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• 简介:

朴素贝叶斯 (Naive Bayes) 算法是机器学习中常见的基本算法之一,它主要被用来做分类任务。其理论基础是基于贝叶斯定理和条件独立性假设的一种分类方法。对于给定的训练数据集:

$$T = \{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$$

首先基于特征条件独立性假设学习联合概率分布 p(X,Y), 然后基于此模型,对于任意的输入 x, 利用贝叶斯定理求出后验概率最大的P(Y|X=x)对应的 y 的取值。

- 基于以上的解释,我们知道:
 - (1) 该算法的理论核心是贝叶斯定理;
 - (2) 它是基于条件独立性假设这个强假设基础之上的,这也是它为什么被称为"朴素"的主要原因。
- Naive Bayes 算法的数学原理:
 - 贝叶斯定理

根据贝叶斯定理,对一个分类问题,给定样本特征 x,样本属于类别 y 的概率 是

$$p(y|x) = \frac{p(x,y) \cdot p(y)}{p(x)}$$

公式中的 x 是特征向量, 假设其维度为 d, 则有

$$p(y|x) = \frac{p(x_1, x_2, \dots, x_d|y) \cdot p(y)}{p(x)}$$

朴素贝叶斯法对条件概率分布做了条件独立性的假设, 于是有

$$p(x_1, x_2, \dots, x_d | y = c_k) = \prod_{i=1}^d p(x_i | y = c_k)$$

$$p(y = c_k|x) = \frac{p(y = c_k) \cdot \prod_{i=1}^d p(x_i|y = c_k)}{p(x)}$$

- 多项式分布模型:
 - 模型假设

$$p(y = c_j) = \pi_j$$

$$p(x|c_j) = p(x_1, x_2, \dots, x_d|y = c_j) = \prod_{i=1}^d p(x_i|c_j)$$

$$= \prod_{i=1}^V \theta_{i|j}^{N(t_i, x)}$$

• 联合概率

$$p(x, y = c_j) = p(c_j) \cdot p(x|c_j) = \pi_j \prod_{i=1}^{\nu} \theta_{i|j}^{N(t_i,x)}$$

• (联合) 似然函数

$$L(\pi, \theta) = \log \prod_{k=1}^{N} p(x_k, y_k)$$

$$= \log \prod_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) p(y_k = c_j) p(x_k | y_k = c_j)$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) \log p(y_k = c_j) p(x_k | y_k = c_j)$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) \log \pi_j \prod_{i=1}^{V} \theta_{i|j}^{N(t_i, x_k)}$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) \left(\log \pi_j + \sum_{i=1}^{V} N(t_i, x_k) \log \theta_{i|j} \right)$$

• 最大似然估计

$$\max_{\pi,\theta} L(\pi,\theta)$$

s. t.
$$\begin{cases} \sum_{j=1}^{C} \pi_{j} = 1 \\ \sum_{i=1}^{V} \theta_{i|j} = 1, j = 1, ..., C \end{cases}$$

> 应用拉格朗日乘数:

$$J = L(\pi, \theta) + \alpha \left(1 - \sum_{j=1}^{C} \pi_{j}\right) + \sum_{j=1}^{C} \beta_{j} \left(1 - \sum_{i=1}^{V} \theta_{i|j}\right)$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_{k} = c_{j}) [\log \pi_{j} + \sum_{i=1}^{V} N(t_{i}, x_{k}) \log \theta_{i|j}] + \alpha \left(1 - \sum_{j=1}^{C} \pi_{j}\right) + \sum_{j=1}^{C} \beta_{j} \left(1 - \sum_{i=1}^{V} \theta_{i|j}\right)$$

• 闭式MLE解

▶ 梯度

$$\frac{\partial J}{\partial \pi_j} = \sum_{k=1}^N I(y_k = c_j) \frac{1}{\pi_j} - \alpha = 0$$

$$\frac{\partial J}{\partial \theta_{i|j}} = \sum_{k=1}^{N} I(y_k = c_j) \frac{N(t_i, x_k)}{\theta_{i|j}} - \beta_j = 0$$

➤ MLE解

$$\pi_{j} = \frac{\sum_{k=1}^{N} I(y_{k} = c_{j})}{\sum_{k=1}^{N} \sum_{j'=1}^{C} I(y_{k} = c_{j})} = \frac{N_{j}}{N}$$

$$\theta_{i|j} = \frac{\sum_{k=1}^{N} I(y_k = c_j) N(t_i, x_k)}{\sum_{k=1}^{N} I(y_k = c_j) \sum_{i'=1}^{V} N(t_i, x_k)}$$

• 拉普拉斯平滑

▶ 目的: 为了防止零概率

$$\pi_{j} = \frac{\sum_{k=1}^{N} I(y_{k} = c_{j}) + 1}{\sum_{j'=1}^{C} \sum_{k=1}^{N} I(y_{k} = c_{j}) + C}$$

$$\theta_{i|j} = \frac{\sum_{k=1}^{N} I(y_k = c_j) N(t_i, x_k) + 1}{\sum_{i'=1}^{V} \sum_{k=1}^{N} I(y_k = c_j) N(t_i, x_k) + V}$$

- 多变量伯努利分布模型:
 - 模型假设

$$p(y = c_j) = \pi_j$$

$$p(x|c_j) = p(t_1, t_2, \dots, t_d|c_j)$$

$$= \prod_{i=1}^{\nu} I(t_i \in x) \cdot \mu_{i|j} + I(t_i \notin x) \cdot (1 - \mu_{i|j})$$

• 联合概率

$$p(x,y=c_j) = \pi_j \prod_{i=1}^{v} I(t_i \in x) \cdot \mu_{i|j} + I(t_i \notin x) \cdot (1 - \mu_{i|j})$$

(联合) 似然函数

$$L(\pi, \mu) = \log \prod_{k=1}^{N} p(x_k, y_k)$$

$$= \sum_{k=1}^{N} \log \sum_{j=1}^{C} I(y_k = c_j) p(x_k, y_k)$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) \log p(c_j) \prod_{i=1}^{V} I(t_i \in x) p(t_i | c_j) + I(t_i \notin x) (1 - p(t_i | c_j))$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{C} I(y_k = c_j) \left(\log \pi_j + \sum_{i=1}^{V} I(t_i \in x_k) \log \mu_{i|j} + I(t_i \notin x_k) \log (1 - \mu_{i|j}) \right)$$

• 最大似然估计

$$\max_{\pi,\mu} L(\pi,\mu)$$

$$s.t.\sum_{j=1}^{C}\pi_{j}=1$$

▶ 应用拉格朗日乘数:

$$\begin{split} J &= L(\pi, \mu) + \alpha \left(1 - \sum_{j=1}^C \pi_j\right) \\ &= \sum_{k=1}^N \sum_{j=1}^C I\left(y_k = c_j\right) \left(\log \pi_j + \sum_{i=1}^V I(t_i \in x_k) \log \mu_{i|j} + I(t_i \notin x) \log(1 - \mu_{i|j})\right) + \alpha \left(1 - \sum_{j=1}^C \pi_j\right) \end{split}$$

• 闭式MLE解

▶ 梯度

$$\frac{\partial J}{\partial \pi_j} = \sum_{k=1}^N I(y_k = c_j) \frac{1}{\pi_j} - \alpha = 0$$

$$\frac{\partial J}{\partial \mu_{i|j}} = \sum_{k=1}^{N} I(y_k = c_j) \left(\frac{I(t_i \in x_k)}{\mu_{i|j}} - \frac{I(t_i \notin x_k)}{1 - \mu_{i|j}} \right) = 0, \forall j = 1, \dots, C.$$

➤ MLE解

$$\pi_{j} = \frac{\sum_{k=1}^{N} I(y_{k} = c_{j})}{\sum_{k=1}^{N} \sum_{j'=1}^{C} I(y_{k} = c_{j'})} = \frac{N_{j}}{N}$$

$$\mu_{i|j} = \frac{\sum_{k=1}^{N} I(y_k = c_j) I(t_i \in x_k)}{\sum_{k=1}^{N} I(y_k = c_j)}$$

• 拉普拉斯平滑

目的:为了防止零概率

$$\pi_j = \frac{\sum_{k=1}^{N} I(y_k = c_j) + 1}{\sum_{j'=1}^{C} \sum_{k=1}^{N} I(y_k = c_j) + C}$$

$$\mu_{i|j} = \frac{\sum_{k=1}^{N} I(y_k = c_j) I(t_i \in x_k) + 1}{\sum_{k=1}^{N} I(y_k = c_j) + 2}$$