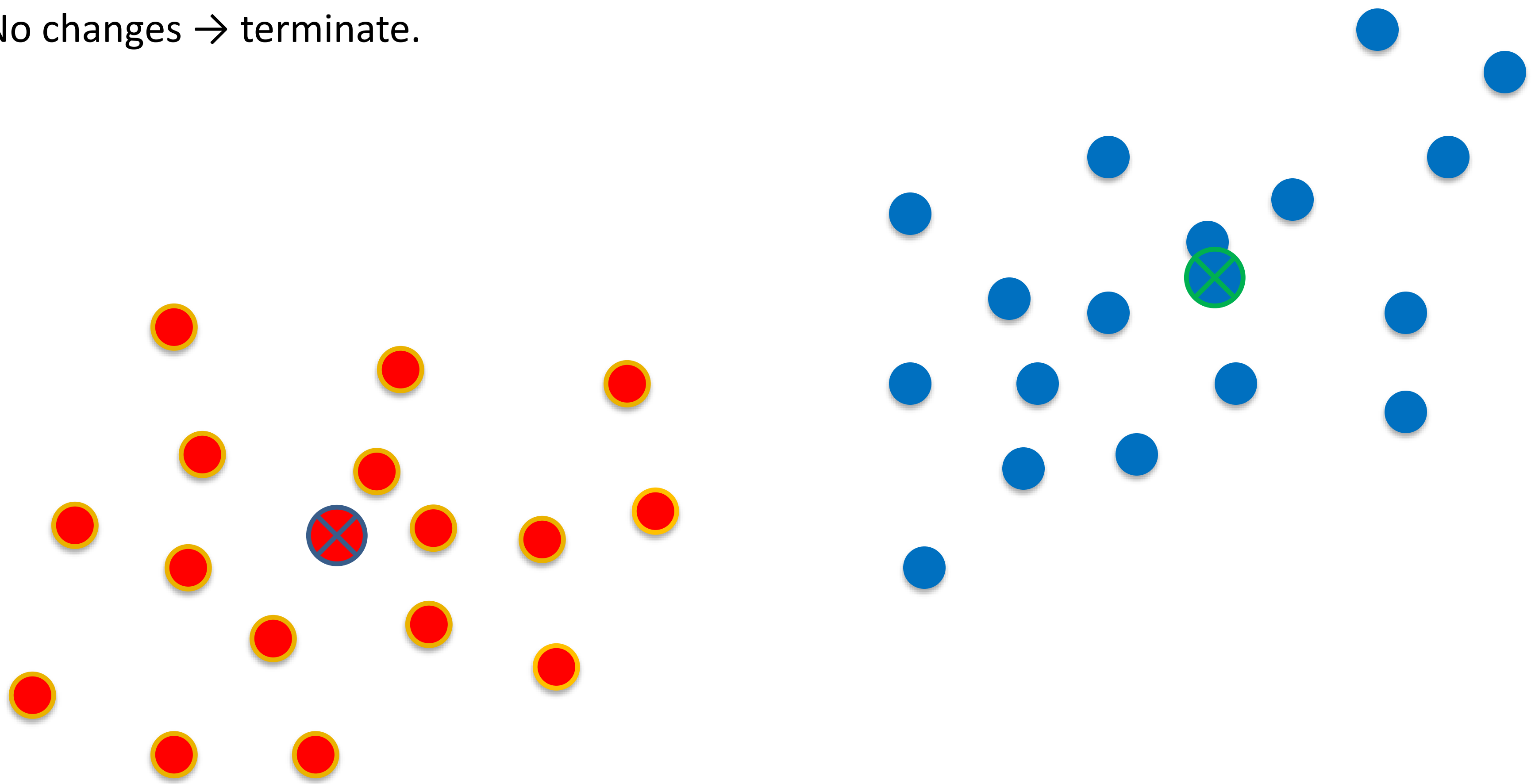
K-means clustering example

Change the cluster center to the average of its assigned points.



K-means clustering example

Assign data points to closest cluster center:
No changes → terminate.

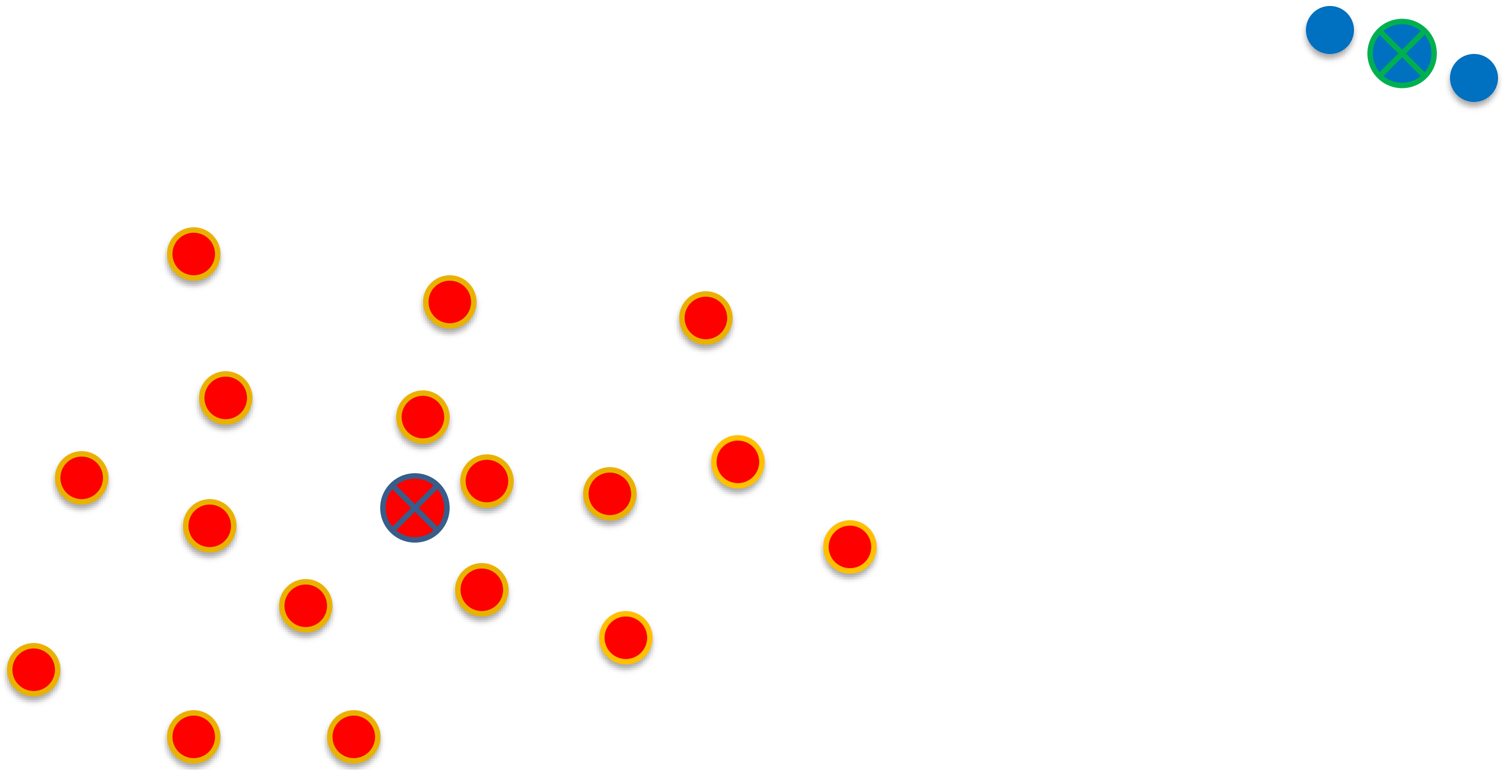


Properties of K-means algorithm

$$D = \{\mathbf{x}^1, \dots, \mathbf{x}^N\} \subset \boldsymbol{X} \subset \mathbf{R}^m$$

- Guaranteed to converge in a finite number of iterations.
- Run-time per iteration:
  K: # clusters; *N*: # data points; *m*: data dim.
  - Assign data points to closest cluster center: O(*KNm*).
  - Change the cluster center to the average of its assigned points: O(*Nm*).
- Non-deterministic: depends on center initialization.
- Requires *K* as a hyper-parameter.

K-means clustering failure case



Measuring the clustering performance

Reconstruction error:

$$\begin{aligned}
\mathbf{x}^1 &\to \mathbf{c}^1 \\
\mathbf{x}^2 &\to \mathbf{c}^1 \\
\mathbf{x}^3 &\to \mathbf{c}^1 \\
\mathbf{x}^4 &\to \mathbf{c}^2 \\
\mathbf{x}^5 &\to \mathbf{c}^2 \\
\mathbf{x}^6 &\to \mathbf{c}^3 \\
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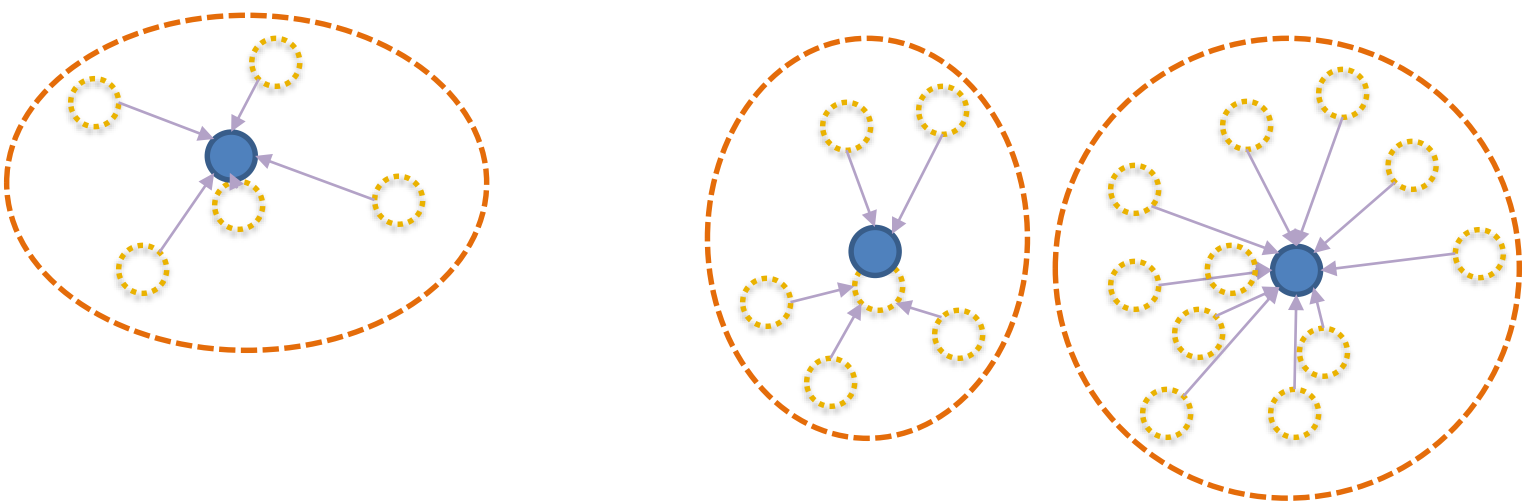
\mathbf{x}^8 &\to \mathbf{c}^3
\end{aligned}$$

$$\begin{aligned}
&\|\mathbf{x}^1 - \mathbf{c}^1\| \\
&\|\mathbf{x}^2 - \mathbf{c}^1\| \\
&\|\mathbf{x}^3 - \mathbf{c}^1\| \\
&\|\mathbf{x}^4 - \mathbf{c}^2\| \\
&\|\mathbf{x}^5 - \mathbf{c}^2\| \\
&\|\mathbf{x}^6 - \mathbf{c}^3\| \\
&\|\mathbf{x}^7 - \mathbf{c}^3\| \\
&\|\mathbf{x}^8 - \mathbf{c}^3\|
\end{aligned}$$

$$\sum_{i=1}^{N} \|\mathbf{x}^i - \mathbf{c}(\mathbf{x}^i)\|$$

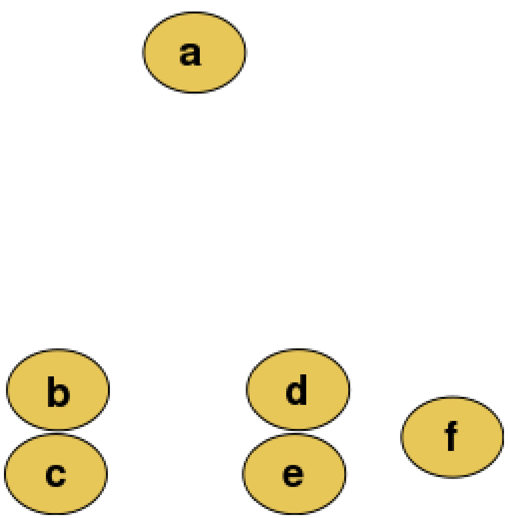
or

$$\sum_{i=1}^{N} \|\mathbf{x}^i - \mathbf{c}(\mathbf{x}^i)\|^2$$

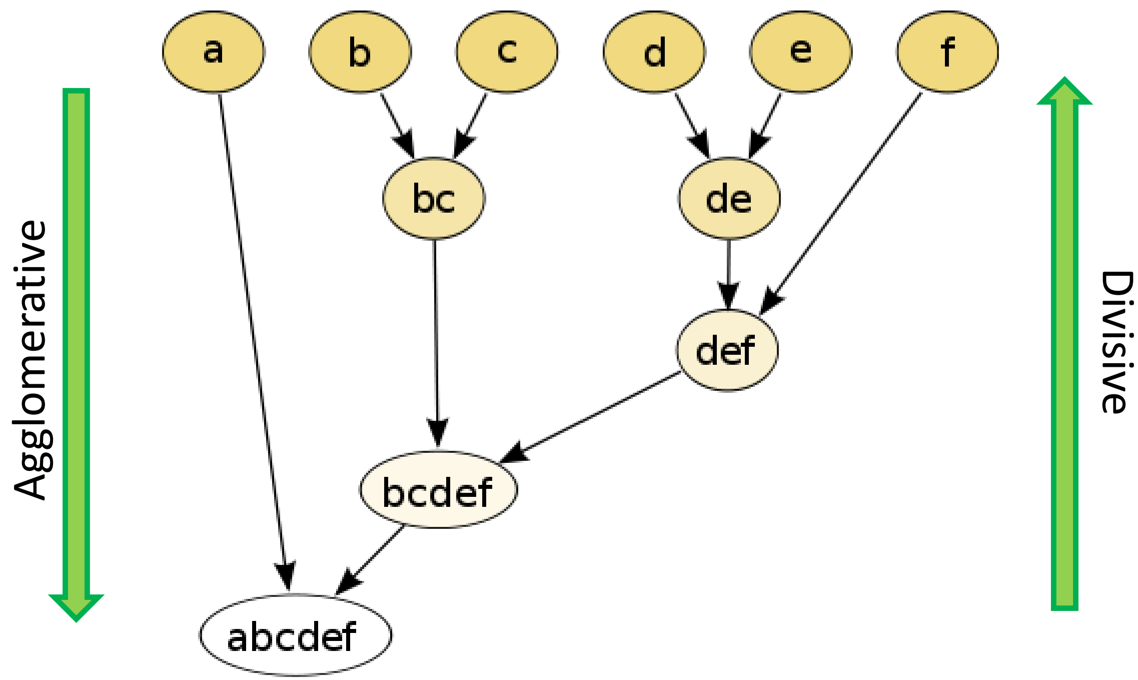


Other clustering approaches: Hierarchical clustering

builds a hierarchy of clusters



Raw data



Clustering tree

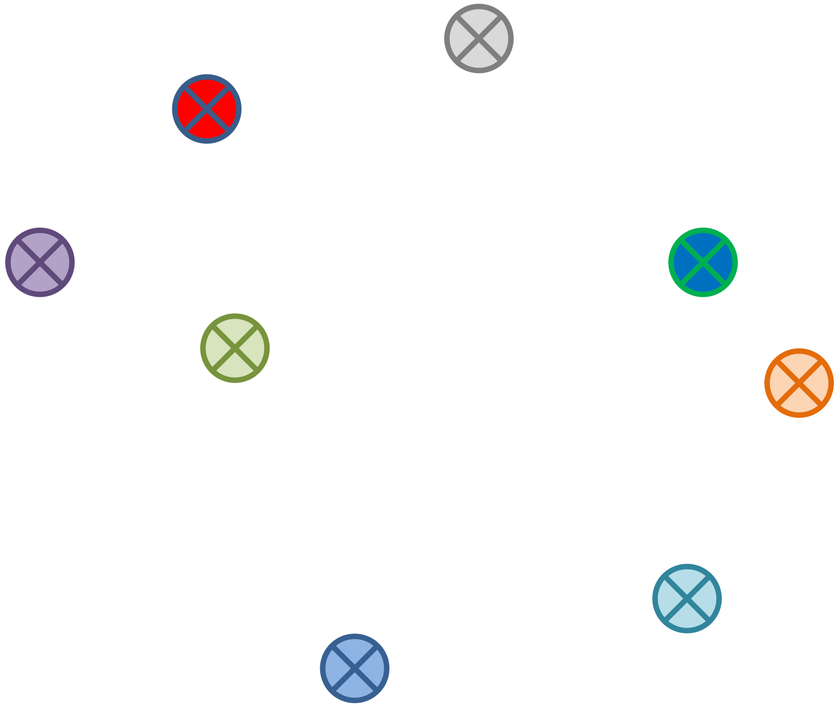
[Wikipedia]

Single-linkage clustering

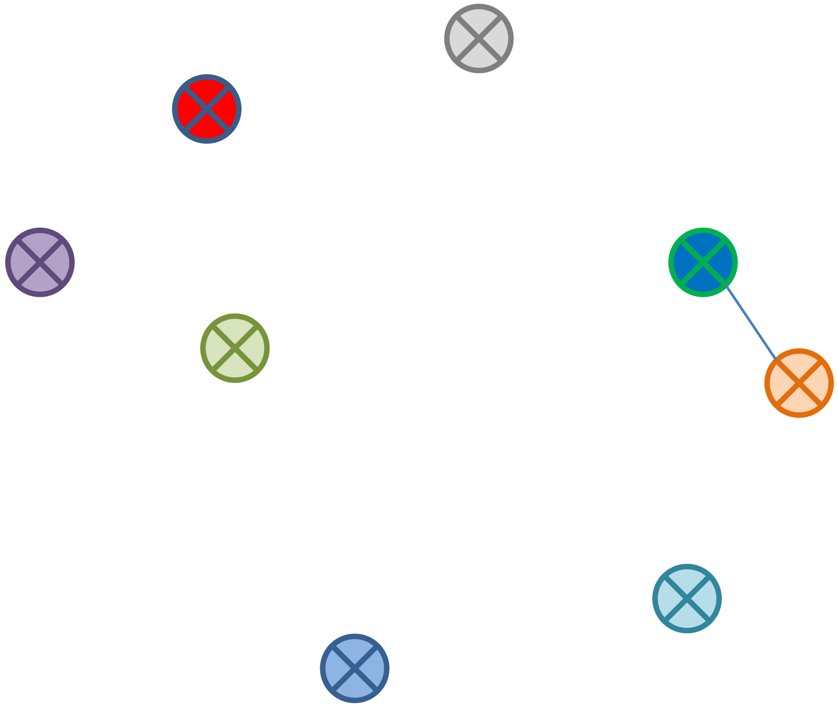
An iterative clustering algorithm

1. Initialize: assign a cluster center to each data point.
2. Iterate
   - Find the two closest pair of cluster centers.
   - Merge the two clusters and define a new center.
3. Stop when # number of clusters < Threshold.

Single linkage clustering example



Single linkage clustering example



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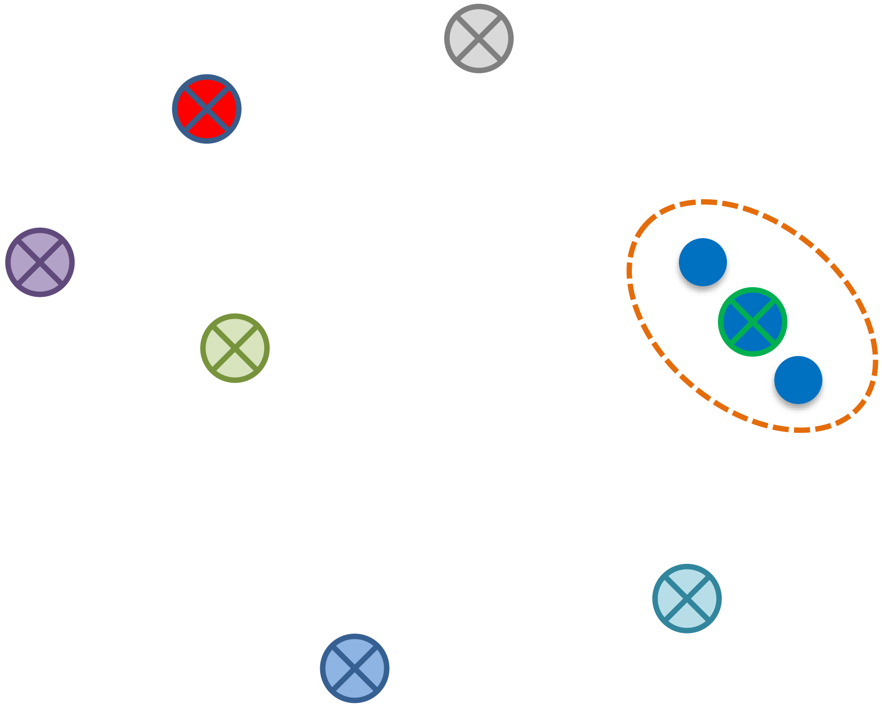

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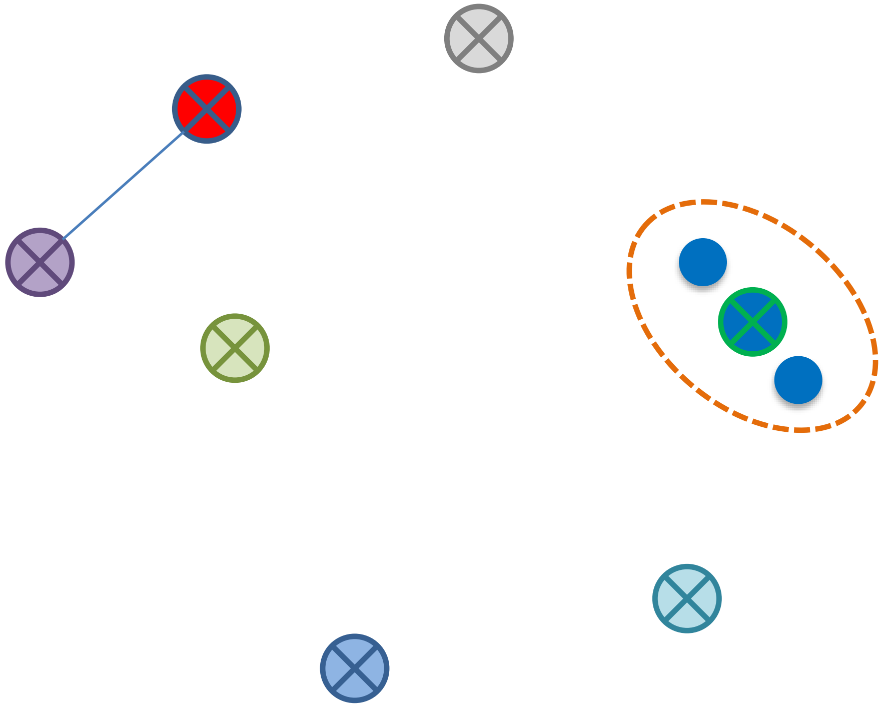

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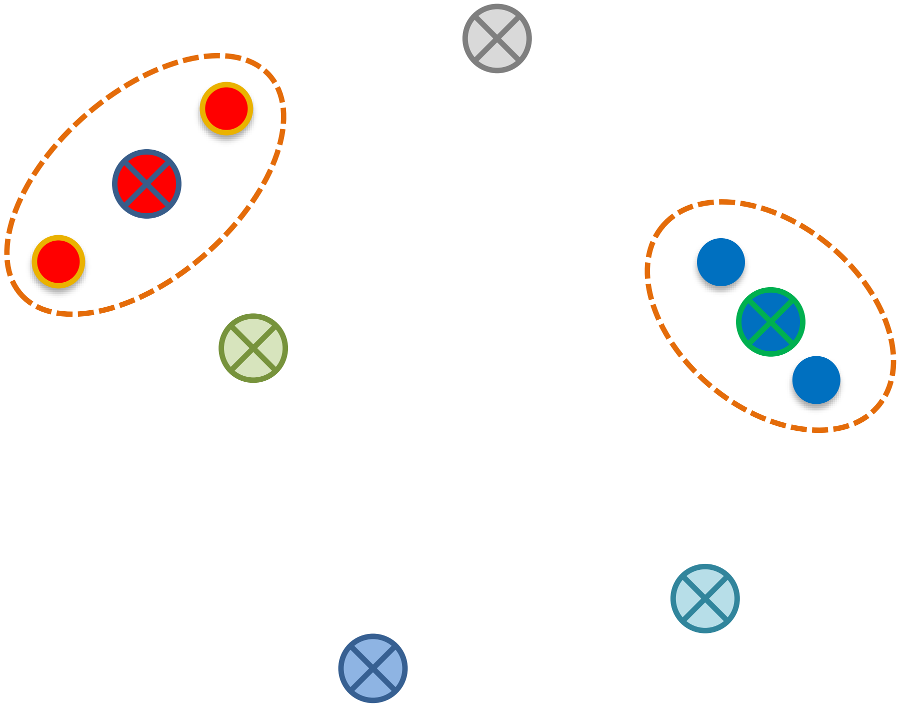

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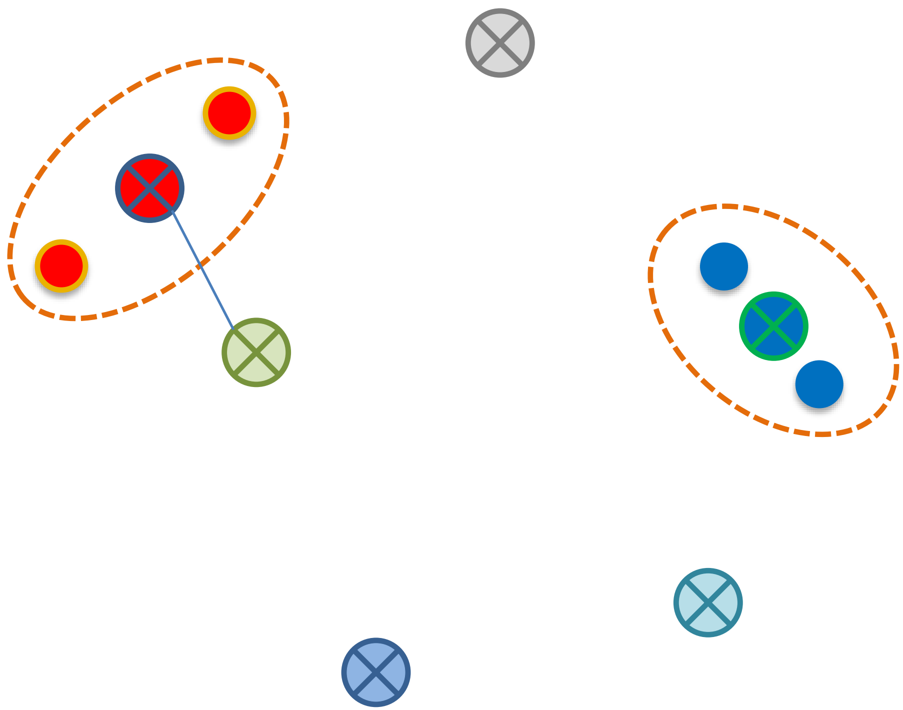

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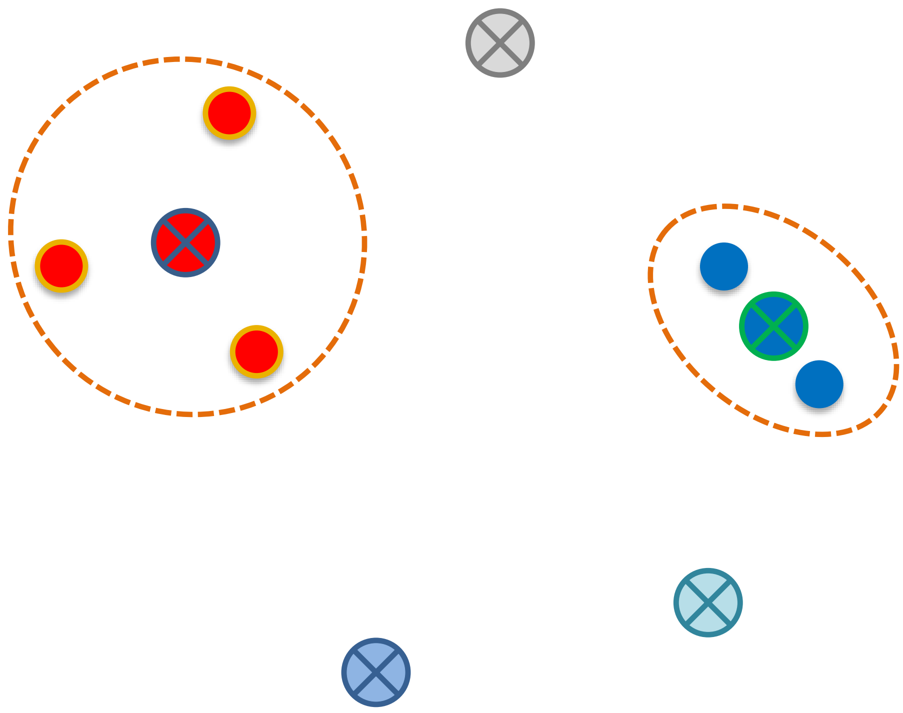

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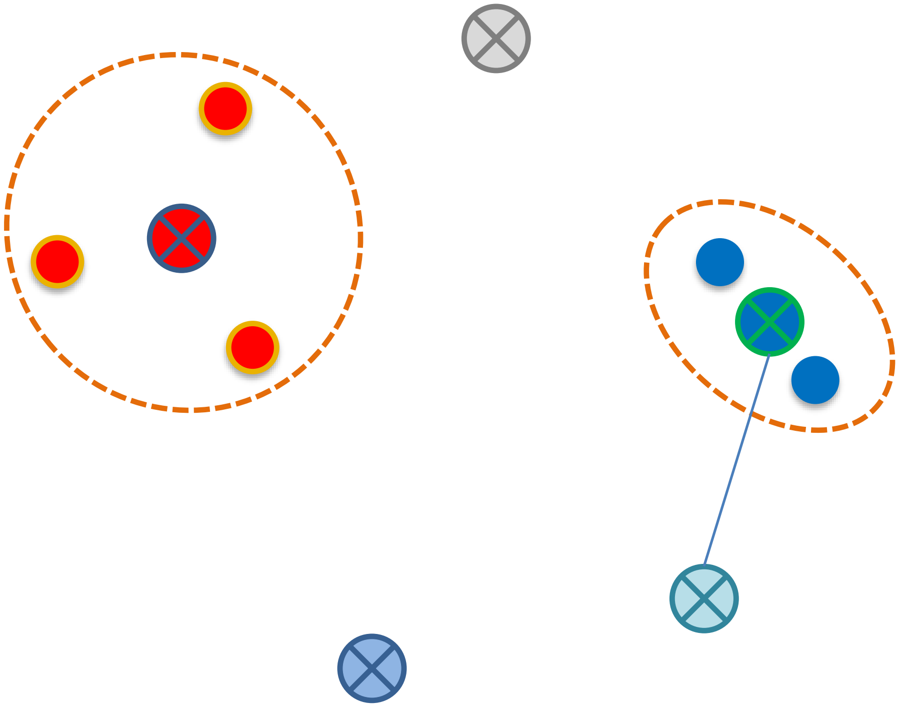

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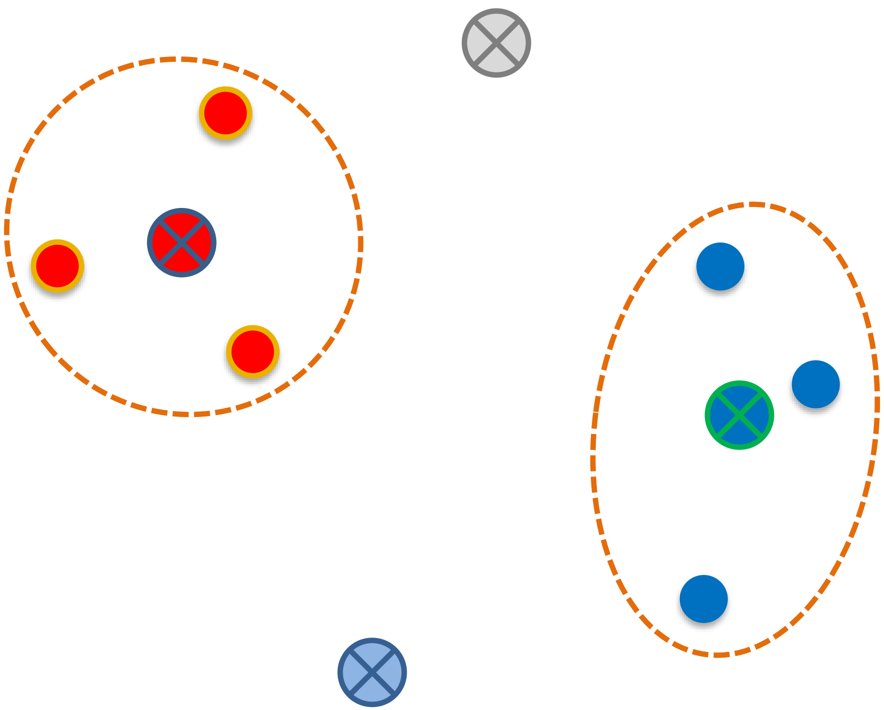
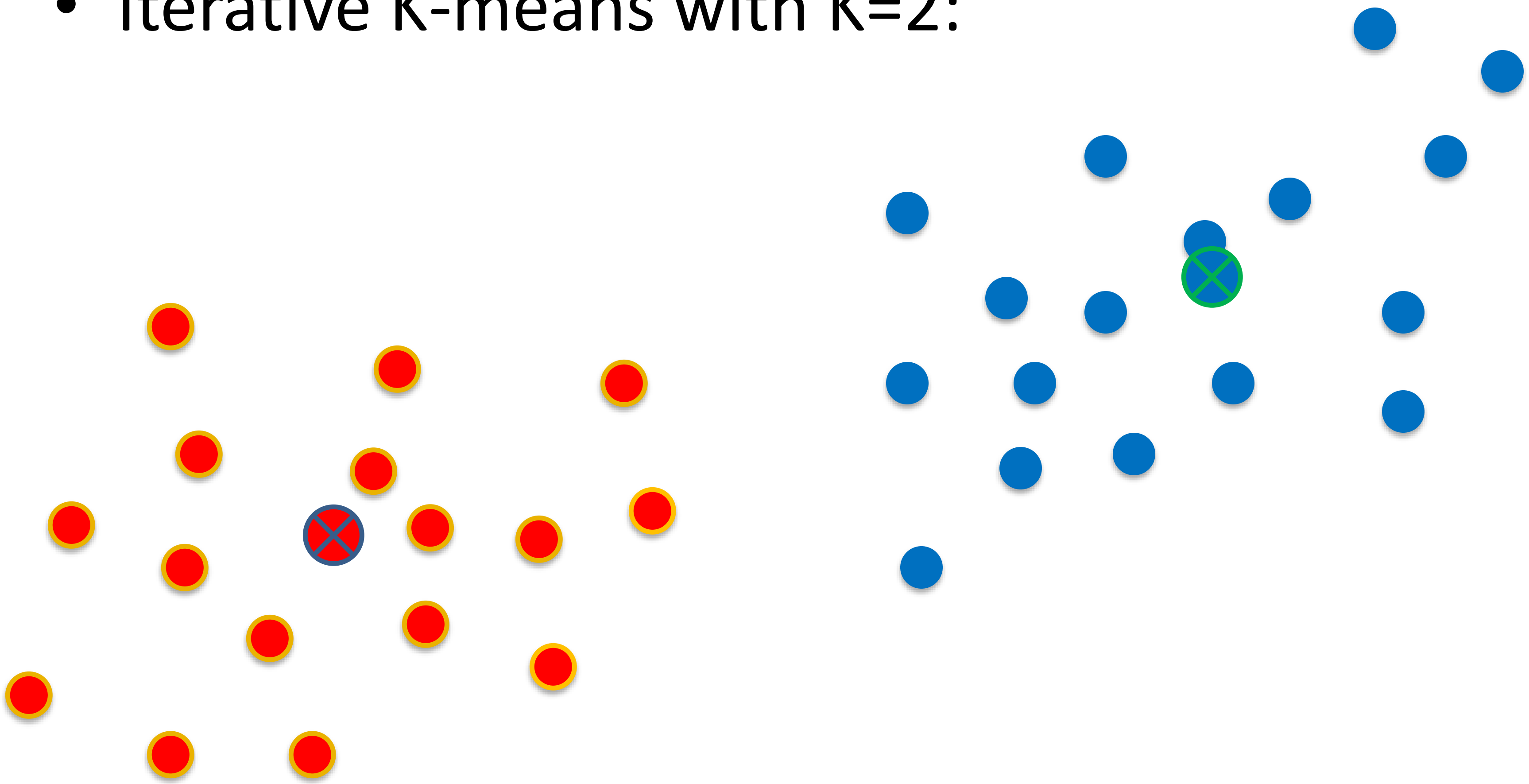


Divisive clustering example

- Iterative K-means with K=2:



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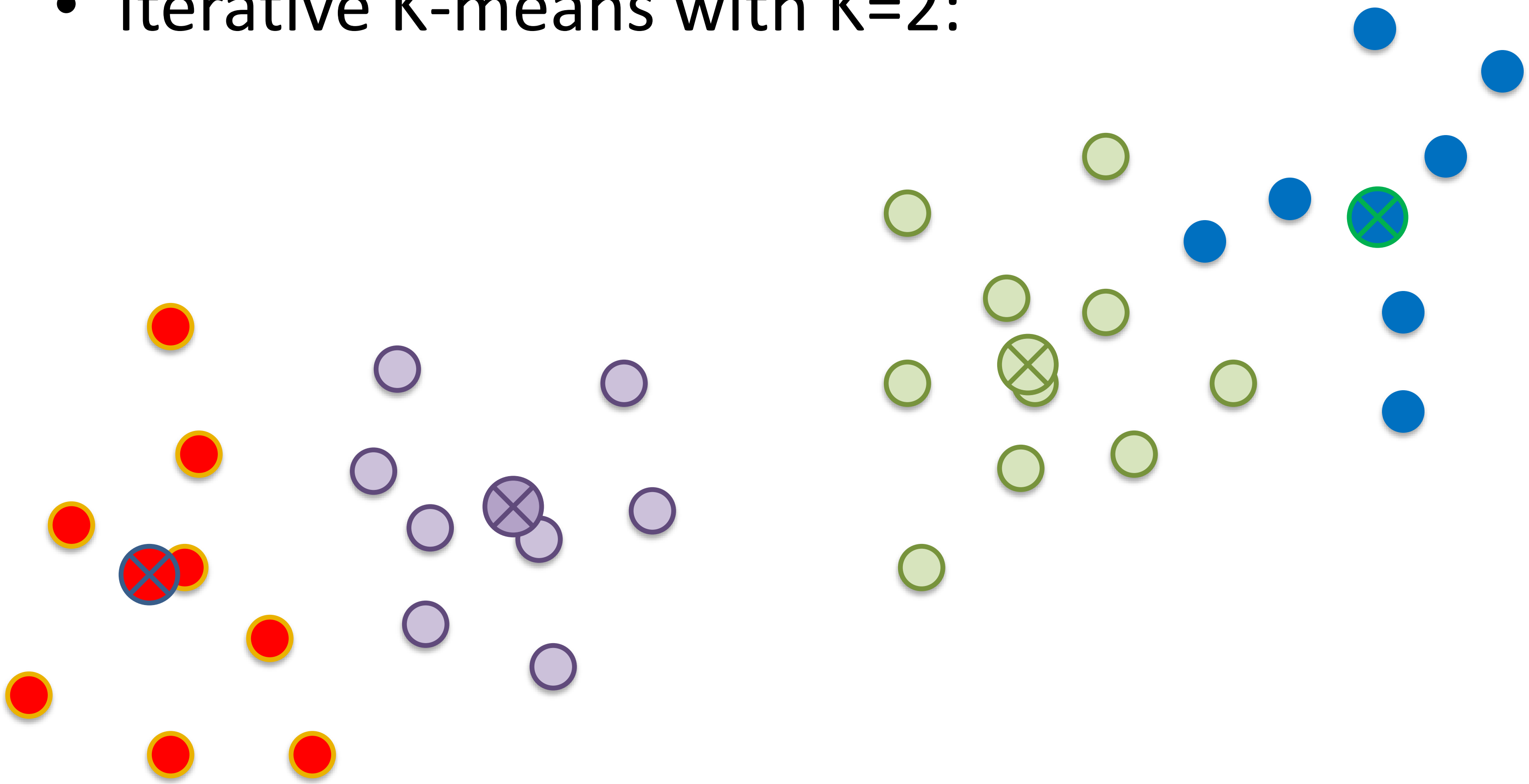
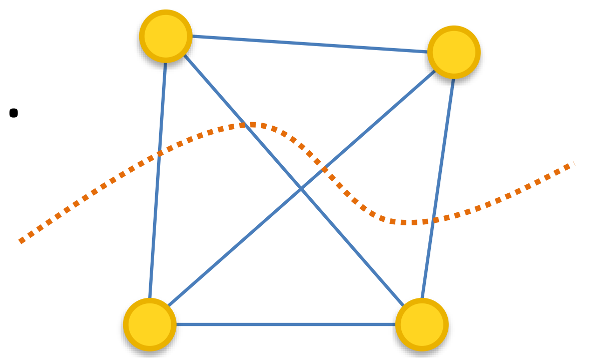


Other clustering approaches: Spectral clustering

- A good clustering algorithm will produce
  - Low intra-cluster distances.
  - High inter-cluster distances.
- Finding such a clustering is NP-hard.



- Spectral clustering approximates the above objective and form a clustering by solving an approximate optimization problem.
- Uses a graph representation of data.

Supervised, unsupervised, semi-supervised learning

- Supervised learning
  - learn from labelled examples:

$$D = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^N, y^N)\}$$

Pairs of input and the corresponding desired output.

- Unsupervised learning
  - learn from unlabelled examples:

$$D = \{\mathbf{x}^1, \dots, \mathbf{x}^N\}$$

Input data only; no desired outputs.

Supervised, unsupervised, semi-supervised learning

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Pairs of input and the corresponding desired output.

- Unsupervised learning
  - learn from unlabelled examples:

$$D = \{\mathbf{x}^1, \dots, \mathbf{x}^N\}$$

Input data only; no desired outputs.

- Semi-supervised learning
  - learn from labelled examples:

$$D = \{(\mathbf{x}^1, y^1), \dots, (\mathbf{x}^N, y^N)\}$$

and unlabelled examples:

$$U = \{\mathbf{x}^{N+1}, \dots, \mathbf{x}^{N+U}\}.$$

Semi-supervised Learning

- In semi-supervised learning, we are given labeled data points

$$D = \{(\mathbf{x}^1, \boxed{y^1}), \ldots, (\mathbf{x}^N, \boxed{y^N})\}$$

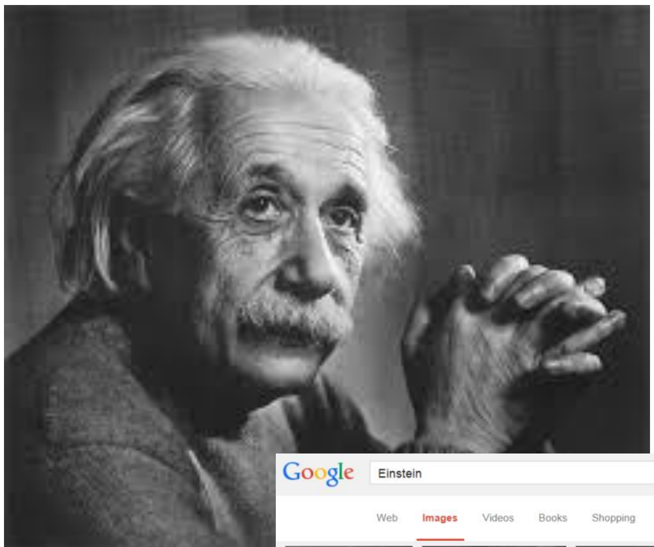
as well as unlabeled data points

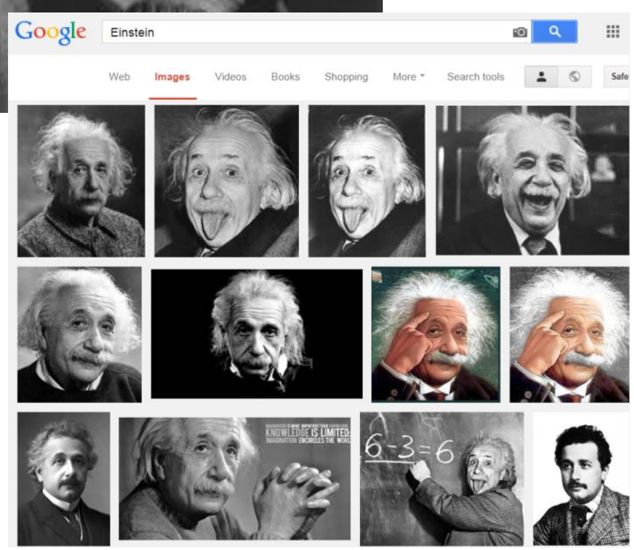
$$U = \{\mathbf{x}^{N+1}, \ldots, \mathbf{x}^{N+1}\}.$$

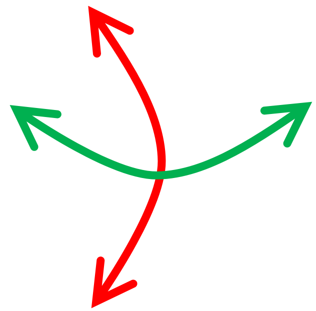
- Our task is to assign labels to U.

Sometimes, called *transductive learning*.

Why semi-supervised learning?



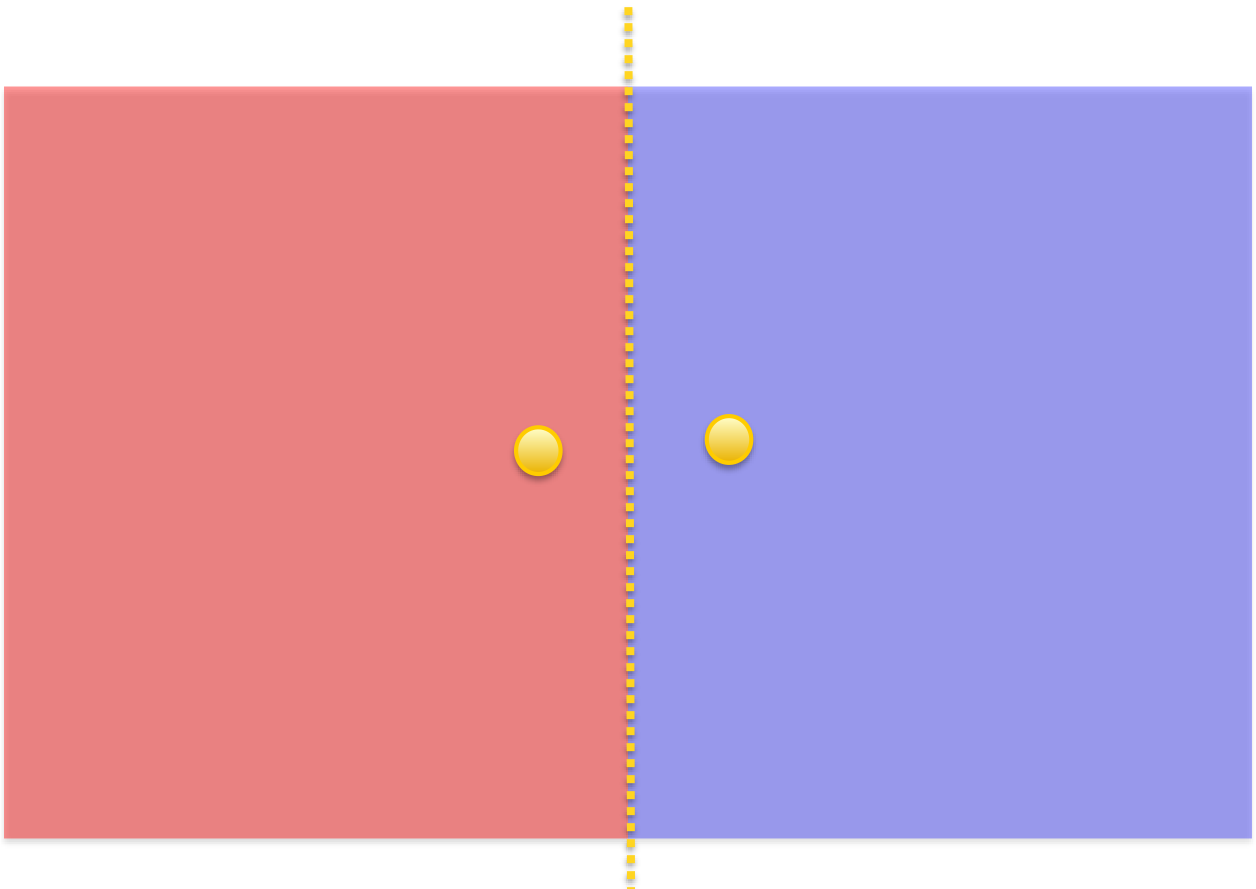




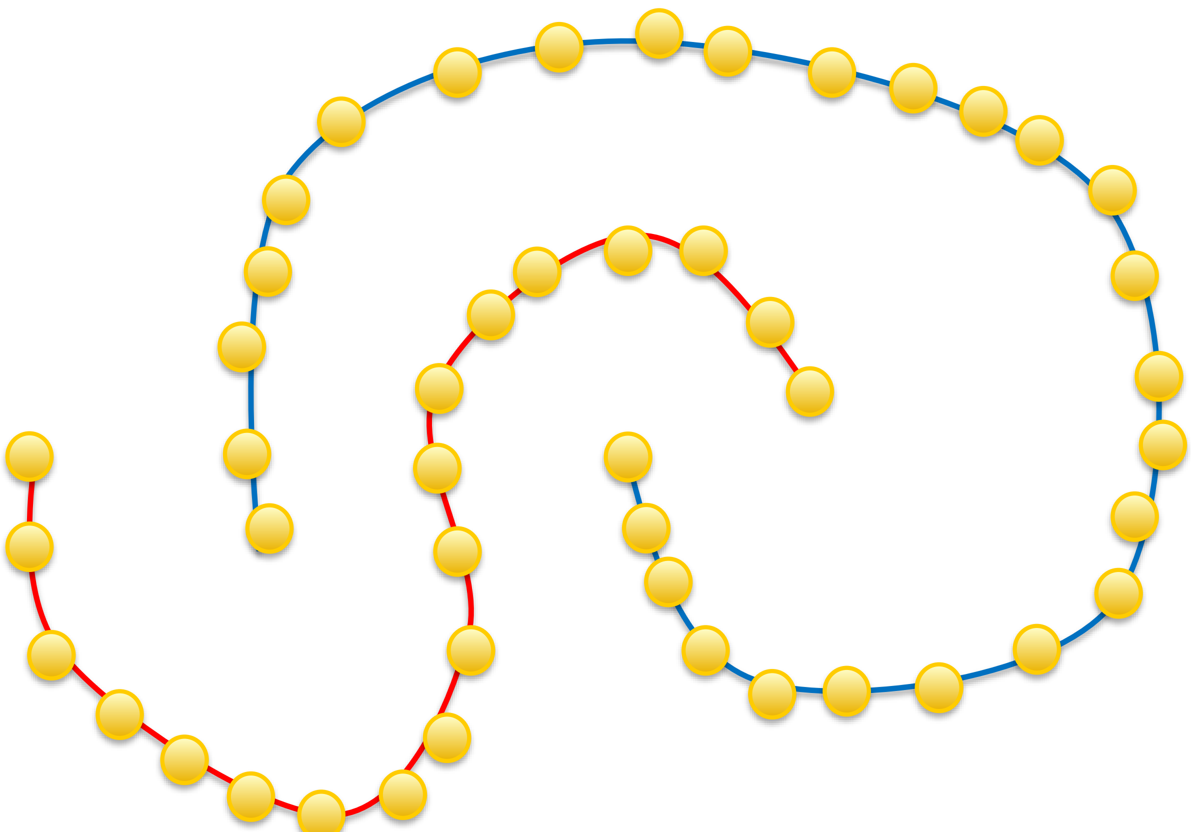
Sometimes, labeling data is difficult; costly.

Obtaining unlabeled data points is easier!

Why semi-supervised learning?

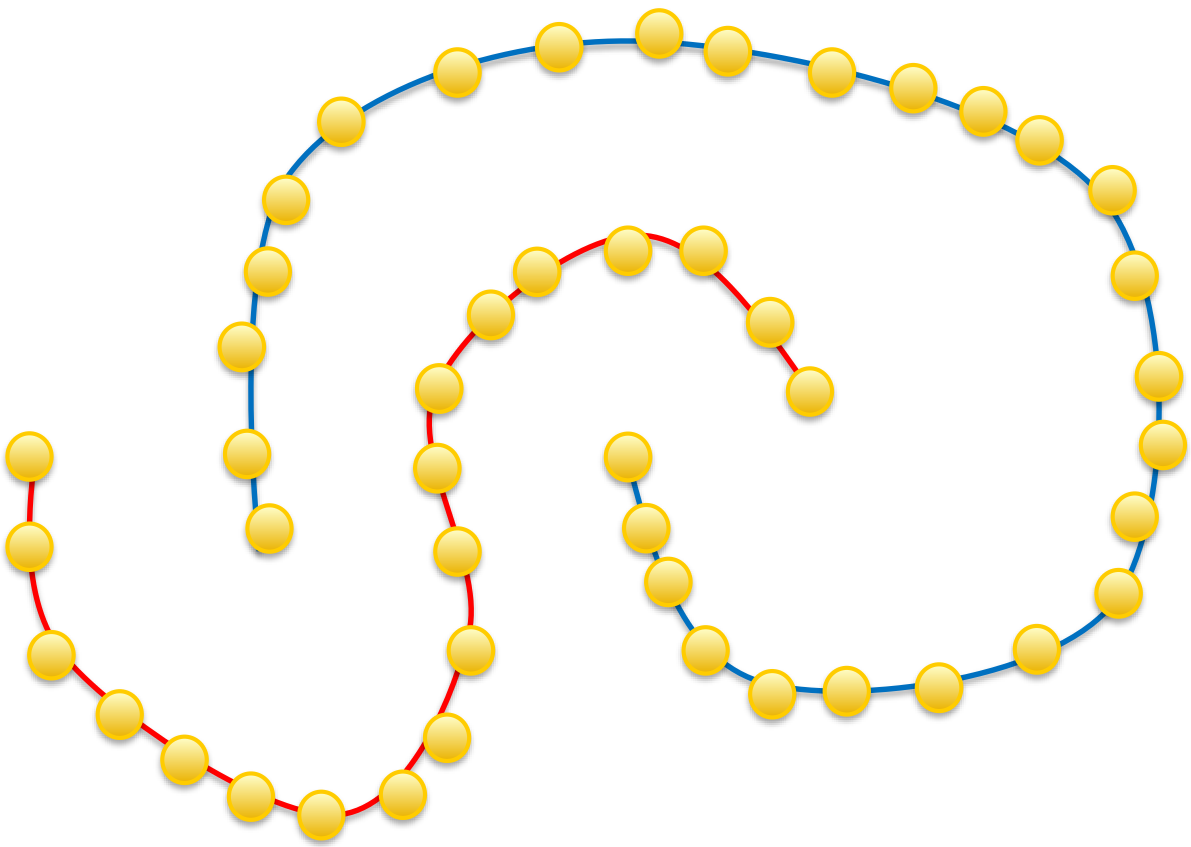


Why semi-supervised learning?



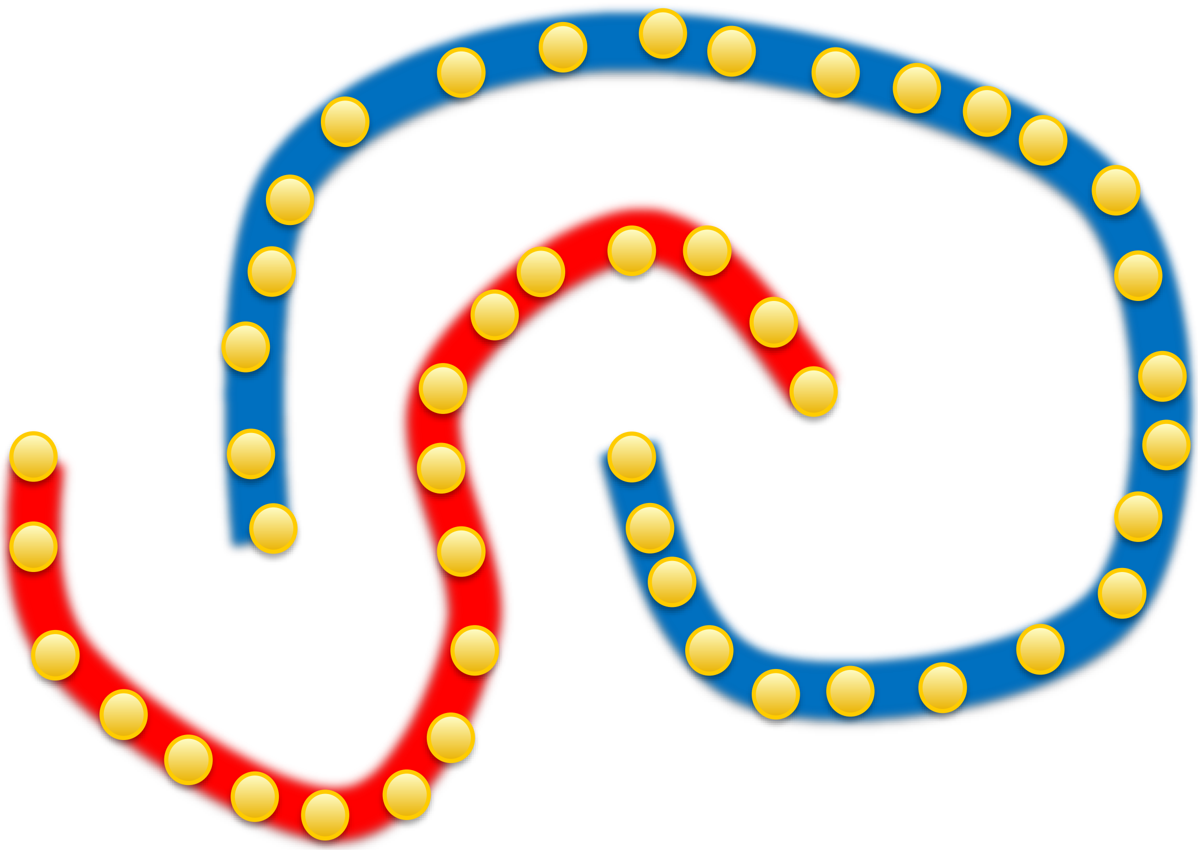
Unlabeled data can provide information on the underlying data generation process.

How to solve semi-supervised learning?



Manifold assumption:
Data are lying on
manifolds.

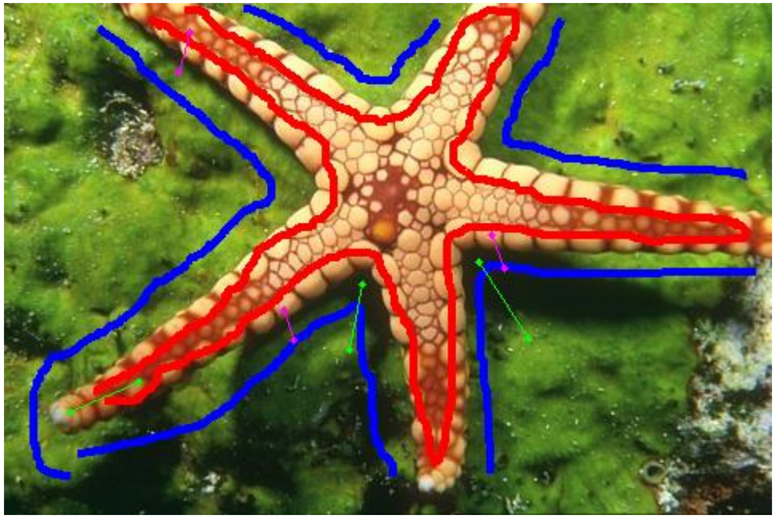
How to solve semi-supervised learning?

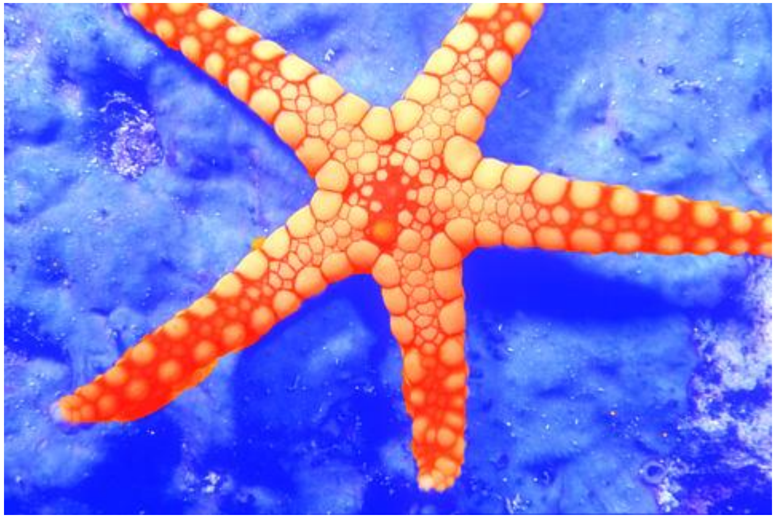


Cluster assumption:
A decision boundary should lie on a low-density region.

Applications: Image colorization

Applications: Interactive image segmentation





Slides references

- David Sontag, *Clustering*, lecture slides.
- Wikipedia article on clustering.