I529: Machine Learning in Bioinformatics (Spring 2017)

# Naïve Bayes Classifiers

Simple (naïve) classification methods based on Bayes rules

### What does Naïve mean?

- "Naïve" refers to the (naïve) assumption that data attributes are independent
- The Bayesian method can still be optimal even when this attribute independency is violated (*Domingos, P., and M. Pazzani.* 1997)

#### Properties of Bayes Classifier

- Combines prior knowledge and observed data: prior probability of a hypothesis multiplied with probability of the hypothesis given the training data
- Probabilistic hypothesis: outputs not only a classification, but a probability distribution over all classes

## **Bayes classifiers**

**Assumption:** training set consists of instances of different classes described  $c_j$  as conjunctions of attributes values

**Task:** Classify a new instance *d* based on a tuple of attribute values into one of the classes  $c_i \in C$ 

Key idea: assign the most probable class  $~~\mathcal{C}_{M\!A\!P}~$  using Bayes Theorem.

 $c_{MAP} = \operatorname{argmax} P(c_j \mid x_1, x_2, \dots, x_n)$ 

 $= \underset{c_{j} \in C}{\operatorname{argmax}} \frac{P(x_{1}, x_{2}, \dots, x_{n} | c_{j})P(c_{j})}{P(x_{1}, x_{2}, \dots, x_{n})}$ = argmax  $P(x_{1}, x_{2}, \dots, x_{n} | c_{j})P(c_{j})$ 

## Parameters estimation

- Use the frequencies in the data (MLE)
- $P(c_j)$ 
  - Can be estimated from the frequency of classes in the training examples.
- *P*(*x*<sub>1</sub>,*x*<sub>2</sub>,...,*x*<sub>n</sub>|*c*<sub>j</sub>)
   O(|*X*|<sup>n</sup>•|*C*|) parameters
  - O(|A|<sup>1</sup>|C|) parameters
- Require large number of training examples
  Independence assumption: attribute values are
- conditionally independent given the target value: *naïve* Bayes.  $P(x, x, ..., x | c_i) = \prod P(x_i | c_i)$

 $P(x_1, x_2, ..., x_n | c_j) = \prod_i P(x_i | c_j)$ 

$$c_{NB} = \arg\max_{c_i \in C} P(c_j) \prod_{i} P(x_i \mid c_j)$$

greatly reduces the number of parameters & data sparseness

## Bayes classification

• An unseen instance is classified by computing the class that maximizes the posterior

 $c_{MAP} = \operatorname*{argmax}_{o \in C} P(c_j \mid x_1, x_2, \dots, x_n)$ 

 When conditioned independence is satisfied, Naïve Bayes corresponds to MAP classification.

$$c_{NB} = \underset{c_{j} \in C}{\operatorname{arg\,max}} P(c_{j}) \prod_{i} P(x_{i} \mid c_{j})$$

Day	Outlook	Temperature	Humidity	Wind	Play Tennis	
Day1	Sunny	Hot	High	Weak	No	
Day2	Sunny	Hot	High	Strong	No	
Day3	Overcast	Hot	High	Weak	Yes	
Day4	Rain	Mild	High	Weak	Yes	
Day5	Rain	Cool	Normal	Weak	Yes	
Day6	Rain	Cool	Normal	Strong	No	
Day7	Overcast	Cool	Normal	Strong	Yes	
Day8	Sunny	Mild	High	Weak	No	
Day9	Sunny	Cool	Normal	Weak	Yes	
Day10	Rain	Mild	Normal	Weak	Yes	
Day11	Sunny	Mild	Normal	Strong	Yes	
Day12	Overcast	Mild	High	Strong	Yes	
Day13	Overcast	Hot	Normal	Weak	Yes	
Day14	Rain	Mild	High	Strong	No	
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Based on the examples in the table, classify the following datum *x*: x=(O=Sunny, T=Cool, H=High, W=strong)• That means: Play tennis or not?  $c_{NB} = \arg\max_{c_j} P(c_j) \prod_i P(x_i|c_j)$   $= \arg\max_{c_j} P(c_j)P(O = sunny|c_j)P(T = cool|c_j)P(H = high|c_j)P(W = strong|c_j)$ • Working: P(PlayTennis = yes) = 9/14 = 0.64 P(PlayTennis = no) = 5/14 = 0.36 P(Wind = strong | PlayTennis = yes) = 3/9 = 0.33 P(Wind = strong | PlayTennis = no) = 3/5 = 0.60etc. P(yes)P(sunny | yes)P(cool | yes)P(high | yes)P(strong | yes) = 0.0053 P(no)P(sunny | no)P(cool | no)P(high | no)P(strong | no) = 0.0206 $\Rightarrow answer : PlayTennis(x) = no$ 









#### Naïve Bayes for sequence classification

- RDP classifier for taxonomic assignment of ribosomal sequences
- A sequence is represented as a bag of k-mers (words)

### **RDP** classifier

- Naïve Bayesian Classifier for Rapid Assignment of rRNA Sequences into the New Bacterial Taxonomy
- The Classifier uses a feature space consisting of all possible 8-base subsequences (words).
  - Word sizes between 6 and 9 bases were tested in preliminary experiments: Sizes of 8 and 9 bases gave nearly identical results, while sizes of 6 and 7 bases were less accurate.
- The position of a word in a sequence is ignored. As with text-based Bayesian classifiers, only those words occurring in the query contribute to the score

## RDP classifier: training

- Word-specific priors:  $W = \{w_1, w_2, ..., w_d\}$ 
  - Given N sequences, let  $n(w_i)$  be the number of sequences containing subsequence  $w_i$ ,  $P_i = [n(w_i) + 0.5]/(N + 1)$  (the likelihood of observing word  $w_i$  in an rRNA sequence).
  - Genus-specific conditional probabilities.
     For genus G with M sequences, let m(w<sub>i</sub>) be the number of these sequences containing word w<sub>i</sub>. The conditional probability that a member of G contains w<sub>i</sub>. P(w<sub>i</sub>|G) = [m(w<sub>i</sub>) + P<sub>i</sub>]/(M + 1).
  - I (gnoring the dependency between words in an individual sequence, the joint probability of observing from genus G a (partial) sequence, S, containing a set of words,  $V = \{V_1, v_2, \dots, v_n\}$  ( $V \subseteq W$ ), was estimated as  $P(S|G) = \prod P(v_i|G)$ .

#### RDP classifier: prediction

- By Bayes' theorem, the probability that an unknown query sequence, S, is a member of genus G is P(G|S) = P(S|G) × P(G)/P(S), where P(G) is the prior probability of a sequence being a member of G and P(S) the overall probability of observing sequence S (from any genus).
- Assuming all genera are equally probable (equal priors), the constant terms *P*(*G*) and *P*(*S*) can be ignored.
- The sequence will be classified as as a member of the genus giving the highest probability score, but we ignore the actual numerical probability estimate.