Data Mining: Clustering and Prediction

Mirek Riedewald

Key Learning Goals

- What is the difference between supervised and unsupervised learning?
- Give an example for a supervised learning algorithm.
- Give an example for an unsupervised learning algorithm.

Key Learning Goals

- Write the pseudo-code for K-means clustering in MapReduce.
- Will the Spark implementation of K-means be significantly faster than the MapReduce implementation? Justify your answer.
- For decision-tree training, explain the parallel counting algorithm for a given set of possible split point candidates using an example.

Introduction

- Data mining can be concisely characterized as "statistics plus computers." Its goals are similar to those of statistical analysis, but the availability of massive computing power enabled novel types of automatic algorithms.
- Han et al. point out that the goal of data mining is the extraction of interesting (non-trivial, implicit, previously unknown and potentially useful) patterns or knowledge from a huge amount of data. [source: Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques, 3rd edition, Morgan Kaufmann, 2011]

Example Applications

- Classification, prediction
  - Will a customer's review of a product be affected by the earlier reviews?
  - Is the incoming credit-card transaction legitimate or fraudulent?
  - What is the probability of observing bird species X, given time of day, weather, climate, human population features, and habitat features?
  - Identify sub-atomic particles from measurements of energy levels in a collider.
  - Predict the income from an ad shown by a search engine for a given keyword search query.
  - Is this email spam or not?
  - How likely is this bank customer to repay the mortgage?
- Clustering
  - What are the main customer groups and what characterizes each group?
  - What are the main categories of users of an online game?
  - Identify groups of viruses with genetic similarity, which are different from other groups of viruses.
- Graph mining
  - How does information spread in a social network?
  - Which people are likely to collaborate in the near future?
  - Which communities do users belong to?
- Association rules
  - What products do people tend to purchase together?

Typical Data Mining Steps: 1. Data Preparation

- In practice, the preparation phase can often take much longer and require more resources than the actual mining phase. There are two major preparation steps: (1) understanding data and domain, and (2) cleaning and pre-processing the data.
- For data mining and its results to be meaningful, the data miner must understand the domain and the given data. This generally requires close collaboration with a domain expert.
  - Understanding the data requires knowing the attributes, their types, and meaning. This includes peculiarities like the encoding of missing data.
  - Summary statistics such as min, max, mean, standard deviation, and quantiles provide valuable insight about the data distribution.
  - Histograms summarize one- and multidimensional distributions, helping uncover skew and correlations.
  - Further insights about relationships between different attributes can be obtained from data summaries such as scatterplots and correlation coefficients.
  - Knowledge about statistical interactions between attributes (called variables in statistics) helps the data miner decide which attributes should be explored jointly, and which can be studied separately.

Typical Data Mining Steps: 1. Data Preparation (Cont.)

- Once the data and problem are sufficiently understood, usually the data needs to be cleaned and pre-processed before data mining can commence.
  - Data cleaning often addresses noise and missing values. A common data-cleaning challenge is to fix the encoding of missing values. Sometimes there exists an explicit NULL value, in other cases it might be encoded as -99, e.g., for an attribute like age for which it is known that negative values are invalid.
  - Data often needs to be integrated from multiple sources. In addition to joining the data, this may require entity resolution. For example, an author might appear as Amy Smith, A. Smith, or Amy B. Smith in different contexts.
  - Depending on problem and data mining method, it might be necessary or beneficial to apply data reduction and transformation such as normalization, Principal Components Analysis, Wavelet transform, Fourier transform, or attribute removal.

Typical Data Mining Steps: 2. Mining the Data

- After proper data preparation, data mining techniques extract the desired information and patterns.
  - For classification and prediction problems, first a model is trained on a subset of the given *labeled* data. Model quality is evaluated on a separate test set. Then the model is used on new inputs to predict the desired output.
    - Popular techniques are decision tree, Random Forest, SVM, artificial neural network (Deep Learning), Bayesian approaches, regression, and boosting.
  - Clustering algorithms such as K-means, hierarchical clustering, and density-based clustering are used to identify groups of similar entities that are different from other groups.
  - Frequent-pattern mining is concerned with identifying frequent itemsets, association rules, and frequent sequences.

Typical Data Mining Steps: 3. Post-Processing

- A data mining model on its own usually is not intelligible. Hence additional tools are used to determine and present what was learned from the data.
- For classification and prediction, there are many possible post-processing tasks:
  - To evaluate the quality of a prediction model, its accuracy or error rate on data representing future input needs to be determined.
  - A classification or prediction model usually is a complex "blackbox" function that returns some output for a given input. Data analysts want to understand the big picture of what the model has learnt. This usually involves identifying (1) the most important variables and their effect on the output, (2) patterns indicating variable interactions, and (3) compact rules explaining the predictions.
- For clustering, analysts verify if the grouping makes sense based on their domain expertise. Usually this also involves finding compact labels or descriptions to express what the entities in the same cluster have in common.
- Visualization of results and patterns found is a powerful tool for humans to gain insights from data mining.

Example

- We take a closer look at Prof. Riedewald's Scolopax system for analysis of big observational data. Screenshots are from its application to a large high-dimensional data set containing reports of bird sightings in North America.
  - This project has been completed, but many other researchers are still working on related challenges.
- Scolopax relied on MapReduce to train models for predicting the probability of observing a species given input features such as location, time, habitat properties, climate features, human population properties and so on.
- Users access it through a standard Web browser. Requests are search queries for interesting patterns. These queries were also processed on a MapReduce cluster, but all results were managed in a distributed key-value store (HBase).

Strong-Trend Search

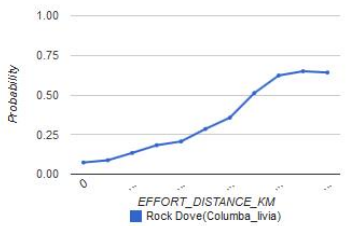
- In the example on the next page, Scolopax was used to identify attributes that potentially have a strong effect on the probability of observing a species.
  - Each plot summarizes the effect of the attribute shown on the x-axis.
  - This effect was computed separately for different attributes, different species, and different geographical regions.
- The summaries are presented to the user ranked by the strength of the estimated effect on the species-observation probability. Since the plots are managed in a key-value store, the user can then interactively browse the result or filter based on properties such as the attribute, species, or region of interest.

Scolopax Query Input | Results

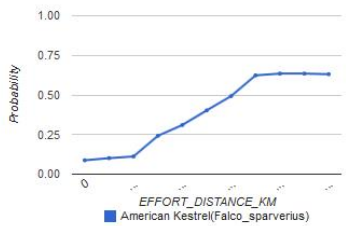
▶ Settings

▶ Filter Results

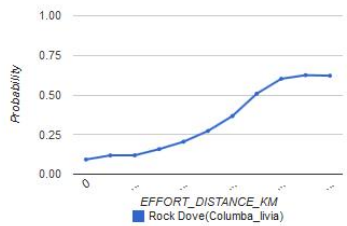
Score: 0.5760106504294036



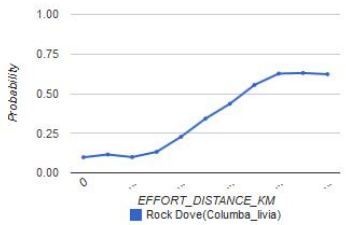
Score: 0.547130735269788



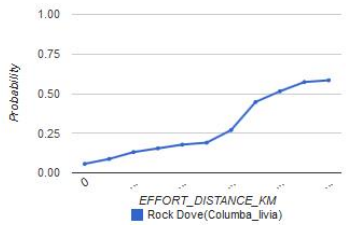
Score: 0.5324868819332683



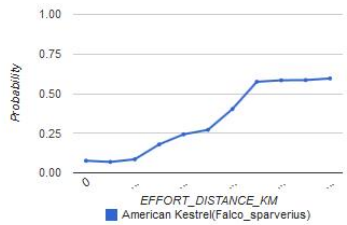
Score: 0.5317512785279156



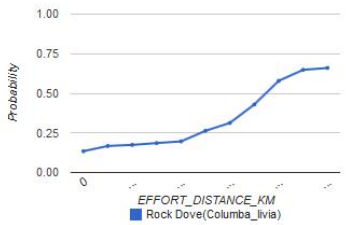
Score: 0.5275223482097153



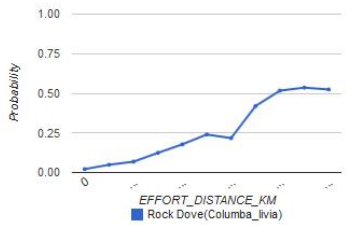
Score: 0.5267399291055254



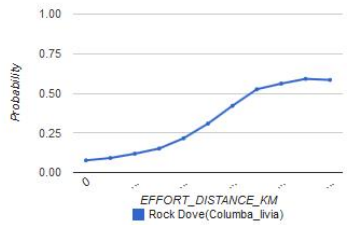
Score: 0.5255142895844727



Score: 0.5143709102805677



Score: 0.514300738939126



Page 1 of 1112 Next Page

Showing 1-9 of 10000 results.

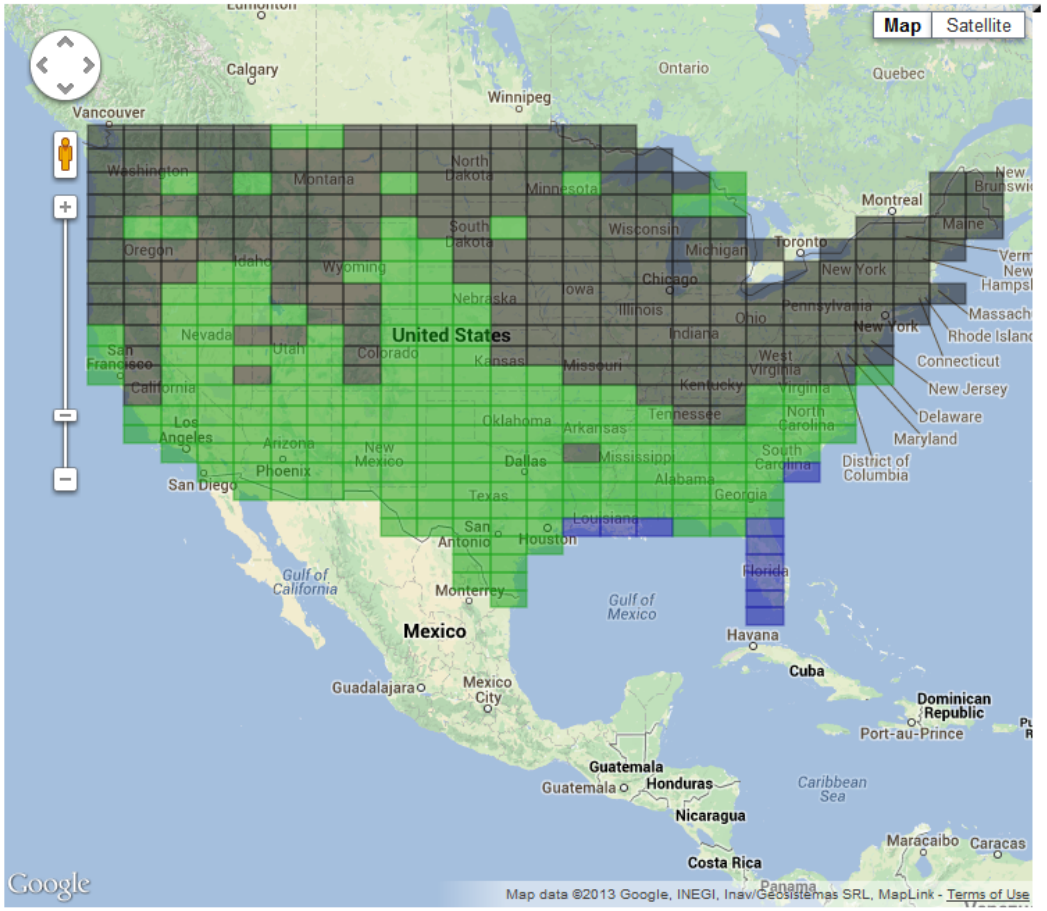
Dynamic-Pattern Discovery

- In the next example, Scolopax uses MapReduce to identify clusters of related summaries. Here clustering was applied to the annual trajectory of a species in different regions.
  - The trajectory is defined by the overall probability of observing the species in different months or weeks of the year.
- The clusters are based on trajectory similarity and do not take geographical location into account. Hence if identified clusters line up with large geographic regions, then they might indicate a pattern caused by some biological process. In the example, the 3 clusters show likely migration behavior:
  - Purple: The tree swallow spends the winter in the southern US (Florida, the Gulf coast, and South Carolina).
  - Green: In spring and fall it migrates north, crossing a horizontal band that ranges from California to the Carolinas.
  - Black: The tree swallow spends the summer in the northern US.

Scolopax Cluster Query Input | Results

<< Previous | Next >>

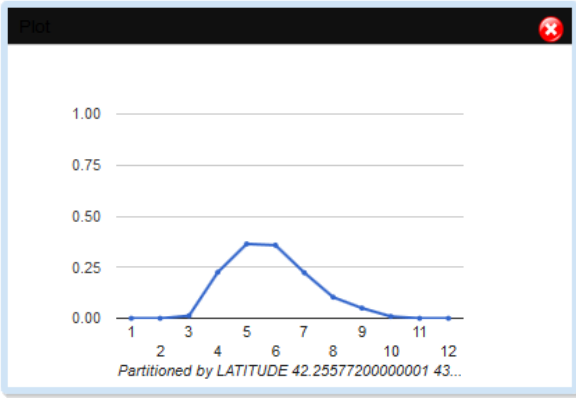
Species: Tachycineta_bicolor
Summary Attribute: MONTH

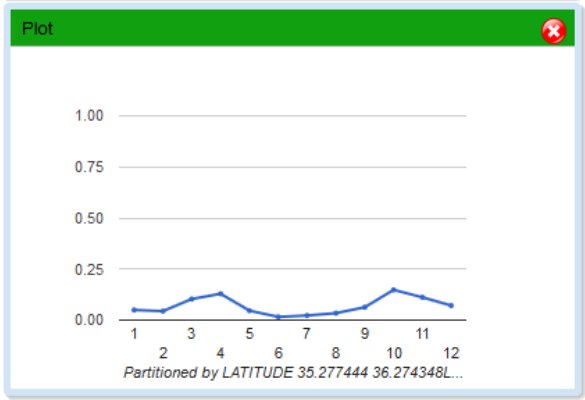


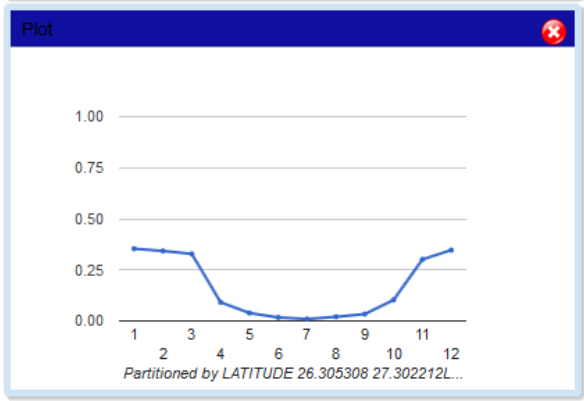
Predefined Queries

- TreeSwallow_US25by25_3clusters
- EastWoodPewee_US25by25_3clusters
- EastBlue_EastWoodPewee_25by25_4cluster
- All_10by20_4clusters

Add Query | Delete Query







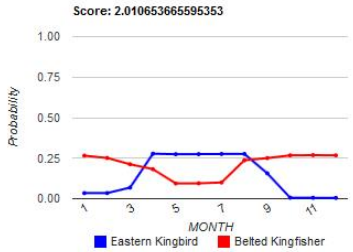
(Anti-)Correlation Search

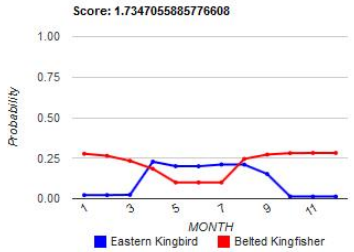
- In this last example, Scolopax relies on MapReduce join algorithms developed by Prof. Riedewald's group to identify relationships between species.
- The example is a join query that searches for pairs of plots with the following properties: the plots are on different species (eastern kingbird and belted kingfisher in the example), but on the same attribute of interest (month in the example) and the same geographical region (the red box on the map highlights one of them for the example).
- The join results are then ranked based on the dissimilarity of the two plots.
  - Note the interesting opposite trends in several of the top-ranked results. Seeing such a result helps the ornithologist identify possible hypotheses about migration patterns or habitat competition.
  - However, we must be careful about false discoveries!

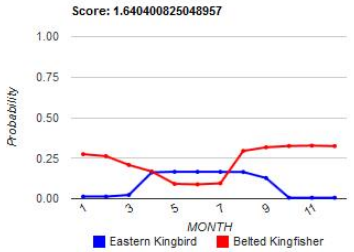
Scolopax Query Input | Results

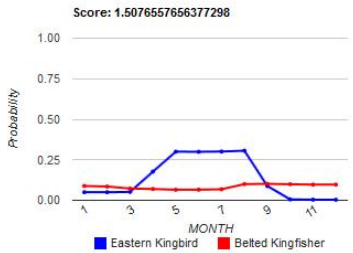
▶ Settings

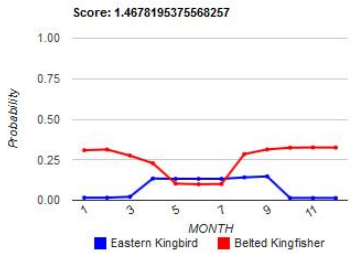
▶ Filter Results

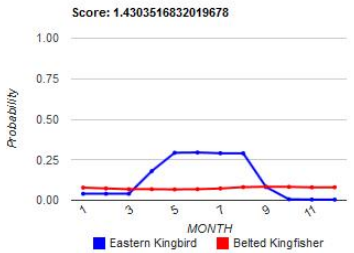


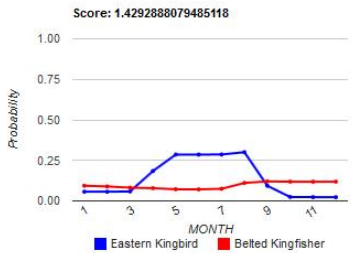


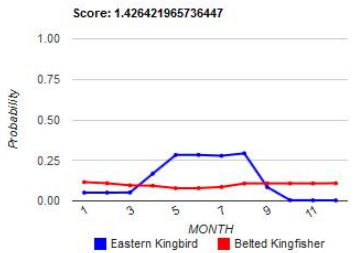


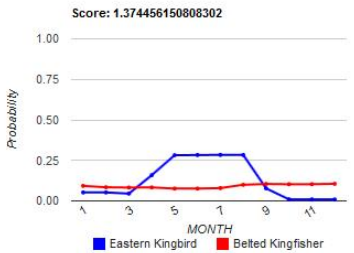












Page 1 of 223 Next Page

Showing 1-9 of 2000 results.

Important Note about Discovery

- Thanks to abundant data and powerful algorithms and hardware, it is now feasible to explore a huge space of possible patterns.
- This increases the risk of discovering spurious patterns, i.e., patterns that arose due to idiosyncrasies or coincidences in the data sample but are not representative of the true distribution.
  - For example, if we measure the ratios between width and height of buildings in Boston, we may find that some of them mirror the ratio of distances between some planets or stars. However, it is unlikely that the architect was indeed influenced by such celestial relationships…
- Scolopax will deliver both real and spurious patterns. It is then up to the domain experts to either (1) apply statistical approaches to limit the probability of false discoveries or (2) collect new data samples specifically designed to verify or refute a hypothesis derived from a discovered pattern.

Parallel Data Mining

- Many mature and feature-rich data mining libraries and products are available. This includes the R system and the Weka open-source Java library. Unfortunately, most data mining solutions are not designed for execution in large distributed systems. This often leaves only the following 3 options:

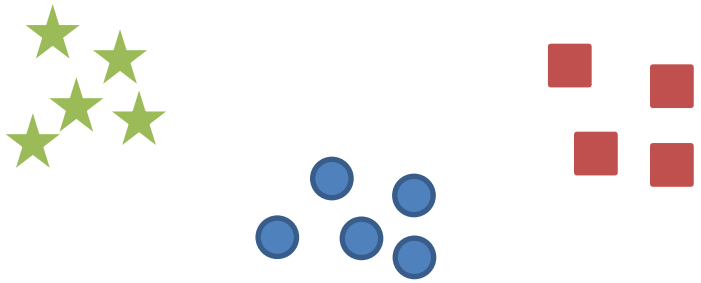
1. Use an existing, but often limited, library of distributed data mining solutions, e.g., Apache Mahout or Spark ML.
2. Design your own distributed version of a data mining algorithm and implemented it in MapReduce or Spark. This tends to be non-trivial, as many data mining algorithms are sophisticated and rely heavily on in-memory computation for performance.
3. Leverage existing mature libraries that were written for in-memory execution on a single machine by using them in a larger ensemble that can be trained and managed in a distributed system. Weka, which is open-source and written in Java, presents itself as an obvious choice for use in Hadoop.

Let us look at two popular types of data mining and machine learning: unsupervised learning and supervised learning.

We start with clustering, which is an unsupervised learning approach.

Clustering

- Clustering is one of the most popular dat mining approaches in practice, because it automatically detects “natural” groups or communities in big data. These clusters could be the end-result. Or they could be used to improve other data mining steps by customizing those steps depending on the cluster membership of an object of interest.
- In general, a cluster is a collection of data objects. The goal of clustering typically is to identify clusters such that objects are similar to one another within the same cluster, but dissimilar to the objects in other clusters.
- Clustering does not require any training data with known cluster membership. Hence it is considered an unsupervised learning method.



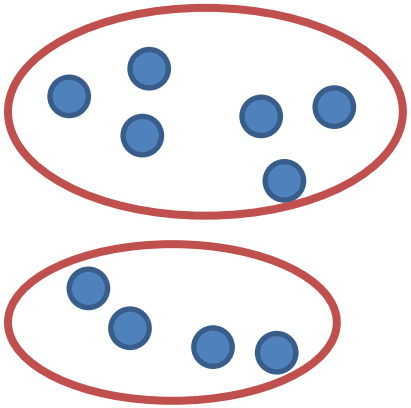
Three clusters based on the Euclidean distances between objects.

Examples of Clustering Applications

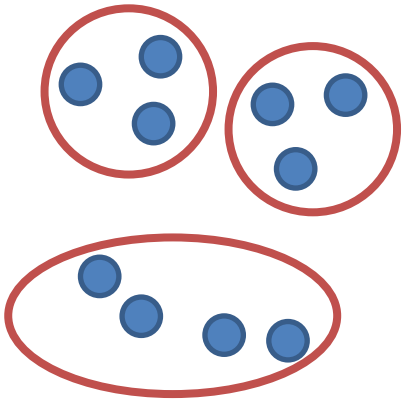
- Marketing: Discover distinct consumer groups based on the products people purchase. Then use this knowledge for targeted marketing.
- Land use: Identify areas of similar land use in an earth observation database.
- City-planning: Identify groups of houses according to house type, value, and location.
- Bird studies: Find species with similar migration behavior.

Ambiguity of Clusters

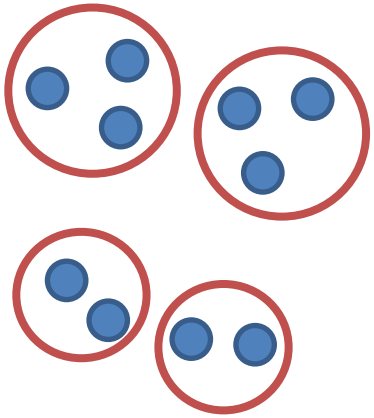
- The notion of what constitutes a cluster is subjective and depends on the preferences of the user.



2 clusters?



3 clusters?



4 clusters?

Distance and Similarity

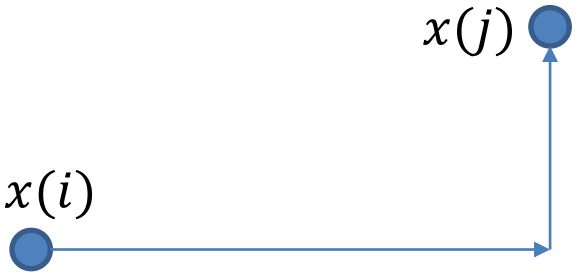
- Clustering is inherently determined by the choice of distance or similarity measure.
  - Consider a dataset of bird-sighting reports. If the distance is measured based on latitude and longitude, then observations made in similar locations will be clustered together. The same data set could instead be clustered based on the weather on the observation day. Now a cluster might contain reports from far-away locations that had similar weather.
- The choice of distance or similarity measure depends on user preferences.
  - Document similarity is usually measured based on the terms they contain.
  - The Minkowski distance is a popular family of distance measures.

Minkowski Distance

- Consider a data set $\{x(1), x(2), \ldots, x(n)\}$ of n d-dimensional data points, i.e., each $x(i)$ is a d-dimensional vector $\big(x_1(i), x_2(i), \ldots, x_d(i)\big)$.
- For $q > 0$, the Minkowski distance between any two data points $x(i)$ and $x(j)$ is defined as

$$\left(\sum_{k=1}^{d} |x_k(i) - x_k(j)|^q\right)^{1/q}$$

- For $q = 1$, it is called the Manhattan distance.
- For $q = 2$, it is called the Euclidean distance.



Intuition for the Manhattan distance: It is the distance of walking from $x(i)$ to $x(j)$ when walking on a rectangular grid of roads—like in Manhattan, New York.

Challenges of Distance Computation

- Since the distance or similarity measure strongly affects the clustering, it should be chosen carefully. Several challenges often must be addressed:
  - Curse of dimensionality
  - Diverse attribute domains
  - Categorical and ordinal attributes

- We discuss each challenge next.

Curse of Dimensionality

- The Minkowski distance between two objects is an aggregate of the differences in the individual dimensions. The more dimensions, the smaller the relative impact of an individual dimension. If there are many noisy attributes, they can bury the distance signal in the combined noise. Other distance measures suffer from similar issues.
  - To address this problem, remove any attribute that is known to be very noisy or not interesting.
- Depending on the attributes considered for the distance computation, the clustering might change significantly.
  - If it is not known which attributes are of most interest, try different subsets and determine experimentally for which of them good clusters are found.

Diverse Attribute Domains

- An attribute with a large domain often dominates the overall distance.
  - Consider Amy, Bill, and Carla with (age, income) combinations (25, $50K), (58, $51K), and (27, $52K). Amy and Carla have very similar age and income, while Bill has similar income, but belongs to a different generation. However, the absolute age difference is in the 30s, while the income difference is in the 1000s, dominating the overall distance.
- This problem can be addressed by scaling and weighting.
  - Scaling: Differences in attribute domains can be addressed by normalizing each domain to [0,1], using a linear transformation. Alternatively, a logarithmic transformation compresses differences between large values more than for small ones.
  - Weighting: Each attribute could be weighted according to its importance. Then the distance is defined as a weighted sum over the contributions in the individual dimensions.
- Choosing the appropriate transformation or weights requires expert knowledge and often involves trial-and-error.

Categorical Attributes

- Categorical attributes encode concepts that have no natural notion of order or numerical difference, making it difficult to choose a distance measure.
  - What is a meaningful distance between brown and black hair color, and how does it compare to the distance between red and blonde?
  - Experts may identify specialized measures, e.g., based on genetic similarity of bird species.
- The distance for a categorical attribute could be set to 0 if the values agree, and to 1 otherwise.
- Alternatively, a categorical attribute can be transformed to a set of binary attributes. For each possible value a binary attribute is created that is set to 1 if the categorical attribute has this value, and to 0 otherwise. This is called one-hot encoding.
  - Consider hair color with values blonde, red, brown, and black. In the transformed data, 4-valued attribute hair color is replaced by 4 binary attributes blonde, red, brown, and black. For a blonde person, they are set to blonde=1, red=0, brown=0, and black=0.

Ordinal Attributes

- Ordinal attributes have a natural notion of order, but not numerical difference. A typical example are ranks in the army and star ratings for products. A product rating of 4 stars is better than 3 stars, but is a 2-star product twice as good as a 1-star product? Would different evaluators agree how to quantify the improvement reflected by one additional star?
  - An ordinal attribute could be treated as a categorical attribute for distance computation. However, this ignores the additional knowledge about the ordering.
  - To preserve the ordering, the values of the ordinal attribute can be mapped to values in range [0,1]. For example, product rating k between 0 and 5 stars can be mapped to k/5. This mapping is based on implicit assumptions about the differences and ratios between ratings; it needs to be approached with care.

Next we explore algorithms that find clusters.

K-means Clustering

- K-means is one of the most popular clustering algorithms. It is comparably simple; therefore it serves as a perfect example for an algorithm that we can implement from scratch for parallel execution.
- K-means has solid mathematical foundations, with a well-defined optimization goal.
- In addition to a distance measure between objects, the user specifies parameter K, the number of clusters to be found. Starting from an initial configuration of K cluster centers, the algorithm iteratively adjusts the centers to improve the clustering.

What is a Cluster Center?

- K-means uses the centroid of a set of objects as their cluster center. Given a set C of objects, their centroid m is defined as $m = \frac{\sum_{x \in C} \boldsymbol{x}}{|C|}$, i.e., m's value in dimension i is the average of the values in the i-th dimension over all objects in C.
  - Consider a set C={(1,1), (2,4), (6,4)} of two-dimensional data points. Its centroid is point ((1+2+6)/3, (1+4+4)/3) = (3,3).
- As the example shows, the centroid does not need to be in C.
- To compute the centroid, addition and division need to be defined for the dimensions. This is guaranteed when working in a vector space. Categorical and ordinal attributes need to be transformed to numerical values.

K-means Algorithm

- The algorithm pseudo-code is shown below.
- For an example execution, see the next page.

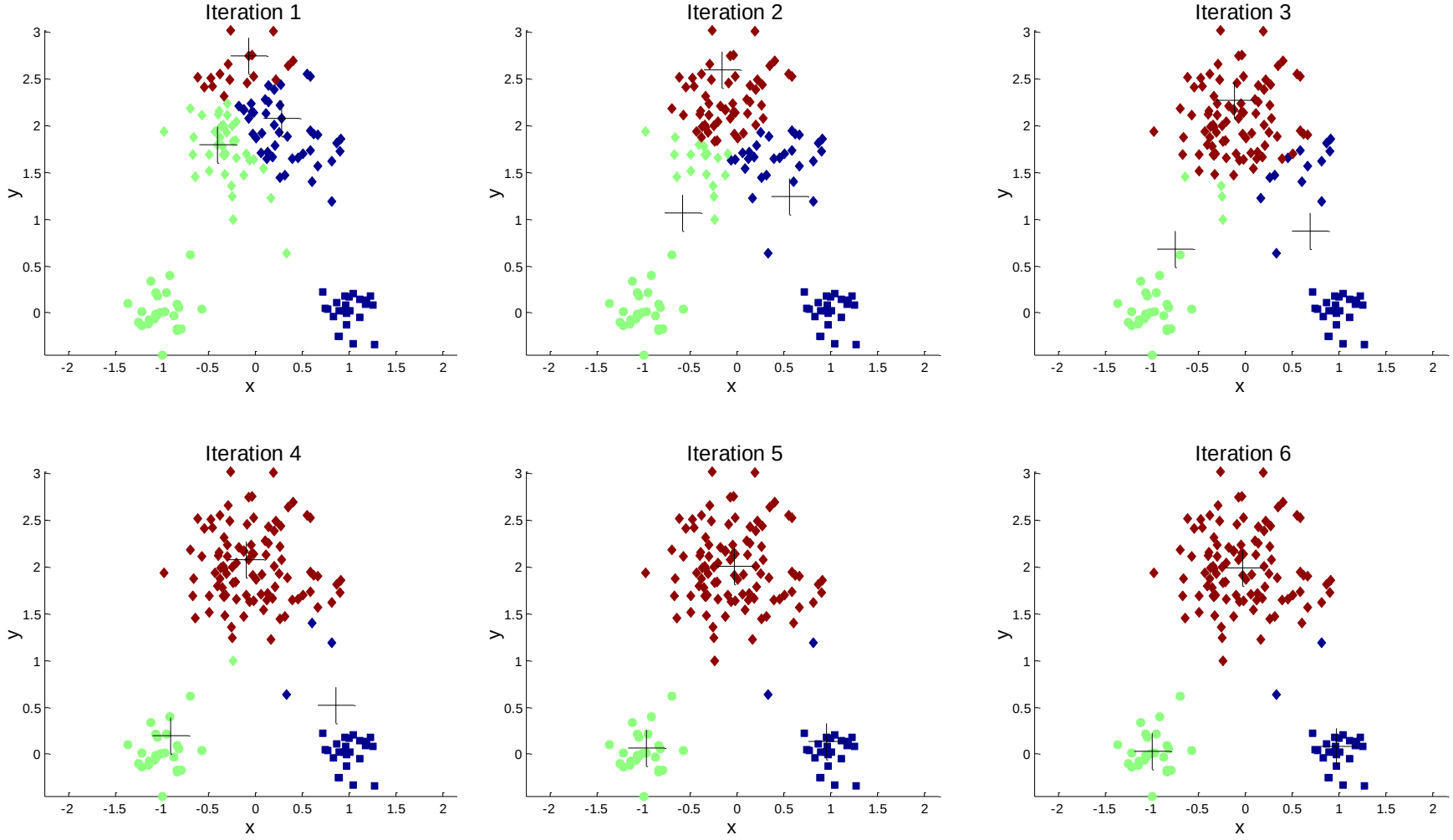
```
// Input: desired number of clusters K, data set D
K-means( K, D ) {

  Centroids = choose K initial centroids

  Repeat until centroids do not change {
    For each x in D do
      Assign x to the nearest centroid in Centroids

    For each C in Centroids do
      Re-compute C based on all data objects assigned to it
  }
}
```

The algorithm performs multiple iterations. In each iteration, first each data object is assigned to the nearest center, then the centers are updated based on this object assignment.



Convergence of K-means: The example shows how cluster centers are adjusted in each iteration. Colors indicate cluster membership for the input data points. Despite starting with all three centers in the big group, K-means automatically pushes the centers out to line up with the “natural” clusters. [from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

K-means Details

- K-means is comparably fast with complexity O(n * K * I * d). Here n denotes the number of input objects, I the number of iterations, and d the number of dimensions (i.e., attributes of the objects).
- Implementing K-means requires two crucial design decisions: selection of the initial centers and choice of distance measure.
  - The initial centers affect the final clustering found. Unfortunately, no existing algorithm guarantees to pick initial centers that result in the best clustering possible. Many heuristics have been proposed, e.g., some try to place the initial centers far away from each other to improve the probability of each turning into the centroid of a different "natural" cluster.
  - A common approach relies on random restarts: Select the initial K centers randomly from the input data and run K-means until convergence. Then repeat for another set of K randomly selected centers, until satisfied with the quality of the best clustering found.
  - For vector spaces, the Euclidean distance is commonly used. Depending on the application one can choose other measures such as cosine similarity or a correlation coefficient.

Evaluating Cluster Quality

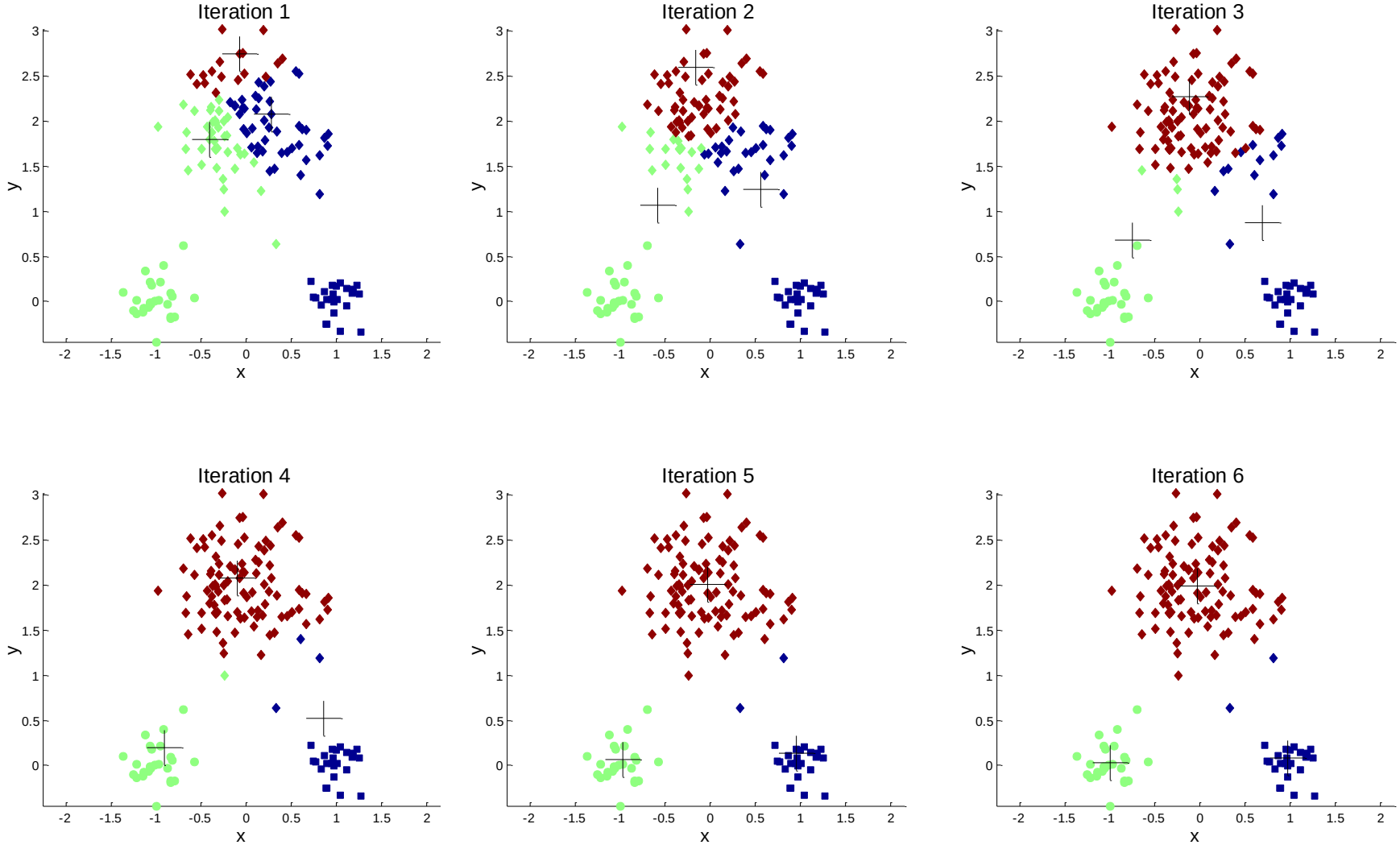
- As an unsupervised learning technique, there is no ground truth about clusters and cluster membership. How can we evaluate the quality of a clustering?
- In K-means, a centroid represents all objects in the cluster. If an object is far from the centroid, then the centroid is a poor representative for it. Hence the quality of a K-means clustering is evaluated based on the "errors" made by representing individual objects with the corresponding cluster centroid. A common error measure in vector space is the Sum of Squared Error (SSE), defined as $\sum_{i=1}^{K} \sum_{x \in C_i} \text{dist}^2(m_i, x)$. Here C_i denotes a cluster and m_i its centroid.
- The goal of K-means it to minimize SSE for a given K.
  - In general, a larger K will result in lower SSE. Hence it is not meaningful to use SSE for comparing 2 clusterings that were obtained for *different* values of K.

K-means Convergence

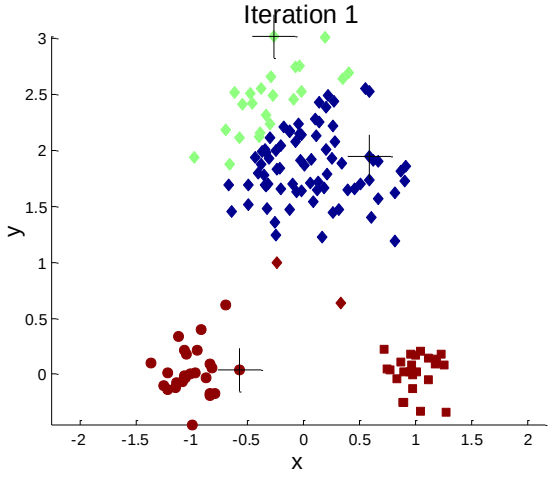
- K-means iterates until all cluster centers stabilize. This raises two questions:
- Will SSE improve in each iteration: Yes, until convergence.
  - Given K cluster centers, K-means assigns each object to the nearest center. If it re-assigns an object x from one cluster to another, x's distance to its cluster center must have decreased, reducing SSE.
  - Given K clusters, K-means updates the centers. It is easy to show that the centroid has a smaller SSE than any other possible center choice. Hence if a cluster centroid is updated, SSE must have decreased.
- Will K-means converge: Yes.
  - There is a finite number of possible partitionings of n objects into K partitions.
  - K-means iterates until the clustering does not change any more. In each iteration, SSE decreases.
  - Since SSE decreases in each iteration, K-means must have reached a new partitioning it has not explored before. So, if it tried to go on forever, it would eventually run out of configurations.

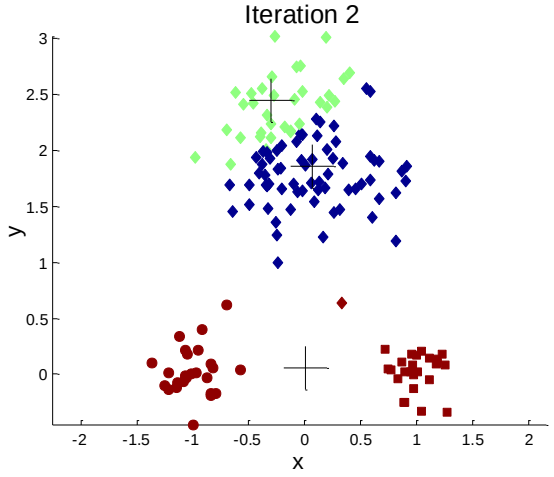
Optimality

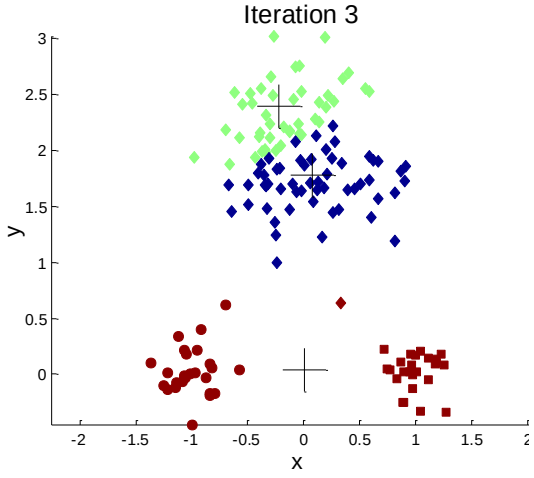
- The previous discussion showed that each iteration of K-means improves SSE until it converges. Unfortunately, this does not mean that it will always find the optimal clustering, i.e., the clustering with the lowest possible SSE for the given data.
- More formally, K-means is guaranteed to converge to a local optimum. Since there are potentially many such local optima, it is not guaranteed to converge to the global optimum.
- The choice of initial cluster centers determines to which local optimum K-means will converge. Let's look at some examples.

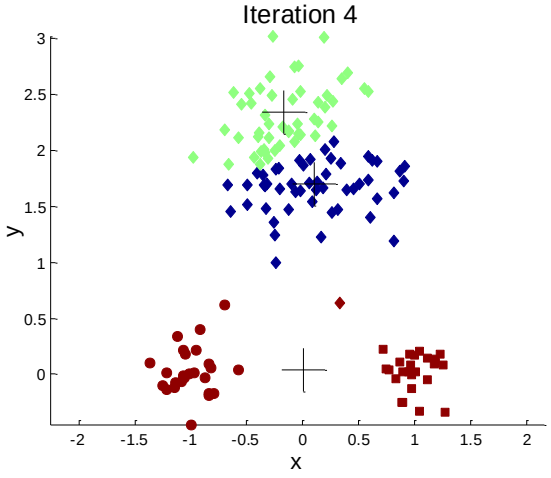


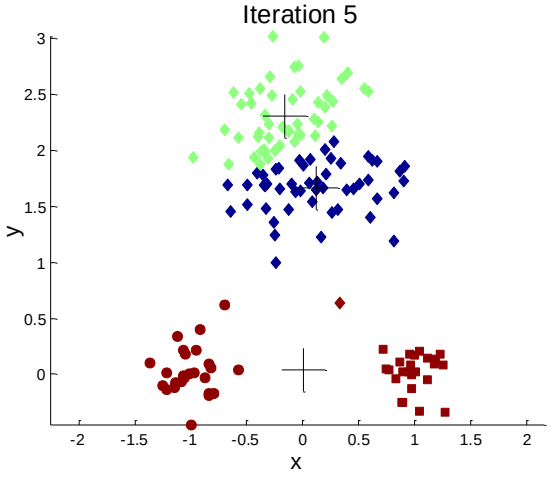
In this example, the initial selection of cluster centers appears poor, because all three centers are in the same “natural” cluster. However, iteration by iteration the centers move in the right direction. [from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]











In this example, the initial selection of cluster centers appears more reasonable as all centers are fairly far apart. Unfortunately, K-means gets trapped in a local optimum that does not correspond to the “natural” clusters. [from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

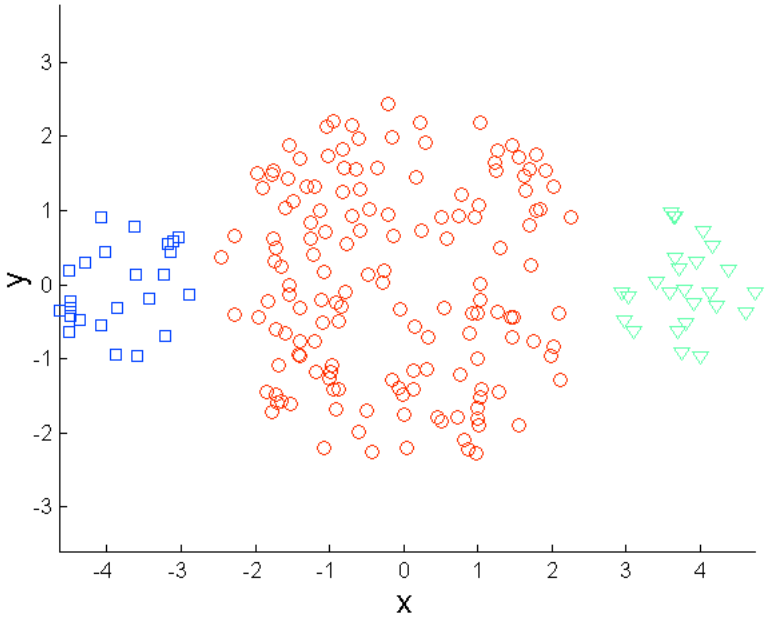
Selecting Initial Cluster Centers

- Since the choice of initial cluster centers determines to which local optimum K-means converges, researchers have explored how to find a good initial configuration. Unfortunately, there is no general solution for this problem.
- Some heuristics attempt to place each initial cluster center in a different “natural” cluster of the data. The probability of finding such a configuration through random selection is extremely low. Hence it is often attempted to place initial centers far apart from each other. This is not guaranteed to work well either.
- Another option is to use a different clustering algorithm that does not need an initial configuration, e.g., hierarchical clustering. The clusters found by that algorithm could inform the choice of initial centers for K-means.
- Even if K-means is lucky in choosing “good” initial cluster centers in different natural clusters, it might converge to a “bad” clustering as we will discuss next.

Limitations of K-means

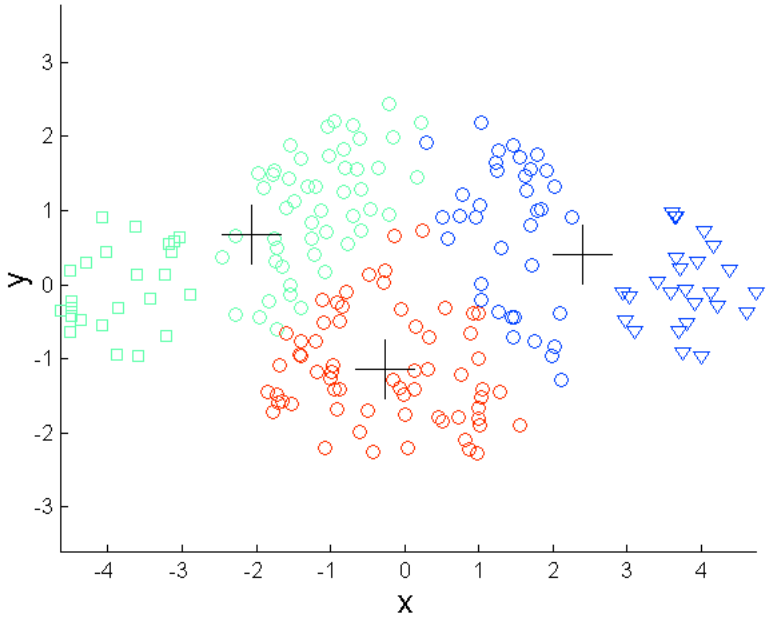
- Assume the user was able to choose the perfect value of K, the right distance measure, and the best initial cluster centers. Would this guarantee that a good clustering is found?
- Unfortunately, there are inherent limitations of K-means that prevent it from finding the “natural” clusters under certain circumstances.
- In particular, K-means has problems when clusters are of differing sizes, densities, or have non-globular shapes—as we illustrate with examples below.

Differing Sizes



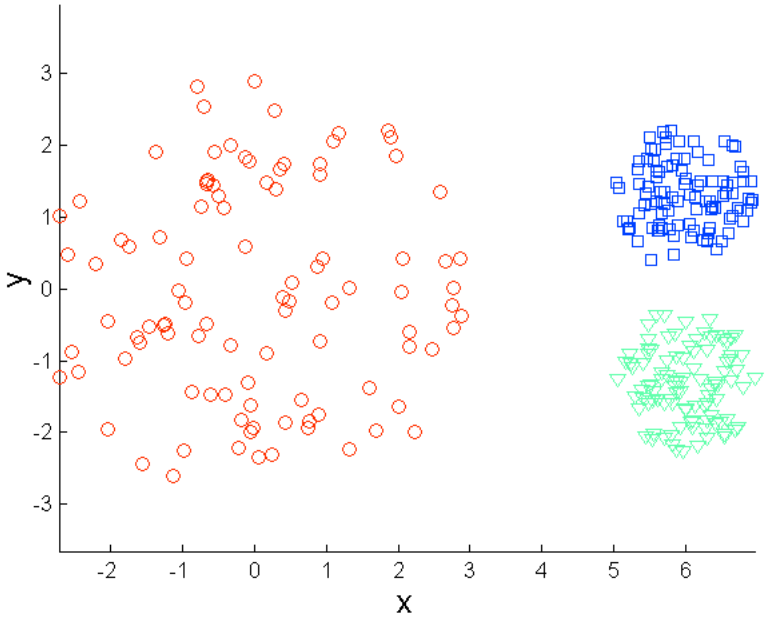
Natural clustering: Intuitively, many users would like to discover the three clusters indicated by point shape and color.

[from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]



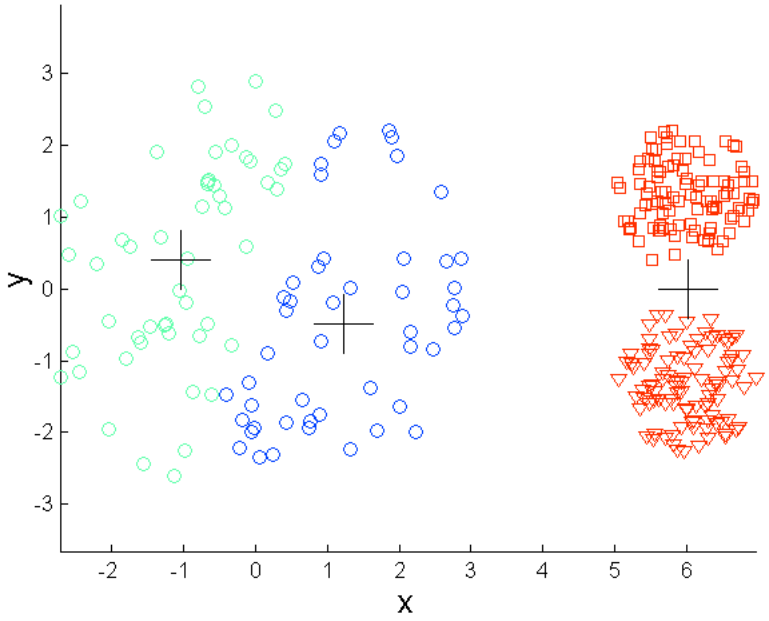
Optimal K-means result: The large natural cluster contains many more points than the small ones. Due to the different diameters of the natural clusters, K-means cannot find them. Even if it started with the perfect cluster centers, it would converge to a clustering as shown, because that minimizes SSE. For instance, note that points on the left fringe of the large cluster are closer to the center of the left small cluster than to the center of the large cluster.

Differing Density



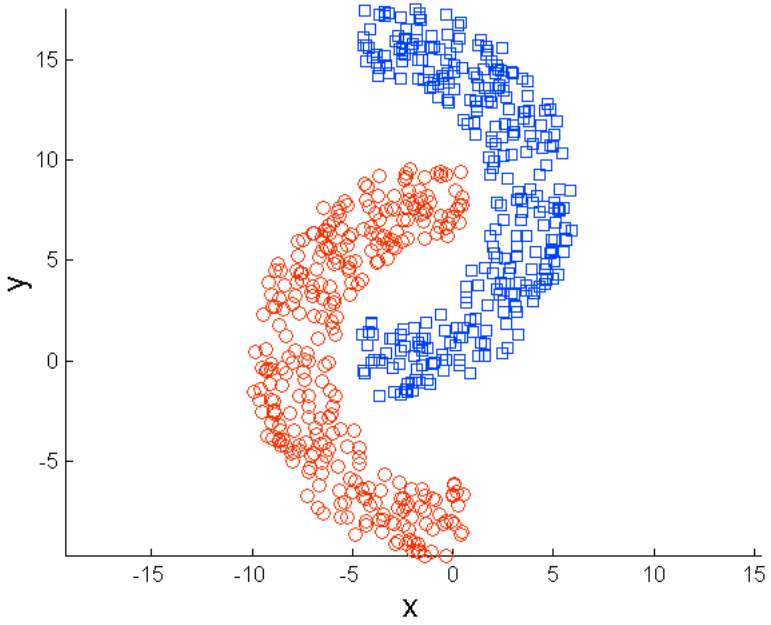
Natural clustering: Intuitively, many users would like to discover the three clusters indicated by point shape and color.

[from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]



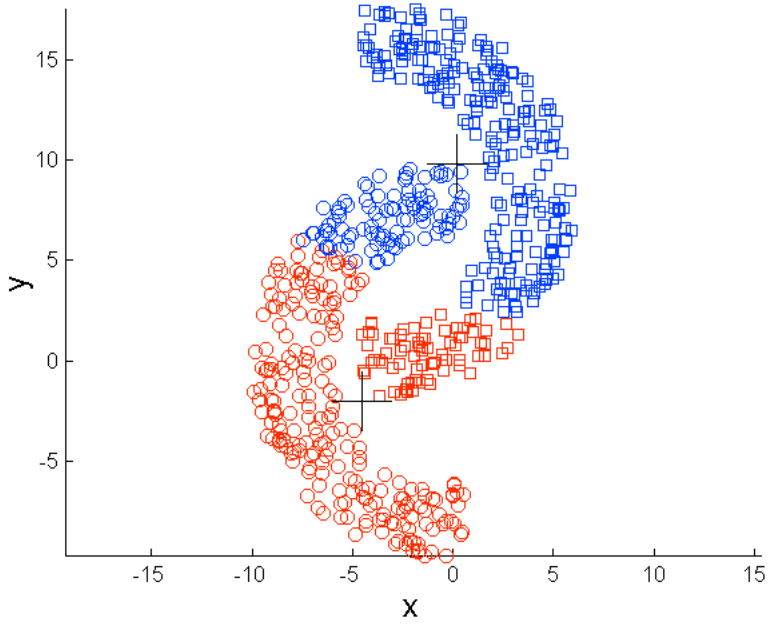
Optimal K-means result: In this example, each of the natural clusters has about the same number of points. However, due to their different densities, the large natural cluster has a much larger diameter than the other two. This results in the same problem as for the previous example with differing sizes.

Non-globular Shapes



Natural clustering: Intuitively, many users would like to discover the two clusters indicated by point shape and color.

[from “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

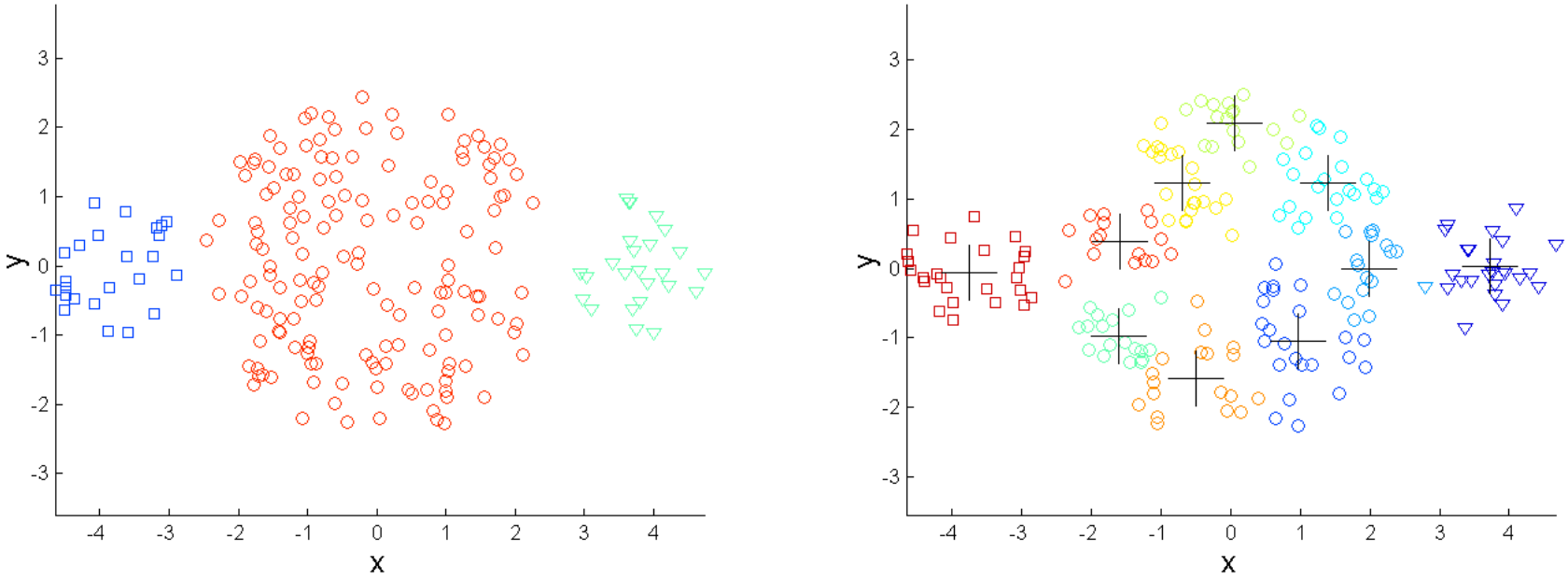


Optimal K-means result: Due to the elongated shape, some points of the left natural cluster are closer to the right natural cluster than to their own center. Again, even if K-means started with the perfect cluster centers, it would still converge to a clustering as shown, because that minimizes SSE.

Addressing K-means Limitations

- There exist solutions for the inherent problems of K-means.
- Choose a different algorithm:
  - Each clustering algorithm is designed for a certain intuitive notion of a cluster. For instance, if the user is looking for clusters based on point density, not based on minimizing SSE, then they should consider an algorithm designed for finding density-based clusters.
- Fix K-means through post-processing:
  - Instead of using the desired K, the user can run K-means for some K' > K. Then the K' clusters found are post-processed by a combination of the following operations:
    - Eliminate small clusters that may represent outliers.
    - Split very large clusters.
    - Merge clusters that are close to each other.

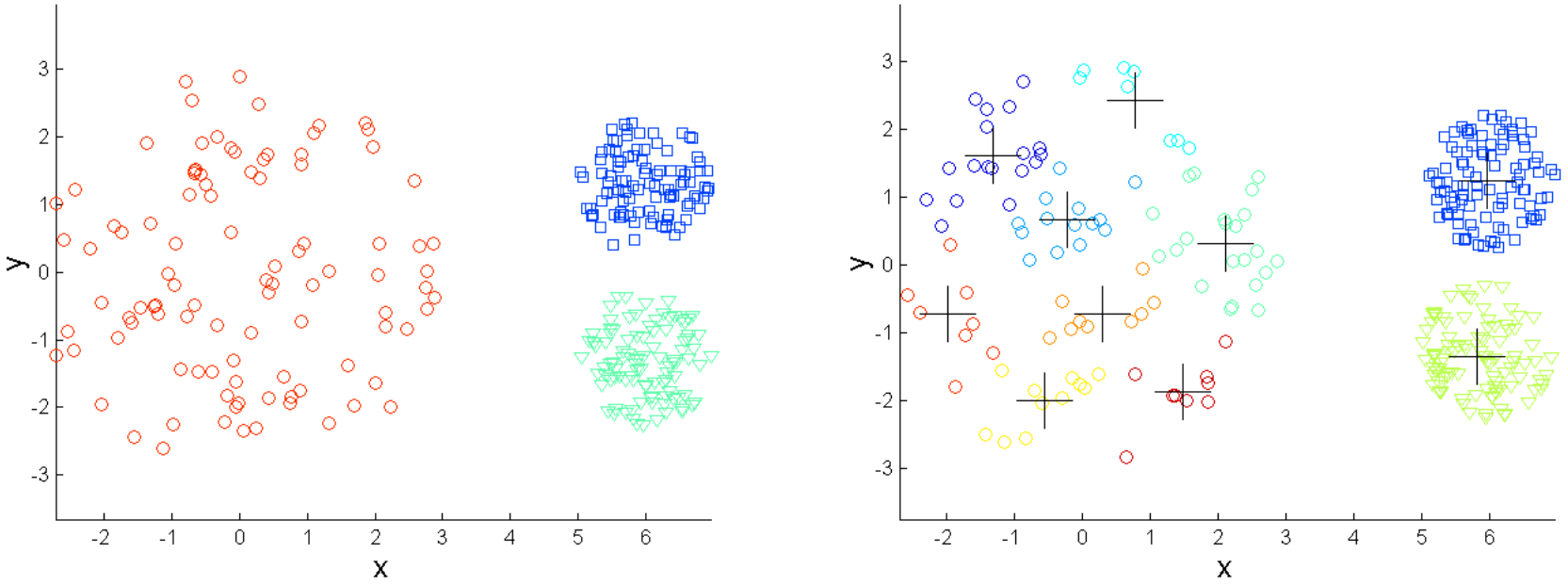
Fixing the Differing-Size Problem



The K-means run for K'=10 found 10 small clusters, each part of one of the three natural clusters. An appropriate post-processing algorithm might be able to combine the 8 small clusters in the middle to form the large natural cluster.

[from "Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

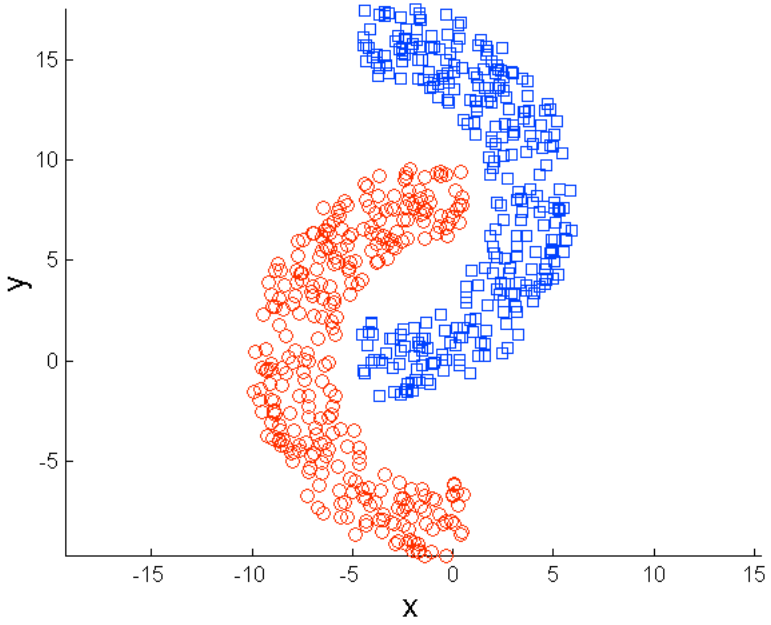
Fixing the Differing-Density Problem

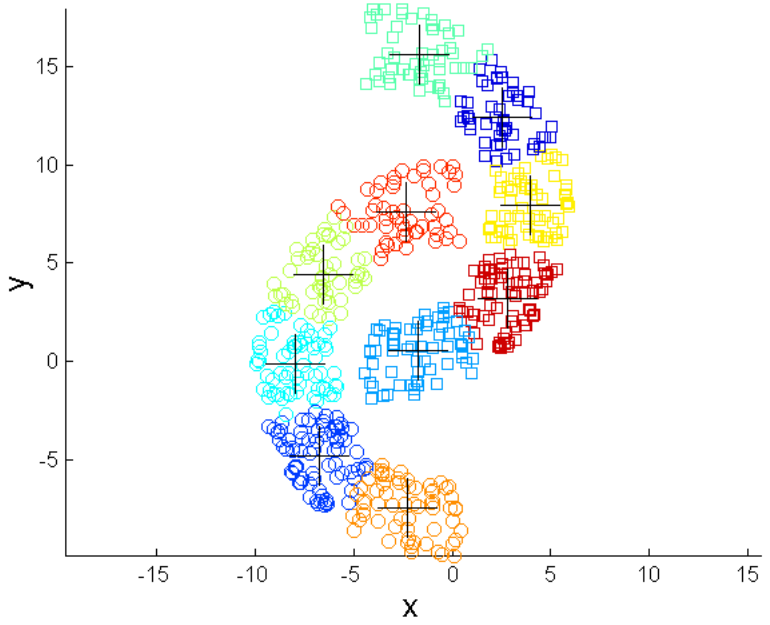


The K-means run for K'=10 found 10 small clusters, each part of one of the three natural clusters. An appropriate post-processing algorithm might be able to combine the 8 small low-density clusters on the left to form the large natural cluster.

[from "Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Fixing the Shape Problem



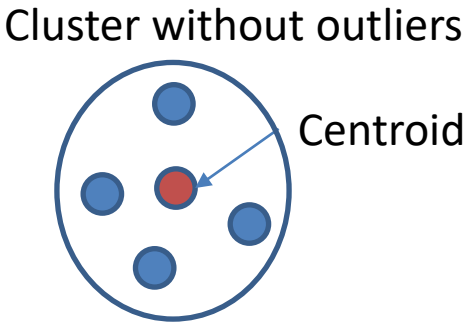


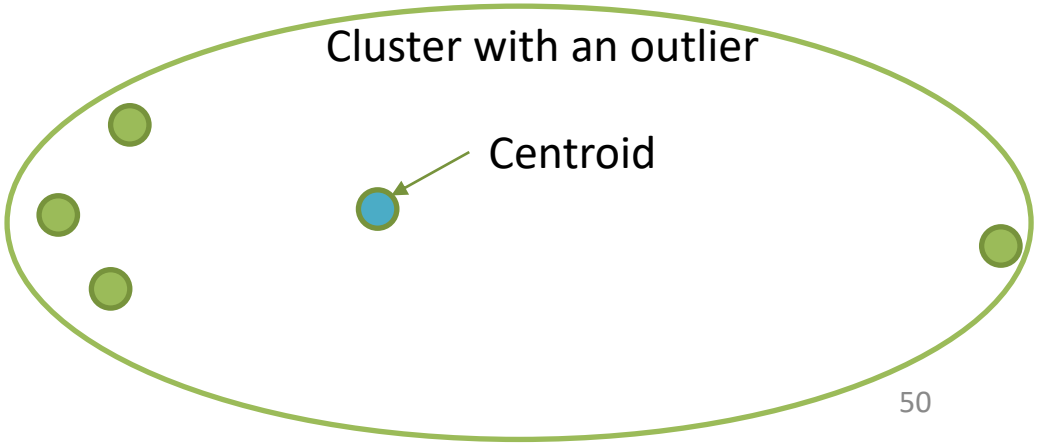
The K-means run for K'=10 found 10 small clusters, each part of one of the two natural clusters. An appropriate post-processing algorithm might be able to combine each group of five adjacent small clusters into the corresponding large natural cluster.

[from "Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

K-Means and Outliers

- K-means is sensitive to outliers, because each centroid is an average of the cluster members. Even a single outlier with a very large value in a dimension can dominate the average.
- This problem is addressed by the K-medoids algorithm. Instead of the centroid, it represents a cluster by its medoid, which is the *most centrally located real object* in a cluster.
  - The algorithm works like K-means, but finding the medoid is computationally more expensive than finding the centroid. For an exact solution, the algorithm would try all objects in the cluster to find the one that minimizes SSE. To reduce cost, it may explore only a randomly selected subset.





Distributed K-Means

- Like other iterative algorithms, e.g., for graph processing, we distinguish between immutable and evolving data. The former should be loaded once and then kept in memory, while the latter potentially needs to be shuffled across the network.
  - For clustering, the set of input objects is fixed. Each task receives a partition of this dataset.
  - Cluster centers can change in each iteration. When centers change, membership of objects in clusters might also change.
- Which data structures do we need to represent the immutable and evolving data?
  - We store the data objects in `Objects` and the cluster centers in `Centers`.

Distributed K-Means (Cont.)

- Each iteration consists of two rounds.
- Round 1:
  - Each task receives a partition of Objects. Spark can re-use these partitions in later iterations.
  - We broadcast Centers to all tasks.
  - The task assigns each object in the partition to the closest center. (Note that centroid computation benefits from combining.)
- Round 2:
  - Each task receives a group of objects that were assigned to the same center. (It might receive multiple such groups.)
  - The task computes the new center for the group by averaging the coordinates of all objects in the group.
- The output of round 2 is the new set of centers.

K-Means in MapReduce

- We implement round 1 as Map and round 2 as Reduce. Centers is broadcast using the file cache. Mappers must read their chunk of Objects anew in every iteration.
- The driver program repeatedly calls this program, putting the new Centers in the file cache after each iteration.

```
Class Mapper {
  Centroids  // Array containing the K cluster centers

  setup()
    Centroids = read centroids from file cache

  map( object o ) {
    closestCenter = Centroids[0]
    minDist = dist(closestCenter, o)

    for i=1 to k-1 {
      if (dist(Centroids[i], o) < minDist))
        closestCenter = Centroids[i]
        minDist = dist(Centroids[i], o)
    }
    emit( closestCenter, o )
  }
}
```

```
reduce( center, [o1, o2,…]) {
  for each object o in inputList {
    update object count
    update coordinate-sum for each dimension
  }

  newCentroid = compute the average
                        for each dimension
  emit ( newCentroid )
}
```

Algorithm Analysis

- In each iteration, the entire Objects file is transferred to Mappers, then from Mappers to Reducers. Reducers write out the (usually small) file with the new centroids, which is broadcast to all Mappers in the next iteration. Like for the iterative graph algorithms, performance suffers from MapReduce's inability to exploit the repetitive structure of the computation.
  - In fact, the MapReduce program executed on many machines can take much longer to finish than the sequential program.

K-Means in Spark

- Spark's ability to maintain data in memory in RDDs or DataSets enables the desired implementation where the object set is kept across iterations.
- If we implement the algorithm from scratch, we need to:
  - Broadcast the new centers to all Executors using broadcast() or create a Scala collection that is automatically sent to all tasks.
  - Keep Objects in an RDD or DataSet. Use cache() or persist() to tell Spark to keep it in memory as much as possible.
  - Use map on Objects, calling a function that for object o emits pair (nearestCenterID, o).
  - Group by nearestCenterID and aggregate each group to compute the average in each dimension.
- For real code (from the Spark 2.4.0 distribution) look at http://khoury.northeastern.edu/home/mirek/code/SparkKMeans.scala
- Or we can just use machine learning library Spark MLlib.

K-Means in MLlib with RDD (from Spark 2.3.2 Documentation)

```
import org.apache.spark.mllib.clustering.{KMeans, KMeansModel}
import org.apache.spark.mllib.linalg.Vectors

// Load and parse the data
val data = sc.textFile("data/mllib/kmeans_data.txt")
val parsedData = data.map(s => Vectors.dense(s.split(' ').map(_.toDouble))).cache()

// Cluster the data into two classes using KMeans
val numClusters = 2
val numIterations = 20
val clusters = KMeans.train(parsedData, numClusters, numIterations)

// Evaluate clustering by computing Within Set Sum of Squared Errors
val WSSSE = clusters.computeCost(parsedData)
println(s"Within Set Sum of Squared Errors = $WSSSE")

// Save and load model
clusters.save(sc, "target/org/apache/spark/KMeansExample/KMeansModel")
val sameModel = KMeansModel.load(sc, "target/org/apache/spark/KMeansExample/KMeansModel")
```

K-Means in Mllib With DataSet (from Spark 2.3.2 Documentation)

```
import org.apache.spark.ml.clustering.KMeans
import org.apache.spark.ml.evaluation.ClusteringEvaluator

// Loads data.
val dataset = spark.read.format("libsvm").load("data/mllib/sample_kmeans_data.txt")

// Trains a k-means model.
val kmeans = new KMeans().setK(2).setSeed(1L)
val model = kmeans.fit(dataset)

// Make predictions
val predictions = model.transform(dataset)

// Evaluate clustering by computing Silhouette score
val evaluator = new ClusteringEvaluator()

val silhouette = evaluator.evaluate(predictions)
println(s"Silhouette with squared euclidean distance = $silhouette")

// Shows the result.
println("Cluster Centers: ")
model.clusterCenters.foreach(println)
```

Alternative Parallel Version

- Often we compute many alternative clusterings for the same data:
  - Usually we do not know the best choice for K, therefore we try different values for it.
  - We also may want to explore different distance measures and initial cluster centers.
- For each K, distance measure, and initial configuration, the clustering can be computed *independently*. This suggests another approach to parallelization: Broadcast the data to all workers and let each task compute a clustering using the sequential K-means algorithm for a different parameter combination.
- In MapReduce we can achieve this by creating a parameter file containing a different parameter combination (K-value, distance measure, and set of initial centers; the latter specified by providing a random seed) in each line. Map reads a line with parameters and computes the corresponding clustering in a single task.
  - Usually the parameter file will be smaller than the default file-split size. To ensure multiple Map tasks, use NLineInputFormat to create small input splits based on lines in the file.
  - Mappers receive the file with the data objects via the file cache.
- The pseudo-code is shown on the next page.

```
// The input file is copied to each worker using the distributed file cache
Class Mapper {
  data D

  setup() {
    D = read input data from file cache
  }

  map( …, parameters p ) {
    // Kmeans() is a sequential implementation of the K-means algorithm
    clustering = Kmeans( D, p )

    emit( p, clustering )
  }
}
```

Now we change gears and look at supervised learning, in particular classification and prediction (a.k.a. regression).

Classification and Prediction

- Classification and prediction are among the most common data mining tasks in practice. The goal is to predict some output of interest for a given input record, for instance:
  - Predict if somebody is likely to repay a mortgage.
  - Predict if a credit-card transaction is fraudulent.
  - Predict if the customer will purchase the product.
  - Predict the probability of observing a certain species in a given environment.
- Classification and prediction are supervised learning methods: They rely on the availability of labeled training data, i.e., records where both input and correct output are known.
- Formally, consider a data set with attributes $X_1,\ldots,X_d$, and Y. From this data, a model is trained, which is a function $f:(X_1,\ldots,X_d)\rightarrow Y$. This function can then be used to predict the unknown output y for a given input record $(x_1,\ldots,x_d)$. For classification problems, Y is a discrete attribute, called the class label. For prediction problems, Y is a continuous attribute.

Classification Example: Labeled Data

- Given a data set of recent graduates, NEU wants to predict for each graduating senior if they will receive a job offer within a year of graduation (column “Job Offer?”).

Training Data

Name	Age	GPA	Major	Job Offer?
Joe	24	3.7	CS	Yes
Amy	28	3.9	CS	Yes
Joe	29	3.3	ECE	Yes
Bill	24	3.1	Bio	No
Beth	22	3.8	Art	No

Test Data

Name	Age	GPA	Major	Job Offer?
Mary	23	4.0	CS	Yes
Joe	24	3.9	Hist	No
Amy	25	3.6	CS	Yes

Classification Example: Induction

- Induction refers to the process of training (or "fitting") a model that captures the relationship between input attributes (name, age, GPA, major) and output (job offer).
- Many different models can be fit to the same training data, some more realistic (Model 1) than others (Model 2). It usually is not that obvious to identify the more realistic model.
  - Models may pick up correlations that are not causal relationships, e.g., the name of a person is not causing the person to get a job offer. This is an idiosyncrasy of the given data.
  - Larger training data protects better against such spurious relationships, e.g., when a Joe or Amy without job offer appear in the data, but it does not eliminate it.

Name	Age	GPA	Major	Job Offer?
Joe	24	3.7	CS	Yes
Amy	28	3.9	CS	Yes
Joe	29	3.3	ECE	Yes
Bill	24	3.1	Bio	No
Beth	22	3.8	Art	No

Model 1: IF (major = CS OR major = ECE)
THEN job = Yes; ELSE job = No

Model 2: IF (name = Joe OR name = Amy)
THEN job = Yes; ELSE job = No

Classification Example: Deduction

- Deduction refers to the process of using the model to make predictions.
- The more meaningful Model 1 gets more of the test records right than Model 2. The fraction of correctly classified test records is called the accuracy of the model.
- To evaluate a model realistically, the test records should not be used for training and should be drawn from the same distribution as future records for which the model will be used to make a prediction.

Name	Age	GPA	Major	Job Offer?
Mary	23	4.0	CS	Yes
Joe	24	3.9	Hist	No
Amy	25	3.6	CS	Yes

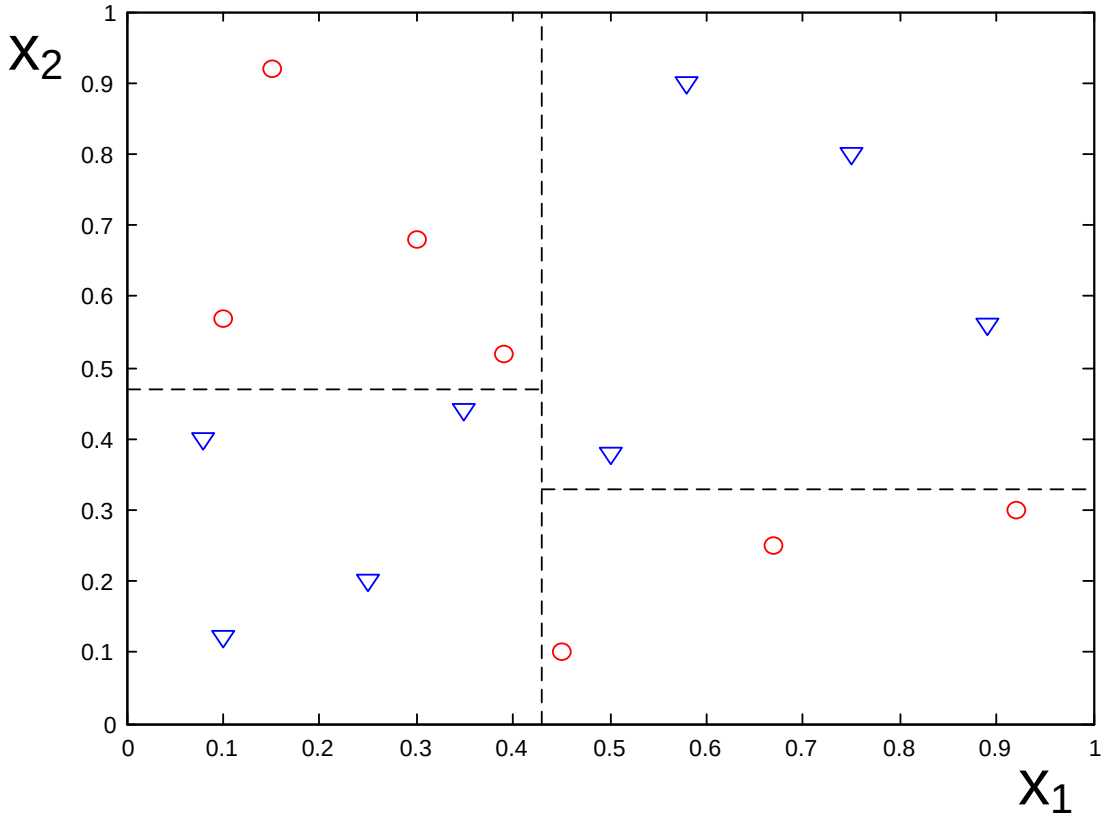
Model 1: IF (major = CS OR major = ECE) THEN job = Yes; ELSE job = No

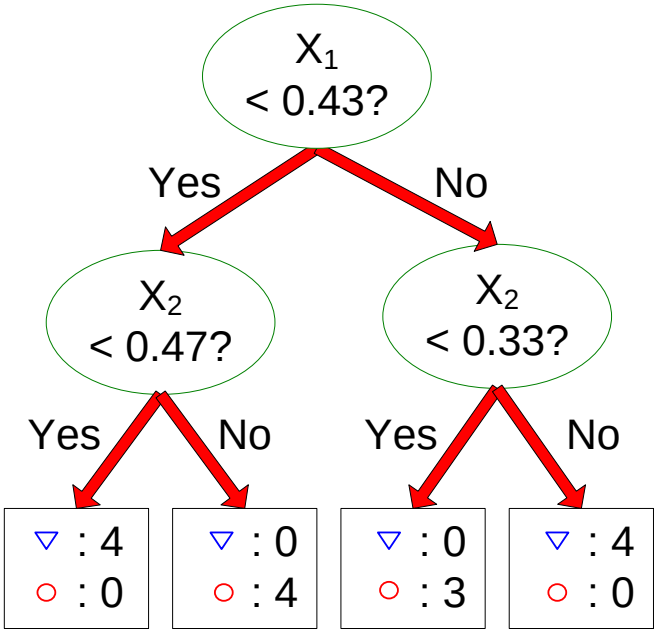
Model 2: IF (name = Joe OR name = Amy) THEN job = Yes; ELSE job = No

Model 1 prediction	Model 2 prediction
Yes	No
No	Yes
Yes	Yes

Decision Trees

- Decision trees are a popular technique for classification problems. A decision tree splits the data space recursively in order to separate the different classes from each other as much as possible.
- The nodes of the tree contain split attributes that guide the search to the appropriate leaf when making a prediction.





The decision tree on the right defines partitions of the data space. The goal of these partitions is to have "pure" leaves, i.e., have ideally only members of a single class in a leaf.

The *decision boundary* is the border between two neighboring regions of different classes. For trees that split on a single attribute at a time, the decision boundary is parallel to the axes.

[Example source: "Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

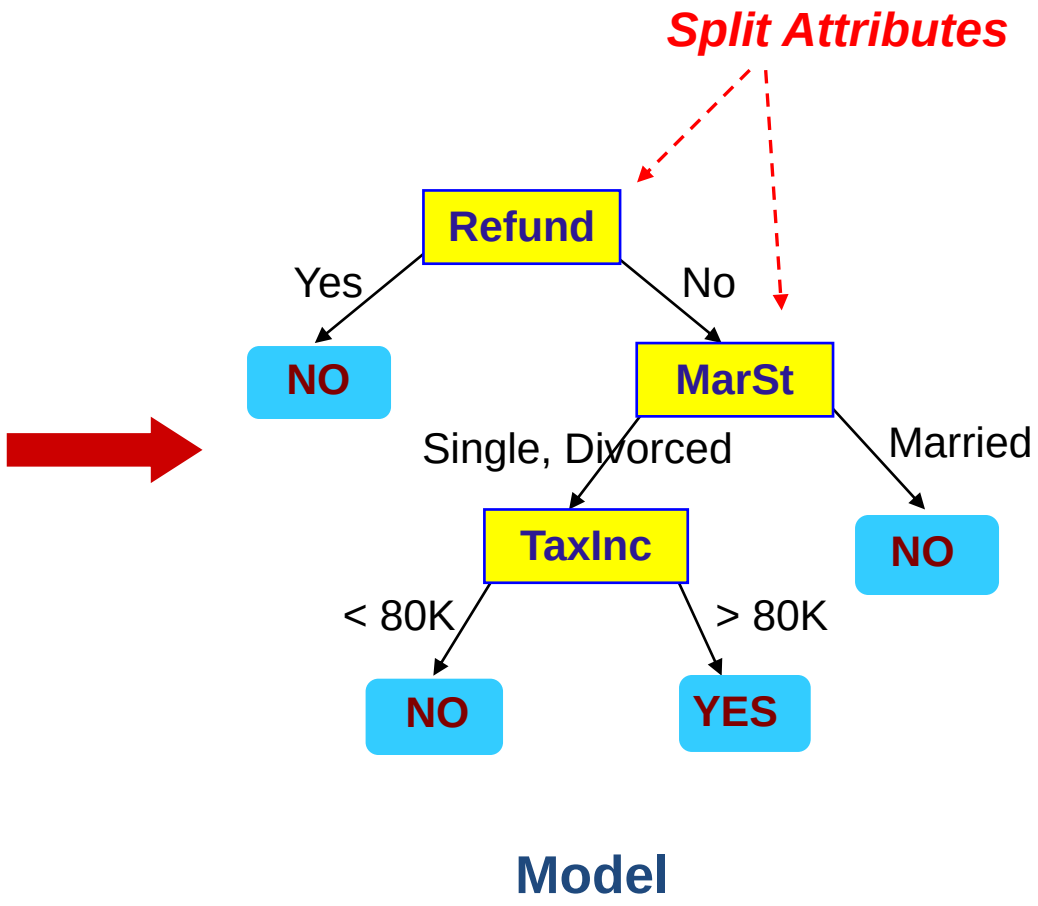
Tree Uniqueness

- For a given data set, there are usually many structurally different trees that achieve similar accuracy on the training data.
- For consistent data, there is more than one tree structure that perfectly represents the entire training data set.
  - Data is consistent if it does not contain two records that have the same input values, but different output.
- We look at two examples next.

Decision Tree That Exactly Represents the Training Data

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data

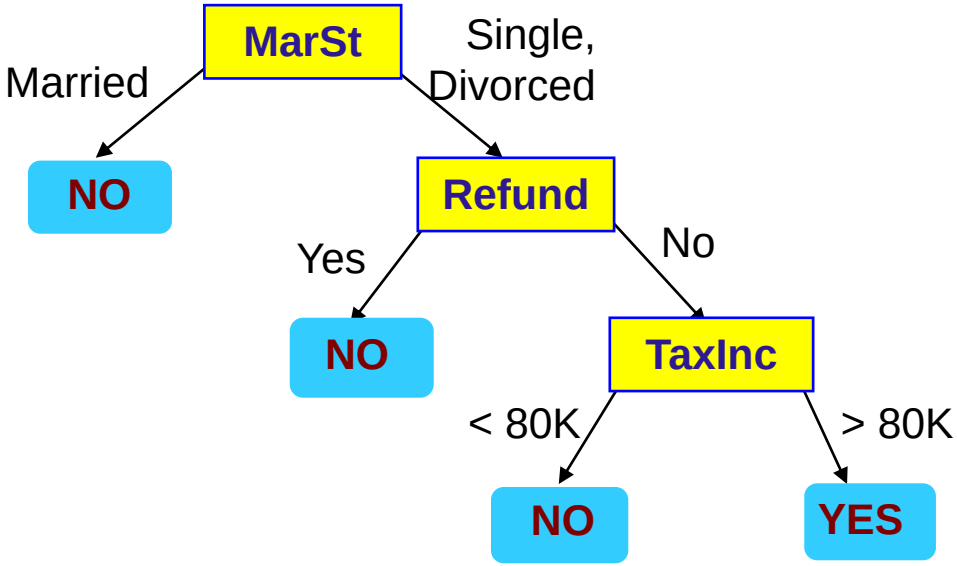


Model

[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

A Different Decision Tree That Exactly Represents the Same Training Data.

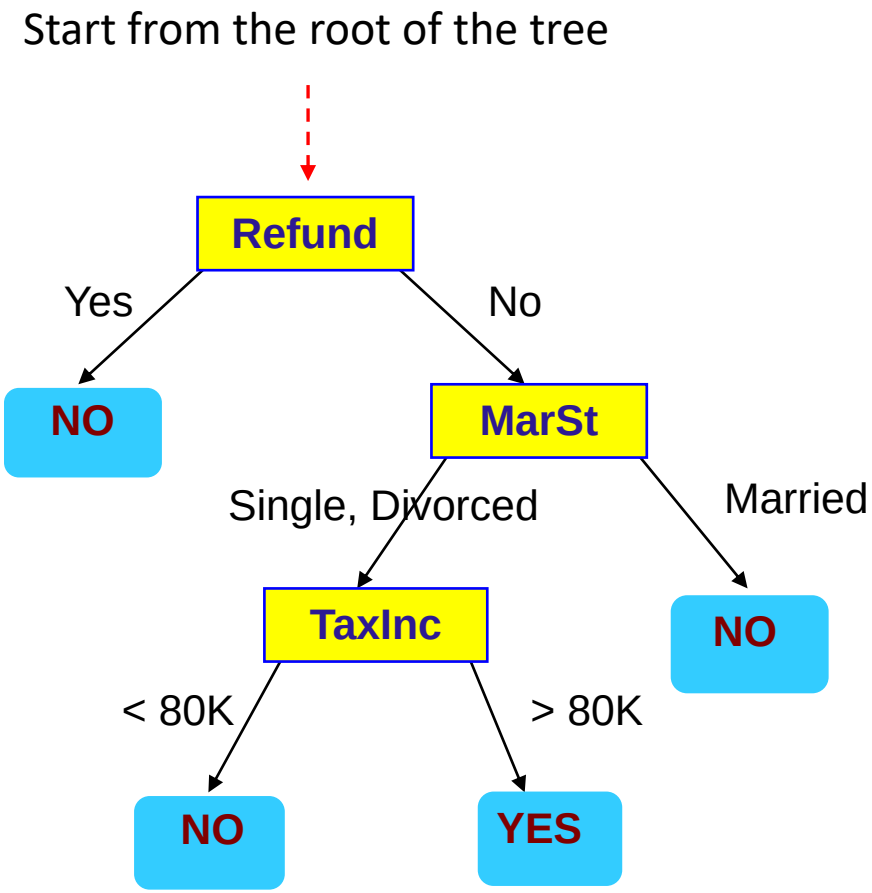
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Making Predictions

- Given a record containing only values for the input attributes, the tree will find the data partition this record falls into. It will then return a class value based on the training records in that partition.
- Tree traversal starts at the root, following the pointer to the next node based on the input value for the node's split attribute.
- Let us look at an example.



Test Data

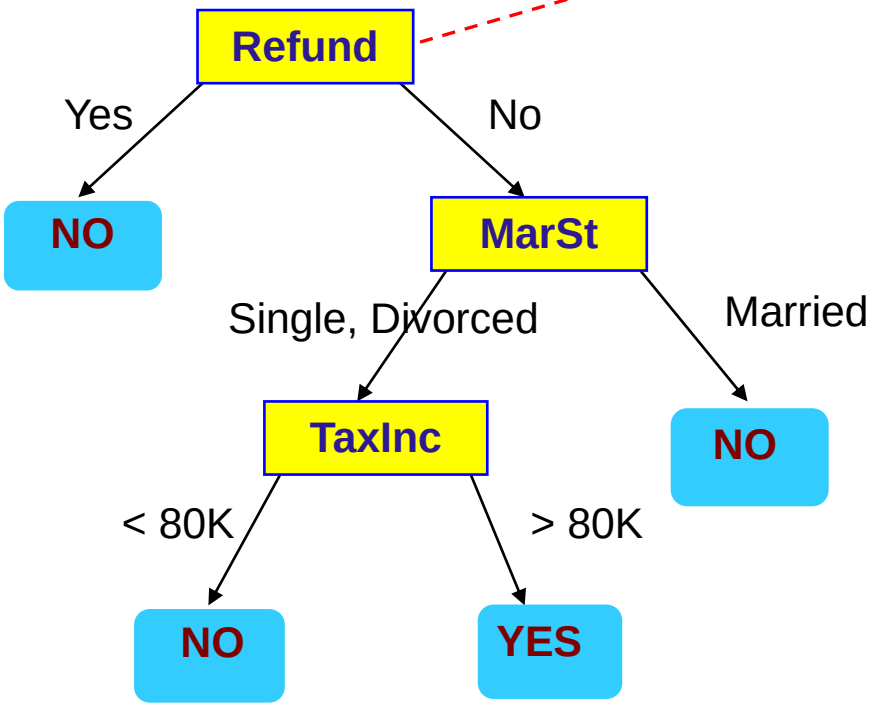
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Check the Refund value to determine which pointer to follow.

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

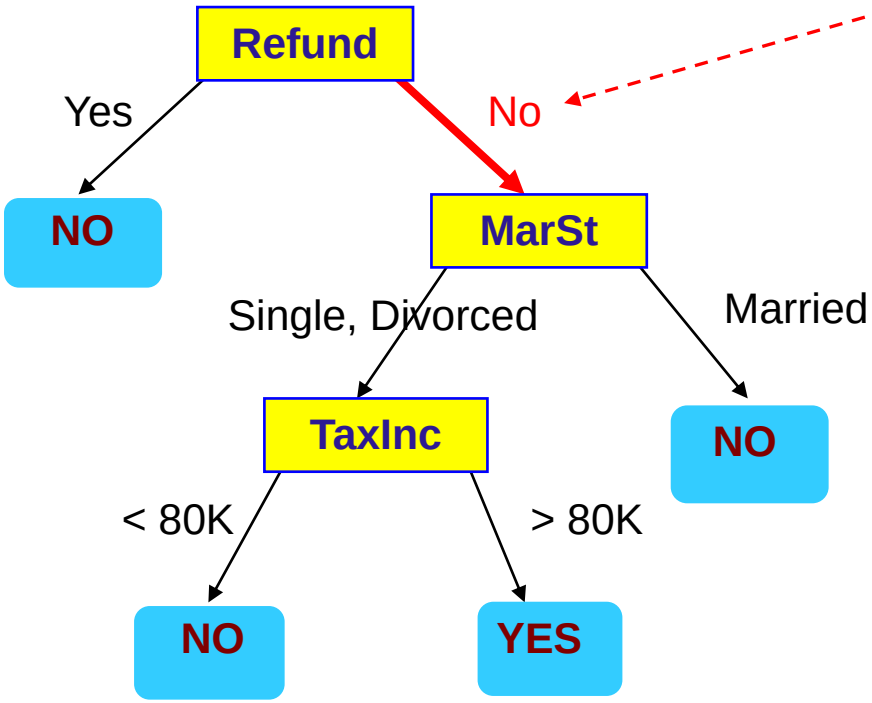


[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Refund = No, therefore follow the right pointer.

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

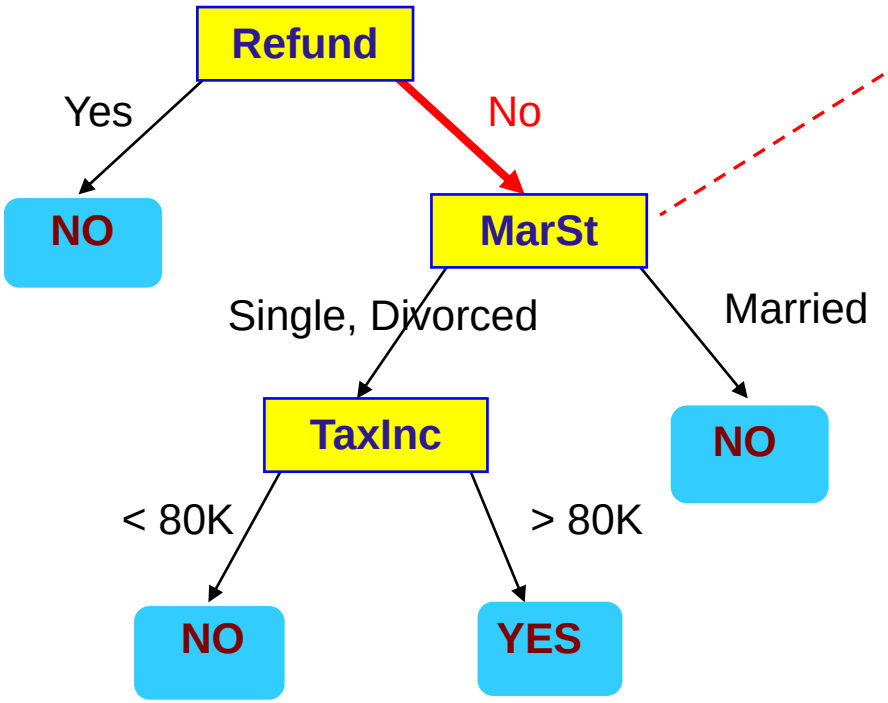


[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Check the Marital Status value to determine which pointer to follow.

Test Data

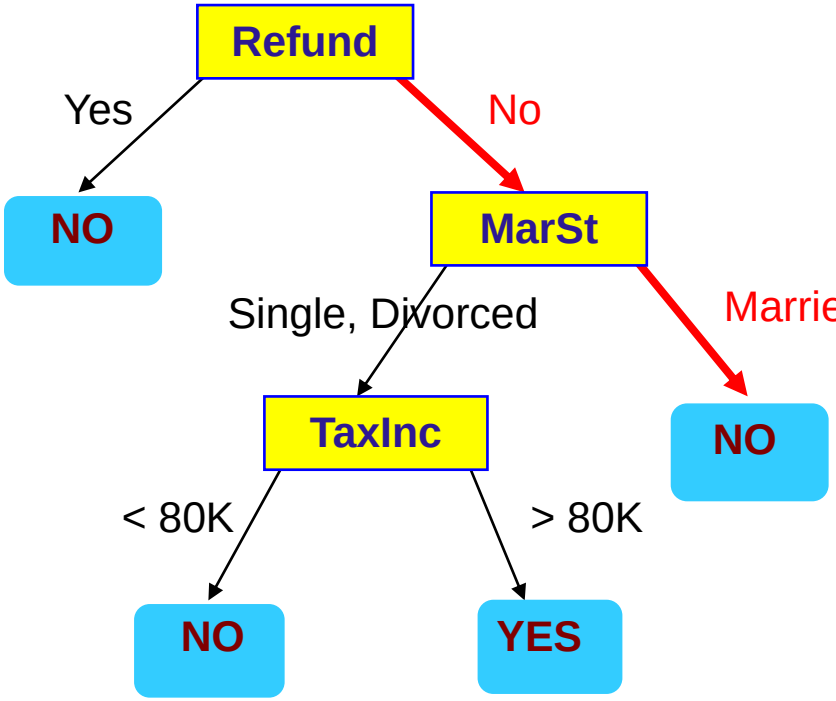
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

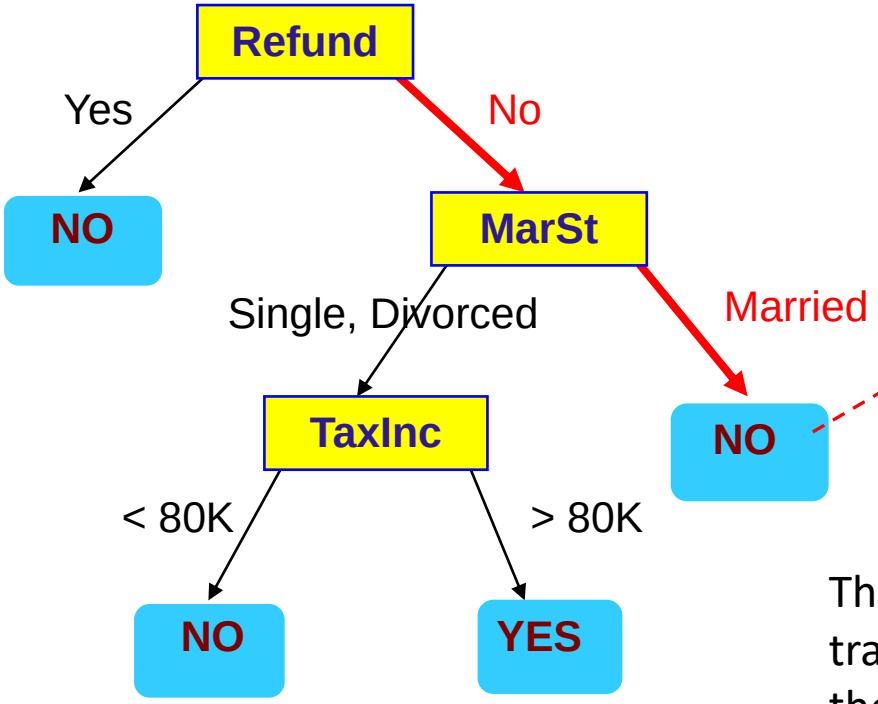


Follow the corresponding pointer to the leaf node.

[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



The reached leaf node only contains training records with Cheat = No. Hence the tree will return Cheat = No as the predicted class.

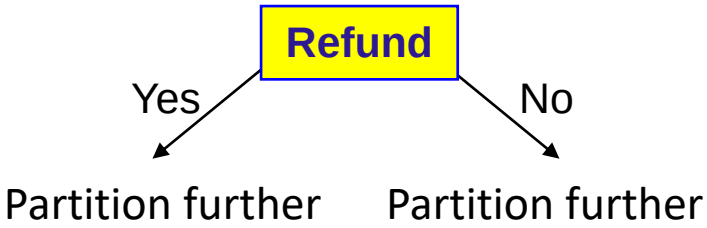
[Example source: “Introduction to Data Mining" by Pang-Ning Tan, Michael Steinbach, and Vipin Kumar. Addison-Wesley, 2006]

Parallel Decision Trees

- For classification and prediction techniques in general, and trees in particular, both induction (model training) and deduction (model use) are potential targets for parallelization.
- Due to their regular structure, trees are easier to parallelize than many other classification techniques.

Parallel Decision Tree Induction

- Tree induction starts with all training records at the root, recursively partitioning the data until a stopping condition is met. For each node, the split predicate, i.e., the condition determining how to partition the data, is selected based on a heuristic such as information gain. Typical stopping conditions are (1) pure node (all records in the node belong to the same class), (2) no split attributes left, and (3) too few records in the partition.
- Trees offer two obvious opportunities for parallel training:
  - A tree node partitions the data space, e.g., records with Refund = Yes go one way, those with Refund = No another. The split decisions in one subtree are independent of those in the other, therefore they can be performed in parallel without communication.
  - To find a node's split predicate, each attribute and its possible split values are explored. The score for each of these candidate predicates can be computed independently, but afterward coordination is required to select the split predicate with the highest score.



```
// This program assumes that each node performs a binary split into "left" and "right" partition
map( nodeID, listOfRecords ) {
 leftPartition = {}; rightPartition = {}

 // Find best split predicate for the node
 for each attribute A
  for each possible split point S
   computeScore( listOfRecords, A, S )
   Keep track of the (A, S) pair with the highest score

 // Let (bestA, bestS) be the winning split predicate. Partition the data according to the split predicate.
 for each record r in listOfRecords
  if satisfiesPredicate(r , (bestA, bestS) )
   leftPartition.add( r )
  else
   rightPartition.add( r )

 // Write the node information containing nodeID, split predicate, and child node IDs to file
 treeFile.write( nodeID, (bestA, bestS), newID(nodeID, left), newID(nodeID, right) )

 // Emit the two partitions for further splitting in the next iteration
 if not stoppingConditionMet( leftPartition )
  emit( newID(nodeID, left), leftPartition )

 if not stoppingConditionMet( rightPartition )
  emit( newID(nodeID, right), rightPartition )
}
```

This algorithm parallelizes computation by training different subtrees concurrently.

MapReduce Program Discussion

- The program uses a breadth-first approach to train the tree layer-by-layer in each iteration.
- Initially the input is the root-node ID and the entire training set. A single Map function call finds the split predicate for the root and partitions the data accordingly. In the next iteration, there are two Map calls—one for each child node of the root. And so on.
- As the computation proceeds, initially the number of different partitions increases, resulting in greater possible parallelism.
- At some point splitting in some branches ends as the stopping condition is met. Hence at some point there will be fewer Map function calls as the tree grows deeper.
- In the beginning each iteration reads the entire input data and writes out the re-partitioned input. As nodes meet the stopping condition, their data records will not be transferred any more, slowly decreasing data transfer as the computation winds down.

Improvements

- In the Map function, finding the best split predicate involves repeated reading of the input records—at least once for each attribute. This will be expensive when the data does not fit in memory. To reduce cost, one can work with a random sample, which usually provides a good approximate score and hence results in splits of similar quality.
- For data sets with a huge number of attributes, e.g., text-analysis applications in information retrieval, one should consider parallelizing the process of finding the best split attribute for a node. However, if different split attributes for the same node are explored in different Map tasks, then Reduce will be needed to find the winner and perform the data partitioning.
- Once the training data at a node fit in memory, the entire subtree could be trained in the map function.

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible “middle” points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible “middle” points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Training data sorted on A

1	2	3	5
+	+	-	-

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible “middle” points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Training data sorted on A

1	2	3	5
+	+	-	-

Split point candidate	1.5
Number of + and - cases going left	+: 1 -: 0
Number of + and - cases going right	+: 1 -: 2

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible "middle" points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Training data sorted on A

1	2	3	5
+	+	-	-

Split point candidate	1.5	2.5
Number of + and - cases going left	+: 1 -: 0	+: 2 -: 0
Number of + and - cases going right	+: 1 -: 2	+: 0 -: 2

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible "middle" points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Training data sorted on A

1	2	3	5
+	+	-	-

Split point candidate	1.5	2.5	4
Number of + and - cases going left	+: 1 -: 0	+: 2 -: 0	+: 2 -: 1
Number of + and - cases going right	+: 1 -: 2	+: 0 -: 2	+: 0 -: 1

Counting for Split Finding

- To find the best split point for attribute A, the data at the current subtree root is sorted on A. then all possible "middle" points between consecutive A-values are explored to find the one with the highest score.
  - The score is determined by a purity measure (e.g., information gain, Gini, gain ratio) for classification, or variance for prediction.

Training data

A	B	Label
2	50	+
5	10	-
1	30	+
3	20	-

Training data sorted on A

1	2	3	5
+	+	-	-

Split point 2.5 is the winner, because it perfectly separates classes + and -.

Split point candidate	1.5	2.5	4
Number of + and - cases going left	+: 1 -: 0	+: 2 -: 0	+: 2 -: 1
Number of + and minus cases going right	+: 1 -: 2	+: 0 -: 2	+: 0 -: 1

Parallel Counting for Split Finding

- Can we count the number of + and – cases going left versus right for all possible split points in parallel?
- We do not want to copy all data records to all tasks. However, if a task only receives some of the records, then it cannot even determine possible split points.
  - In the example, assume task 0 only receives the records with A-values 1 and 3. Then the middle point would be 2, not 1.5. Intuitively, task 0 cannot determine the correct split candidates, because it is missing some of the data.
- Range-partitioning would help, but can we find a cheaper solution?

Parallel Counting with Predefined Split Points

- What if each task knew all possible split points from the beginning? If all tasks count the left and right class distribution for the same split candidates, then it is easy to find the total counts.
  - In the example, assume each task was told to check split points 1.5 and 3.5.

Round 1, task 0

Training data partition

A	B	Label
2	50	+
5	10	-

Round 1, task 1

Training data partition

A	B	Label
1	30	+
3	20	-

Parallel Counting with Predefined Split Points

- What if each task knew all possible split points from the beginning? If all tasks count the left and right class distribution for the same split candidates, then it is easy to find the total counts.
  - In the example, assume each task was told to check split points 1.5 and 3.5.

Round 1, task 0

Training data partition

A	B	Label
2	50	+
5	10	-

Round 1, task 1

Training data partition

A	B	Label
1	30	+
3	20	-

Output:

1.5: left(+: 0, -: 0), right(+: 1, -: 1)

3.5: left(+: 1, -: 0), right(+: 0, -: 1)

Parallel Counting with Predefined Split Points

- What if each task knew all possible split points from the beginning? If all tasks count the left and right class distribution for the same split candidates, then it is easy to find the total counts.
  - In the example, assume each task was told to check split points 1.5 and 3.5.

Round 1, task 0

Training data partition

A	B	Label
2	50	+
5	10	-

Output:
1.5: left(+: 0, -: 0), right(+: 1, -: 1)
3.5: left(+: 1, -: 0), right(+: 0, -: 1)

Round 1, task 1

Training data partition

A	B	Label
1	30	+
3	20	-

Output:
1.5: left(+: 1, -: 0), right(+: 0, -: 1)
3.5: left(+: 1, -: 1), right(+: 0, -: 0)

Parallel Counting with Predefined Split Points

- What if each task knew all possible split points from the beginning? If all tasks count the left and right class distribution for the same split candidates, then it is easy to find the total counts.
  - In the example, assume each task was told to check split points 1.5 and 3.5.

Round 1, task 0

Training data partition

A	B	Label
2	50	+
5	10	-

Output:
1.5: left(+: 0, -: 0), right(+: 1, -: 1)
3.5: left(+: 1, -: 0), right(+: 0, -: 1)

Round 1, task 1

Training data partition

A	B	Label
1	30	+
3	20	-

Output:
1.5: left(+: 1, -: 0), right(+: 0, -: 1)
3.5: left(+: 1, -: 1), right(+: 0, -: 0)

Round 2 then groups by split point and aggregates the counts as:
1.5: left(+: 1, -: 0), right(+: 1, -: 2)
3.5: left(+: 2, -: 1), right(+: 0, -: 1)

How Well Does This Work?

- Data can be partitioned in any way, without duplication, and both round 1 and round 2 parallelize well. However, if round 2 has multiple tasks, then a third round is needed to find the split with the best score.
- How do we select the split-point candidates for an attribute A?
  - We can pick evenly-spaced values from A's domain. More candidates result in higher computation cost but increase the probability of finding a good split point. In the example, the optimal split is missed, because no candidate between 3 and 5 was tried.
  - To not miss the optimal splits, we could sort the input on A and use all middle values between consecutive A-values. This adds extra sort cost and often produces too many candidates, resulting in high cost during the parallel counting phase.
- For more information, see [Biswanath Panda, Joshua S. Herbach, Sugato Basu, and Roberto J. Bayardo. PLANET: Massively Parallel Learning of Tree Ensembles with MapReduce. Proc. Int. Conf. on Very Large Data Bases (VLDB), 2009]. This is the algorithm on which Spark's tree implementation in MLlib is based.

Parallel Decision Tree Deduction

- For a single test record, parallelizing deduction will usually not be efficient. Even for large trees, it would be faster to access nodes in a file instead of running multiple MapReduce iterations.
- Parallel deduction becomes viable if predictions are made for a huge set of test records. The tree model can broadcast to all worker machines; then each Map call independently computes the prediction for a test record.

```
// The file with the decision tree is made available through the file cache
Class Mapper {
  tree

  setup()
    tree = load tree from file cache

  map( test record r ) {
    output = tree.makePrediction( r )
    emit( r, output)
  }
}
```

Decision Trees in Spark

- We can again rely on MLlib for a ready-to-use solution. Look at the source code to see how it is implemented.
  - The code below shows excerpts from the example in the Spark 2.3.2 documentation.

```
// spark.ml
val dt = new DecisionTreeClassifier()
  .setLabelCol("indexedLabel")
  .setFeaturesCol("indexedFeatures")

// Chain indexers and tree in a Pipeline.
val pipeline = new Pipeline()
  .setStages(Array(labelIndexer, featureIndexer,
    dt, labelConverter))

// Train model. This also runs the indexers.
val model = pipeline.fit(trainingData)

// Make predictions.
val predictions = model.transform(testData)
```

```
// spark.mllib
val model = DecisionTree.trainClassifier(trainingData,
numClasses, categoricalFeaturesInfo,
  impurity, maxDepth, maxBins)

// Evaluate model on test instances and compute test
error
val labelAndPreds = testData.map { point =>
  val prediction = model.predict(point.features)
  (point.label, prediction)
}
```

Other Classification and Prediction Methods

- In addition to decision trees, numerous other classification and prediction techniques have been proposed. Many are complex and hence not easy to parallelize. The following is a list of popular techniques:
  - Support Vector Machines (SVMs)
  - Artificial Neural Networks (ANNs)/Deep Learning
  - Nearest Neighbor
  - Naïve Bayes
  - Bayesian networks
  - Regression.

Summary

- Data mining techniques are crucial tools for discovering hidden patterns in big data. Unfortunately, many techniques are complex. Available implementations often are highly optimized for centralized in-memory processing.
- For some of the simpler techniques such as K-means clustering and decision trees, parallel implementations can be designed with reasonable effort.
- As a fallback, when the input data is too big to fit in memory, create an in-memory sample and then apply an existing centralized implementation. While not perfect, this often gives a good approximation of the desired results. And it can be parallelized easily by exploring different samples and/or model parameter settings on different worker machines.

References

- Data mining textbook: Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques, 3rd edition, Morgan Kaufmann, 2011
- Biswanath Panda and Joshua S. Herbach and Sugato Basu and Roberto J. Bayardo. PLANET: Massively Parallel Learning of Tree Ensembles with MapReduce. Proc. Int. Conf. on Very Large Data Bases (VLDB), 2009
  - https://scholar.google.com/scholar?cluster=11753975382054642310&hl=en&as_sdt=0,22