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3253 - Analytic Techniques and Machine Learning

Module 4: Clustering and Unsupervised Learning

Course Plan

Module Titles
Module 1 – Introduction to Machine Learning
Module 2 – End to End Machine Learning Project
Module 3 – Classification
Module 4 – Current Focus: Clustering and Unsupervised Learning
Module 5 – Training Models and Feature Selection
Module 6 – Support Vector Machines
Module 7 – Decision Trees and Ensemble Learning
Module 8 – Dimensionality Reduction
Module 9 – Introduction to TensorFlow
Module 10 – Introduction to Deep Learning and Deep Neural Networks
Module 11 – Distributing TensorFlow, CNNs and RNNs
Module 12 – Final Assignment and Presentations (no content)

Learning Outcomes for this Module

- Distinguish and describe unsupervised learning
- Identify clustering concepts
- Become familiar with clustering algorithms:
  k-means, DBSCAN, hierarchical

Topics for this Module

- **4.1** Unsupervised learning
- **4.2** Clustering
- **4.3** k-Means clustering
- **4.4** DBSCAN clustering
- **4.5** Hierarchical clustering
- **4.6** Resources and Wrap-up

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Module 4 – Section 1

Unsupervised Learning

Supervised vs. Unsupervised Learning

- Algorithms used to build classifiers need supervised data examples
- The input data to the learner consists of examples $(x_1, y_1), \dots (x_n, y_n)$
- An example (x_i, y_i) shows the correct response y_i to the input x_i
- In unsupervised ML the learner does not have labels, only examples $x_1, \dots, x_n$

Unsupervised Learning

- A clustering algorithm will still produce an output $C(x) = c$ given an input x
- However, there is no way to know if the output is correct or not
- The learning algorithm does not optimize a cost function based on labels
- But some classification algorithms do optimize a cost function based on the input examples $x_1, \ldots, x_n$

Unsupervised Algorithms

- Tasks to consider:
  - Reduce dimensionality
  - Find clusters
  - Model data density
  - Find hidden causes

- Key utility
  - Compress data
  - Detect outliers
  - Facilitate other learning

Unsupervised Algorithms

- Approaches in unsupervised learning fall into three classes:
  - Dimensionality reduction: represent each input case using a small number of variables (e.g., principal components analysis, factor analysis, independent components analysis)
  - Clustering: represent each input case using a prototype example (e.g. k-means, mixture models)
  - Density estimation: estimating the probability distribution over the data space

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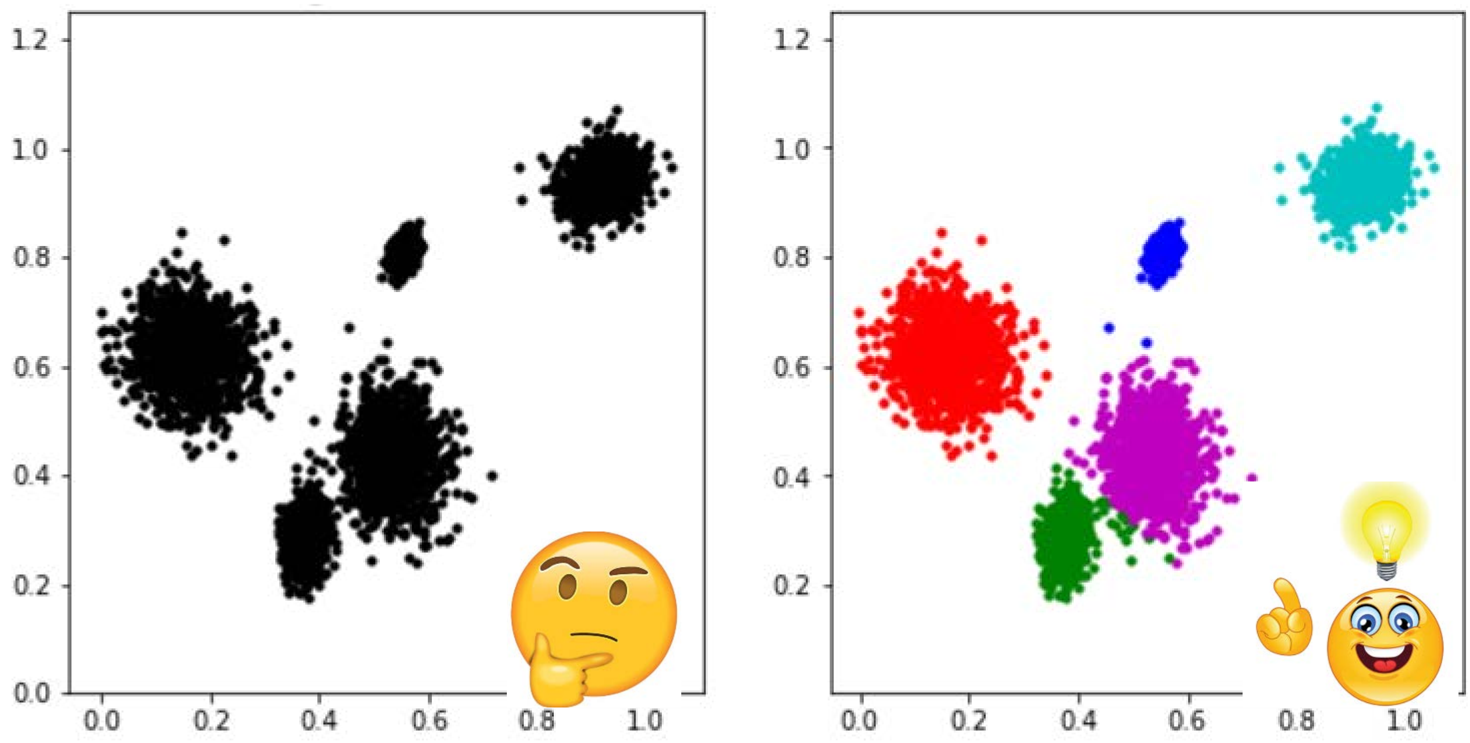
Module 4 – Section 2

Clustering

Clustering Goal

- The aim is to group points (examples) into a small number of clusters



Clustering Goal (cont'd)

- Similar examples should go to a same cluster; while different examples should be in different clusters
- There are many different clustering methods
- The clustering algorithm also learns how to assign a cluster to an example seen later
- Applications:
  - Automatic topic detection of documents
  - Customer segmentation
  - Variable selection

Clustering Algorithms

- Input: n vectors, m-dimensional, represent the objects to be clustered:
- Can start with object themselves (e.g. documents), but need a vector representation

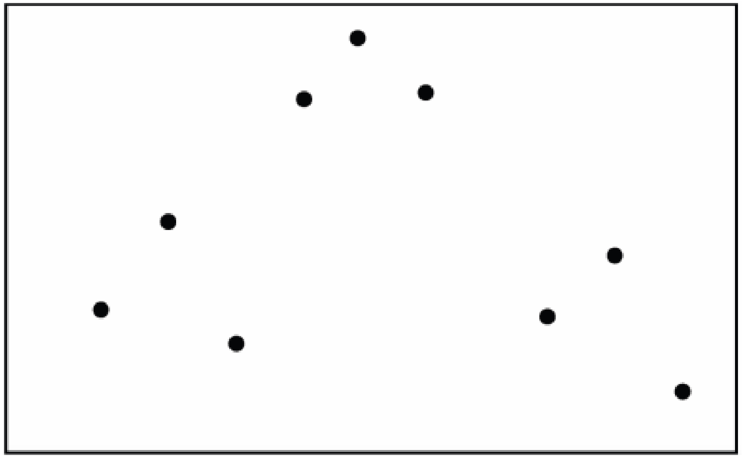
  Document → vector of word counts
- Vectors have same (fixed length) but clustering can be done over sequences of different length (the matrix of distances is needed)

More on Clustering

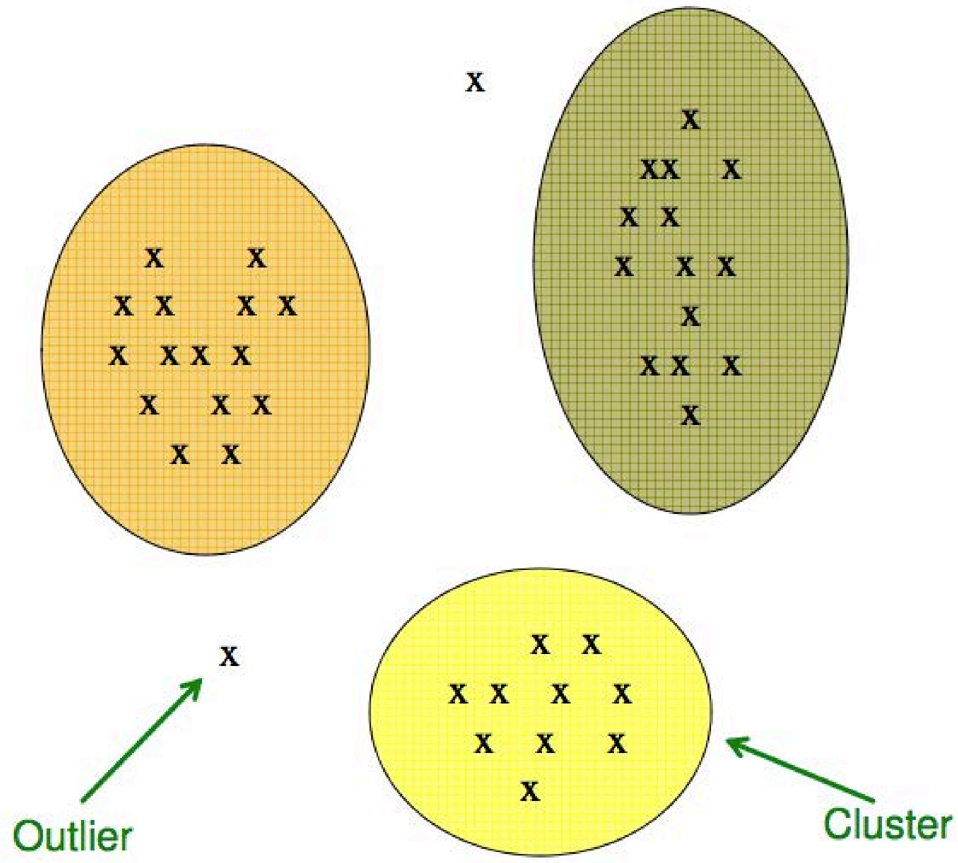
- Motivation: prediction; lossy compression; outlier detection
- We assume that the data was generated from a number of different classes. The aim is to cluster data from the same class together.
  - How many classes?
  - Why not put each datapoint into a separate class?
  - What is the objective function that is optimized by sensible clustering?

More on Clustering (cont'd)

- Assume the data {x(1), . . . , x(N)} lives in a Euclidean space, $x(n) \in Rd$
- Assume the data belongs to K classes (patterns)
- How can we identify those classes (data points that belong to each class)?



Clustering and Outliers



J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

Clustering and Feature Selection

- An important part of building models is feature selection
- Many variables could be available to predict a target, but many of them could carry no information about the target
- There are many method for feature selection: univariate methods, regularization, feature importance, etc.
- Clustering the features (columns, instead of rows) is a way to reduce the dimensionality by picking a representative on each cluster
- Python Scikit-Learn provides this with FeatureAgglomeration

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Module 4 – Section 3

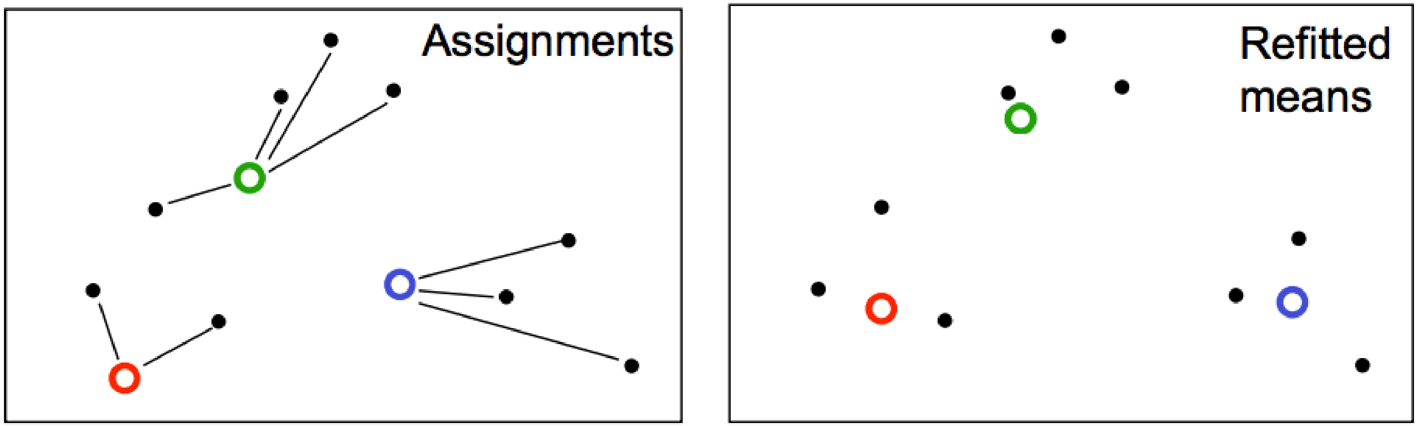
K-Means

k-means Algorithm

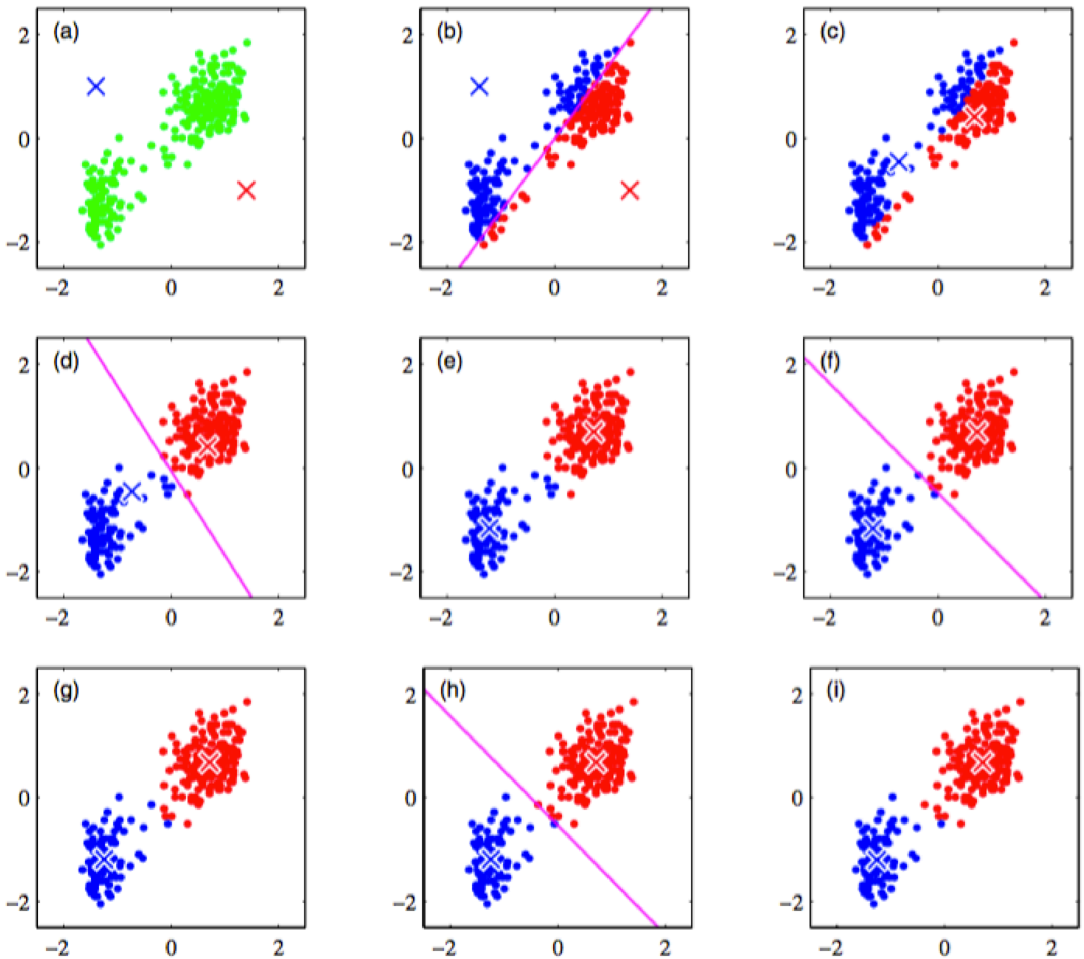
- Input: vectors $S = \{x^{(1)}, \dots, x^{(n)}\}$
  $k =$ number of desired clusters
- Output: a partition of S into k clusters, and the clusters' average (centroid)
- Goal: $S_1, \dots, S_k$ should minimize the square distances between each example x_i and its closest centroid $c(x_i)$: $\sum_{j=1}^{n} \left|\left|x_i - c(x_i)\right|\right|^2$
- Lloyd's algorithm finds (a good enough) solution

k-means

- Initialization: randomly initialize cluster centers
- The algorithm iteratively alternates between two steps:
  - Assignment step: Assign each data point to the closest cluster
  - Refitting step: Move each cluster center to the center of gravity of the data assigned to it



k-means (cont'd)



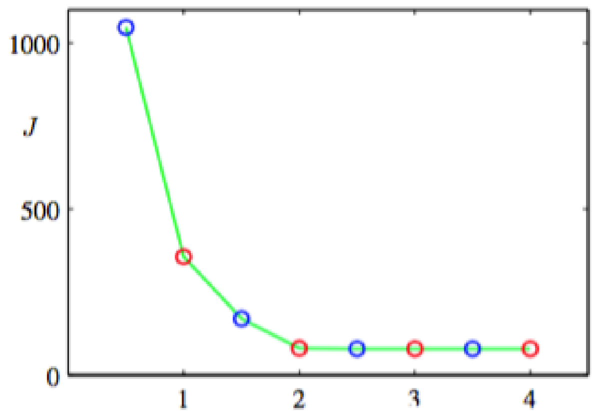


Figure 9.2 Bishop

Figure 9.1 Bishop

k-means Algorithm

- Steps:

  0) Start with a set of k centroids (random points from S)

  1) Assign each point to the centroid to which it is closest: this defines clusters

  2) Update the centroids as the mean within each cluster

  3) Repeat (1) and (2) until the centroids change is very small (threshold)

JavaScript implementation of K-means algorithm

K-means clustering animations

k-means Optimization

Find cluster centers m and assignments r to minimize the sum of squared distances of data points $\{x^{(n)}\}$ to their assigned cluster centers

$$\min_{\{\mathbf{m}\},\{\mathbf{r}\}} J(\{\mathbf{m}\},\{\mathbf{r}\}) = \min_{\{\mathbf{m}\},\{\mathbf{r}\}} \sum_{n=1}^{N}\sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

$$\text{s.t.} \sum_k r_k^{(n)} = 1, \forall n, \quad \text{where} \quad r_k^{(n)} \in \{0,1\}, \forall k, n$$

where $r_k^{(n)} = 1$ means that $x^{(n)}$ is assigned to cluster k (with center m_k)

k-means Algorithm

- k is a hyper-parameter: input to the algorithm. User specifies it.
- Sometimes the value for k is known for the application (e.g. the goal is to find 5 segments)
- The value of k can be data-driven:
  - inertia:
  - inertia/inertia2
  - silhouette

k-means for Image Segmentation

k-means Challenges

- High-dimensional spaces look different:
  - Almost all pairs of points are at about the same distance
- There is nothing to prevent k-means getting stuck at local minima.

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Module 4 – Section 4

DBSCAN Clustering

DBSCAN Clustering

- k-means clusters tend to be delimited by convex regions

- Both k-means and hierarchical clusters assign a cluster to every point
  - outliers are forced to belong to a cluster

DBSCAN Clustering (cont'd)

- DBSCAN is an algorithm that allows:
  - clusters with non-convex shapes
  - outlier detection
- Other algorithms allow non-convex shaped clusters:
  - agglomerative with ward linkage
  - spectral clustering
- Demo:

DBSCAN Clustering (cont'd)

- Parameters:
  - *min_samples* (non-negative integer)
  - *epsilon* (positive number)
- A core point is a point that has at least *min_samples* points within *epsilon* distance
- Core points are determined first
- Core points belonging to a cluster are computed iteratively:
  - take a core point
  - find all core points within *epsilon* distance
  - repeat until no more core points exist within *epsilon*
  - continue creating other clusters until no core points exists
- Non-core points:
  - Add to each cluster non-core points within *epsilon* distance from a core point
- Points that do not belong to any cluster are outliers
- Note that the number of clusters is not decided by the user

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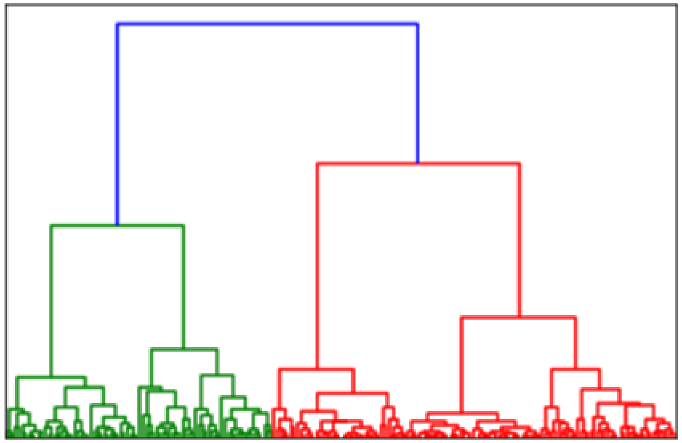
Module 4 – Section 5

Hierarchical Clustering

Hierarchical Clustering

- A bottom-up hierarchical clustering starts with as many clusters as points, and merges them iteratively
- Steps:
  - 0) Make each data point a distinct cluster
  - 1) Find the two closest clusters and merge them
  - 2) Repeat (1) until all points belong to one single cluster



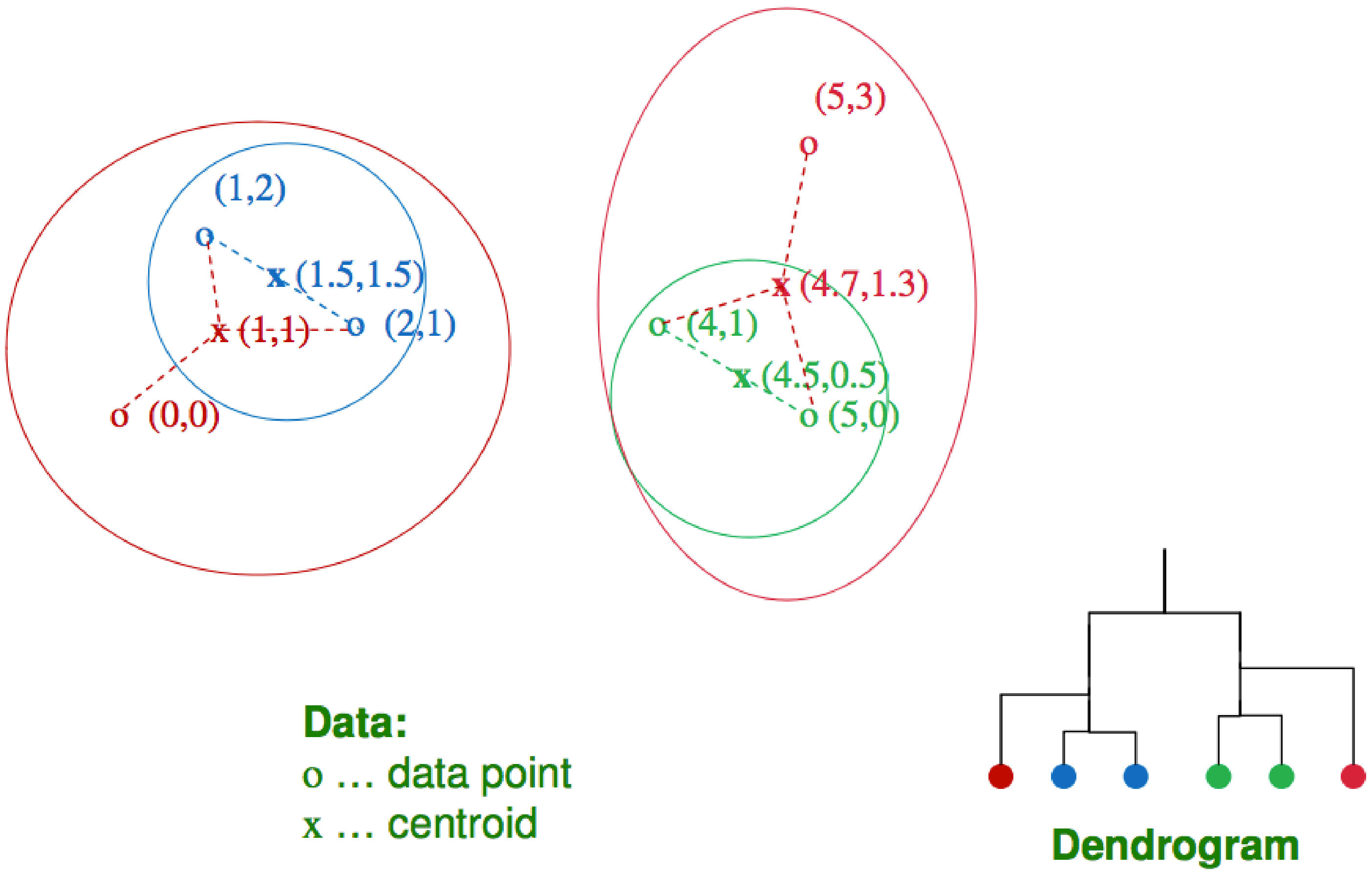
Hierarchical Clustering (cont'd)

- Key operation: Repeatedly combine two nearest clusters
- How to represent a cluster of many points?
  - Key problem: As you merge clusters, how do you represent the "location" of each cluster, to tell which pair of clusters is closest?
  - Euclidean case: each cluster has a centroid = average of its (data) points
- How to determine "nearness" of clusters?
  - Measure cluster distances by distances of centroids

Hierarchical Clustering (cont'd)

- There are different ways to determine the 2 clusters that are joined in each step:
  - Ward's method: minimize variance
  - average: minimize average distance between every pair of points (one in each cluster)
  - complete: minimize maximum distance between a pair of points, one in each cluster
- The user decides the number of clusters to use

Hierarchical Clustering Example



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Module 4 – Section 6

Resources and Wrap-up

Resources

- Clustering:
- Data Science from Scratch, Joel Grus
- An Introduction to Statistical Learning, James, G.; Witten, D.; Hastie, T.; Tibshirani, R

Homework

- Complete the notebook in the assignments section for this week
- Submit your solution here
- Make sure you rename your notebook to
  - W4_UTORid.ipynb
  - Example: W4_adfasd01.ipynb

Next Class

- Training Models and Features Selection
- Reading Hands-on ML (Chapter 4)

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Any questions?

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Thank You

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