CMSC 724: Data Mining

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Outline

Data Mining

- Going beyond the “query-response” model
  - “Tell me what is interesting in this huge dataset” ?
  - Also called “knowledge discovery”
- Many applications
  - Marketing, fraud detection etc. . .
- Much work in the Machine Learning and Statistics literature
- Three of the most common problems addressed in the area:
  - Clustering
  - Association Rules
  - Classification

Outline

Association Rules

- Consider “market basket” data
  - Each “transaction” contains the list of “items” bought by a customer in one visit
  - Not normalized (transactions contain diff no. of items)
  - Example:
    - *(customer1, “2/2/2 5pm”, “milk”, “bread”, ...)*
    - *(customer2, “2/3/2 5:10pm”, “milk”, “coffee”, ...)*

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  - Example:
    - *(customer1, "2/2/2 5pm", "milk", "bread", ...)*
    - *(customer2, "2/3/2 5:10pm", "milk", "coffee", ...)*
- Association Rule: $X \implies Y$, with conf c%, support s%
  - Confidence: c% of all tuples that contain X contain Y
  - Support: s% of all tuples in the table contain $X \cup Y$
  - X and Y are sets of items ("itemsets"), with $X \cap Y = \phi$

Association Rule Mining

- Goal:
  - Find all association rules with at least a given confidence (say 90%) and a given support (say 5%)

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  - Find all association rules with at least a given confidence (say 90%) and a given support (say 5%)
- Fast Algorithms for Mining Association Rules; Rakesh Agrawal and Ramakrishnan Srikant; VLDB 2004
  - Presented an algorithm called “Apriori”
    - *For finding the itemsets with the specified support*
  - Probably the first “scalable” data mining paper
  - One of the highest cited papers in all of CS
  - Came out of Database literature, not Machine Learning

Basic Apriori Algorithm

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- Observation: A set X cannot have sufficient support if $Y \subset X$ doesn't have sufficient support

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- Observation: A set X cannot have sufficient support if $Y \subset X$ doesn't have sufficient support
- Algorithm:
  1. Start by counting all items that occur in 5% transactions (say $\{I_1\}$, $\{I_2\}$, $\{I_3\}$)
  2. Generate a set of candidates for the next step by combining the above itemsets ($\{I_1, I_2\}$, $\{I_1, I_3\}$, $\{I_2, I_3\}$)
  3. Make another pass and check if the candidate itemsets appear in 5% transactions (say $\{I_1, I_2\}$, $\{I_1, I_3\}$ appear)
  4. Repeat steps 2 and 3. (In the example, there are no more candidate sets. $\{I_1, I_2, I_3\}$ cannot occur in 5% transactions, because $\{I_2, I_3\}$ doesn't).

Association Rule Mining

- Basic Apriori Algorithm:
  - Step 2 done using SQL queries and self-joins
    - Essentially a self-join between the itemsets found at previous step
    - Number of joins limited (and size of the relations decreases)
  - More efficient algorithms presented in the paper

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  - Step 2 done using SQL queries and self-joins
    - Essentially a self-join between the itemsets found at previous step
    - Number of joins limited (and size of the relations decreases)
  - More efficient algorithms presented in the paper
- Much more work on this topic since that paper
  - 5197 citations on Google Scholar
    - Compare with: Garey and Johnson (18226) or Introduction to algorithms (13786)

Outline

Clustering

- Given a set of tuples and k, group them into k "clusters"
  - So that some distance metric is minimized
- Unsupervised: You are only given k
- Cluster IDs have no intrinsic meaning (though one can be provided later)
- Commonly used distance metrics:
  - For numerical data: *Euclidean* distance, *Manhatten* distance, L_∞ distance
  - For categorical data: Map to reals

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  - For categorical data: Map to reals
- Number of clusters ?
  - The algorithms find exactly k clusters
  - Too many clusters not very useful
  - Trying to have few clusters results in large diameters

Clustering

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  - k-means: The center of a cluster is the “mean” of the points assigned to it
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    - k-center: minimizes the largest distance between a point and its cluster head
    - k-median: minimizes the sum of distances between points and their cluster heads

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    - k-median: minimizes the sum of distances between points and their cluster heads
- The latter two considered harder
- *Facility Location Problem:* The number of centers is not fixed, but there is a cost to choose a new center

Clustering

- “k-means” algorithm
  - At any point, have k “centroids”, one for each cluster
  - Initially, choose k of the points randomly to be centroids
  - Assign each point in the dataset to the closest cluster centroid
  - Recompute the cluster centroids to be the “means” of the points assigned to that cluster
  - Repeat till convergence

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  - Repeat till convergence
- Guaranteed to converge, usually within a few iterations
- Not optimal, finds a local minima (there are too many local minimas in the solution space)
- Also somewhat sensitive to the initial choice of centrois
- EM Algorithm: Expectation-Maximization Algorithm

Clustering

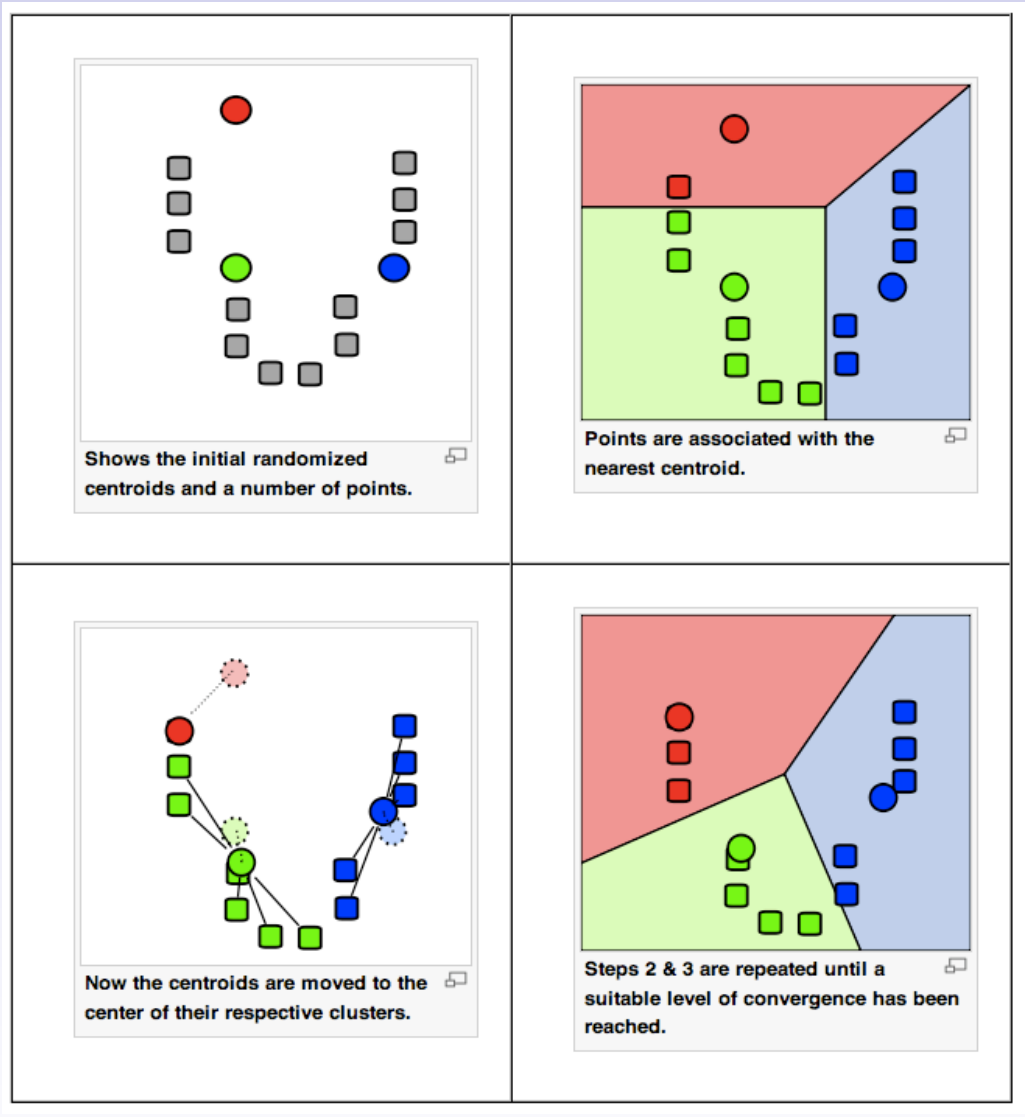

Figure: K-Means Illustration (From Wikipedia Article)

BIRCH: Scalable Clustering

- Algorithms like *k-means* not suitable for large datasets
- BIRCH provides a one-pass algorithm for clustering
- Supports a variety of distance metrics between clusters and across clusters

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- Algorithms like *k-means* not suitable for large datasets
- BIRCH provides a one-pass algorithm for clustering
- Supports a variety of distance metrics between clusters and across clusters
- Key notions:
  - Given a set of points, $\overrightarrow{X_i}$, three terms capture all of their important properties:
    - $CF = (n, \Sigma\overrightarrow{X_i}, \Sigma\overrightarrow{X_i}^2)$ (Clustering feature)
    - Everything else (the distance metrics) can be computed using these, assuming you treat them as a unit
    - Easy to compute if two groups of points are merged
    - Also called “sufficient statistics”
  - There may exist distance metrics for which this won’t hold (e.g. median-based metrics)

BIRCH: Scalable Clustering

- CF-Tree
  - Height-balanced Tree
  - A node contains at most B entries of form $[CF_i, child_i]$
    - $child_i$: pointer to the i^{th} child
    - CF_i: Clustering feature of all points grouped below $child_i$
  - Leaves: Same except that the diameter of the points must be below a threshold T

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- Basic Algorithm:
  - Build the CF-Tree incrementally as the data is scanned
    - May have to adjust the threshold so that the tree fits in memory
  - Do a clustering using the final CF-Tree (using any clustering algorithm)

BIRCH: Scalable Clustering

- Points to note:
  - Helps to imagine a “bottom-up” algorithm for clustering
    - Can think of each of the leaves as a “sub-cluster”
    - First we create fixed sized sub-clusters from the data (Phase 1)
    - Note: Leaf $\neq$ sub-cluster
    - Then do the clustering on the sub-clusters (Phase 3)

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    - Then do the clustering on the sub-clusters (Phase 3)
  - The CF-Tree has no "ordering" on the leaves
    - Same data point, if duplicated, may end up in different leaves
  - The clustering at the sub-clusters is final
    - Once two points are put together in a single sub-cluster, no way to separate them
    - Since we have "lost" the original points

BIRCH: Scalable Clustering

- Points to note:
  - Adjusting the threshold: requires very little extra memory
  - Outliers:
    - Can cause problems
    - Each outlier must be in a separate sub-cluster
    - BIRCH handles this by spooling them to disk or throwing them out

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    - BIRCH handles this by spooling them to disk or throwing them out
  - How are the points assigned to the clusters ?
    - At the end, we get a set of cluster centroids
    - Another pass is required to assign a “cluster-id” to the data points
    - Or can do it on demand (when the user asks for some point)

Outline

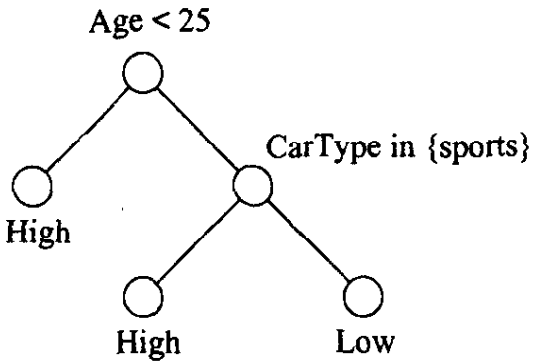
Classification

- Assign tuples to pre-defined labels (high/med/low “risk”)
- Supervised learning task: Usually given the labels for a set of tuples
- Usually based on some statistical model
- Commonly used techniques
  - Decision trees: A (usually) binary tree that you can traverse for each tuple
  - Bayesian classifiers (e.g. Naive Bayes)
  - Support vector machines etc. . .
- Much work on scaling these up in the Database literature

Decision Trees

rid	Age	Car Type	Risk
0	23	family	High
1	17	sports	High
2	43	sports	High
3	68	family	Low
4	32	truck	Low
5	20	family	High

(a) Training Set



(b) Decision Tree

- Learning decision trees:
  - Given: A set of tuples and their classes
  - Goal: Find the best decision tree of limited size
    - How to define “Best” ? *Misclassifies fewest training tuples*
    - Why limited size ?? Otherwise becomes too specific and not very useful (overfitting).
- NP-Hard problem.

Decision Trees

- Algorithm Overview:
  - Find *(attr, value)* pair that differentiates between the labels in the training data the best
    - Different metrics: *information gain*, *Gini index*
  - Set that as the root
  - Split the dataset in two parts and recurse
  - At the end, prune the decision tree found so that it is not very large

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  - At the end, prune the decision tree found so that it is not very large
- Key algorithmic/scalability challenges:
  1. Finding the best "split point" for very large training sets
     - Need to evaluate the information gain or Gini index many times
  2. Splitting the dataset
  3. How to parallelize

Aside: Evaluating Splits

- Original tuples: *S = (a, 1, HIGH), (a, 2, HIGH), (b, 1, LOW), (b, 2, LOW)*
  - Schema: (attr1, attr2, class label)
- Based on Gini Index Gain:
  - Gini Index: $G(p) = 1 - \Sigma p_i^2$, where p is a distribution
    - Equals zero only if all tuples have the same class label
    - Here we use the distribution on the class labels
  - $Gini(S) = 1 - 0.5^2 - 0.5^2$
  - If S split in S_1 and S_2, the gain =

$$Gini(S) - (\frac{|S_1|}{|S|} Gini(S_1) + \frac{|S_2|}{|S|} Gini(S_2))$$

  - Maximize this value over all possible splits (in this case, the split on attr1)

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- Based on Information Gain: Replace $G(p)$ with $H(p)$

SPRINT: A Scalable Parallel Algorithm

- Key ideas: Maintain several sorted lists
  - Can be easily split into two parts

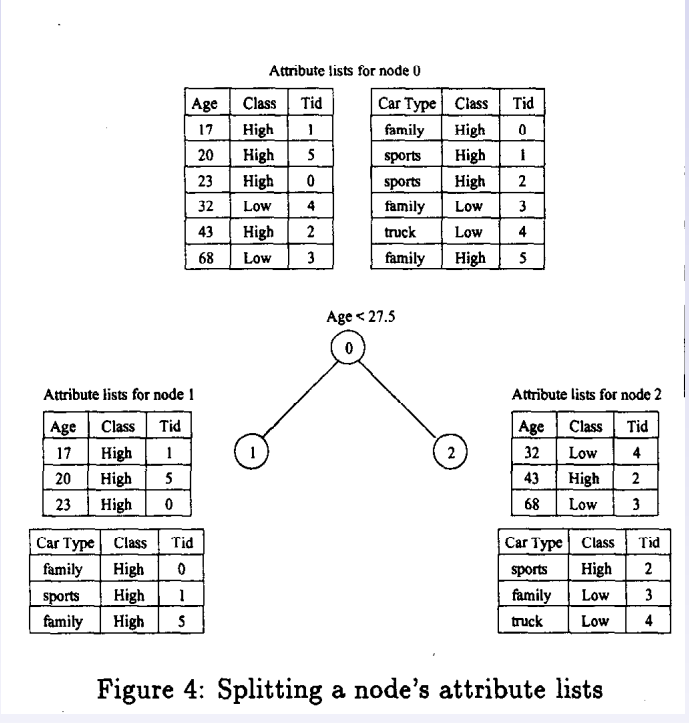

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Figure 4: Splitting a node's attribute lists

- Construct histograms to quickly compute the Gini index
  - Can be done with sorted attribute lists in one pass
- Can be parallelized using "parallel sort" techniques

Outline

Naive Bayes Classifiers

- Important class of classifiers to know about; simple; widely-used
- Given a data point, $\overrightarrow{x} = \{x_1, \cdots, x_d\}$, the probability that it belongs to class c is given by:
  - $p(class = c|\overrightarrow{x}) = \frac{p(c)p(\overrightarrow{x}|c)}{p(\overrightarrow{x})}$ (Bayes Rule)

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- To pick the class with the maximum $p(c|\overrightarrow{x})$, we instead pick the class with the maximum:
  - $p(c)p(\overrightarrow{x}|c)$
  - $= p(c)p(x_1|c)p(x_2|c)\cdots p(x_d|c)$ (assume Independence)

Naive Bayes Classifiers

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- Also, we learn $p(c)$ for all c from training data
- Note: Very few parameters $\Longrightarrow$ not much training data required

Naive Bayes Classifiers

- We learn $p(x|c)$ for all x and all c from training data
- Also, we learn $p(c)$ for all c from training data
- Note: Very few parameters $\implies$ not much training data required
- Given a new data point $\overrightarrow{x}$:
  - Compute $p(c)p(x_1|c)p(x_2|c)\cdots p(x_d|c)$
  - Pick the class label with the largest value

Outline

Data Mining Models + Query Evaluation

- Data mining: Specialized algorithms
  - Typically run outside the database
  - The results might be added back in
  - Not very efficient (recall MauveDB motivation)
- Goal: Closer integration of mining models into a DBMS

Data Mining Models + Query Evaluation

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  - Typically run outside the database
  - The results might be added back in
  - Not very efficient (recall MauveDB motivation)
- Goal: Closer integration of mining models into a DBMS
- Specifically:
  - Allow querying the “model output” as normal attributes
  - “where risk = High” (“risk” is the predicted class label)
  - Similarly in MauveDB, allow querying output of regression models

Data Mining Models + Query Evaluation

- Efficient Evaluation of Queries with Mining Predicates; Chaudhuri et al.
- Classification/Clustering Models
  - Allow querying the “class labels” directly
- Language Support ?
  - MS Analysis Server allows defining classification models directly and allows querying
  - IBM Intelligent Miner (IM) also supports such functionality
  - Can think of these as “model-based views” as well

Support in MS Analysis Server

```
CREATE MINING MODEL Risk_Class          %Name of Model
(
Customer_ID LONG KEY,                   %source column
Gender TEXT DISCRETE,                   %source column
Risk TEXT DISCRETE PREDICT,             %prediction column
Purchases DOUBLE DISCRETIZED(),         %source column
Age DOUBLE DISCRETIZED,                 %source column
))
USING [Decision_Trees_101]              %Mining Algorithm
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```
SELECT D.Customer_ID, M.Risk
FROM [[Risk_Class] M
PREDICTION JOIN
(SELECT Customer_ID, Gender, Age, sum(Purchases) as SP
  FROM Customers D Group BY Customer_ID, Gender, Age
  ON M.Gender = D.Gender
  and M.Age = D.Age
  and M.Purchases = t.SP
  Where M.Risk = ‘low”
```

Data Mining Models + Query Evaluation

- Query (abusing notation):
  - select * from [Risk-Class] M where M.risk = “low”
- Naive Approach
  - Extract all rows that satisfy the rest of the predicates (none in this case)
  - Apply the model to each row to predict the risk, and then check whether = “low”

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- Naive Approach
  - Extract all rows that satisfy the rest of the predicates (none in this case)
  - Apply the model to each row to predict the risk, and then check whether = “low”
- Issues:
  - Must do a seq scan and apply to all tuples (in this case)
  - Can we do better ?
- Aside:
  - Assumption that the model is to be applied for every tuple separately

Approximate Predicates

- Add predicates to the query that are guaranteed to not change the answer
- Simple example:
  - select * from R where $R.a = 10$
- Change to
  - select * from R where $R.a = 10$ and $R.a$ betn 9 and 11
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    - No use, but...
  - select * from R where $R.a = 10$ and $R.b = 10$
    - IF it is known that $R.a = R.b$ (maybe through a *function dependency*)
    - Faster to evaluate if there is an index on $R.b$ (but not on $R.a$)
    - Commonly done in most query optimizers

Approximate Predicates

- Similar ideas have been exploited before
  - E.g. bounding rectangles in R+-Trees
- Query optimizers infer new predicates to add to the given predicates
  - Using transitivity, functional dependencies etc. . .
  - Not approximate though

Approximate Predicates

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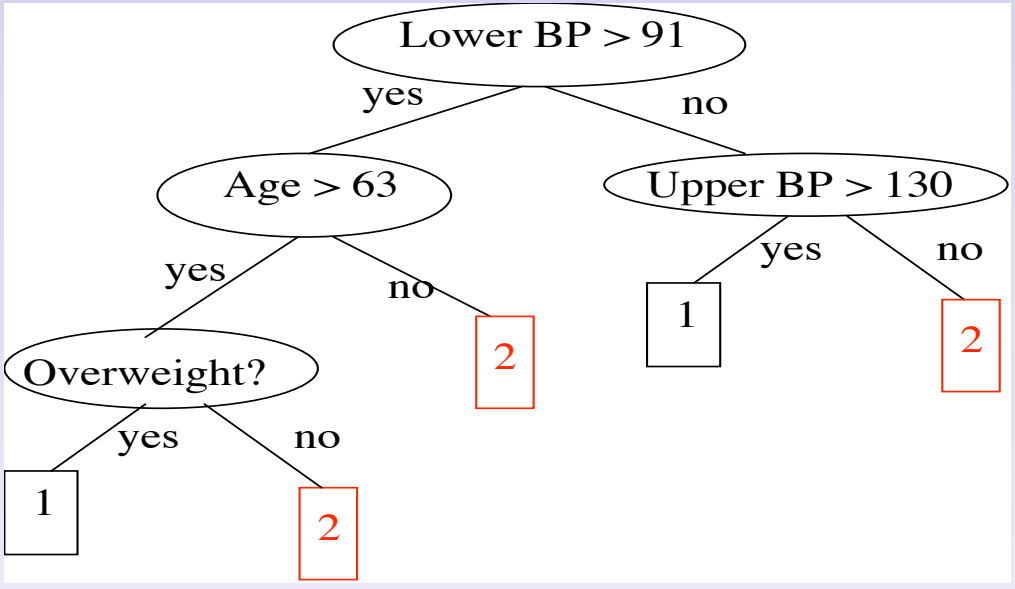
  - E.g. bounding rectangles in R+-Trees
- Query optimizers infer new predicates to add to the given predicates
  - Using transitivity, functional dependencies etc...
  - Not approximate though
- In general, to add predicate $P2$ to the query:
  - select * from R where $P1$
- We must have that:
  - $P1 \implies P2$
  - Not necessary the other way around
- Why ?
  - $P2$ might permit better access methods (indexes etc)

Mining Predicates: Decision Trees



- For a query: “label = 2”, find all leaves, find the predicate corresponding to it, and take a disjunction

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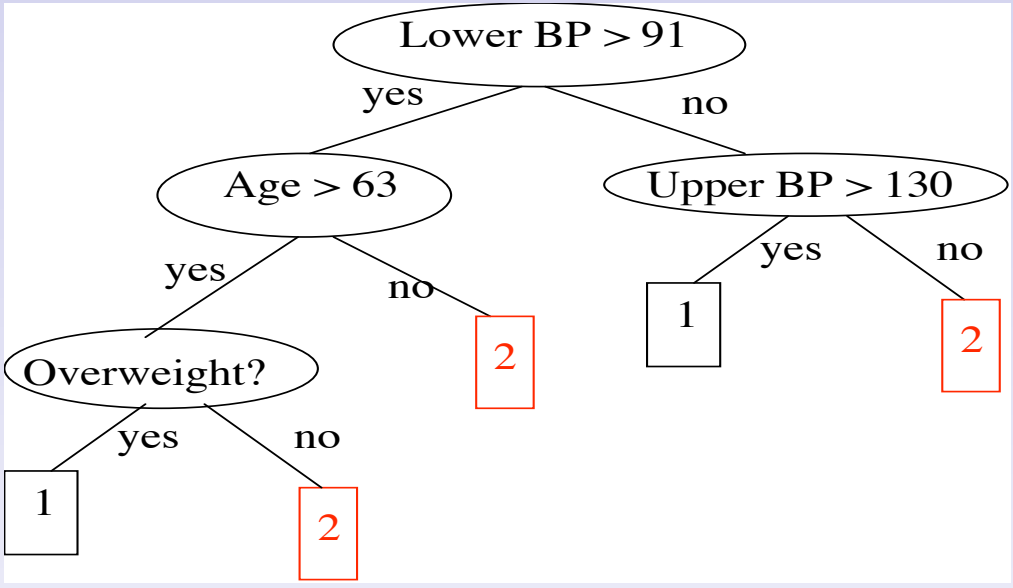

- For a query: “label = 2”, find all leaves, find the predicate corresponding to it, and take a disjunction
  - (LowerBP > 91 and Age > 63 and Overweight = no) $\vee$
  - (LowerBP > 91 and Age < 63) $\vee$
  - (LowerBP <= 91 and UpperBP <= 130)

Mining Predicates: Any classifier. . .

- Consider a predicate: “label = 1”
- Let d be the number of attributes/dimensions
- Imagine the d-dimensional hyperrectangle, where all points are marked as T or F
  - T $\rightarrow$ “label = 1”

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- Let d be the number of attributes/dimensions
- Imagine the d-dimensional hyperrectangle, where all points are marked as T or F
  - T $\rightarrow$ “label = 1”
- Cover all T’s using a set of hyperrectangles
- Use them as the predicates
  - Typically many ways of doing this
  - Want to limit the number of rectangles
    - So could be approximate
- If small No. of dimensions, could do this exhaustively
  - Only needs to be done once for each label
- But generally, must find more efficient ways

Mining Predicates: Any classifier. . .

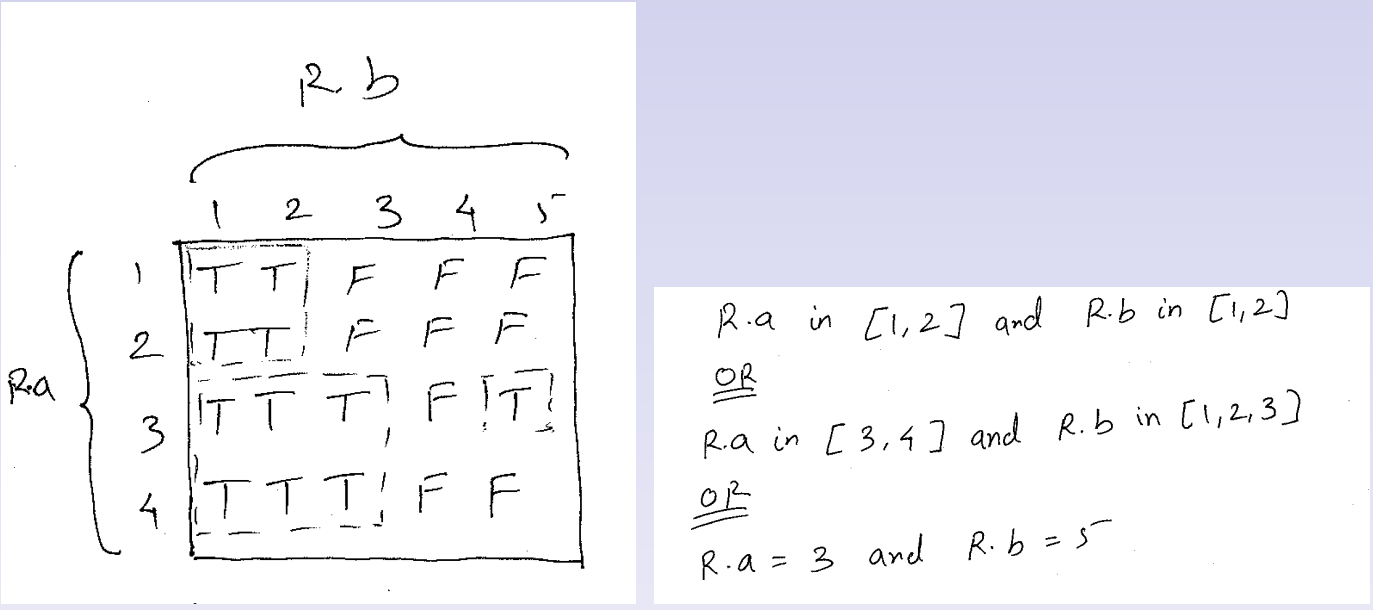

Figure: Mining Predicates: Creating a predicate for any classifier

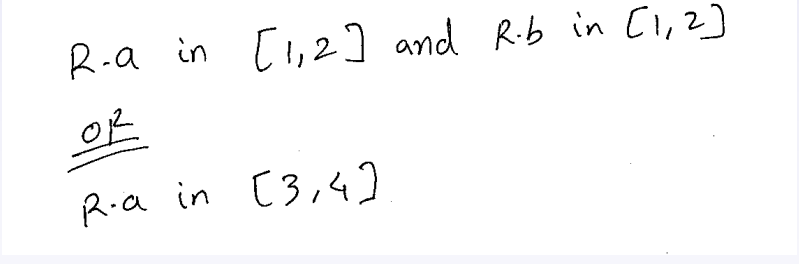

Figure: Mining Predicates: Approximating the predicate constructed in previous figure

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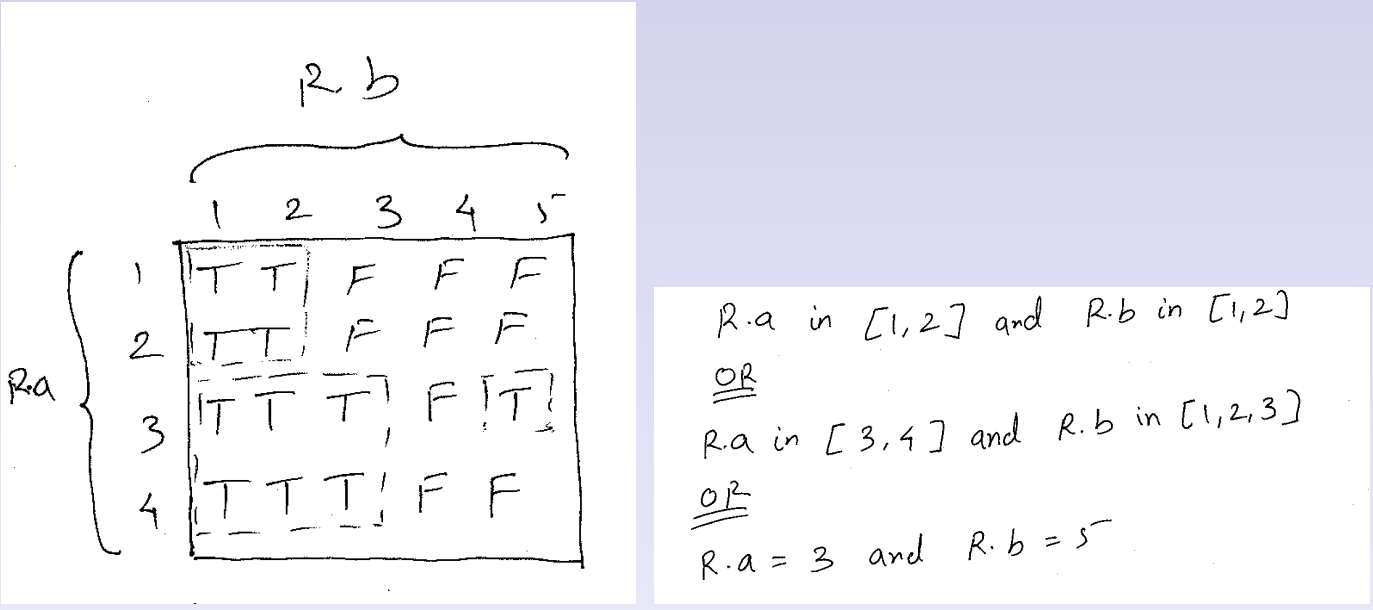

Figure: Mining Predicates: Creating a predicate for any classifier

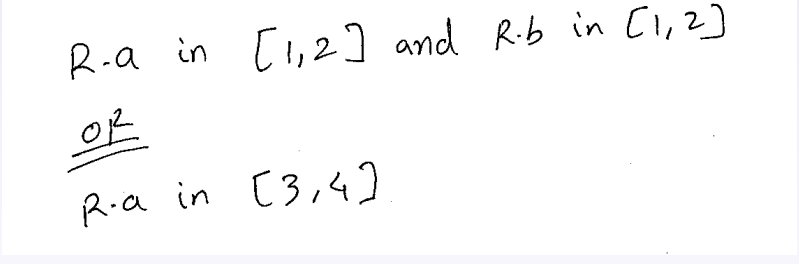

Figure: Mining Predicates: Approximating the predicate constructed in previous figure

Mining Predicates: Clustering

- Typically new points classified using their distance to the centroids
- The space gets split into convex polyhedrons
- Other types of clustering-based classifiers can be handled similarly, or using the algorithm for Naive Bayes

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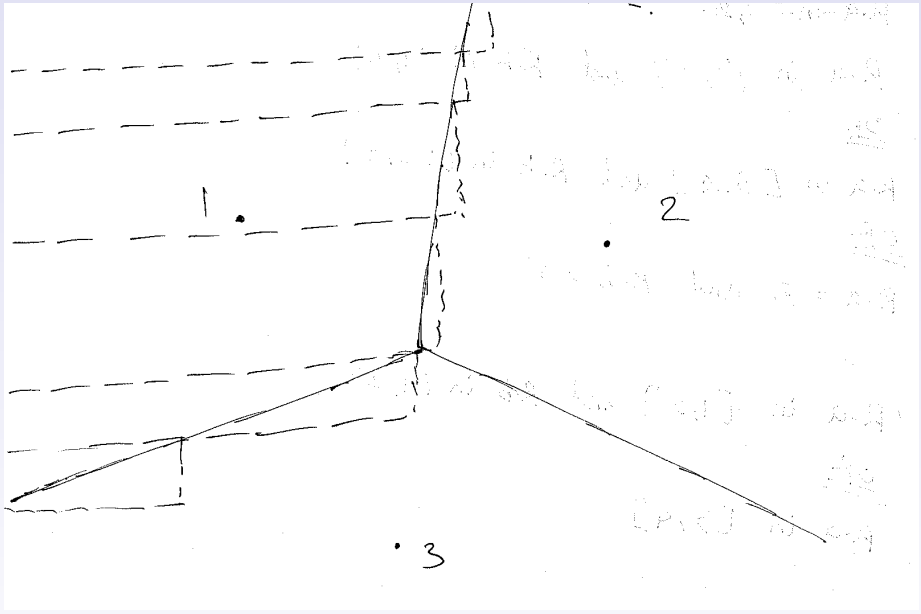

Figure: Mining Predicates: Creating a predicate for a clustering-based classifier

Mining Predicates: Naive Bayes Classifiers

- Option 1: Enumerate the hyperspace and find the covering rectangles
- Option 2: Use the properties of the classifer to find the covering rectangles efficiently
- Can quickly check if a class c:
  - Holds for all the points in a hyperrectangle (MUST-WIN)
  - Holds for no point in a hyperrectangle (MUST-LOSE)
  - Holds for some points (AMBIGUOUS)

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- Start with the hyperrectangle covering the entire space
- Subdivide until all hyperrectangles fall in one of the first two categories
- A “threshold” parameter used to get an approximate but small set of rectangles
  - In which case, some rectangles remain AMBIGUOUS

Mining Predicates: Further Thoughts

- Can be extended to handle some other types of predicates as well

Mining Predicates: Further Thoughts

- Can be extended to handle some other types of predicates as well
- Optimizers are not perfect
  - May not like adding too many new predicates
  - Too much complexity $\Longrightarrow$ sequential scan
  - Also selectivity estimates will get messed up
    - By definition, highly-correlated predicates
- Very specific to the specific types of models being used
  - How to generalize ?