

Classification

KNN Classifier, Naive Bayesian Classifier

Outline

1 KNN Classifier

2 Naive Bayesian Classifier

k-Nearest-Neighbor classifiers

- First introduced in early 1950s
- Distance metrics
 - Generally Euclidean distance is used when the values are continuous
 - Hamming distance for categorical/nominal values

Algorithm idea



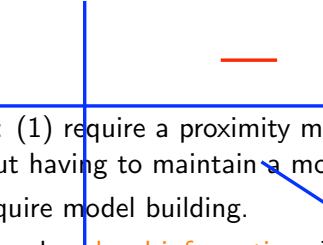
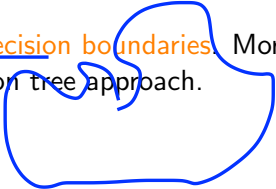
- Let k be the number of nearest neighbors and D be the set of training examples
 - **for** each test example $z = (\mathbf{x}', y')$, do
 - Compute $d(\mathbf{x}, \mathbf{x}')$, the distance between z and every example $(\mathbf{x}, y) \in D$
 - Select $D_z \subseteq D$, the set of k closest training examples to z
 - $y' = \operatorname{argmax}_v \sum_{(x_i, y_i) \in D_z} I(v == y_i)$ // Majority voting
 - **end for**
- v : a class label
- y_i : the class label for one of the NNs
- I : indicate function that returns value 1 if its argument is true and 0 otherwise.

Discussions

- Computation can be **costly** if the number of training examples is large.
- **Efficient indexing techniques** are available to find the nearest neighbors of a test example.
- **Sensitive k** : reduce the impact of k is to weight the influence of a NN \mathbf{x}_i : $w_i = \frac{1}{d(\mathbf{x}', \mathbf{x}_i)^2}$
Distance-weighted voting:

$$y' = \underset{(x_i, y_i) \in D_z}{\operatorname{argmax}_v} \sum w_i \times I(v == y_i)$$

Characteristics

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- Instance-based learning: (1) require a proximity measure (2) make predictions without having to maintain a model
 - Lazy learner: do not require model building.
 - Predictions are made based on local information. Thus, it is quite susceptible to noise.
 - Can produce arbitrarily shaped decision boundaries. More flexible compared with the decision tree approach.
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References


- Hui Ding, Goce Trajcevski, Peter Scheuermann, Xiaoyue Wang, Eamonn J. Keogh: **Querying and mining of time series data: experimental comparison of representations and distance measures**. PVLDB 1(2):1542-1552 (2008)
- Abdullah Mueen, Eamonn J. Keogh, Neal Young: **Logical-shapelets: an expressive primitive for time series classification**. KDD 2011:1154-1162.
- Minh Nhut Nguyen, Xiao-Li Li, See-Kiong Ng: **Positive Unlabeled Learning for Time Series Classification**. IJCAI2011: 1421-1426.

KNeighborsClassifier – Python scikit-learn 0.22.1

```
class sklearn.neighbors.KNeighborsClassifier(  
    n_neighbors=5, weights='uniform', algorithm='auto',  
    leaf_size=30, p=2, metric='minkowski',  
    metric_params=None, n_jobs=None, **kwargs)
```

- **n_neighbors**: Number of neighbors to use by default for kneighbors queries.
- **p**: Power parameter for the Minkowski metric. When $p = 1$, this is equivalent to using `manhattan_distance (l1)`, and `euclidean_distance (l2)` for $p = 2$. For arbitrary p , `minkowski_distance (l_p)` is used.
- **Metric**: the distance metric to use. The default metric is `minkowski`, and with $p=2$ is equivalent to the standard Euclidean metric.

Naive Bayesian Classifier

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- **Non-deterministic** relationship between attribute set and the class label.
 - Reason 1: noisy data
 - Reason 2: complex factors
 - **Probabilistic relationships** between attribute set and the class label.
 - Bayesian classifiers: a probabilistic framework for solving classification problems.

Bayes Theorem

■ Conditional probability

$$P(C|A) = \frac{P(A, C)}{P(A)}$$
$$P(\underline{A}|C) = \frac{P(A, C)}{P(C)}$$

■ Bayes theorem

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

Example of Bayes Theorem

- Given:
 - A doctor knows that meningitis causes stiff neck 50% of the time
 - Prior probability of any patient having meningitis is $1/50,000$
 - Prior probability of any patient having stiff neck is $1/20$
- If a patient has stiff neck, what's the probability he/she has meningitis?

Example of Bayes Theorem

- Given:
 - A doctor knows that meningitis causes stiff neck 50% of the time
 - Prior probability of ~~any patient~~ having meningitis is $1/50,000$
 - Prior probability of any patient having stiff neck is $1/20$
- If a patient has stiff neck, what's the probability he/she has meningitis?
- Solve this problem:
 - M: a patient has meningitis
 - S: a patient has stiff neck
 - $P(S|M) = 50\%$, $P(M) = 1/50,000$, $P(S) = 1/20$, $P(M|S) = ?$

$$P(M|S) = \frac{P(S|M)P(M)}{P(S)} = \frac{(1/2) \cdot (1/50,000)}{1/20} = \frac{20}{100,000} = 0.0002$$

Bayesian Classifiers

- Consider each attribute and class label as random variables
- Given a record with attributes (A_1, A_2, \dots, A_n)
 - Goal is to predict class C
 - Specifically, we want to find the value of C that maximizes $P(C|A_1, A_2, \dots, A_n)$
- Can we estimate $P(C|A_1, A_2, \dots, A_n)$ directly from data?

Bayesian Classifiers – approach

- Compute the **posterior probability** $P(C|A_1, A_2, \dots, A_n)$ for **all values of C** using the Bayes theorem

$$P(C|A_1, A_2, \dots, A_n) = \frac{P(A_1, A_2, \dots, A_n|C)P(C)}{P(A_1, A_2, \dots, A_n)}$$

- Choose value of **C that maximizes** $P(C|A_1, A_2, \dots, A_n)$

$$\equiv \text{maximize } P(A_1, A_2, \dots, A_n|C)P(C)$$

- How to estimate $P(A_1, A_2, \dots, A_n|C)$?

Naive Bayes Classifier

$$P(A_1, A_2) = P(A_1) P(A_2)$$

$$P(A_1, A_2) = P(A_1) P(A_2|A_1)$$

- Assume independence among attributes A_i when class is given

$$\underline{P(A_1, A_2, \dots, A_n | C_j)} = \underline{P(A_1 | C_j) P(A_2 | C_j) \dots P(A_n | C_j)}$$

- Can estimate $P(A_i | C_j)$ for all A_i and C_j .
- New point is classified to C_j if $P(C_j) \prod P(A_i | C_j)$ is maximal.

Estimate Probabilities from Data

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

 $P(C)$ $P(C=Yes) = 3/10$ $P(C=No) = 7/10$

- Class: $P(C = C_i) = \frac{N_i}{N}$
- Discrete attributes: $P(A_i = a_i | C = C_j) = \frac{N_{ij}}{N_j}$
 - N_{ij} : # of instances having attribute $A_i = a_i$ and belonging to class C_j
 - N_j : # of instances belonging to class C_j
- $P(\text{No}) = 0.7, P(\text{Yes}) = 0.3$
- $P(\text{Status} = \text{Married} | \text{No}) = \frac{4}{7}, P(\text{Refund} = \text{Yes} | \text{Yes}) = 0$

Estimate Probabilities from Data – continuous attributes

- **Discretize** the range into bins
 - one ordinal attribute per bin
- **Two-way split**: $(A < v)$ or $(A \geq v)$
 - 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 μ and standard deviation σ)
 - Once probability distribution is known, can use it to estimate the conditional probability

$$P(A_i|c_j) = \frac{1}{\sqrt{2\pi}\sigma_{ij}} \exp^{-\frac{(A_i - \mu_{ij})^2}{2\sigma_{ij}^2}}$$

- μ_{ij} : estimated as sample mean of A_i for all training records with class c_j .
- σ_{ij} : estimated as sample variance s^2 of all training records with class c_j .

Estimate Probabilities from Data – Example

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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$$P(A_i|c_j) = \frac{1}{\sqrt{2\pi}\sigma_{ij}} \exp^{-\frac{(A_i - \mu_{ij})^2}{2\sigma_{ij}^2}}$$

For (Income, Class=No)

Sample mean: $\frac{125+100+70+120+60+220+75}{7} = 110$

Sample variance: 2975

$$P(\text{Income} = 120|\text{No}) = \frac{1}{\sqrt{2\pi}(54.54)} \exp^{-\frac{(120-110)^2}{2(2975)}} = 0.0072$$

Example of Naive Bayes Classifier – Example 1

A₁

Given a test record: $X=(\text{Refund}=\text{No}, \text{Married}, \text{Income}=120\text{K})$

$$P(\text{Refund} = \text{Yes}|\text{No}) = 3/7$$

$$P(\text{Refund} = \text{No}|\text{No}) = 4/7$$

$$P(\text{Refund} = \text{Yes}|\text{Yes}) = 0$$

$$P(\text{Marital Status} = \text{Single}|\text{No}) = 2/7$$

$$P(\text{Marital Status} = \text{Divorced}|\text{No}) = 1/7$$

$$P(\text{Marital Status} = \text{Married}|\text{No}) = 4/7$$

$$P(\text{Marital Status} = \text{Single}|\text{Yes}) = 2/3$$

$$P(\text{Marital Status} = \text{Divorced}|\text{Yes}) = 1/3$$

$$P(\text{Marital Status} = \text{Married}|\text{Yes}) = 0$$

$$P(\text{Class} = \text{Yes}) = 0.3$$

$$P(\text{Class} = \text{No}) = 0.7$$

For taxable income

If class=No: Sample mean=110, variance=2975

If class=Yes: Sample mean=90, variance=25

$$P(\text{CIA1}=\text{No}, \text{A2}=\text{M}, \text{A3}=120\text{K})$$

$$\sim P(\text{A1}=\text{No}|\text{C}) P(\text{A2}=\text{MIC}) P(\text{A3}=120\text{K}|\text{C}) P(\text{C})$$

$$P(\text{A1}=\text{No}|\text{C}=\text{Y}) P(\text{A2}=\text{MIC}=\text{Y}) P(\text{A3}=120\text{K}|\text{C}=\text{Y}) P(\text{C}=\text{Y})$$

>

$$P(\text{A1}=\text{No}|\text{C}=\text{N}) P(\text{A2}=\text{MIC}=\text{N}) P(\text{A3}=120\text{K}|\text{C}=\text{N}) P(\text{C}=\text{N})$$

Example 1 (cont.)

$$\begin{aligned}P(X|Class = No) &= P(Refund = No|No) * P(Married|No) * P(Income = 120K|No) \\&= 4/7 * 4/7 * 0.0072 \\&= 0.0024\end{aligned}$$

$$\begin{aligned}P(X|Class = Yes) &= P(Refund = No|Yes) * P(Married|Yes) * P(Income = 120K|Yes) \\&= 1 * 0 * 1.2 * 10^{-9} \\&= 0\end{aligned}$$

Since $\underline{P(X|No) * P(No)} > \underline{P(X|Yes) * P(Yes)}$
 $P(No|X) > P(Yes|X) \rightarrow \text{class} = \text{No}$

$P(Married|Yes) = 0$. If one of the conditional probability is zero, then the entire expression becomes zero.

Naive Bayes Classifier – Probability estimation for Zero conditional probability

- Original: $P(A_i = a_i | C = C_j) = \frac{N_{ij}}{N_j}$
- Laplace: $P(A_i = a_i | C = C_j) = \frac{N_{ij}+1}{N_j+c}$
- m-estimate: $P(A_i = a_i | C = C_j) = \frac{N_{ij}+mp}{N_j+m}$
- N_{ij} : the number of instances with attribute value a_i and belonging to a class C_j
- N_j : the number of instances belonging to a class C_j
- c : total number of classes
- p : prior probability for the positive class C_j
- m : parameter

E.g., use m -estimate: $m = 3$ and $p = 0.3$ (prior for positive class Yes)

$$P(\text{Marital Status}=\text{Married}|\text{Yes})=\frac{0+0.3*3}{3+3} = \frac{0.9}{6}$$

Example of Naive Bayes Classifier – Example 2

Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

Example 2 (cont.)

Give test case:

Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
	yes	no	yes	no	?

- A: attributes
- M: mammals
- N: non-mammals

Class M: $P(\text{GB}=\text{Yes}|\text{M}) P(\text{CF}=\text{No}|\text{M}) P(\text{LW}=\text{yes}|\text{M}) P(\text{HL}=\text{no}|\text{M}) \cdot P(\text{M})$

Class N: $P(\text{GB}=\text{Yes}|\text{N}) P(\text{CF}=\text{No}|\text{N}) P(\text{LW}=\text{yes}|\text{N}) P(\text{HL}=\text{no}|\text{N}) \cdot P(\text{N})$

Example 2 (cont.)

- $P(M) = \frac{7}{20}, P(N) = \frac{13}{20}$
- $P(GB = Y|M) = \frac{6}{7}, P(GB = N|M) = \frac{1}{7}$
- $P(Can Fly = Y|M) = \frac{1}{7}, P(Can Fly = N|M) = \frac{6}{7}$
- $P(Live in Water = Y|M) = \frac{2}{7}, P(Live in Water = N|M) = \frac{5}{7}$
- $P(Have Legs = Y|M) = \frac{5}{7}, P(Have Legs = N|M) = \frac{2}{7}$

$$\begin{aligned}
 P(X|M) &= P(GB = Y|M) * P(Can Fly = N|M) * P(Live in Water = Y|M) \\
 &\quad * P(Have Legs = N|M) \\
 &= 6/7 * 6/7 * 2/7 * 2/7 = 0.06
 \end{aligned}$$

$$\begin{aligned}
 P(X|N) &= P(GB = Y|N) * P(Can Fly = N|N) * P(Live in Water = Y|N) \\
 &\quad * P(Have Legs = N|N) \\
 &= 1/13 * 10/13 * 3/13 * 4/13 = 0.0042
 \end{aligned}$$

$$P(X|M) * P(M) = 0.06 * 7/20 = 0.021$$

$$P(X|N) * P(N) = 0.0042 * 13/20 = 0.0027$$

Since $P(X|M) * P(M) > P(X|N) * P(N)$, class = Mammals

Naive Bayes Classifier (Summary)

- Robust to isolated **noise** points
- 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)

References

- Chapter 4: Introduction to Data Mining (2nd Edition) by Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, and Vipin Kumar
- KNN classifier: <https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html>
- Naive Bayes classifier: https://scikit-learn.org/stable/modules/naive_bayes.html