Outline

1. What is Classification?
2. k Nearest Neighbors and Nearest Centroids
3. Naïve Bayes
4. Decision Trees
5. Evaluating Classification
6. The Overfitting Problem
7. Rule Learning
8. Other Classification Approaches
9. Parameter Tuning
A Couple of Questions

• What is this?
• Why do you know?
• How have you come to that knowledge?
Introductory Example

• Learning a new concept, e.g., "Tree"

/tree/
/tree/
/tree/
/not a tree/
/not a tree/
/not a tree/
Introductory Example

• Example: learning a new concept, e.g., "Tree"
  – we look at (positive and negative) examples
  – ...and derive a *model*
    • e.g., "Trees are big, green plants"

• Goal: Classification of new instances

*Warning:* Models are only approximating examples! Not guaranteed to be correct or complete!
What is Classification?

• Classic programming:
  – if more than 10 orders/year and more than $100k spent
    set customer.isPremiumCustomer = true

• The prevalent style of programming computers
  – works well as long as we know the rules
  – e.g.: what makes a customer a premium customer?
What is Classification?

- Sometimes, it's not so easy
- E.g., due to missing knowledge
  - if customer is likely to order a new phone
    send advertisement for new phones
- E.g., due to difficult formalization as an algorithm
  - if customer review is angry
    send apology
What is Classification?

• A different paradigm:
  – User provides computer with examples
  – Computer finds model by itself
  – Notion: the computer *learns* from examples (term: *machine learning*)

• Example
  – labeled examples of angry and non-angry customer reviews
  – computer finds model for telling if a customer is angry
Classification: Formal Definition

• Given:
  – a set of labeled records, consisting of
    • data fields (a.k.a. attributes or features)
    • a class label (e.g., true/false)

• Generate
  – a function f(r)
    • input: a record
    • output: a class label
  – which can be used for classifying previously unseen records

• Variants:
  – single class problems (e.g., only true/false)
  – multi class problems
  – multi label problems (more than one class per record, not covered in this lecture)
  – hierarchical multi class/label problems (with class hierarchy, e.g., product categories)
What is Classification?

• Classification is a *supervised* learning problem
  – i.e., given labeled data, learn a prediction function for those labels

http://dilbert.com/strip/2013-02-02
The Classification Workflow

<table>
<thead>
<tr>
<th>Tid</th>
<th>Attrib1</th>
<th>Attrib2</th>
<th>Attrib3</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>Large</td>
<td>125K</td>
<td>No</td>
</tr>
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<td>6</td>
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<td>60K</td>
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<tr>
<td>7</td>
<td>Yes</td>
<td>Large</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Small</td>
<td>85K</td>
<td>No</td>
</tr>
<tr>
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<td>10</td>
<td>No</td>
<td>Small</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Training Set

<table>
<thead>
<tr>
<th>Tid</th>
<th>Attrib1</th>
<th>Attrib2</th>
<th>Attrib3</th>
<th>Class</th>
</tr>
</thead>
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<td>?</td>
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<tr>
<td>13</td>
<td>Yes</td>
<td>Large</td>
<td>110K</td>
<td>?</td>
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<td>Small</td>
<td>95K</td>
<td>?</td>
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<tr>
<td>15</td>
<td>No</td>
<td>Large</td>
<td>67K</td>
<td>?</td>
</tr>
</tbody>
</table>

Unseen Records

11
Classification Applications – Examples

- Attributes: a set of symptoms (headache, sore throat...)
  - class: does the patient suffer from disease X?

- Attributes: the values in your tax declaration
  - class: are you trying to cheat?

- Attributes: your age, income, debts, ...
  - class: are you getting credit by your bank?

- Attributes: the countries you phoned with in the last 6 months
  - class: are you a terrorist?
Classification Applications – Examples

• Attributes: words in a product review
  – Class: Is it a fake review?

• Attributes: words and header fields of an e-mail
  – Class: Is it a spam e-mail?
Classification Applications – Examples

• A controversial example
  – Class: whether you are searched by the police
  – Class: whether you are selected at the airport for an extra check

http://lubbockonline.com/stories/030609/loc_405504016.shtml
Classification Algorithms

• Recap:
  – we give the computer a set of labeled examples
  – the computer learns to classify new (unlabeled) examples

• How does that work?
k Nearest Neighbors

- Problem
  - find out what the weather is in a certain place
  - where there is no weather station
  - how could you do that?
**k Nearest Neighbors**

- **Idea:** use the average of the nearest stations
- **Example:**
  - 3x sunny
  - 2x cloudy
  - result: sunny
- **Approach is called**
  - “k nearest neighbors”
  - where k is the number of neighbors to consider
  - in the example: k=5
  - in the example: “near” denotes geographical proximity
k Nearest Neighbors

• Further examples:
  • Is a customer going to buy a product?
    → have similar customers bought that product?
  • What party are you going to vote for?
    → what party do your (closest) friends/family members vote for?
  • Is a film going to win an oscar?
    → have similar films won an oscar?

• and so on...
Experiment

• Try to predict: do you want to watch “Finding Dory”?

• Binary attributes: have you watched these 2016 films?
  – The Revenant
  – The Hateful Eight
  – The BFG (Big Friendly Giant)
  – X-Men: Apocalypse
  – Anomalisa
  – The Jungle Book
  – Jason Bourne
  – Kung Fu Panda 3
  – Zootopia
Recap: Similarity and Distance

- **k Nearest Neighbors**
  - requires a notion of similarity (i.e., what is “near”?)

- **Review: similarity measures for clustering**
  - similarity of individual data values
  - similarity of data points

- **Think about scales and normalization!**

- **Which similarity measure was used in our experiment?**
  - we could have used different ones
  - probably with different results
Nearest-Neighbor Classifiers

- Requires three things
  - The set of stored records
  - A distance metric to compute distance between records
  - The value of $k$, the number of nearest neighbors to retrieve
Nearest-Neighbor Classifiers

- To classify an unknown record:
  - Compute distance to each training record
  - Identify k nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record
    - by taking majority vote
    - by weighing the vote according to distance
Definition of the k Nearest Neighbors

The k nearest neighbors of a record $x$ are data points that have the k smallest distance to $x$.

(a) 1-nearest neighbor  
(b) 2-nearest neighbor  
(c) 3-nearest neighbor
Choosing a Good Value for 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: Test k values between 1 and 10.
Discussion of K-Nearest Neighbor

- Often very accurate

- ... but slow as training data needs to be searched

- Can handle decision boundaries which are not parallel to the axes

- Assumes all attributes are equally important
  - Remedy: Attribute selection or using attribute weights
Decision Boundaries of a k-NN Classifier

- \( k=1 \)
- Single noise points have influence on model
Decision Boundaries of a k-NN Classifier

- $k=3$
- Boundaries become smoother
- Influence of noise points is reduced
Applying the Model
Contrast: Nearest Centroids

- a.k.a. Rocchio classifier
- Training: compute centroid for each class
  - center of all points of that class
  - like: centroid for a cluster
- Classification:
  - assign each data point to nearest centroid
- RapidMiner:
  - available in Mannheim RapidMiner Toolbox Extension

Sounds pretty much just like k-NN, huh?
k-NN vs. Nearest Centroid

• Basic problem: two circles
  – Both k-NN and Nearest Centroid are rather perfect
k-NN vs. Nearest Centroid

- Some data points are mislabeled
  - k-NN loses performance
  - Nearest Centroid is stable
k-NN vs. Nearest Centroid

- One class is significantly smaller than the other
  - k-NN loses performance
  - Nearest Centroid is stable
**k-NN vs. Nearest Centroid**

- Outliers are contained in the dataset
  - k-NN is stable
  - Nearest Centroid loses performance
k-NN vs. Nearest Centroid

• k-NN
  – slow at classification time (linear in number of data points)
  – requires much memory (storing all data points)
  – robust to outliers

• Nearest Centroid
  – fast at classification time (linear in number of classes)
  – requires only little memory (storing only the centroids)
  – robust to label noise
  – robust to class imbalance

• Which classifier is better?
  – that strongly depends on the problem at hand!
Bayes Classifier

• Based on Bayes Theorem
• Thomas Bayes (1701-1761)
  – British mathematician and priest
  – tried to formally prove the existence of God
• Bayes Theorem
  – important theorem in probability theory
  – was only published after Bayes' death
Conditional Probability and Bayes Theorem

• A probabilistic framework for solving classification problems

• Conditional Probability:

\[
P(C|A) = \frac{P(A,C)}{P(A)}
\]

\[
P(A|C) = \frac{P(A,C)}{P(C)}
\]

• Bayes theorem:

\[
P(C|A) = \frac{P(A|C)P(C)}{P(A)}
\]
Conditional Probability and Bayes Theorem

• Bayes Theorem
  – Computes one conditional probability $P(C|A)$ out of another $P(A|C)$
  – given that the base probabilities $P(A)$ and $P(C)$ are known

• Useful in situations where $P(C|A)$ is unknown
  – while $P(A|C)$, $P(A)$ and $P(C)$ are known or easy to determine/estimate

• Example:
  – Given a symptom, what's the probability that I have a certain disease?
Example of Bayes Theorem

• ELISA Test
  – the most common test for HIV

• Numbers:
  – If you're infected, ELISA shows a positive result with p=99.9%
  – If you're not infected, ELISA shows a negative result with p=99.5%

• Assume you have a positive test
  – What's the probability that you're infected with HIV?

• Make a guess!
Example of Bayes Theorem

• We want to know $P(HIV|pos)$
  – Bayes theorem:
    \[
    P(HIV|pos) = \frac{P(pos|HIV)P(HIV)}{P(pos)}
    \]

• We still need $P(pos)$
  – the probability of a positive test
    \[
    P(pos) = P(pos|HIV \lor \neg HIV) = P(pos|HIV) \cdot P(HIV) + P(pos|\neg HIV) \cdot P(\neg HIV)
    \]

• Putting the pieces together:
  \[
  P(HIV|pos) = \frac{P(pos|HIV)P(HIV)}{P(pos|HIV) \cdot P(HIV) + P(pos|\neg HIV) \cdot P(\neg HIV)}
  \]

0.1% in Germany
Example of Bayes Theorem

• Now: numbers

\[
P(HIV|pos) = \frac{P(pos|HIV) \cdot P(HIV)}{P(pos|HIV) \cdot P(HIV) + P(pos|\neg HIV) \cdot P(\neg HIV)}
\]

\[
= \frac{0.999 \cdot 0.001}{0.999 \cdot 0.001 + 0.005 \cdot 0.999} = 0.167
\]

• That means:
  – at more than 80% probability, you are still healthy, given a positive test!

• Reason:
  – low overall apriori probability of being HIV positive
Example of Bayes' Theorem

$$P(\text{I'm near the ocean} \mid \text{I picked up a seashell}) = \frac{P(\text{I picked up a seashell} \mid \text{I'm near the ocean}) P(\text{I'm near the ocean})}{P(\text{I picked up a seashell})}$$

Statistically speaking, if you pick up a seashell and don't hold it to your ear, you can probably hear the ocean.

http://xkcd.com/1236/
Bayesian Classifiers

• Consider each attribute and class label as random variables

• Given a record with attributes \((A_1, A_2, \ldots, A_n)\)
  – Goal is to predict class \(C\)
  – Specifically, we want to find the value of \(C\) that maximizes \(P(C| A_1, A_2, \ldots, A_n)\)

• Can we estimate \(P(C| A_1, A_2, \ldots, A_n)\) directly from the data?
Bayesian Classifiers

• Approach:
  – compute the probability $P(C \mid A_1, A_2, \ldots, A_n)$ for all values of $C$ using the Bayes theorem

$$P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C)P(C)}{P(A_1 A_2 \ldots A_n)}$$

  – Choose value of $C$ that maximizes $P(C \mid A_1, A_2, \ldots, A_n)$

  – Equivalent to choosing value of $C$ that maximizes $P(A_1, A_2, \ldots, A_n \mid C) P(C)$

• How to estimate $P(A_1, A_2, \ldots, A_n \mid C)$?
Naïve Bayes Classifier

• Assume independence among attributes $A_i$ when class is given:
  
  – $P(A_1, A_2, \ldots, A_n | C_j) = P(A_1 | C_j) \cdot P(A_2 | C_j) \cdots P(A_n | C_j)$

  – Can estimate $P(A_i | C_j)$ for all $A_i$ and $C_j$

  – New point is classified to $C_j$ if $P(C_j) \cdot \prod P(A_i | C_j)$ is maximal
How to Estimate Probabilities from Data?

- Class: \( P(C) = \frac{N_c}{N} \)
  - e.g., \( P(\text{No}) = \frac{7}{10} \), \( P(\text{Yes}) = \frac{3}{10} \)

- For discrete attributes:
  \[ P(A_i | C_k) = \frac{|A_{ik}|}{N_c} \]
  - where \(|A_{ik}|\) is number of instances having attribute \(A_i\) and belongs to class \(C_k\)
  - Examples:
    \[ P(\text{Status}=\text{Married}|\text{No}) = \frac{4}{7} \]
    \[ P(\text{Refund}=\text{Yes}|\text{Yes})=0 \]
How to Estimate Probabilities from Data?

• For continuous attributes:
  – **Discretize** the range into bins
    • one binary attribute per bin
    • violates independence assumption
  – **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 \(P(A_i|c)\)
How to Estimate Probabilities from Data?

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Evade</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
<td>Married</td>
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<td>No</td>
</tr>
<tr>
<td>3</td>
<td>No</td>
<td>Single</td>
<td>70K</td>
<td>No</td>
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<tr>
<td>4</td>
<td>Yes</td>
<td>Married</td>
<td>120K</td>
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<td>95K</td>
<td>Yes</td>
</tr>
<tr>
<td>6</td>
<td>No</td>
<td>Married</td>
<td>60K</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>Yes</td>
<td>Divorced</td>
<td>220K</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>No</td>
<td>Single</td>
<td>85K</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>No</td>
<td>Married</td>
<td>75K</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>No</td>
<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

- Normal distribution:

\[ P(A_i \mid c_j) = \frac{1}{\sqrt{2\pi\sigma_{ij}^2}} e^{-\frac{(A_i - \mu_j)^2}{2\sigma_{ij}^2}} \]

- One for each \((A_i, c_i)\) pair

- For (Income, Class=No):
  - If Class=No
    - sample mean = 110
    - sample variance = 2975

\[
P(\text{Income} = 120 \mid \text{No}) = \frac{1}{\sqrt{2\pi (54.54)}} e^{-\frac{(120-110)^2}{2(2975)}} = 0.0072
\]
How to Estimate Probabilities from Data?

• Example visualization:
  – normal distribution
  – mean = 110
  – variance = 2975

• $P(\text{Income}=120|\text{No}) = 0.0072$
Example of Naïve Bayes Classifier

Given a Test Record:

\[ X = (\text{Refund} = \text{No}, \text{Married}, \text{Income} = 120\text{K}) \]

naive Bayes Classifier:

\[
P(\text{Refund}=\text{Yes}|\text{No}) = \frac{3}{7}
\]
\[
P(\text{Refund}=\text{No}|\text{No}) = \frac{4}{7}
\]
\[
P(\text{Refund}=\text{Yes}|\text{Yes}) = 0
\]
\[
P(\text{Refund}=\text{No}|\text{Yes}) = 1
\]
\[
P(\text{Marital Status}=\text{Single}|\text{No}) = \frac{2}{7}
\]
\[
P(\text{Marital Status}=\text{Divorced}|\text{No}) = \frac{1}{7}
\]
\[
P(\text{Marital Status}=\text{Married}|\text{No}) = \frac{4}{7}
\]
\[
P(\text{Marital Status}=\text{Single}|\text{Yes}) = \frac{2}{7}
\]
\[
P(\text{Marital Status}=\text{Divorced}|\text{Yes}) = \frac{1}{7}
\]
\[
P(\text{Marital Status}=\text{Married}|\text{Yes}) = 0
\]

For taxable income:

If class=No: sample mean=110
sample variance=2975

If class=Yes: sample mean=90
sample variance=25

\[
P(X|\text{Class}=\text{No}) = P(\text{Refund}=\text{No}|\text{Class}=\text{No})
\times P(\text{Married}| \text{Class}=\text{No})
\times P(\text{Income}=120\text{K}| \text{Class}=\text{No})
= \frac{4}{7} \times \frac{4}{7} \times 0.0072 = 0.0024
\]

\[
P(X|\text{Class}=\text{Yes}) = P(\text{Refund}=\text{No}| \text{Class}=\text{Yes})
\times P(\text{Married}| \text{Class}=\text{Yes})
\times P(\text{Income}=120\text{K}| \text{Class}=\text{Yes})
= 1 \times 0 \times 1.2 \times 10^{-9} = 0
\]

Since \( P(X|\text{No})P(\text{No}) > P(X|\text{Yes})P(\text{Yes}) \)
Therefore \( P(\text{No}|X) > P(\text{Yes}|X) \)
\[ \Rightarrow \text{Class} = \text{No} \]
Handling missing values

- Missing values may occur in training and classification examples
- **Training:** Instance is not included in frequency count for attribute value-class combination.
- **Classification:** Attribute will be omitted from calculation.
- **Example:**

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Evade</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>No</td>
<td>?</td>
<td>120k</td>
<td>?</td>
</tr>
</tbody>
</table>

Likelihood of “yes” = 1 * (1.2 * 10^{-9}) = 1.2 * 10^{-9}
Likelihood of “no” = 4/7 * 0.0072 = 0.0041
From Likelihoods to Probabilities

• A person can either evade or not
  – so why do the likelihoods not add up to 1?

• Recap: \[ P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C)P(C)}{P(A_1 A_2 \ldots A_n)} \]

We have ignored the denominator so far!
  – however, it is the same for all classes
  – so we can simply normalize to 1:

Likelihood of “yes” = 1 * (1.2 * 10^{-9}) = 1.2 * 10^{-9}
Likelihood of “no” = 4/7 * 0.0072 = 0.0041
\[ P(\text{“yes”}) = 1.2 \times 10^{-9} / (1.2 \times 10^{-9} + 0.0041) = 0.0000003 \]
\[ P(\text{“no”}) = 0.0041 / (1.2 \times 10^{-9} + 0.0041) = 0.9999997 \]
Zero Frequency Problem

• If one of the conditional probabilities is zero, then the entire expression becomes zero.
• And it is not unlikely that an exactly same data point has not yet been observed.
• Probability estimation:

Original: \[ P(A_i | C) = \frac{N_{ic}}{N_c} \]

Laplace: \[ P(A_i | C) = \frac{N_{ic} + 1}{N_c + c} \]

- \( c \): number of classes
Naïve Bayes in RapidMiner
Naïve Bayes in RapidMiner

### Attribute Parameter Distribution Table

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Parameter</th>
<th>no</th>
<th>yes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlook</td>
<td>value=rain</td>
<td>0.392</td>
<td>0.331</td>
</tr>
<tr>
<td>Outlook</td>
<td>value=overcast</td>
<td>0.014</td>
<td></td>
</tr>
<tr>
<td>Outlook</td>
<td>value=sunny</td>
<td>0.581</td>
<td></td>
</tr>
<tr>
<td>Outlook</td>
<td>value=unknown</td>
<td>0.014</td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>mean</td>
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</tr>
<tr>
<td>Temperature</td>
<td>standard deviation</td>
<td>7.893</td>
<td></td>
</tr>
<tr>
<td>Humidity</td>
<td>mean</td>
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<td></td>
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<td>Humidity</td>
<td>standard deviation</td>
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<tr>
<td>Wind</td>
<td>value=true</td>
<td>0.589</td>
<td></td>
</tr>
<tr>
<td>Wind</td>
<td>value=false</td>
<td>0.397</td>
<td></td>
</tr>
<tr>
<td>Wind</td>
<td>value=unknown</td>
<td>0.014</td>
<td></td>
</tr>
</tbody>
</table>

![Distribution Graph](image)
Naïve Bayes in RapidMiner

<table>
<thead>
<tr>
<th>Row No.</th>
<th>Play</th>
<th>confidence(no)</th>
<th>confidence(yes)</th>
<th>prediction(Play)</th>
<th>Outlook</th>
<th>Temperature</th>
<th>Humidity</th>
<th>Wind</th>
</tr>
</thead>
<tbody>
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**classifier is quite sure**

**classifier is not sure**
Decision Boundary of Naive Bayes Classifier

- Usually larger coherent areas
- Soft margins with uncertain regions
- Arbitrary (often curved) shapes
Naïve Bayes (Summary)

• Robust to isolated noise points
  – they have a small impact on the probabilities

• Handle missing values by ignoring the instance during probability estimate calculations

• Robust to irrelevant attributes

• Independence assumption may not hold for some attributes
  – Use other techniques such as Bayesian Belief Networks (BBN)
Why Naïve Bayes?

• Recap:
  – we assume that all the attributes are independent

• This does not hold for many real world datasets
  – e.g., persons: sex, weight, height
  – e.g., cars: weight, fuel consumption
  – e.g., countries: population, area, GDP
  – e.g., food: ingredients
  – e.g., text: word occurrences ("Barack", "Obama")
  – ...

Naïve Bayes Discussion

• Naïve Bayes works surprisingly well.
  – even if independence assumption is clearly violated
  – Classification doesn’t require accurate probability estimates as long as maximum probability is assigned to correct class

• However: Adding too many redundant attributes will cause problems
  – Solution: Select attribute subset as Naïve Bayes often works as well or better with just a fraction of all attributes.

• Technical advantages:
  – Learning Naïve Bayes classifiers is computationally cheap as probabilities can be estimated doing one pass over the training data
  – Storing the probabilities does not require a lot of memory
Comparison kNN and Naïve Bayes

• Computation
  – Naïve Bayes is often faster

• Naïve Bayes uses *all* data points
  – Naive Bayes is less sensitive to label noise
  – k-NN is less sensitive to outliers

• *Redundant* attributes
  – are less problematic for kNN

• *Irrelevant* attributes
  – are less problematic for Naïve Bayes
  – attribute values equally distributed across classes
    → same factor for each class

• In both cases
  – attribute pre-selection makes sense (see Data Mining II)
Lazy vs. Eager Learning

- k-NN, and Naïve Bayes are all “lazy” methods
- They do not build an explicit model!
  - “learning” is only performed on demand for unseen records
- Nearest Centroid is a simple “eager” method

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Lazy vs. Eager Learning

• We have seen three of the most common techniques for lazy learning
  – k nearest neighbors
  – Naïve Bayes
• ...and a very simple technique for eager learning
  – Nearest Centroids

• We will see eager learning in the next lectures
  – where explicit models are built
  – e.g., decision trees
  – e.g., rule sets
Questions?