Naive Bayes Classifier

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Machine Learning Techniques

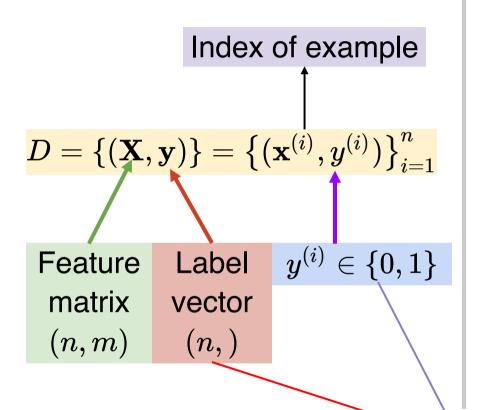
Introduction

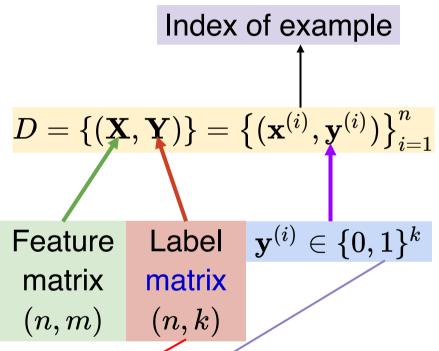
- Generative counterpart of logistic regression.
- Uses Bayes theorem for calculating probability of a sample belonging to a class.
- Makes strong (naive) conditional independence assumption between the features given a label.
- Simple yet very powerful classifier that is used extensively in applications like document classification and spam filtering.

Part 1: Training Setup

Binary classification

Multiclass classification





Spot the difference!

Part 2: Model

Naive Bayes' assumption

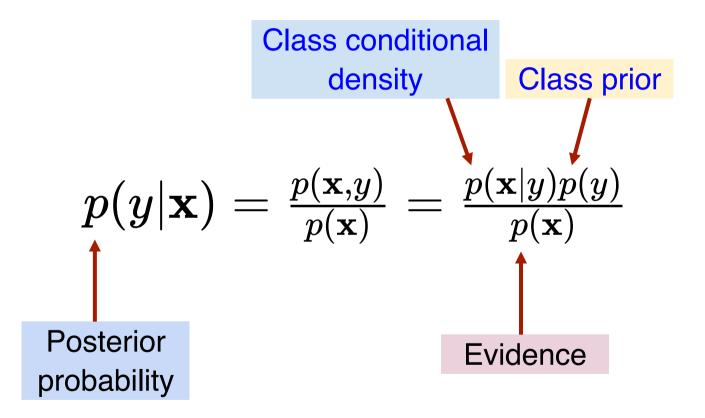
Naive Bayes classifier makes a strong conditional independence assumption:

Features are conditionally independent given the label.

It enables us to express joint probability of features given label as product of probabilities of individual features given label:

$$p(x_1, x_2, \dots, x_m | y) = p(x_1 | y) \ p(x_2 | y) \dots p(x_m | y) = \prod_{j=1}^m p(x_j | y)$$

NB classifier predicts probability, $p(y|\mathbf{x})$, of class label, y, given a feature vector \mathbf{x} , using Bayes' theorem



With Naive Bayes assumption, posterior probability $p(y|\mathbf{x})$ becomes

$$p(y=y_c|\mathbf{x}) = rac{p(\mathbf{x}|y_c) \; p(y_c)}{p(\mathbf{x})}$$

Rewriting
$$p(\mathbf{x}|y) = p(x_1, x_2, \dots, x_m|y)$$
 and $p(\mathbf{x}) = p(x_1, x_2, \dots, x_m)$

$$=rac{p(x_1,x_2,\ldots,x_m|y_c)\;p(y_c)}{p(x_1,x_2,\ldots,x_m)}$$

Expressing denominator as a sum over all k labels.

$$=rac{p(x_1,x_2,\ldots,x_m|y_c)\;p(y_c)}{\sum_{r=1}^k\,p(x_1,x_2,\ldots,x_m,y_r)}$$

$$=rac{p(x_1,x_2,\ldots,x_m|y_c)\;p(y_c)}{\sum_{r=1}^k p(x_1,x_2,\ldots,x_m,y_r)}$$

Rewriting the denominator after applying the chain rule

$$\sum_{r=1}^k p(x_1, x_2, \dots, x_m, y_r) = \sum_{r=1}^k p(x_1, x_2, \dots, x_m | y_r) p(y_r)$$

$$=rac{p(x_1,x_2,\ldots,x_m|y_c)\;p(y_c)}{\sum_{r=1}^k p(x_1,x_2,\ldots,x_m|y_r)p(y_r)}$$

Rewriting numerator and denominator following conditional independence assumption $p(x_1, x_2, \dots, x_m | y) = p(x_1 | y) p(x_2 | y) \dots p(x_m | y)$

$$p(y=y_c|\mathbf{x}) = rac{p(y_c)p(x_1|y_c)p(x_2|y_c)\dots p(x_m|y_c)}{\sum_{r=1}^k p(y_r)p(x_1|y_r)p(x_2|y_r)\dots p(x_m|y_r)}$$

$$p(y = y_c | \mathbf{x}) = rac{p(y_c) p(x_1 | y_c) p(x_2 | y_c) \dots p(x_m | y_c)}{\sum_{r=1}^k p(y_r) p(x_1 | y_r) p(x_2 | y_r) \dots p(x_m | y_r)}$$

Rewriting numerator and denominator compactly

$$=rac{p(y_c)\prod_{j=1}^m p(x_j|y_c)}{\sum_{r=1}^k p(y_r)\prod_{j=1}^m p(x_j|y_r)}$$

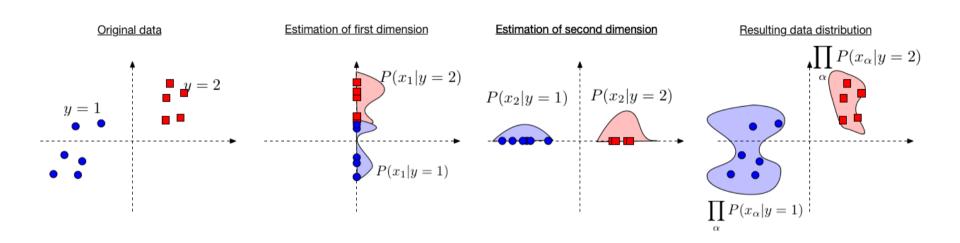
Parameters of naive Bayes classifier

$$p(y=y_c|\mathbf{x}) = rac{p(y_c)\prod_{j=1}^m p(x_j|y_c)}{\sum_{r=1}^k p(y_r)\prod_{j=1}^m p(x_j|y_r)}$$
 k prior $k imes m$ class conditional $\{p(y_1), p(y_2), \dots, p(y_k)\}$ densities $\{p(x_1|y_r), p(x_2|y_r), \dots, p(x_m|y_r)\}$

m conditional densities per class and there are k such classes.

The number of parameters for each conditional density vary and depends on its mathematical form.

NB schematic



Credits: https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote05.html

Modeling conditional densities: $p(x_i|y)$

- Depends on the nature of the feature x_i :
 - Binary feature e.g. word is present or not
 - categorical feature is generalization of binary.
 - Multinomial feature e.g. word count c_i as features with additional constraint that $\sum_{i=1}^{m} c_i = l$, the length of the sequence they represent.
 - Continuous feature Features are real numbers. e.g. area of an apartment in sq. feet.

Modeling $p(x_j|y_c)$

Probability distribution used for modeling $p(x_j|y_c)$ depends on the nature of the feature x_i :

- Categorical feature: $p(x_j|y_c) \sim \mathrm{Cat}(e,\mu_{j1c},\mu_{j2c},\ldots,\mu_{jec})$
- Binary feature: $p(x_j|y_c) \sim \mathrm{Bernoulli}(\mu_{jc})$
- ullet Continuous feature: $p(x_j|y_c) \sim \mathcal{N}(\mu_{jc},\sigma_{jc})$
- Multinomial feature: $p(\mathbf{x}|y_c) \sim ext{Multinomial}(l, \mu_{1c}, \mu_{2c}, \dots, \mu_{mc})$

Note: we need to estimate parameters of relevant distributions, one for each feature, for each class label.

Let \mathbf{w} be the set of all parameters: priors as well as class conditional densities

Bernoulli Distribution

When x_j is a binary feature, we use Bernoulli distribution to model the class conditional density: $p(x_j|y_c)$

Parameterized by $\mu_i c$, $p(x_i|y_c)$ is calculated as follows:

$$\bullet \ \ p(x_j=1|y_c)=\mu_{jc}$$

•
$$p(x_j = 0|y_c) = 1 - \mu_{jc}$$

Combine these two equations into a compact form as follows:

$$p(x_j|y_c;\mu_{jc}) = \mu_{jc}^{x_j} (1-\mu_{jc})^{(1-x_j)}$$

Verify that the compact form and earlier form are equivalent.

When
$$x_j=1$$
, $\mu_{jc}^{1}(1-\mu_{jc})^{(1-1)}=\mu_{jc}^{1}(1-\mu_{jc})^{0}=\mu_{jc}$ and $x_j=0$, $\mu_{jc}^{0}(1-\mu_{jc})^{(1-0)}=\mu_{jc}^{0}(1-\mu_{jc})^{1-0}=1-\mu_{jc}$

For $s \leq m$ binary features and k classes, we will have $k \times s$ parameters for s Bernoulli distributions.

Categorical Distribution

When x_j is a categorical feature i.e. it takes one of the e>2 discrete values [e.g. $\{\text{red}, \text{green}, \text{blue}\}$ or roll of a dice], we use categorical distribution to model the class conditional density $p(x_j|y_c)$.

Let $v = \{v_1, v_2, \dots, v_e\}$ be the set of e discrete values.

For discrete set v, $p(x_j|y_c)$ is parameterized by the |v|, that is # events in v and probability of each event $\mu_{j1c}, \mu_{j2c}, \ldots, \mu_{jec}$ such that $\sum_{g=1}^e \mu_{jqc} = 1$

For $x_j = v_q$ such that $v_q \in v$:

$$p(x_j = v_q | y_c; e, \mu_{j1c}, \mu_{j2c}, \dots, \mu_{jec}) = \mu_{jqc}$$

Let $\mu_{\mathbf{jc}} = [\mu_{j1c}, \mu_{j2c}, \dots, \mu_{jec}]$ be the parameter vector for $p(x_j|y_c)$

 $p(x_j|y_c)$ can be written in a compact form as follows:

$$p(x_j|y_c;e,\mu_{\mathbf{jc}}) = \mu_{j1c}^{{}_{\mathbf{1}}(x_j=v_1)} \mu_{j2c}^{{}_{\mathbf{1}}(x_j=v_2)} \dots \mu_{jec}^{{}_{\mathbf{1}}(x_j=v_e)}$$

where
$$\mathbf{1}(x_j=v_q)=1 ext{ if } x_j=v_q ext{ else } 0$$

Verify that the compact form is equivalent to the following:

$$egin{align} p(x_j = v_1 | y_c; e, \mu_{\mathbf{jc}}) &= \mu_{j1c} \ p(x_j = v_2 | y_c; e, \mu_{\mathbf{jc}}) &= \mu_{j2c} \ &dots \ p(x_j = v_e | y_c; e, \mu_{\mathbf{jc}}) &= \mu_{jec} \ \end{pmatrix}$$

Total parameters =
$$k imes \sum_{j=1}^m |v_j|$$

Multinomial Distribution

When \mathbf{x} is count vector i.e. each component x_j is a count of appearance in the object it represents and $\sum x_j = l$, which is the length of the object, we use multinomial distribution to model $p(\mathbf{x}|y_c)$.

Used for modelling documents that are represented by the word counts.

It is parameterized by the length of object l and probability of features $\{x_1, \ldots, x_m\}$: $\mu_{1c}, \ldots, \mu_{mc}$.

The probability of $p(\mathbf{x}|y_c)$ such that $\sum_{j=1}^m x_j = l$ is given by:

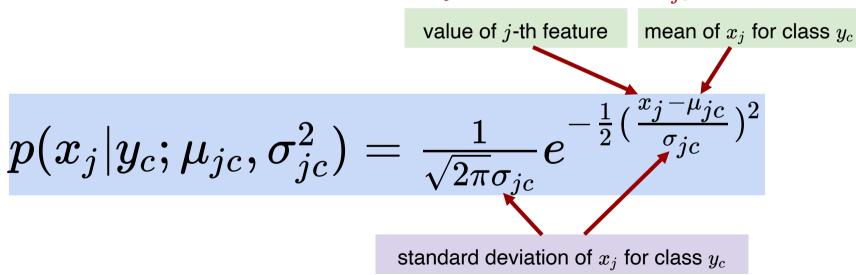
$$p(\mathbf{x}|y_c; l, \mu_{1c}, \mu_{2c}, \dots, \mu_{mc}) = rac{n!}{x_1! \dots x_m!} \prod_{j=1}^m \mu_{jc}^{x_j}$$

Total parameters = $k \times m$

Gaussian Distribution

When x_j is a continuous feature i.e. it takes a real value, we use gaussian (or normal) distribution to model the class conditional density $p(x_i|y_c)$.

It is parameterised by the mean μ_{jc} and variance σ_{jc}^2 .



This is 1-D gaussian distribution. It models class conditional density for a single feature.

Multivariate Gaussian Distribution

Alternately, we can use multivariate gaussian distribution to represent $p(\mathbf{x}|y)$ with parameters mean vector $\mu_{m\times 1}$ and covariance matrix $\Sigma_{m\times m}$.

In NB setting, since the features are conditionally independent of one another, all entries of Σ except diagonal are zero.

• The diagonal entries represent variance of that feature i.e. $\Sigma_{jj} = \sigma_i^2$

$$p(\mathbf{x}|y;\mu,\Sigma) = rac{1}{\sqrt{(2\pi)^m|\Sigma|}} \mathrm{exp}\left(-rac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)
ight)$$

Total parameters = $k \times 2m$

Once we learn parameters of different conditional densities, we use them to infer class label for new example.

Inference

We assign a class label y_c to a new example ${\bf x}$ that maximizes the posterior probability.

Let w be the set of all paramaters.

$$y = ext{argmax}_{y_c} p(y_c|\mathbf{x};\mathbf{w})$$

Using the definition of posterior probability

$$= ext{argmax}_{y_c} rac{p(\mathbf{x}|y_c; \mathbf{w}) \ p(y_c; \mathbf{w})}{p(\mathbf{x}; \mathbf{w})}$$

Since $p(\mathbf{x}; \mathbf{w})$ is independent of y_c , we ignore denominator from this computation

$$= ext{argmax}_{y_c} p(\mathbf{x}|y_c;\mathbf{w}) p(y_c;\mathbf{w})$$

$$= ext{argmax}_{y_c} p(\mathbf{x}|y_c;\mathbf{w}) p(y_c;\mathbf{w})$$

Expanding $p(\mathbf{x}|y_c;\mathbf{w})$ with naive Bayes assumption, we get

$$= ext{argmax}_{y_c} \left(\prod_{j=1}^m p(x_j|y_c; \mathbf{w})
ight) p(y_c; \mathbf{w})$$

This equation involves multiplication of small numbers, there is a risk of underflow in this calculation:

$$y = ext{argmax}_{y_c} \left(\sum_{j=1}^m \log p(x_j|y_c; \mathbf{w})
ight) + \log p(y_c; \mathbf{w})$$

For a new example, \mathbf{x} , we assign a class label y_c that yields max value among all $y = \{y_1, \dots, y_k\}$.

The following equation is useful for getting the class label. It does not return the probability of an example belonging to class y_c .

$$y = \mathop{\mathrm{argmax}}_{y_c} \left(\sum_{j=1}^m \log p(x_j|y_c; \mathbf{w})
ight) + \log p(y_c; \mathbf{w})$$

In case, we want the probability, we should use the following equation

$$p(y_c|\mathbf{x};\mathbf{w}) = rac{p(\mathbf{x}|y_c;\mathbf{w}) \ p(y_c;\mathbf{w})}{p(\mathbf{x};\mathbf{w})}$$

This calculation should also be performed in log space.

Part 3: Loss function

Likelihood describes joint probability of observed data D given the parameter \mathbf{w} for the chosen statistical model.

$$L(\mathbf{w}) = p(D; \mathbf{w}) = p(\mathbf{X}, \mathbf{y}; \mathbf{w})$$

Since training examples are i.i.d., we can express this as a product of probability of individual samples:

$$L(\mathbf{w}) = \prod_{i=1}^n p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})$$

For mathematical and computational convenience, we calculate log likelihood by taking log on both the sides:

$$\log L(\mathbf{w}) = \log \left(\prod_{i=1}^n p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})
ight)$$

The product becomes sum in the log space.

$$l(\mathbf{w}) = \sum_{i=1}^n \log \left(p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})
ight)$$

Log likelihood is defined as

$$l(\mathbf{w}) = \sum_{i=1}^n \log \left(p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})
ight)$$

Our job is to find the parameter vector \mathbf{w} such that the $l(\mathbf{w})$ is maximized.

Equivalently we can minimize the negative log likelihood (NLL) to maintain uniformity with other algorithms:

$$egin{aligned} J(\mathbf{w}) &= -l(\mathbf{w}) \ &= -\sum_{i=1}^n \log\left(p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})
ight) \end{aligned}$$

$$l(\mathbf{w}) = \sum_{i=1}^n \log \left(p(\mathbf{x}^{(i)}, y^{(i)}; \mathbf{w})
ight)$$

Simplifying with naive Bayes assumptions of conditional independence of features given label:

$$=\sum_{i=1}^n \log \left(\left(\prod_{i=1}^m p(\mathbf{x}_j^{(i)}|y^{(i)};\mathbf{w})
ight) \; p(y^{(i)};\mathbf{w})
ight)$$

Applying log on product makes it summation in log.

$$= \sum_{i=1}^n \left(\sum_{i=1}^m \log p(x_j^{(i)}|y^{(i)}; \mathbf{w})
ight) + \log p(y^{(i)}; \mathbf{w})$$

Rearranging

$$=\sum_{i=1}^n \log p(y^{(i)}; \mathbf{w}) + \sum_{i=1}^n \sum_{j=1}^m \log p(x_j^{(i)}|y^{(i)}; \mathbf{w})$$

$$l(\mathbf{w}) = \sum_{i=1}^n \log p(y^{(i)}; \mathbf{w}) + \sum_{i=1}^n \sum_{i=1}^m \log p(x_j^{(i)}|y^{(i)}; \mathbf{w})$$

The calculation of $p(x_j^{(i)}|y^{(i)})$ depends on the probability distribution of the features.

Part 4: Optimization for parameter estimation

The parameter estimation by maximizing the log likelihood function is carried out with the following three steps:

- 1. Calculate partial derivation of log likelihood function w.r.t. each parameter.
- 2. Set the partial derivative to 0, which is the condition at maxima.
- 3. Solve the resulting equation to obtain the parameter value.

Since $p(x_j|y)$ depends on the choice of probability distribution, we will discuss parameter estimation for different distributions separately.

Estimating prior probability: p(y)

The total number of parameters to be estimated is equal to the number of class labels k - one prior per label.

$$p(y=y_c)=rac{\sum_{i=1}^n 1(y^{(i)}=y_c)}{n}$$

Note that
$$1(y^{(i)} = y_c) = 1$$
 when $y^{(i)} = y_c$ else 0.

The prior probability for class y_c is equal to the ratio of the number of examples with label y_c to the total number of examples in the training set n.

Estimating class conditional densities

Bernoulli distribution

$$l(\mathbf{w}) = \sum_{i=1}^n \log p(y^{(i)}; \mathbf{w}) + \sum_{i=1}^n \sum_{j=1}^m \log p(x_j^{(i)}|y^{(i)}; \mathbf{w})$$

Recall $p(x_j|y_c;w_{jc})=w_{jc}^{x_j}(1-w_{jc})^{(1-x_j)}$, substituting this in $l(\mathbf{w})$

$$=\sum_{i=1}^n \log w_{y^{(i)}} + \sum_{i=1}^n \sum_{j=1}^m \log \left(w_{jy^{(i)}}^{x_j^{(i)}} (1-w_{jy^{(i)}})^{1-x_j^{(i)}}
ight)$$

Distributing log into the bracket - multiplication turns into addition

$$=\sum_{i=1}^n \log w_{y^{(i)}} + \sum_{i=1}^n \sum_{j=1}^m x_j^{(i)} \log w_{jy^{(i)}} + (1-x_j^{(i)}) \log (1-w_{jy^{(i)}})$$

Parameters for label y_r : $\mathbf{w} = w_{1r}, w_{2r}, \dots, w_{mr}$

(Step 1) calculate $\frac{\partial l(\mathbf{w})}{\partial w_{in}}$ and set it to 0.

$$rac{\partial l(\mathbf{w})}{\partial w_{jy_r}} = rac{\partial}{\partial w_{jy_r}} \left(\sum_{i=1}^n \log w_{y^{(i)}} + \sum_{i=1}^n \sum_{j=1}^m x_j^{(i)} \log w_{jy^{(i)}} + (1-x_j^{(i)}) \log \left(1-w_{jy^{(i)}}
ight)
ight)$$

Applying derivative to individual terms in the loss equation.

$$=\sum_{i=1}^n rac{\partial}{\partial w_{jy_r}} {
m log} \ w_{y^{(i)}} + \sum_{i=1}^n \sum_{j=1}^m rac{\partial}{\partial w_{jy_r}} \left(x_j^{(i)} {
m log} \ w_{jy^{(i)}} + (1-x_j^{(i)}) {
m log} \ (1-w_{jy^{(i)}})
ight)$$

The derivatives of the first term and all terms where $y^{(i)} \neq y_r$ are 0. Retaining terms where $y^{(i)} = y_r$.

$$=\sum_{i=1}^n 1(y^{(i)}=y_r) rac{\partial}{\partial w_{jy_r}} \left(x_j^{(i)} {\log w_{jy_r}} + (1-x_j^{(i)}) {\log \left(1-w_{jy_r}
ight)}
ight)$$

$$=\sum_{i=1}^n 1(y^{(i)}=y_r) \left(rac{x_j^{(i)}}{w_{jy_r}} - rac{1-x_j^{(i)}}{1-w_{jy_r}}
ight)$$

(Step 2) Setting $\frac{\partial l(\mathbf{w})}{\partial w_{in}}$ to 0.

$$rac{\partial l(\mathbf{w})}{\partial w_{jy_r}} = \sum_{i=1}^n 1(y^{(i)} = y_r) \left(rac{x_j^{(i)}}{w_{jy_r}} - rac{(1-x_j^{(i)})}{(1-w_{jy_r})}
ight) = 0$$

(Step 3) Solving it further with algebraic manipulation:

$$egin{split} \sum_{i=1}^n 1(y^{(i)} = y_r) \left(rac{x_j^{(i)}}{w_{jy_r}} - rac{(1-x_j^{(i)})}{(1-w_{jy_r})}
ight) &= 0 \ \sum_{i=1}^n 1(y^{(i)} = y_r) \left(x_j^{(i)} (1-w_{jy_r}) - (1-x_j^{(i)}) w_{jy_r}
ight) &= 0 \ \sum_{i=1}^n 1(y^{(i)} = y_r) \left(x_j^{(i)} - w_{jy_r}
ight) &= 0 \ \sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)} &= \sum_{i=1}^n 1(y^{(i)} = y_r) w_{jy_r} \end{split}$$

This yields:

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)}}{\sum_{i=1}^n 1(y^{(i)} = y_r)}$$

examples with label y_r and $x_j = 1$

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)}}{\sum_{i=1}^n 1(y^{(i)} = y_r)}$$
 # examples with label y_r

What if
$$\sum_{i=1}^{n} 1(y^{(i)} = y_r) x_j^{(i)} = 0$$
?

Leads to $w_{jy_r} = 0$, which would mean $p(x_j|y_r) = 0$

Leads to $p(y=y_r|\mathbf{x})=0$ since $p(x_j|y_r)=0$

Fixing problem with zero count

Laplace smoothing: We can correct it by adding +1 to numerator and +2 to denominator (1 for each value of feature: $x_i \in \{0,1\}$).

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)} + 1}{\sum_{i=1}^n 1(y^{(i)} = y_r) + 2}$$

In general, we can add +c to numerator and +2c to denominator. c is a hyperparameter that helps control overfitting.

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)} + c}{\sum_{i=1}^n 1(y^{(i)} = y_r) + 2c}$$

However too high value of c leads to underfitting.

Categorical distribution

$$w_{jvy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) \ 1(x_j^{(i)} = v)}{\sum_{i=1}^n 1(y^{(i)} = y_r)}$$

In plain english, this is ratio of number of examples with label y_r and $x_j = v$ to the total number of training examples with label y_r .

Parameters:

$$\mathbf{w} = \{w_{111}, \dots, w_{1e1}, \dots, w_{m11}, \dots, w_{me1}, \dots, w_{mek}\}$$

Incorporating smoothing, we obtain

$$w_{jvy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) \ 1(x_j^{(i)} = v) + c}{\sum_{i=1}^n 1(y^{(i)} = y_r) + ce}$$

Smoothing factor c is a hyperparameter and c=1 leads to Laplace smoothing.

Multinomial distribution

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) \, x_j^{(i)}}{\sum_{i=1}^n 1(y^{(i)} = y_r) \sum_{j=1}^m x_j^{(i)}}$$

In plain english, this is ratio of number of training examples where x_j appears with label y_r to the sum of feature values in training examples with label y_r .

Incorporating smoothing, we obtain

$$w_{jy_r} = rac{\sum_{i=1}^n 1(y^{(i)} = y_r) \ x_j^{(i)} + c}{\sum_{i=1}^n 1(y^{(i)} = y_r) \sum_{j=1}^m x_j^{(i)} + cm}$$

Smoothing factor c is a hyperparameter and c=1 leads to Laplace smoothing.

Gaussian/Normal distribution

Let n_r be the number of examples of class y_r

$$n_r = \sum_{i=1}^n 1(y^{(i)} = y_r)$$

There are two parameters per feature $\{\mu_j, \sigma_i^2\}$ per label.

$$egin{align} \mu_{jr} &= rac{1}{n_r} \sum_{i=1}^n 1(y^{(i)} = y_r) x_j^{(i)} \ \sigma_{jr}^2 &= rac{1}{n_r} \sum_{i=1}^n 1(y^{(i)} = y_r) (x_j^{(i)} - \mu_{jr})^2 \ \end{array}$$

Part 5: Evaluation

Evaluation

Classification evaluation measures with cross validation and test set:

- Confusion matrix
- Precision/recall/F1 score
- AUC ROC/PR curve