Data Mining and Analysis: Fundamental Concepts and Algorithms

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Chapter 18: Probabilistic Classification

Bayes Classifier

Let the training dataset $\mathbf{D}$ consist of n points $\mathbf{x}_i$ in a d-dimensional space, and let y_i denote the class for each point, with $y_i \in \{c_1, c_2, \ldots, c_k\}$.

The Bayes classifier estimates the posterior probability $P(c_i|\mathbf{x})$ for each class c_i, and chooses the class that has the largest probability. The predicted class for $\mathbf{x}$ is given as

$$\hat{y} = \arg\max_{c_i} \{P(c_i|\mathbf{x})\}$$

According to the Bayes theorem, we have

$$P(c_i|\mathbf{x}) = \frac{P(\mathbf{x}|c_i) \cdot P(c_i)}{P(\mathbf{x})}$$

Because $P(\mathbf{x})$ is fixed for a given point, Bayes rule can be rewritten as

$$\hat{y} = \arg\max_{c_i} \{P(c_i|\mathbf{x})\} = \arg\max_{c_i} \left\{ \frac{P(\mathbf{x}|c_i)P(c_i)}{P(\mathbf{x})} \right\} = \arg\max_{c_i} \big\{ P(\mathbf{x}|c_i)P(c_i) \big\}$$

Estimating the Prior Probability: $P(c_i)$

Let $\mathbf{D}_i$ denote the subset of points in $\mathbf{D}$ that are labeled with class c_i:

$$\mathbf{D}_i = \{\mathbf{x}_j \in \mathbf{D} \mid \mathbf{x}_j \text{ has class } y_j = c_i\}$$

Let the size of the dataset $\mathbf{D}$ be given as $|\mathbf{D}| = n$, and let the size of each class-specific subset $\mathbf{D}_i$ be given as $|\mathbf{D}_i| = n_i$.

The prior probability for class c_i can be estimated as follows:

$$\hat{P}(c_i) = \frac{n_i}{n}$$

Estimating the Likelihood: Numeric Attributes, Parametric Approach

To estimate the likelihood $P(\mathbf{x}|c_i)$, we have to estimate the joint probability of $\mathbf{x}$ across all the d dimensions, i.e., we have to estimate $P\big(\mathbf{x} = (x_1, x_2, \ldots, x_d)|c_i\big)$.

In the parametric approach we assume that each class c_i is normally distributed, and we use the estimated mean $\hat{\boldsymbol{\mu}}_i$ and covariance matrix $\widehat{\boldsymbol{\Sigma}}_i$ to compute the probability density at $\mathbf{x}$

$$\hat{f}_i(\mathbf{x}) = \hat{f}(\mathbf{x}|\hat{\boldsymbol{\mu}}_i, \widehat{\boldsymbol{\Sigma}}_i) = \frac{1}{(\sqrt{2\pi})^d \sqrt{|\widehat{\boldsymbol{\Sigma}}_i|}} \exp\left\{ -\frac{(\mathbf{x} - \hat{\boldsymbol{\mu}}_i)^T \widehat{\boldsymbol{\Sigma}}_i^{-1} (\mathbf{x} - \hat{\boldsymbol{\mu}}_i)}{2} \right\}$$

The posterior probability is then given as

$$P(c_i|\mathbf{x}) = \frac{\hat{f}_i(\mathbf{x}) P(c_i)}{\sum_{j=1}^{k} \hat{f}_j(\mathbf{x}) P(c_j)}$$

The predicted class for $\mathbf{x}$ is:

$$\hat{y} = \arg\max_{c_i} \left\{ \hat{f}_i(\mathbf{x}) P(c_i) \right\}$$

Bayes Classifier Algorithm

BayesClassifier ($\mathbf{D} = \{(\mathbf{x}_j, y_j)\}_{j=1}^{n}$):

for $i = 1, \ldots, k$ **do**

  $\mathbf{D}_i \leftarrow \left\{\mathbf{x}_j \mid y_j = c_i, j = 1, \ldots, n\right\}$ `// class-specific subsets`

  $n_i \leftarrow |\mathbf{D}_i|$ `// cardinality`

  $\hat{P}(c_i) \leftarrow n_i/n$ `// prior probability`

  $\hat{\boldsymbol{\mu}}_i \leftarrow \frac{1}{n_i} \sum_{\mathbf{x}_j \in \mathbf{D}_i} \mathbf{x}_j$ `// mean`

  $\mathbf{Z}_i \leftarrow \mathbf{D}_i - \mathbf{1}_{n_i} \hat{\boldsymbol{\mu}}_i^T$ `// centered data`

  $\widehat{\boldsymbol{\Sigma}}_i \leftarrow \frac{1}{n_i} \mathbf{Z}_i^T \mathbf{Z}_i$ `// covariance matrix`

return $\hat{P}(c_i), \hat{\boldsymbol{\mu}}_i, \widehat{\boldsymbol{\Sigma}}_i$ *for all* $i = 1, \ldots, k$

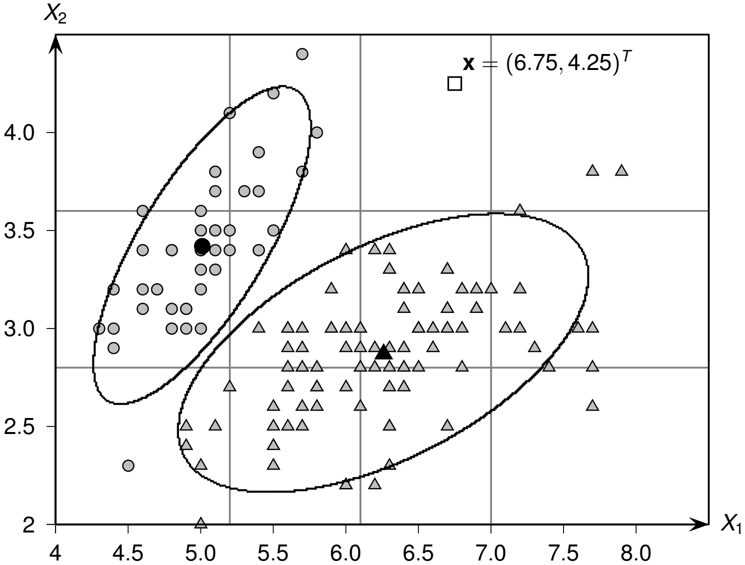
Testing ($\mathbf{x}$ **and** $\hat{P}(c_i)$, $\hat{\boldsymbol{\mu}}_i$, $\widehat{\boldsymbol{\Sigma}}_i$, **for all** $i \in [1, k]$):

$\hat{y} \leftarrow \arg\max_{c_i} \left\{ f(\mathbf{x} | \hat{\boldsymbol{\mu}}_i, \widehat{\boldsymbol{\Sigma}}_i) \cdot P(c_i) \right\}$

return $\hat{y}$

Bayes Classifier: Iris Data

X_1:`sepal length` versus X_2:`sepal width`



Bayes Classifier: Categorical Attributes

Let X_j be a categorical attribute over the domain $dom(X_j) = \{a_{j1}, a_{j2}, \ldots, a_{jm_j}\}$. Each categorical attribute X_j is modeled as an m_j-dimensional multivariate Bernoulli random variable $\mathbf{X}_j$ that takes on m_j distinct vector values $\mathbf{e}_{j1}, \mathbf{e}_{j2}, \ldots, \mathbf{e}_{jm_j}$, where $\mathbf{e}_{jr}$ is the rth standard basis vector in $\mathbb{R}^{m_j}$ and corresponds to the rth value or symbol $a_{jr} \in dom(X_j)$.

The entire d-dimensional dataset is modeled as the vector random variable $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_d)^T$. Let $d' = \sum_{j=1}^{d} m_j$; a categorical point $\mathbf{x} = (x_1, x_2, \ldots, x_d)^T$ is therefore represented as the d'-dimensional binary vector

$$\mathbf{v} = \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_d \end{pmatrix} = \begin{pmatrix} \mathbf{e}_{1r_1} \\ \vdots \\ \mathbf{e}_{dr_d} \end{pmatrix}$$

where $\mathbf{v}_j = \mathbf{e}_{jr_j}$ provided $x_j = a_{jr_j}$ is the r_jth value in the domain of X_j.

Bayes Classifier: Categorical Attributes

The probability of the categorical point $\mathbf{x}$ is obtained from the joint probability mass function (PMF) for the vector random variable $\mathbf{X}$:

$$P(\mathbf{x}|c_i) = f(\mathbf{v}|c_i) = f\big(\mathbf{X}_1 = \mathbf{e}_{1r_1}, \ldots, \mathbf{X}_d = \mathbf{e}_{dr_d} \,|\, c_i\big)$$

The joint PMF can be estimated directly from the data $\mathbf{D}_i$ for each class c_i as follows:

$$\hat{f}(\mathbf{v}|c_i) = \frac{n_i(\mathbf{v})}{n_i}$$

where $n_i(\mathbf{v})$ is the number of times the value $\mathbf{v}$ occurs in class c_i.
However, to avoid zero probabilities we add a *pseudo-count* of 1 for each value

$$\hat{f}(\mathbf{v}|c_i) = \frac{n_i(\mathbf{v}) + 1}{n_i + \prod_{j=1}^{d} m_j}$$

Discretized Iris Data: `sepal length` and `sepal width`

Bins	Domain
$[4.3, 5.2]$	Very Short (a_{11})
$(5.2, 6.1]$	Short (a_{12})
$(6.1, 7.0]$	Long (a_{13})
$(7.0, 7.9]$	Very Long (a_{14})

(a) Discretized `sepal length`

Bins	Domain
$[2.0, 2.8]$	Short (a_{21})
$(2.8, 3.6]$	Medium (a_{22})
$(3.6, 4.4]$	Long (a_{23})

(b) Discretized `sepal width`

Class-specific Empirical Joint Probability Mass Function

	Class: c_1	X_2 Short ($\mathbf{e}_{21}$)	Medium ($\mathbf{e}_{22}$)	Long ($\mathbf{e}_{23}$)	$\hat{f}_{X_1}$
X_1	Very Short ($\mathbf{e}_{11}$)	1/50	33/50	5/50	39/50
	Short ($\mathbf{e}_{12}$)	0	3/50	8/50	13/50
	Long ($\mathbf{e}_{13}$)	0	0	0	0
	Very Long ($\mathbf{e}_{14}$)	0	0	0	0
	$\hat{f}_{X_2}$	1/50	36/50	13/50	

	Class: c_2	X_2 Short ($\mathbf{e}_{21}$)	Medium ($\mathbf{e}_{22}$)	Long ($\mathbf{e}_{23}$)	$\hat{f}_{X_1}$
X_1	Very Short ($\mathbf{e}_{11}$)	6/100	0	0	6/100
	Short ($\mathbf{e}_{12}$)	24/100	15/100	0	39/100
	Long ($\mathbf{e}_{13}$)	13/100	30/100	0	43/100
	Very Long ($\mathbf{e}_{14}$)	3/100	7/100	2/100	12/100
	$\hat{f}_{X_2}$	46/100	52/100	2/100	

Iris Data: Test Case

Consider a test point $\mathbf{x} = (5.3, 3.0)^T$ corresponding to the categorical point (`Short, Medium`), which is represented as $\mathbf{v} = \begin{pmatrix}\mathbf{e}_{12}^T & \mathbf{e}_{22}^T\end{pmatrix}^T$.

The prior probabilities of the classes are $\hat{P}(c_1) = 0.33$ and $\hat{P}(c_2) = 0.67$. The likelihood and posterior probability for each class is given as

$$\hat{P}(\mathbf{x}|c_1) = \hat{f}(\mathbf{v}|c_1) = 3/50 = 0.06$$
$$\hat{P}(\mathbf{x}|c_2) = \hat{f}(\mathbf{v}|c_2) = 15/100 = 0.15$$
$$\hat{P}(c_1|\mathbf{x}) \propto 0.06 \times 0.33 = 0.0198$$
$$\hat{P}(c_2|\mathbf{x}) \propto 0.15 \times 0.67 = 0.1005$$

In this case the predicted class is $\hat{y} = c_2$.

Iris Data: Test Case with Pesudo-counts

The test point $\mathbf{x} = (6.75, 4.25)^T$ corresponds to the categorical point (`Long`, `Long`), and it is represented as $\mathbf{v} = \begin{pmatrix} \mathbf{e}_{13}^T & \mathbf{e}_{23}^T \end{pmatrix}^T$.

Unfortunately the probability mass at $\mathbf{v}$ is zero for both classes. We adjust the PMF via pseudo-counts noting that the number of possible values are $m_1 \times m_2 = 4 \times 3 = 12$.

The likelihood and prior probability can then be computed as

$$\hat{P}(\mathbf{x}|c_1) = \hat{f}(\mathbf{v}|c_1) = \frac{0+1}{50+12} = 1.61 \times 10^{-2}$$
$$\hat{P}(\mathbf{x}|c_2) = \hat{f}(\mathbf{v}|c_2) = \frac{0+1}{100+12} = 8.93 \times 10^{-3}$$
$$\hat{P}(c_1|\mathbf{x}) \propto (1.61 \times 10^{-2}) \times 0.33 = 5.32 \times 10^{-3}$$
$$\hat{P}(c_2|\mathbf{x}) \propto (8.93 \times 10^{-3}) \times 0.67 = 5.98 \times 10^{-3}$$

Thus, the predicted class is $\hat{y} = c_2$.

Bayes Classifier: Challenges

The main problem with the Bayes classifier is the lack of enough data to reliably estimate the joint probability density or mass function, especially for high-dimensional data.

For numeric attributes we have to estimate $O(d^2)$ covariances, and as the dimensionality increases, this requires us to estimate too many parameters.

For categorical attributes we have to estimate the joint probability for all the possible values of $\mathbf{v}$, given as $\prod_j |\text{dom}(X_j)|$. Even if each categorical attribute has only two values, we would need to estimate the probability for 2^d values. However, because there can be at most n distinct values for $\mathbf{v}$, most of the counts will be zero.

Naive Bayes classifier addresses these concerns.

Naive Bayes Classifier: Numeric Attributes

The naive Bayes approach makes the simple assumption that all the attributes are independent, which implies that the likelihood can be decomposed into a product of dimension-wise probabilities:

$$P(\mathbf{x}|c_i) = P(x_1, x_2, \ldots, x_d|c_i) = \prod_{j=1}^{d} P(x_j|c_i)$$

The likelihood for class c_i, for dimension X_j, is given as

$$P(x_j|c_i) \propto f(x_j|\hat{\mu}_{ij}, \hat{\sigma}_{ij}^2) = \frac{1}{\sqrt{2\pi}\hat{\sigma}_{ij}} \exp\left\{-\frac{(x_j - \hat{\mu}_{ij})^2}{2\hat{\sigma}_{ij}^2}\right\}$$

where $\hat{\mu}_{ij}$ and $\hat{\sigma}_{ij}^2$ denote the estimated mean and variance for attribute X_j, for class c_i.

Naive Bayes Classifier: Numeric Attributes

The naive assumption corresponds to setting all the covariances to zero in $\widehat{\mathbf{\Sigma}}_i$, that is,

$$\mathbf{\Sigma}_i = \begin{pmatrix} \sigma_{i1}^2 & 0 & \dots & 0 \\ 0 & \sigma_{i2}^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \\ 0 & 0 & \dots & \sigma_{id}^2 \end{pmatrix}$$

The naive Bayes classifier thus uses the sample mean $\hat{\boldsymbol{\mu}}_i = (\hat{\mu}_{i1}, \dots, \hat{\mu}_{id})^T$ and a *diagonal* sample covariance matrix $\widehat{\mathbf{\Sigma}}_i = diag(\sigma_{i1}^2, \dots, \sigma_{id}^2)$ for each class c_i. In total $2d$ parameters have to be estimated, corresponding to the sample mean and sample variance for each dimension X_j.

Naive Bayes Algorithm

NAIVEBAYES $(\mathbf{D} = \{(\mathbf{x}_j, y_j)\}_{j=1}^{n})$:

for $i = 1, \ldots, k$ **do**

  $\mathbf{D}_i \leftarrow \{\mathbf{x}_j \mid y_j = c_i, j = 1, \ldots, n\}$ // class-specific subsets

  $n_i \leftarrow |\mathbf{D}_i|$ // cardinality

  $\hat{P}(c_i) \leftarrow n_i/n$ // prior probability

  $\hat{\boldsymbol{\mu}}_i \leftarrow \frac{1}{n_i} \sum_{\mathbf{x}_j \in \mathbf{D}_i} \mathbf{x}_j$ // mean

  $\mathbf{Z}_i = \mathbf{D}_i - \mathbf{1} \cdot \hat{\boldsymbol{\mu}}_i^T$ // centered data for class c_i

  for $j = 1, .., d$ **do** // class-specific variance for X_j

    $\hat{\sigma}_{ij}^2 \leftarrow \frac{1}{n_i} Z_{ij}^T Z_{ij}$ // variance

  $\hat{\boldsymbol{\sigma}}_i = \left(\hat{\sigma}_{i1}^2, \ldots, \hat{\sigma}_{id}^2\right)^T$ // class-specific attribute variances

return $\hat{P}(c_i), \hat{\boldsymbol{\mu}}_i, \hat{\boldsymbol{\sigma}}_i$ for all $i = 1, \ldots, k$

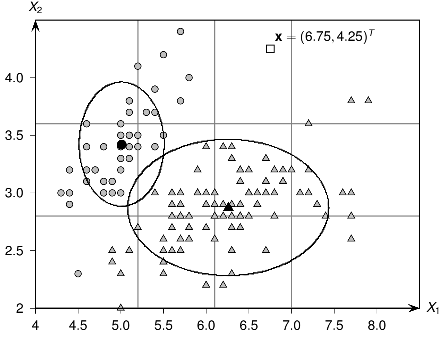
TESTING ($\mathbf{x}$ **and** $\hat{P}(c_i)$, $\hat{\boldsymbol{\mu}}_i$, $\hat{\boldsymbol{\sigma}}_i$, **for all** $i \in [1, k]$):

$$\hat{y} \leftarrow \arg\max_{c_i} \left\{ \hat{P}(c_i) \prod_{j=1}^{d} f(x_j | \hat{\mu}_{ij}, \hat{\sigma}_{ij}^2) \right\}$$

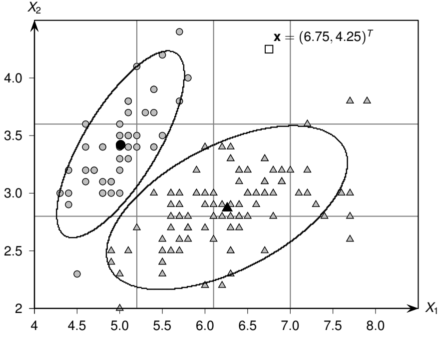
return $\hat{y}$

Naive Bayes versus Full Bayes Classifier: Iris 2D Data

X_1:`sepal length` versus X_2:`sepal width`



(a) Naive Bayes



(b) Full Bayes

Naive Bayes: Categorical Attributes

The independence assumption leads to a simplification of the joint probability mass function

$$P(\mathbf{x}|c_i) = \prod_{j=1}^{d} P(x_j|c_i) = \prod_{j=1}^{d} f\left(\mathbf{X}_j = \mathbf{e}_{jr_j} \,|\, c_i\right)$$

where $f(\mathbf{X}_j = \mathbf{e}_{jr_j}|c_i)$ is the probability mass function for $\mathbf{X}_j$, which can be estimated from $\mathbf{D}_i$ as follows:

$$\hat{f}(\mathbf{v}_j|c_i) = \frac{n_i(\mathbf{v}_j)}{n_i}$$

where $n_i(\mathbf{v}_j)$ is the observed frequency of the value $\mathbf{v}_j = \mathbf{e}_j r_j$ corresponding to the r_jth categorical value a_{jr_j} for the attribute X_j for class c_i.

If the count is zero, we can use the pseudo-count method to obtain a prior probability. The adjusted estimates with pseudo-counts are given as

$$\hat{f}(\mathbf{v}_j|c_i) = \frac{n_i(\mathbf{v}_j) + 1}{n_i + m_j}$$

where $m_j = |dom(X_j)|$.

Nonparametric Approach: *K* Nearest Neighbors Classifier

We consider a non-parametric approach for likelihood estimation using the nearest neighbors density estimation.

Let $\mathbf{D}$ be a training dataset comprising n points $\mathbf{x}_i \in \mathbb{R}^d$, and let $\mathbf{D}_i$ denote the subset of points in $\mathbf{D}$ that are labeled with class c_i, with $n_i = |\mathbf{D}_i|$.

Given a test point $\mathbf{x} \in \mathbb{R}^d$, and K, the number of neighbors to consider, let r denote the distance from $\mathbf{x}$ to its Kth nearest neighbor in $\mathbf{D}$.

Consider the d-dimensional hyperball of radius r around the test point $\mathbf{x}$, defined as

$$B_d(\mathbf{x}, r) = \left\{\mathbf{x}_i \in \mathbf{D} \mid \; \delta(\mathbf{x}, \mathbf{x}_i) \leq r\right\}$$

Here $\delta(\mathbf{x}, \mathbf{x}_i)$ is the distance between $\mathbf{x}$ and $\mathbf{x}_i$, which is usually assumed to be the Euclidean distance, i.e., $\delta(\mathbf{x}, \mathbf{x}_i) = \|\mathbf{x} - \mathbf{x}_i\|_2$. We assume that $|B_d(\mathbf{x}, r)| = K$.

Nonparametric Approach: *K* Nearest Neighbors Classifier

Let K_i denote the number of points among the K nearest neighbors of $\mathbf{x}$ that are labeled with class c_i, that is

$$K_i = \left\{\mathbf{x}_j \in B_d(\mathbf{x}, r) \mid y_j = c_i\right\}$$

The class conditional probability density at $\mathbf{x}$ can be estimated as the fraction of points from class c_i that lie within the hyperball divided by its volume, that is

$$\hat{f}(\mathbf{x}|c_i) = \frac{K_i/n_i}{V} = \frac{K_i}{n_i V}$$

where $V = \text{vol}(B_d(\mathbf{x}, r))$ is the volume of the d-dimensional hyperball.
The posterior probability $P(c_i|\mathbf{x})$ can be estimated as

$$P(c_i|\mathbf{x}) = \frac{\hat{f}(\mathbf{x}|c_i)\hat{P}(c_i)}{\sum_{j=1}^{k} \hat{f}(\mathbf{x}|c_j)\hat{P}(c_j)}$$

However, because $\hat{P}(c_i) = \frac{n_i}{n}$, we have

$$\hat{f}(\mathbf{x}|c_i)\hat{P}(c_i) = \frac{K_i}{n_i V} \cdot \frac{n_i}{n} = \frac{K_i}{nV}$$

Nonparametric Approach: *K* Nearest Neighbors Classifier

The posterior probability is given as

$$P(c_i|\mathbf{x}) = \frac{\frac{K_i}{nV}}{\sum_{j=1}^{k} \frac{K_j}{nV}} = \frac{K_i}{K}$$

Finally, the predicted class for $\mathbf{x}$ is

$$\hat{y} = \arg\max_{c_i} \{P(c_i|\mathbf{x})\} = \arg\max_{c_i} \left\{\frac{K_i}{K}\right\} = \arg\max_{c_i} \{K_i\}$$

Because K is fixed, the KNN classifier predicts the class of $\mathbf{x}$ as the majority class among its K nearest neighbors.

Iris Data: K Nearest Neighbors Classifier