## **Managing Big Data Classification: Alternative Methods**

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Reminder of the classification problem Given a collection of records **(training set )**

› Each record contains a set of *attributes*, one of the attributes is (always) the *class*.

 Find a *model* **for class attribute** as a function of the values of other attributes.

 Goal: **previously unseen** records should be **assigned a class** as accurately as possible.

# A big picture of classification methods



### Alternative methods

 Rule-based classifiers k-Nearest Neighbors (k-NN) **• Naïve Bayes** 

### Rule-based classifiers

- **Classify records** by using a collection of **"if…then…" rules**
- General form of rule: **(***Condition***)**  *y*
	- › where
		- *Condition* is a **conjunctions (logical AND/)** of attributes
		- *y* is the **class label**
	- › *LHS*: rule **antecedent or condition (Left-hand side)**
	- › *RHS*: rule **consequent (Right-hand side)**
	- › **Examples** of classification rules:

**(Blood Type=Warm) (Lay Eggs=Yes) Birds**

**Antecedent/LHS Consequent/RHS**

## Rule-based classifier (Example)



**Records (also called**  *instances***)**

**Set of rules for above dataset**

**R1: (Give Birth = no)**  $\land$  (Can Fly = yes)  $\rightarrow$  Birds **R2: (Give Birth = no)**  $\wedge$  (Live in Water = yes)  $\rightarrow$  Fishes **R3: (Give Birth = yes) (Blood Type = warm) Mammals R4: (Give Birth = no)**  $\wedge$  (Can Fly = no)  $\rightarrow$  Reptiles **R5: (Live in Water = sometimes) Amphibians**

Applying rule-based classifier Say that a rule *r* **covers an instance or record x** if the **attributes** of the instance **satisfy the condition of the rule (result TRUE)**

R1: (Give Birth = no)  $\land$  (Can Fly = yes)  $\rightarrow$  Birds R2: (Give Birth = no)  $\wedge$  (Live in Water = yes)  $\rightarrow$  Fishes R3: (Give Birth = yes)  $\land$  (Blood Type = warm)  $\rightarrow$  Mammals R4: (Give Birth = no)  $\land$  (Can Fly = no)  $\rightarrow$  Reptiles R5: (Live in Water = sometimes)  $\rightarrow$  Amphibians **Set of rules**



Above rules cover instances (look at conditions):

**The rule R1 covers a instance "hawk" => Bird ( class )** 

**The rule R3 covers the instance "grizzly bear" => Mammal (class)**

# Measuring "quality" of rule?

- **Assume classification rule A → y**, where A an expression of any number on conjunctions on attributes, y class attribute and a dataset D
- **Coverage of a rule:**
	- › **Fraction of records** that **satisfy only the antecedent** (LHS or expression A) of a rule

*Coverage*(r) =  $\frac{|A|}{|D|}$ ,

 $|A|$  = number of inst. satisf. antecedent,

 $|D|$  = number of inst. in dataset

### **Accuracy of rule**

› **Fraction of records** that **satisfy both the antecedent and consequent of a rule**

 $Accuracy(r) = \frac{|A \cap y|}{|A|}$ ,

 $|A \cap y|$  = number of inst. satisf. antecedent and consequent

# Measuring "quality" of rule? Examples

- Rule: **(Status=Single) No**
	- $\geq$  Coverage of rule = 4/10 = 40%
	- $\rightarrow$  Accuracy of rule = 2/4 = 50%
- Rule: **(Refund=Yes) Yes**
	- Coverage of rule =  $3/10 = 30\%$
	- Accuracy rule =  $0/3 = 0\%$
- Rule: **(Status=Married) (TaxInc. < 70k)**   $\rightarrow$  No
	- Coverage of rule =  $1/10 = 10\%$
	- Accuracy or fule =  $1/1 = 100\%$
- Rule: **(Refund=No) (TaxInc. > 65K) Yes**
	- Coverage of rule =  $6/10 = 60\%$
	- Accuracy or rule =  $3/6 = 50\%$



**Dataset, |D|=10**

### How do rules work?

**• Rules are triggered by each instance i.e. starts the** execution. Example:

**R1:** (Give Birth = no)  $\land$  (Can Fly = yes)  $\rightarrow$  Birds

**R2:** (Give Birth = no)  $\land$  (Live in Water = yes)  $\rightarrow$  Fishes

**R3:** (Give Birth = yes)  $\land$  (Blood Type = warm)  $\rightarrow$  Mammals

**R4:** (Give Birth = no)  $\land$  (Can Fly = no)  $\rightarrow$  Reptiles

**R5:** (Live in Water = sometimes)  $\rightarrow$  Amphibians



What rules are triggered by the above data?

- **A lemur triggers rule R3, so it is classified as a mammal**
- **A turtle triggers both R4 and R5**
- **A dogfish shark triggers none of the above rules**

### Characteristics of rules

### **Mutually exclusive rules**

- › Classifier contains mutually exclusive rules if the rules are independent of each other
- › Every record is covered by at most one rule

### **Exhaustive rules**

› Classifier (i.e. set of rules) has **exhaustive coverage** if it **accounts for every possible combination** of attribute values

Each record is covered by at least one rule

# Examples of characteristics

### Example



R1: (Body Temp = cold)  $\rightarrow$  Not mammal R2: (Body Temp = warm)  $\land$  (Gives birth = yes)  $\rightarrow$  Mammal R3: (Body Temp = warm)  $\land$  (Gives birth = no)  $\rightarrow$  Not mammal

**This rule set is i) mutual exclusive and ii) exhaustive**

## **Building classification rules**

### Two ways

- › **Direct Method**
	- **Extract rules directly from training data**
	- Algorithms: RIPPER, CN2, Holte's 1R

### › **Indirect Method**

- **Extract rules from other classification models** (e.g. decision trees, neural networks, etc).
- Algorithms: C4.5rules

## Direct method

Sequential covering algorithm

- 1. Start from an empty rule
- 2. Grow a rule using **the Learn-One-Rule function**
	- Grow a rule, by **adding attributes in a greedy way**
- 3. Remove training records covered by the rule
- 4. Repeat Step (2) and (3) until stopping criterion is met

### Direct method

Sequential covering algorithm

- › Extracts rule for each value of class sequentially.
- › Learn-one-rule returns one new rule based on its efficiency:
	- Large positive rate
	- Small negative rate
- How are rules "grown"?

# Example of Sequential Covering





(i) Original Data (ii) Step 1

**Start by finding instances with attributes/conditions that have great positive cover by rule. Remove these instances**

# Example of Sequential Covering



(iii) Step 2

R1 R2

(iv) Step 3

**Continue finding the next rule which covers as much of the space as possible.**

### Strategies for growing rules

 How do rules grow i.e. get "bigger" by enclosing more conditions?

- Two Strategies
	- › **General to specific**
	- › **Specific to general**

# Strategies for growing rules



# Strategies for growing rules

### **Specific to general**



### **1. Select one random instance**

2. Create rule out of instance, by forming conjunctions **from attributes of instance** 

3. **Start removing conjunctions** until it starts covering negative instances

## Summary of Direct Method

### Grow **a single rule**

- Using general-to-specific or specificto general strategies
- **Remove Instances** satisfying rule
- Prune the rule (if necessary)
- **Add rule** to Current Rule Set
- **⊙ Repeat**

## Indirect Method Use Decision Tree to extract rules



 Add rules by **forming conjunctions at each node**. **Braches/Paths to leaves represent one rule**

## Indirect Method - Example



**R1:** (Refund=Yes)  $\rightarrow$  No **R2:** (Refund=No)  $\land$  (MarSt=Married)  $\rightarrow$  No **R3:** (Refund=No)  $\land$  (MarSt = Single, Divorced)  $\land$  (TaxInc < 80K)  $\rightarrow$  Yes

# Advantages of Rule based classifiers

- As **highly expressive** as decision trees
- Easy to **interpret**
- Easy to **generate**
- Can classify new instances **rapidly**
- Performance **comparable to decision trees**

## k-Nearest Neighbors

## Instance-based classifiers



**also** 

- **Instance based classifier?**
	- **Just store** the training records forever
	- **Do not process** training records at all to learn something (in contrast to e.g. decision trees)
	- **Use stored training records** to predict class label of unseen

#### Unseen Case



### Instance-based classifiers

- Instance-based are among the simplest classifiers in existens
- Examples methods:
	- › **Rote-learner**
		- **Memorizes (i.e. stores)** entire training data and performs **classification only** if attributes of record **match** one of the training examples **exactly**
	- › **k-Nearest neighbor (k-NN)**
		- Uses **k "closest" points (nearest neighbors)** for performing classification
			- **For categorical class vars: majority vote** of k closest points

Nearest Neighbor Classifiers Basic idea of k-NN (aka duck-typing): › If it **walks like a duck**, **quacks like a duck**, then **it's probably a duck**



# k-Nearest Neighbors Classifiers

- Outline of k-NN algorithm (quite simple)
	- › **Calculate distance** between **new (unclassified) record** and **all other records in dataset (training set)**
	- › Find the **k records in dataset with the closest distances to new record**
		- **k is always given, input of algorithm**
	- › **Look** at the **class of these k nearest records**
	- › If **majority** of the k records **belong to class C**, then **new record** is assigned **class C (one way)**
		- **k** usually chosen odd
	- › k-NN is a **non-parametric method** (in contrast to decision trees)
		- **Non-parametric?** Does not care at all about he distribution of records

## **k-Nearest Neighbor Classifiers**

### $\overline{\bullet}$  Historical note

› One of the **earliest methods** to classify records (and one of the simplest)

1956

## Nearest-Neighbor (NN) Classifiers



- NN **requires three things**
	- The **set of stored records**
	- **Distance Metric to compute** distance between records
	- The **value of** *k*, the number of nearest neighbors to retrieve
	- To classify an unknown record:
		- Compute **distance to all other training records**
		- Identify *k* **nearest neighbors i.e. smallest distance**
			- Use **class labels of nearest neighbors** to determine the class label of unknown record (e.g., by taking **majority vote**)

## **Defining Neighbors**



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor **k=1 k=2 k=3**

k-Nearest Neighbors of a record x are data points that have **the k smallest distance to x**

# 1 nearest-neighbor

#### 1-NN (k=1) **aka Voronoi Diagram**

**If unknown record falls in this area, then class of unknown record is the class of training record defining the area**

**In a Voronoi diagram: -Points are training records -Areas represent "regions" where the training record is the closest point and hence defines the class**

> **Training records**



# Nearest Neighbor Classification

- Based on the **notion of distance** between records (or "points")
- How to **calculate distance between records?** 
	- › **Many, many ways depending on attribute types and objective**
- For **records with numerical attributes**, variations of the Minkowski distance:

$$
d(x,y) = \sqrt{\sum_{k=1}^n |(x_k - y_k)|^r}
$$

Nearest Neighbor Classification If **r=1**, Minkowski distance becomes the Manhattan distance

$$
d(p,q) = \sum_{i=1}^k |p_i - q_i|
$$

... where **p**, **q** vectors i.e.  $\left[\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, ..., \mathbf{p}_k\right)$ **of numericals**.

### Nearest Neighbor Classification If **r=2**, Minkowski distance becomes the **Euclidean distance**

$$
d(p,q)=\sqrt{\sum_{i=k}^k (p_i-q_i)^2}
$$

... where **p**, **q** vectors i.e.  $\left[\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, ..., \mathbf{p}_k\right)$ **of numericals**.
- **3 most popular distance measures** in use for numerical records in k-NN:
	- **1. Euclidean** distance
	- **2. Manhattan** or **City block** distance
	- **3. Supremum or L<sub>n</sub> norm**, i.e. Minkowski distance when  $\mathbf{r} \rightarrow \infty$ . What does that mean?
		- **As r** $\rightarrow \infty$ , the Minkowski formula is **dominated by the term with the biggest difference**
		- A fancy way of saying: "*ignore all other attributes/dimensions except the ones with the biggest difference*".





**Solution: Normalize the vectors to unit length**

Curse of dimensionality

› In general when large number of attributes present, **all records become close i.e. distances shrink**.

- What about records with **nominal attributes?**
	- › E.g. (blue, Spaghetti, skirt)
	- › Compute **Overlap (or Hamming) measure**:

$$
d(p,q) = \sum_{i=1}^m d(p_i,q_i)
$$

… where **p, q** vectors with nominal values  $d(p_i, q_i) = 1$  if  $p_i \ll q_i$  and  $d(p_i, q_i) = 0$  if  $p_i = q_i$ i.e. distance is 1 if they differ and 0 otherwise

### **Nearest Neighbor Classification** - Overlap measure example



**Training records/dataset – stored permanently**

 Classification of new data? Based on overlap (Hamming) distances:

- › If k=1, then new record belongs to **class B**
- › If k=2, then new record belongs to **classes A or B (?)**
- › If k=3, then new record belongs to **class A**
- › If k=4, then new record belongs to **class A**

- Overlap (Hamming) distance **not the only way** to measure distance **for nominal attributes**
- More clever ways to calculate distances of nominal attributes, which give much better results
	- › For example **Value Difference Measure VDM**

Value Difference Measure

- › Takes into consideration the class(!)
- › Gives much better results than the Hamming distance
- › Defined as:

$$
d(p,q) = \sum_{i=1}^n |P(c_i|p) - P(c_i|q)|^n
$$

#### … where **p, q nominal values**, **n=number of classes**, **P(ci|p) = probability of class c<sup>i</sup> given the presence of value p (Bayesian prob.)**

**Note:** The **Modified Value Difference Measure** does **not raise to power n** the difference.

- Example of VDM
	- › Assume cars sold in various colors: **red**, **green**, **blue** etc
	- › For Overlap measure, difference between **red and green** is the same as the difference **red and blue**

› However, **red and blue cars may sell more**  than green cars which somehow implies that **red is closer to blue than to green**

- VDM aims to capture this
- Measures always depend on the objective!

- How to calculate **distance** when vectors have **numerical and nominal attributes** (mixed data types) ?
	- › e.g. **(43, blue, Married, 50901, Good, Peking Duck, 0.87)** ?
	- › **Not always an easy task!**
	- › **Find yourself** one measure that makes sense
		- You can come up with your own **that makes sense for your context**
		- Although there are many available e.g. Gower's General Similarity Coefficient
	- › You may also **combine different measures into a single measure. E.g.**
		- Euclidean distance for numerical attributes
		- Other measure for nominal values
		- Combine (somehow) the above two

### • In general

- › **You design** your own distance measure function
- › Put your knowledge of the domain in
- › **Reason about what makes things similar and what not**
	- Depends on the domain, objective etc

- Aren't there **any properties that the distance function must have**? Yes there are
- A metric or distance function D(·, ·) for all points x, y and z, must satisfy the following properties:
	- $\triangleright$  **Nonnegativity**:  $D(x, y) \ge 0$
	- $\triangleright$  **Reflexivity:**  $D(x, y) = 0$  if and only if  $x = y$
	- $\triangleright$  **Symmetry:**  $D(x, y) = D(y, x)$
	- **Triangle inequality:**  $D(x,y)+D(y,z) \ge D(x,z)$

#### Example of k-nn: ordinal and nominal values **Training records (stored)** Credit risk data



**Class**

 How would Maria who is **single, high-income earner, and low in debt be classified**? Record for Maria: *(Low, High, No)* 

- Assume **k=3**
- Proper distance metric?
	- Using Overlap (Hamming): 0=same, 1=different and sum



#### Maria: **(Low, High, No, ????)**

**Step 1.** 

**Calculate distance of Maria from all other records of the training set.** **d(Maria, Joe) = 1 + 0 + 1 = 2 d(Maria, Amber) = 0 + 0 + 1 = 1 d(Maria, Harry) = 0 + 0 + 0 = 0 d(Maria, Lindsay) = 1 + 1 + 1 = 3 d(Maria, Kaley) = 0 + 1 + 0 = 1**

#### Assume **k=3**

• Proper distance metric?

Using Overlap (Hamming): 0=same, 1=different and sum



Maria: **(Low, High, No, ????)**

**Step 2. Sort distances in ascending order**  **d(Maria, Harry) = 0 d(Maria, Amber) = 1 d(Maria, Kaley) = 1 d(Maria, Joe) = 2 d(Maria, Lindsay) = 3**

#### Assume **k=3**

● Proper distance metric?

Using Overlap (Hamming): 0=same, 1=different and sum



Maria: **(Low, High, No, ????)**

**Step 3.** 

**Keep the k closest records to Maria (here, k=3)**

**d(Maria, Harry) = 0 d(Maria, Amber) = 1 d(Maria, Kaley) = 1**



The **k-neighborhood of Maria**

#### Assume **k=3**

● Proper distance metric?

Using Overlap (Hamming): 0=same, 1=different and sum



Maria: **(Low, High, No, ????)**

**Step 4.** 

**Look at the class of the 3 closest record to Maria**

**d(Maria, Harry) Poor (=class of Harry) d(Maria, Amber) Good (=class of Amber) d(Maria, Kaley) Poor (=class of Kaley)**

#### Assume **k=3**

● Proper distance metric?

Using Overlap (Hamming): 0=same, 1=different and sum



Maria: **(Low, High, No, POOR)**

**Step 5.** 

**Assign to Maria the most frequent class (majority vote)**

**d(Maria, Harry) Poor d(Maria, Amber) Good d(Maria, Kaley) Poor**

**Class of Maria: POOR**

### Example MVDM

### Calculate distances using the **Modified** value difference metric (MVDM)



**Class**

**d(Single, Married)** = | P(Yes|Single) – P(Yes|Married) | + |P(No|Single) –  $P(No|Married)$  | = |  $(2/10)/(4/10)$  –  $(0/10)/(4/10)$  | +  $(2/10)/(4/10)$  –  $(4/10)/(4/10)$  = 1

**d(Single, Divorces)** = | 2/4 – 1/2 | + | 2/4 –  $1/2$  | = 0

**d(Married, Divorced)** =  $| 0/4 - 1/2 | + | 4/4 - 1/4|$  $1/2$  | = 1

**d(Refund=Yes, Refund=No)** =  $\sqrt{0/3} - \frac{3}{7}$  | + | 3/3 – 4/7 | = **6/7**

#### Example of k-nn: ordinal and nominal values **Training records (stored)** Credit risk data

**Class**



 How would Maria who is **single, high-income earner, and low in debt be classified**? **NOTE: Using MVDM**

Record for Maria: *(Low, High, No)* 

Assume **k=3**

### Distance metric?

› Using **MVDM**



#### **Step 1.**

**Calculate distance of Maria from all other records of the training set using MVDM. Hence calculate first differences between nominal values of all attributes.**

Maria: **(Low, High, No, ????)**

**Dept?: d(High, Low) = |P(Good|High) – P(Good|Low) | + |P(Poor|High) – P(Poor|Low)| = |1/2 – 1/3| + |1/2 – 2/3| = 0.33333**

**Incomme? d(High, Low) = |P(Good|High) – P(Good|Low)| + |P(Poor|High) – P(Poor|Low)| = |(2/5)-(0/5)| + |(1/5)-(2/5)| = 0.6**

**Married?d(Yes, No) = |P(Good|Yes) – P(Good|No)| + |P(Poor|Yes) – P(Poor|No)| = |(1/2) – 0| + ||(1/2) – 1 | = 1**

Proper distance metric?

Using **MVDM** 



#### Maria: **(Low, High, No, ????)**

**Step 2.** 

**Calculate actual distances. Based on previous slide**

**d(Maria, Harry) = d(Low, Low) + d(High, High) + d(No, No) = 0 d(Maria, Amber) = d(Low,Low) + d(High, High) + d(No,Yes) = 0 + 0 + 1 = 1 d(Maria, Kaley) = d(Low, Low) + d(High,Low) + d(No,Yes) = 0 + 0.6 + 1 = 1.6 d(Maria, Joe) = d(Low,High) + d(High,High) + d(No,Yes) = 0.333 + 0 + 1 = 1.333 d(Maria, Lindsay) = d(Low,High) + d(High,Low) + d(No,Yes) = 0.333 + 0.6 + 1 = 1.933**

Proper distance metric?

**Using MVDM** 



#### Maria: **(Low, High, No, ????)**

**Step 3. Sort distances in ascending order**

#### **d(Maria, Harry) = 0 d(Maria, Amber) = 1 d(Maria, Joe) = = 1.333 d(Maria, Kaley) = 1.6 d(Maria, Lindsay) = 1.933**

Proper distance metric?

Using **MVDM** 



Maria: **(Low, High, No, ????)**

**Step 4.** 

**Keep the k (=3) closest records to Maria**

**d(Maria, Harry) = 0 d(Maria, Amber) = 1 d(Maria, Joe) = = 1.333**

- Proper distance metric?
	- Using **MVDM**



Maria: **(Low, High, No, ????)**

**Step 5.** 

**Get class of the k (=3) closest records to Maria**

 $d(Maria, Harry) = 0 \rightarrow Poor (=class of Harry)$ **d(Maria, Amber) = 1 Good (=class of Amber)**  $d(Maria, Joe) = 1.333 \rightarrow Good (=class of Joe)$ 

- Proper distance metric?
	- Using **MVDM**



Maria: **(Low, High, No,** *Good***)**

**Step 6.** 

**Assign to Maria the most frequent class (majority vote)**

 $d(Maria, Harry) = 0 \rightarrow Poor$ **d(Maria, Amber) =**  $1 \rightarrow$  **Good d(Maria, Joe) = 1.333 → Good** 



- How to reach decision based on k nearest neighbors?
	- › Many different approaches
		- **Un-weighted votes**: count simply the most frequent class among k nearest neighbors
		- **Distance weighted votes:** weigh each vote by some factor that takes into consideration e.g. the distance
			- Hence, records further away have less influence in the voting process

Choosing the value of k:

- › If **k** is **too small**, sensitive to **noise points**
- › If **k** is too **large**, neighborhood **may include points from other classes**
- › **Rule of thumb: k ~= sqrt(number of observations)**



#### **Very important! Scaling issues for numerical attributes**

- › Attributes may **have to be scaled** to prevent distance measures from being dominated by one of the attributes
- › Example:
	- height of a person may vary from 1.5m to 1.8m
	- weight of a person may vary from 90lb to 300lb
	- income of a person may vary from \$10K to \$1M
	- Assume **all above in record data**. Difference in **income a lot greater** than **height difference**, which **influences (dominates) the distance measure**.
	- In **practice**, all numerical attributes are usually **scaled to the (0,1) range (other ranges possible too)**

- Why scaling Example
	- › Assume vector representing visitors/customer to a website with attributes: **Age, Income, Number of visits .**
	- **Jim: (75, 55000, 35)** => Jim is old and visits site often

**k-NN distance measure may calculate that Alice is closest to Jim, because income dominates**

**Alice: (22, 54000, 0)** => Alice is young and never

visited the site

**But this does not sound "reasonable". Other attributes differences have been masked by income**

### Nearest Neighbor Classification  $\circ$  How to scale? Many different ways › Calculate what portion of the range a value accounts for (called **min-max normalization**)



…where **"Old value"** current value of an attribute, **xminimum** = the minimum value of the attribute and **xmaximum** = the maximum value of the attribute Ranges from 0 to 1. Do this for all attributes.

- How to scale? Many different ways
	- Express each value in **terms of z scores** i.e. how many std. deviations  $\sigma$  it is away from the mean of attribute (called **standardization**):

$$
z_{val} = \frac{(val - \overline{y_{val}})}{\sigma}
$$

…where **"val"** a value of an attribute, **= mean of attribute y for which val is a value** and **σ the std deviation of attribute y** Ranges aprox. from -3 to 3 Apply this to all numerical attributes

### k-NN classifiers are **lazy learners**

- › It does **not build models explicitly**
	- **Instead stores training data and computes distances every time (wtf!). Does not build model.**
- › Unlike eager learners such as decision tree induction and rule-based systems
- › Classifying unknown records **is relatively expensive**
	- **Always compute again distances instances for each new record**
- Decision Trees/Rule-based are **eager learners**
	- They **build model out of training data**

### kNN prone to **overfitting** › Overfitting when k small (k=1). Why?

#### **When k small** then

classification prone to noise. E.g consider a space where most points are class A, few class B. Test records **happens to be near record of class B.** If k=1 probably misclassified as B, which is counterintuitive.

# Nearest Neighbor implementation in R

- Using the iris dataset to classify different species of iris plant
	- › 3 species: **virginica**, **setosa**, **versicolor**
	- › Determine species (class) based on some characteristics, length and width- of petals and sepals. **Will use k-nn algorithm**





**Iris virginica Iris setosa**





**Iris versicolor**

### $k$ -NN in R

#### **The k-NN algorithm in R**

#includes the class package, containing the necessary functions for k-nn library(class)

#Add the Iris dataset. Note: iris dataset is build-in and comes with R data(iris)

#Take a quick look at the data (peek at data) head(iris)

# Something strange things can be seen. The iris dataset is sorted on class. i.e. # 50 first records are all the same species, next 50 are the same etc. # This does not help us in getting a good training dataset which should contain # a good mix of each species. # Hence, first shuffle iris dataset. There are many ways to do it, but this is one

# Initialize random number generator set.seed(9850) # Get 150 random numbers from 0 to 1 from a uniform distribution gp <- runif(nrow(iris)) # Now, use the outcome of order on gp, to get the rankings of the random numbers # and use these to shuffle iris records iris <-iris[order(gp),] #Take a look at the values of each attribute. summary(iris) # There is an issue. Attributes have different ranges. This may introduce bias. So, # try to normalize each value of attribute in the range 0 to 1. One easy way to do # this is to normalize is to use min-max normalization : # new value = (old value – col min())/ (col max() – col min() ) . To do this, we will use a # function. Makes things easier. …Continued on next slide…

### $k$ -NN in R

```
# Continued from previous slide
# Define a function to normalize all attributes. Yes, in R you can define function and
# store the definition of function in variables (whaaaat???)
norm \le function(x){ return( (x-min(x)) / (max(x)-min(x)) ) }
# Now normalize each attribute by applying norm i.e. make each value from 0 to 1
iris[,"Sepal.Length"] <- norm(iris$Sepal.Length) 
iris[,"Sepal.Width"] <- norm(iris$Sepal.Width) 
iris[,"Petal.Length"] <- norm(iris$Petal.Length)
iris[, "Petal.Width"] <- norm(iris$Petal.Width)
#Take a look at the data again
summary(iris)
# Looks cool! Create now training dataset We will use first 129 records as training
# set and the rest as testing set
iris train \leq iris[1:129,]iris test \leq - iris[130:150,]# Single out, i.e. keep separately the class of each record. This will help us make 
# some tests easier. Also, the R function for knn requires it.
iris train target \le-iris[1:129, 5]iris test target \le-iris[130:150, 5]
# This is advance ninja techniques vol 4: without the next lines, R;s knn function
# goes berserk.
iris train <-iris train[, -5]
```
iris test  $\le$ -iris test[, -5]

# Now we are ready to apply the k-NN algorithm. See next slide…
#### k-NN in R

# Continued from previous slide # Call R's knn function which does our job. Set as k the square root of # number of records in dataset (a rule of thumb)

model1 <- knn(train=iris train, test=iris test, cl=iris train target, k=13)

# Ok done! At this point we have calculated the k-nearest neighbors # and assigned class by majority vote for each one of the records in the iris test # dataset. I.e. we have predicted a class for each record in the testing set.

# Print the confusion matrix to see how our model has performed table(iris test target, model1)

#### Complexity of k-NN?

- Suppose we have **training set of size d** and **dimension d and require k closest neighbors**
	- › Complexity to compute distance to one training record: **O(d)**
	- › Complexity to compute distance to all training records: **O(nd)**
	- › Complexity to find k closest distances: **O(nk)**
	- › Total time (complexity): **O(nd + nk)**
	- › **For large training set (usually the case) expensive!**

# K-NN: Possible if class is continuous

#### Classification

*y* = most common class in set {y<sub>1</sub>,..., *y* ˆ $\hat{y}$  = most common class in set  $\{y_1, ..., y_K\}$ 

#### ● Regression

$$
\hat{y} = \frac{1}{K} \sum_{k=1}^{K} y_k
$$

In regression, take the **average of values of k nearest neighbors**. This will be the "class" or dependent value for unknown record

### K-NN: Possible if class is continuous

#### Weighted by distance › Classification

 $\{ D(\mathbf{x}, \mathbf{x}_{1}) y_{1},..., D(\mathbf{x}, \mathbf{x}_{K}) y_{K}\}$  $\hat{y}$  = most common class in wieghted set

› Regression

$$
\hat{y} = \frac{\sum_{k=1}^{K} D(x, x_k) y_k}{\sum_{k=1}^{K} D(x, x_k)}
$$

# Advantages/Disadvantages of k-NN?

- Advantages
	- › "Learning" is very, very fast
		- If you can call it "learning" (well, it's not learning actually)
	- › Can "learn" complex target functions/models easily
		- Because **there is no model** to learn.
	- Does not lose any information
		- Compare with decision tree
- Disadvantages
	- **Computationally expensive**, slow query time i.e. slow to classify unknown records
		- Due to **number of times the distance** has to be calculated training sets generally large
	- **Requires lots of storage** 
		- Not a problem anymore (in 1956 was great problem)
	- › Easily **fooled by irrelevant attributes** (most important problem) Curse of dimensionality.
		- **Signal of important attributes may be masked by the noise of many irrelevant attributes**

# Naïve Bayes Classifiers

#### Naïve Bayes classifiers

#### Naïve Bayes classifiers?

- › A **probabilistic framework** for solving classification problems
	- **Probabilistic?** Calculate some probabilities and decide class based on these
	- Record belongs to a class with some probability
		- Can calculate probability for any class (!)
		- We don't assert with certainty the class a record belongs to
- › Based on **conditional probabilities**
- **Based on Bayes theorem**

#### Preliminaries

● Conditional probability

› **Probability of event A** given that **event B has occurred**

> $P(A|B) =$  $P(A \cap B)$  $P(B)$



**Tells us how the probability of events A and B occurring wrt Ω (S). Measures how big/pct the common area is between A and B with respect**   $\mathbf{to} \Omega$  (S)

**Tells us the probability of event A given that B occurred. Measures how big/pct the common area between A and B with respect to B**

- Bayes theorem
	- › Tells us how **conditions** are **related to events:**

$$
P(A|B) = \frac{P(B|A)P(A)}{P(B)}
$$

 Derives straight from conditional probabilities:

 $P(A|B) =$  $P(A \cap B)$  $P(B)$ , but since  $P(B|A) =$  $P(A \cap B)$  $P(B)$  $\rightarrow$  P(A  $\cap$  B) = P(B|A)P(A hence  $P(A|B) =$  $P(B|A)P(A)$  $P(B)$ 

 $\bullet$  Intuitively understanding the elements in Bayes' theorem

$$
P(A|B) = \frac{P(B|A)P(A)}{P(B)}
$$

- **P(A)**: Prior belief. Probability of event A before seeing any data. The hypothesis.
- **P(B|A)**: Likelihood. Probability of the data if event B is true
- **P(B)**: Data evidence. Marginal probability of the data
- **P(A|B)**: Posterior probability. Probability of event A after having seen data of event B

#### Bayes theorem

- › Alternative forms of Bayes' theorem, based on **Law of Total Probability**
- › **Law of total probability?** Assume space Ω is  $\mathsf{p}$  artitioned into n partitions  $\mathsf{A}_{\mathsf{i}}$  such that  $\mathsf{A}_{\mathsf{i}} \cap \mathsf{A}_{\mathsf{j}} = \mathsf{p}$ **ø** (**mutual exclusive**) and ∪ **A<sup>i</sup> = Ω** (**exhaustive**), then probability of event B occurring is:

$$
P(B) = \sum_{i=1}^{n} P(A_i \cap B) = \sum_{i=1}^{n} P(B|A_i) P(A_i)
$$

# **Bayes Theorem** Bayes theorem

› Visualizing **Law of Total Probability**



- Bayes theorem
	- › **Based on Law of total probability**, Bayes theorem becomes:

 $P(A|B) =$  $P(B|A)P(A)$  $\sum_{i=1}^n P(B|A_i)P(A_i)$ 

…assuming that **space B is partitioned in n partitions A<sup>i</sup>** with the same properties (i.e. A<sup>i</sup> mutual exclusive and exhaustive)

Examples of Bayes theorem (quite counterintuitive)

Assume the following:

- › Breast cancer affects 1% of women
- › A test (e.g. mammogram) detects breast cancer 80% if the person has breast cancer
- › 9.1% of the test detects breast cancer when the person has not cancer (false positive)
- › **Question: Given that a woman takes the test and the test reveals cancer (i.e. indicated that the woman has cancer) what is the probability that she really has cancer?**

Examples of Bayes theorem (quite counterintuitive)

What do we have?

- › **P(has breast cancer)** = 0.01
- › **P(Test says br. cancer | has br. cancer)** = 0.8
- › **P(Test says br. cancer | has not br. cancer)** = 0.096
- › For the woman which took the test and it revealed breast cancer, we are actually looking for this:
	- **P(has breast cancer | test says br. cancer) = ?**
		- The basic idea here is that **it's different for a test to say it**  and **actually having it!**

# Examples of Bayes theorem (quite counterintuitive)

#### Applying Bayes Theorem

 $P(has\ br\cdot cancer\ |\ test\ says\ br\cdot cancer) =$  $P(test$  says br. cancer | has br. cancer) $P(has\ br\ .\ cancer)$ P(test says br. cancer)

**P(test says br. Cancer | has br. Cancer)** known = 0.8, **P(has br. cancer)** also known = 0.01 . For **P(test says br. cancer)** we can **apply the Law of total probability**: we have two partitions -br. Cancer and no br. Cancer- that are mutual exclusive and exhaustive and "test says br. cancer" crosses both areas. **Hence** 

**P(test says br. cancer)** = P(test says br. cancer | has cancer)P(has cancer) + P(test says br. cancer | has no cancer)P(has no cancer) =  $0.8*0.01 + 0.096*(1 (0.01) = 0.10304$ 

Answering the question:

**P(has br. Cancer | test says br. Cancer) = (0.8\*0.01)/0.10304 = 0.077 (or 7.7%)** NOTE: Quite small chance, even test came out positive for breast cancer.

- Assume that **X** are all the values of some attributes of a record r  $(x_1, x_2, x_3, ..., x_d)$ and **Y** the class label of the record
	- › Note: **X** will stand in next sections as the **set of all values of attributes of a record (except class of course)**
- Further assume that the **class label Y is non-deterministically related to X**
	- **Non-deterministically?** Simply means you can not associate values of X with a particular value of Y with certainty 100%

- Then, we can **treat X and Y as random variables and calculate P(Y | X)** i.e. the probability that record r, with these values X on its attributes belongs to class Y.
	- › The problem of **classifying record r** becomes **then to find Y (class) that maximizes P(Y|X)**
- This is the **main idea of Bayesian classifiers**

- **P(Y|X)** known as **posterior probability**
- **P(Y)** known as **prior probability**
- As with all classification methods, 2 phases
	- › **Training phase**: Try to calculate P(Y|X) based on the records of the training set
	- › **Testing phase:** Given a record X' with unknown class, and **find P(Y'|X') which maximizes this probability**. If Y' maximizes, say record X' belongs to class Y'

#### How to compute P(Y|X) ?

- › More clearly **P(Y|X)** is actually **P(Y|x<sup>1</sup>** ∩ **x<sup>2</sup>** ∩ **x<sup>3</sup>** ∩ **…** ∩ **x<sup>d</sup> ) where xi values on attributes of record with dimension d. (Remember X attribute values)**
- › Use **Bayes Theorem** to **calculate posterior probability**:

 $P(Y|X) =$  $P(X|Y)P(Y)$  $P(X)$ 

#### How to compute P(Y|X) ?

 $P(Y|X) =$  $P(X|Y)P(Y)$  $P(X)$ 

…calculates posterior probability **based on prior probability P(Y), conditional dependence P(X|Y)** and **P(X) called the evidence.** Now, **given a record r**, with **unknown class Y**, in order to see which class it belongs, try to **maximize P(Y|X)** or **maximize P(X|Y)P(Y)** since <u>P(X) for record r always constant (and not always</u> computable). Record belongs to class Y that maximizes this probability,

#### How to calculate P(Y|X)?

- › It's **easy to calculate prior P(Y)** based on training set
- › Calculating **P(X|Y) not that easy**.
	- Note: For record r with dimension d and attribute values (x1, x2, x3, … ,xd ), **P(X|Y) = P(x<sup>1</sup>** ∩ **x<sup>2</sup>** ∩ **x<sup>3</sup>** ∩ **…**  ∩ **x<sup>d</sup> | Y)**
- › Bayes classifiers **differ in their way** they deal with calculating P(X|Y) and what assumptions they make
	- **Naïve Bayes classifier**
	- Artificial Neural Networks (ANN)

### Naïve Bayes Classifier

 **Naïve Bayes classifier assumes** that the attributes X of record r are **conditionally independent of class Y. I.e.**

 $P(X|Y = y) = P(x_1 \cap x_2 \cap \dots \cap x_d | Y = y) = | P(x_i | Y = y)$  $\boldsymbol{i}$ =1  $\boldsymbol{d}$ 

In Naïve Bayes, new record r is classified to **class y if**  $P(y)$   $\Pi P(x_i | Y=y)$  is maximal.

#### Naïve Bayes Classifier

- Conditional independence
	- › Let there be **three events X, Y, Z**. We say that event **X is conditionally independent of Z given Y** when:

**P(X|Y** ∩ **Z) = P(X|Y) or equivalent P(X** ∩ **Z | Y) = P(X|Y)P(Z|Y)**

# Naïve Bayes Classifier for discrete attrik



 For discrete attributes:  $\Rightarrow$  P(Y) = N<sub>y</sub> / N, Y class attributé **P(Yes) = 3/10 P(No) = 7/10** › **P(Xi|Y<sup>k</sup> ) = |Xik| / Nyk** Where  $|X_{ik}|$  number of attributes having value x<sub>i</sub> and belong to class  $\mathsf{Y}_\mathsf{k}$  . E.g. **P(Status=Married|No) = 4/7**

Naïve Bayes Classifier for qualitative attributes - applying naïve Bayes example



**Class!**

Assume all attributes categorical. Assume conditional independence of class

 Given record **X =(M2, N3, Q1).** What is it's class?

- $\sqrt{P(R1)} = 1/3$  $\text{P(R2)} = 2/3$
- › **Calculate P(R1|X)** . Note: Can't and don't need to calculate P(X). P(X|R1)P(R1)= P(M2|R1)P(N3|R1)P(Q1|R1)P( R1) =1\*(1/2)\*(1/2)(1/3)= *0.083*
- › **Calculate P(R2|X).**  P(M2|R2)P(N3|R2)P(Q1|R2)P(  $R2$ ) = (1/4)\*(1/4)\*(1/4)\*(2/3)=*0.0104* › **Since P(R1|X) > P(R2|X), record X belongs to class R1**

#### Naïve Bayes Classifier for qualitative attributes - applying naïve Bayes example

#### Training data





Assume

- › A: all attributes of unknown record
- › M: Mammals
- › N: Non-Mammal

 **P(A|M) =**   $(\overline{6}/7)^*(\overline{6}/7)^*(2/7)^*(2/7)$ = **0.06**

- **P(A|N)** = **0.0042**
- **P(A|M)\*P(M) = 0.021**
- **P(A|N)\*P(N) = 0.0027**
- **•** Hence, since **P(A|M)\*P(M) > P(A|N)\*P(N)** unknown is classified as "Mammal" .

**Unknown record. Find class**

# Naïve Bayes Classifier: Continuous attributes

#### For continuous attributes:

- › **Discretize** the range into bins
	- one **ordinal attribute** per bin (e.g. poor, good, better, very good etc. **Note: have ordering**)
	- violates independence assumption
		- Discretization may mask discriminating factors of attribute (loss of information)
- › **Two-way split: (A < v) or (A > v)**
	- choose only one of the two splits as new attribute
- › **Probability density estimation:**
	- Assume **attribute follows a normal distribution**
	- Use data to estimate parameters of distribution (e.g., **mean** and **standard deviation**)
	- Once probability distribution is known, **can use it to estimate the conditional probability P(Ai|c)**

# Naïve Bayes Classifier: Continuous attributes

- Probability density estimation method
	- › Assume every continuous attribute normally distributed.
	- › Calculate mean, variance **for each attribute given class**
	- › Calculate **P(xi|Y<sup>j</sup> ) for each (x<sup>i</sup> , Y<sup>j</sup> )** pair as follows, using the normal distribution's PDF:

$$
P\big(x_i\big|Y_j\big)=\frac{1}{\sqrt{2\pi\sigma_{ij}^2}}e^{-\frac{\big(x_i-\mu_{ij}\big)^2}{2\sigma_{ij}^2}}
$$

# Naïve Bayes Classifier: Continuous attributes

#### PDF of normal distribution of attributes assumption in Naïve Bayes



Some notes: The **PDF (Probability Density Function)** does not calculate probabilities(!). For continuous variable X **P(X=x<sup>0</sup> ) = 0**. The PDF tells us the "density" at this point i.e. **how common are samples (i.e. observed values) at exactly this value X=x**<sup>0</sup>

$$
P(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}
$$

# **continuous**



#### Training Data

- Assume Income (cont. var) normally distributed
- $\circ$  Calculate P(x<sub>i</sub> | c<sub>i</sub>) for each pair  $(x_i|c_i)$  using normal distribution's PDF
- To do this, calculate for each class (yes/no), mean and variance
	- **For Class=no** 
		- **Sample mean μ of "no" class = 110K**  (add all income where class=no and divide by # of "no" classes). Note: will use value 110, as we take each income as measured in K. i.e. 125 instead of 125000 (125K)
		- **Sample variance σ<sup>2</sup> of "no" class = 2975**

**P(Income=120 | No) =** 

54.54 $\sqrt{2\pi}$ 

 $\mathbf{1}$ 

 $\boldsymbol{e}$ 

 $(120-110)^2$  $2*2975 = 0.0072$ 

#### Naïve Bayes Classifier: Example with unknown record

#### **Conditional prob for discrete attributes from training data**

#### naive Bayes Classifier:

P(Refund=Yes|No) = 3/7  $P(Refund=NolNo) = 4/7$ P(Refund=Yes|Yes) = 0 P(Refund=No|Yes) = 1 P(Marital Status=Single|No) = 2/7 P(Marital Status=Divorced|No)=1/7 P(Marital Status=Married|No) = 4/7 P(Marital Status=Single|Yes) = 2/7 P(Marital Status=Divorced|Yes)=1/7 P(Marital Status=Married|Yes) = 0

#### For taxable income: If class=No: sample mean=110 sample variance=2975 If class=Yes: sample mean=90 sample variance=25

**Data needed to calculate continuous variables assuming normal distribution, via PDF**

- Assume previous training data
- We are given **new, unclassified record X=(No, Married, 120K). Class=?? Mixed: discrete and continuous attributes.**
- Calculate P(X|Class=No) and P(X|Class=Yes) for record X
- **P(X|Class=No) =**  P(Ref=No|No)\*P(Married|No)\*P(120 K|Class=No) =  $(4/7)*(4/7)*0.0072 =$ **0.0024**
- **P(X|Class=Yes) =**  P(Ref=No|Class=Yes)\*P(Married| Class=Yes)\*P(Income=120K|  $Class=Yes$  = 1  $\times$  0  $\times$  1.2  $\times$  10<sup>-9</sup> = 0
- Calculate now P(X|Class=No)\*P(No) and P(X|Class=Yes)\*P(Yes)
	- $P(X|Class=No)*P(No) = 0.0024*(7/10) =$ 0.00168
		- $P(X|Class=Yes)*P(Yes) = 0$
- **Since P(X|Class=No)\*P(No) > P(X|Class=Yes)\*P(Yes), given record X is classified as "No"**

# Naïve Bayes Classifier improvements

- **If one of the conditional probability is zero**, then the entire expression becomes zero
- Other probability estimation:

Original : 
$$
P(A_i | C) = \frac{N_{ic}}{N_c}
$$
  
\nLaplace :  $P(A_i | C) = \frac{N_{ic} + 1}{N_c + c}$   
\nm-estimate :  $P(A_i | C) = \frac{N_{ic} + mp}{N_c + m}$ 

c: number of classes p: prior probability m: parameter

#### Naïve Bayes in R

#Includes functions for Naïve Bayes library(e1071)

#We will be using the Congressional Voting Records Data Set #From: http://archive.ics.uci.edu/ml/datasets/Congressional+Voting+Records

#First read the data. Note the dataset HAS NO headers, hence set header to FALSE. #We well add headers later. NOTE: Change your path to data appropriately! voteData = read.csv("house-votes-84.data", header=FALSE) attach(voteData)

#Add headers to data. Makes working with dataset easier colnames(voteData) <- c("party", "infants", "water-cost", "budgetRes", "PhysicianFr", "ElSalvador", "ReligSch", "AntiSat", "NicarAid", "Missile", "Immigration", "CorpCutbacks", "EduSpend", "RightToSue", "Crime", "DFExports", "SAExport")

#Take a quick look at the data. Is everything ok? head(voteData)

#Looks fine. We are now ready to train our model and derive our Naïve Bayes #classifier. We want to predict the party based on how a congress delegate #has voted on various issues. NaiveBayesModel <- naiveBayes (party  $\sim$  ., data = voteData)

#Done! Model created. Variable NaiveBayesModel contains now our naïve bayes model #as it resulted from the training data (voting records dataset) #Now, try to predict the party based on the voting history of some congressman. See next slide

#### Naïve Bayes in R

#Now, try to apply the Naïve Bayes model to an unknown record.

#Add a new unknown record to existing voteData. Note that first attribute (party) has #value ? meaning we don't know it and try to quess it from all the other #attributes. NOTE: we will get a warning but we ignore it.  $voteData[ntow(voteData)+1, 1 < -$ c("?","n","n","y","y","y","n","n","y","n","n","y","n","y","y","y","y")

#Apply Naive Bayes model to unknown record i.e. to last record that was #added to voteData unknownRecordClass = predict(NaiveBayesModel, voteData[nrow(voteData), ])

#Now unknownRecordClass has the class i.e. party predicted for unknown record. #Let's see it unknownRecordClass

#You can also plot it (sigh) plot(unknownRecordClass)

#### Naïve Bayes - Summary

#### **Advantages**

- › **Robust** to **isolated noise points**
- › Can handle missing values by ignoring the instance during probability estimate calculations
- › **Robust** to **irrelevant attributes**

#### **Disadvantages**

- Assumption: **class conditional independence**, which may cause loss of accuracy
- › **Independence assumption may not hold** for some attribute. Practically, dependencies exist among variables
	- Use other techniques such as Bayesian Belief Networks (BBN)
## Appendices

## Appendix B: Bibliography

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