CS M146: Introduction to Machine Learning
Clustering

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The instructor gratefully acknowledges Sriram Sankaraman (UCLA) for some of the materials and organization used in these slides, and many others who made their course materials freely available online.

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Unsupervised Learning

- Supervised learning used labeled data pairs (**x**, y) to learn a function $f : X \rightarrow Y$
  - But, what if we don't have labels?

- No labels = **unsupervised learning**
- Only some points are labeled = **semi-supervised learning**
  - Labels may be expensive to obtain, so we only get a few

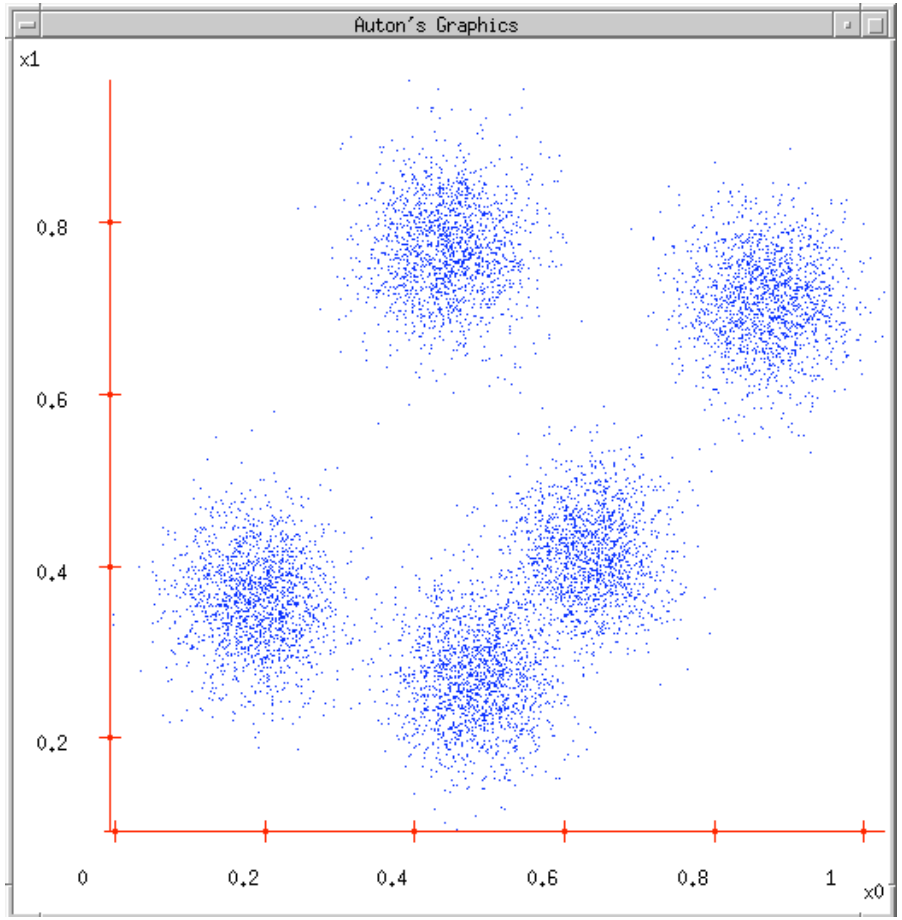
- **Clustering** is the unsupervised grouping of data points. It can be used for **knowledge discovery**.

k-means Clustering

Some material adapted from slides by Andrew Moore, CMU.

Visit http://www.autonlab.org/tutorials/ for
Andrew's repository of Data Mining tutorials.

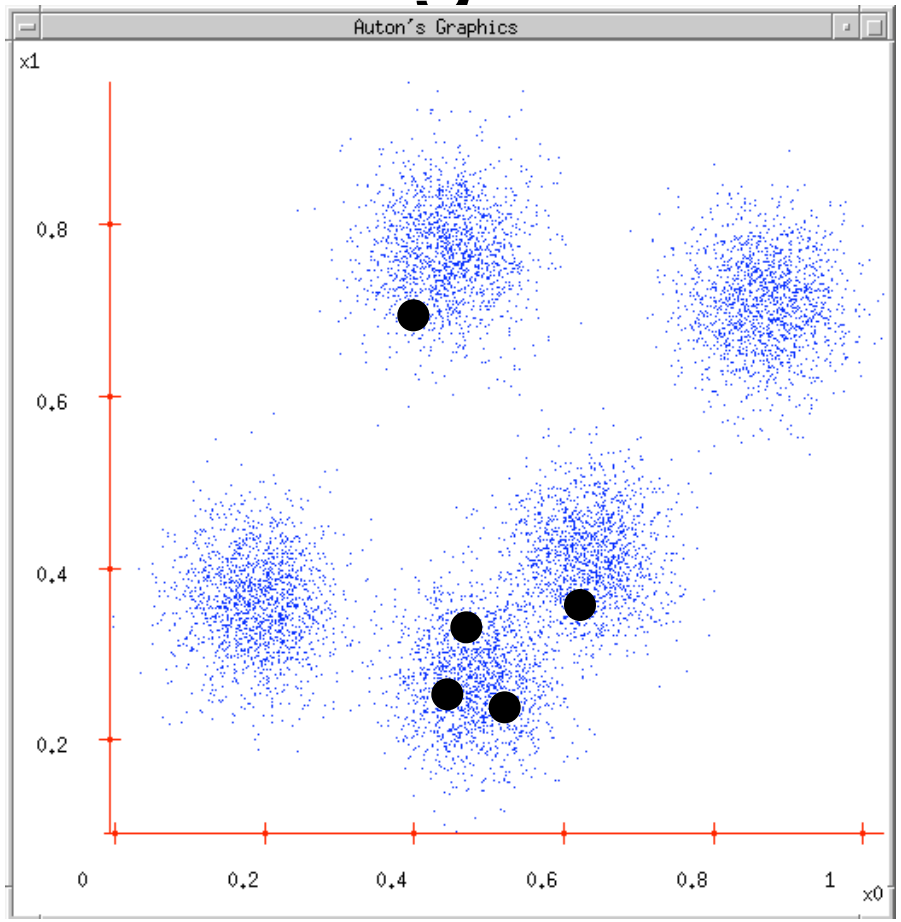
Clustering Data



k-means Clustering

k-means(k, X)

- Randomly choose k cluster center locations (centroids)
- Loop until convergence
  - Assign each point to the cluster of the closest centroid
  - Re-estimate the cluster centroids based on the data assigned to each cluster



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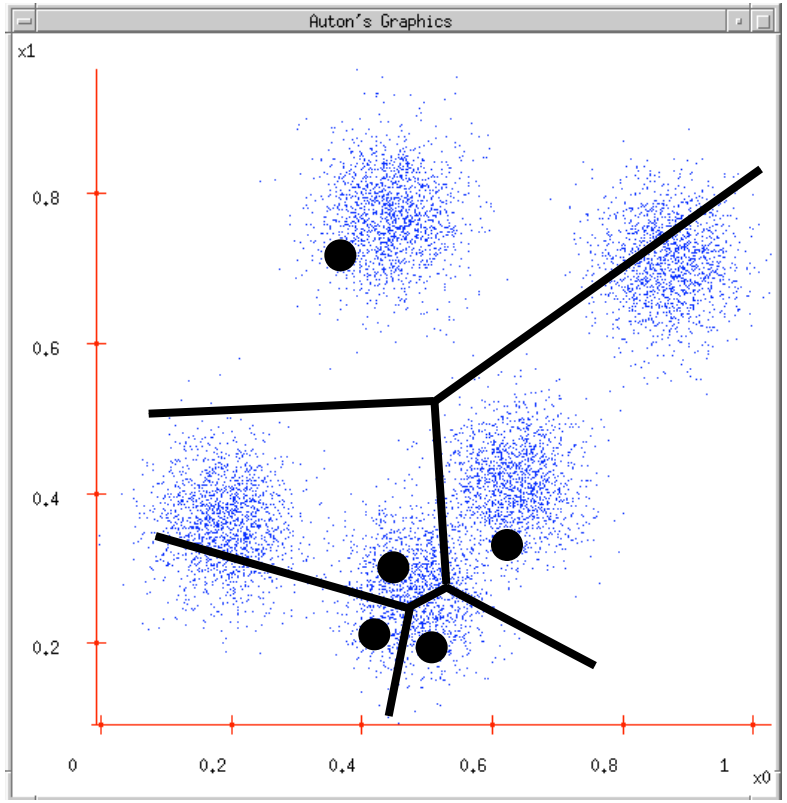

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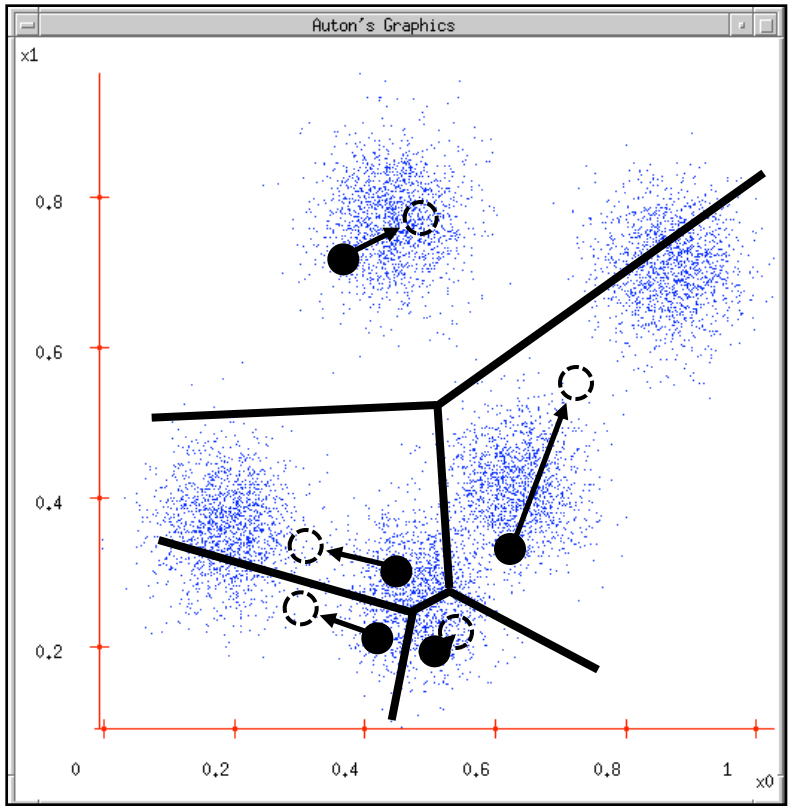
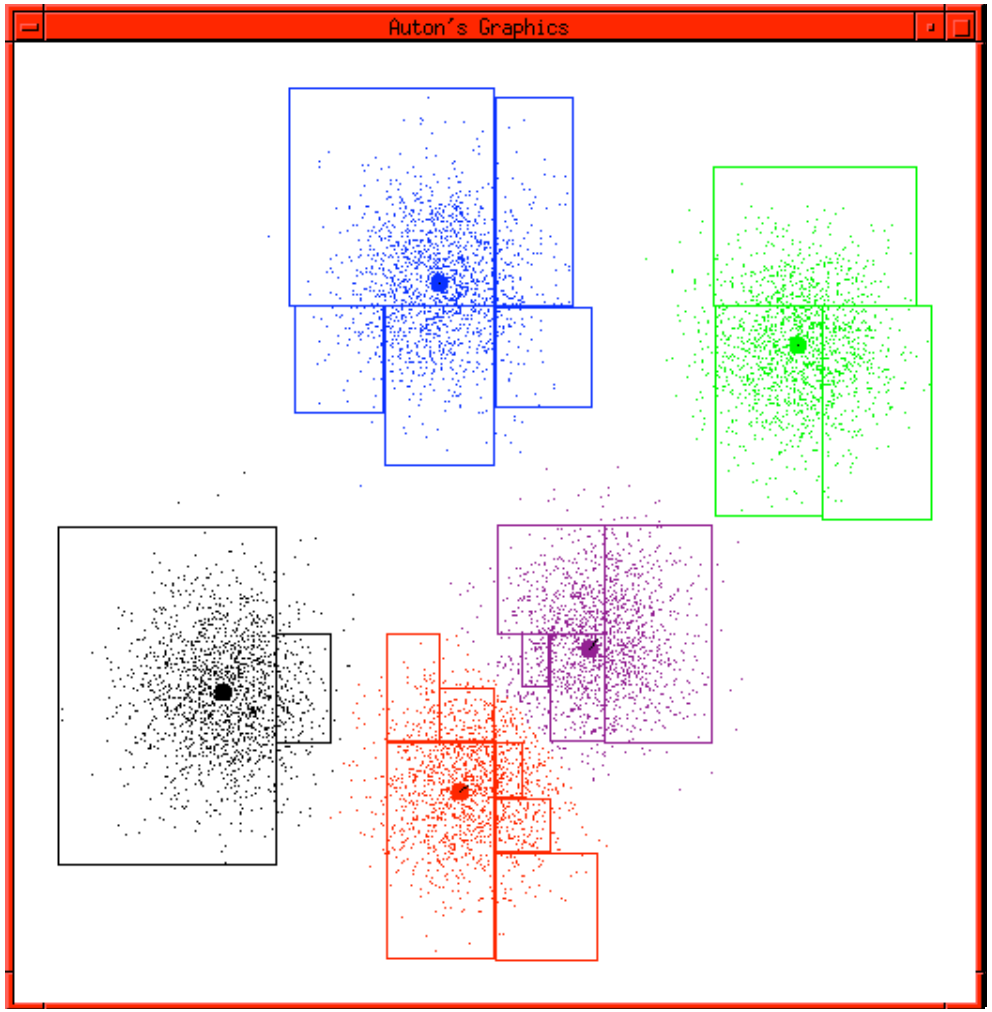


k-means Animation



Example generated by Andrew Moore using Dan Pelleg's super-duper fast k-means system:

Dan Pelleg and Andrew Moore. Accelerating Exact k-means Algorithms with Geometric Reasoning. Proc. Conference on Knowledge Discovery in Databases 1999.

Pseudocode

Inputs: Training set of n datapoints $\{\boldsymbol{x}^{(i)}\}$, number of clusters k

- **Step 1:** Initialize cluster centroids $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \cdots, \boldsymbol{\mu}_k$
- **Step 2:**

    Loop until convergence: {

        For every point i, assign it to a cluster

        $$c_i := \arg\min_j \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j \right\|_2^2$$

        For every cluster j, re-estimate its centroid

        $$\boldsymbol{\mu}_j := \frac{\sum_{i=1}^{n} 1\{c_i = j\} \boldsymbol{x}^{(i)}}{\sum_{i=1}^{n} 1\{c_i = j\}}$$

    }

Output: clusters for training points $c_{1:n}$, cluster centers for test points $\boldsymbol{\mu}_{1:k}$

k-means Objective Function

- k-means optimizes the following objective function:

$$\arg\min_{\boldsymbol{S}} \sum_{i=1}^{k} \sum_{\boldsymbol{x} \in S_i} \|\boldsymbol{x} - \boldsymbol{\mu}_i\|_2^2$$

  where $\boldsymbol{S} = \{S_1, \cdots, S_k\}$ is a partitioning over $X = \{x^{(1)}, \cdots, x^{(n)}\}$ such that $X = \cup_{i=1}^{k} S_i$ and $\boldsymbol{\mu}_i = \text{mean}(S_i)$

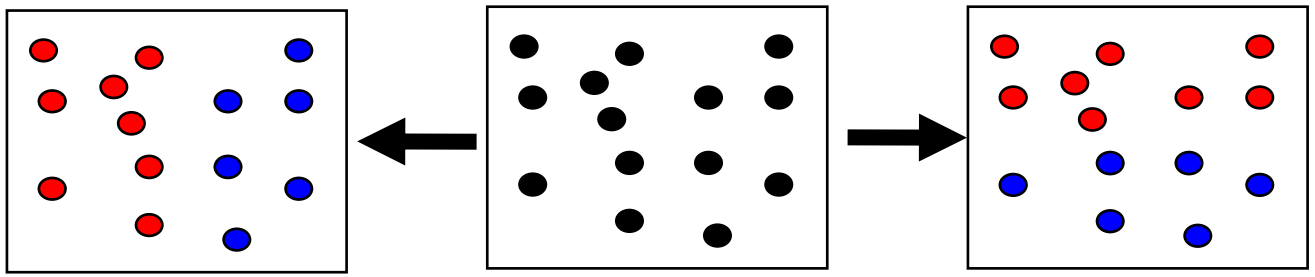
- Non-convex optimization problem. Solving it is NP-hard
- Convergence criteria for k-means: no change in objective value
- k-means is guaranteed to converge to a local optima
  - Worst case: Exponential in the number of data points
  - In practice, very fast to converge

Problems with k-means

- Very sensitive to the initial points
  - Do many runs of k-means, each with different initial centroids
- Must manually choose k
  - Validating the optimal k is not direct
    - Note that this requires a downstream performance measure
- Sensitive to outliers
  - k-median: Instead of computing mean in Step 2, compute median

Evaluating Clustering

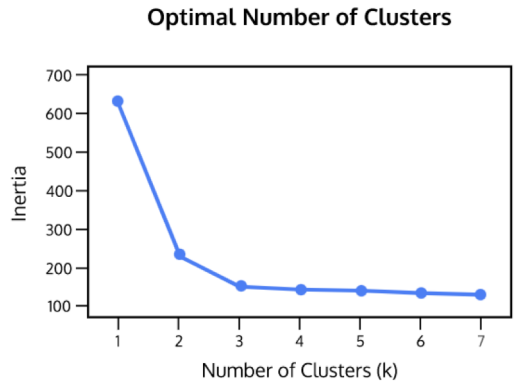
- Ambiguity in evaluating clustering. Which cluster is better?



- Performance metrics of clustering are often tied to a downstream task
  - E.g., human interpretability, classification (requires labels)

Evaluating Clustering

- Unsupervised evaluation: Low inertia **and** low k is desirable
  - **Inertia:** Sum of squared distances of datapoints to cluster centers
  - Tradeoff with number of clusters k: As k increases, inertia decreases



- Rule of thumb: choose k at which drop in inertia slows down (e.g., k=3 in the above figure)

Summary

- k-means clustering

    Hard assignment of points into k clusters

    Alternates between cluster assignment and centroid estimation

    Evaluation is tricky