

CSC380: Principles of Data Science

Predictive Modeling and Classification 3

Xinchen Yu

Midterm score curving

$$new = score + \sqrt{1 - score}$$

origin_scores	new_scores
38	45.87400787401181
39	46.810249675906654
40	47.74596669241483
41	48.681145747868605
42	49.61577310586391
43	50.54983443527075
44	51.48331477354788
45	52.41619848709566
46	53.348469228349536
47	54.28010988928052
48	55.211102550927976
49	56.14142842854285
50	57.071067811865476
51	58.0
52	58.92820323027551
53	59.855654600401046
54	60.782329983125265
55	61.70820393249937
56	62.633249580710796

origin_scores	new_scores
63	69.08276253029823
64	70.0
65	70.91607978309962
66	71.8309518948453
67	72.74456264653803
68	73.65685424949238
69	74.56776436283002
70	75.47722557505166
71	76.3851648071345
72	77.29150262212919
73	78.19615242270663
74	79.09901951359278
75	80.0
76	80.89897948556636
77	81.79583152331271
78	82.69041575982342
79	83.58257569495584
80	84.47213595499957
81	85.35889894354068

new_scores	origin_scores
86.24264068711929	82
87.12310562561765	83
88.0	84
88.87298334620742	85
89.74165738677394	86
90.605551275464	87
91.46410161513775	88
92.3166247903554	89
93.16227766016839	90
94.0	91
94.82842712474618	92
95.64575131106459	93
96.44948974278317	94
97.23606797749979	95
98.0	96
98.73205080756888	97
99.41421356237309	98
100.0	99
100.0	100

Estimating current scores

- Assignments: 36%
- Midterm: 20%
- Project: 14%
- Final Exam: 20%
- Participation: 10%
- 7 homeworks, drop the lowest one.
 - Each 6 points
 - e.g., 6 * 120/130 = 5.54 -- if a homework total points are 130 and you got 120

Model Evaluation

Confusion Matrix

Suppose our classifier distinguishes between cats and non-cats.

We can make the following table called **confusion matrix**:

Predicted class Actual class	Cat	Non-cat
Cat	6 true positives	2 false negatives
Non-cat	1 false positive	3 true negatives

It tells us if classifier is biased towards certain mistakes (False Positives, False Neg.)

Good for investigating opportunities to improve the classifier.

Evaluating Classifiers - Precision

PREDICTED

	POSITIVE	NEGATIVE
POSITIVES	TRUE POSITIVES	FALSE NEGATIVES
NEGATIVE	FALSE POSITIVES	TRUE NEGATIVES

Precision: dividing the true positives by anything that was predicted as a positive.

TRUE POSITIVES

TRUE POSITIVES + FALSE POSITIVES

Evaluating Classifiers - Recall

PREDICTED

	POSITIVE	NEGATIVE
POSITIVES	TRUE POSITIVES	FALSE NEGATIVES
NEGATIVE	FALSE POSITIVES	TRUE NEGATIVES

Recall (or True Positive Rate): dividing the true positives by anything that should have been predicted as positive.



Evaluating Classifiers

F1 score symmetrically represents both precision and recall in one metric.

$$F_1 = rac{2}{ ext{recall}^{-1} + ext{precision}^{-1}} = 2 \cdot rac{ ext{precision} \cdot ext{recall}}{ ext{precision} + ext{recall}} = rac{ ext{tp}}{ ext{tp} + rac{1}{2}(ext{fp} + ext{fn})}$$

- This is the *harmonic mean* of precision and recall
 - harmonic_mean(x,y)

$$\frac{1}{\frac{1}{2}(\frac{1}{x}+\frac{1}{y})}$$

• Gives equal importance to precision and recall – F1 may not be best when you care about one more than the other (e.g., in medical tests we care about recall)

Evaluation in Scikit-Learn

Evaluation functions live in metrics

<pre>metrics.confusion_matrix(y_true, y_pred, *)</pre>	Compute confusion matrix to evaluate the accuracy of a classification.
<pre>metrics.dcg_score(y_true, y_score, *[, k,])</pre>	Compute Discounted Cumulative Gain.
<pre>metrics.det_curve(y_true, y_score[,])</pre>	Compute error rates for different probability thresholds.
<pre>metrics.f1_score(y_true, y_pred, *[,])</pre>	Compute the F1 score, also known as balanced F-score or F-measure.
<pre>metrics.fbeta_score(y_true, y_pred, *, beta)</pre>	Compute the F-beta score.
<pre>metrics.hamming_loss(y_true, y_pred, *[,])</pre>	Compute the average Hamming loss.
<pre>metrics.hinge_loss(y_true, pred_decision, *)</pre>	Average hinge loss (non-regularized).
<pre>metrics.jaccard_score(y_true, y_pred, *[,])</pre>	Jaccard similarity coefficient score.
<pre>metrics.log_loss(y_true, y_pred, *[, eps,])</pre>	Log loss, aka logistic loss or cross-entropy loss.
<pre>metrics.matthews_corrcoef(y_true, y_pred, *)</pre>	Compute the Matthews correlation coefficient (MCC).
<pre>metrics.multilabel_confusion_matrix(y_true,)</pre>	Compute a confusion matrix for each class or sample.
<pre>metrics.ndcg_score(y_true, y_score, *[, k,])</pre>	Compute Normalized Discounted Cumulative Gain.
<pre>metrics.precision_recall_curve(y_true,)</pre>	Compute precision-recall pairs for different probability thresholds.
metrics.precision_recall_fscore_support()	Compute precision, recall, F-measure and support for each class.
<pre>metrics.precision_score(y_true, y_pred, *[,])</pre>	Compute the precision.
<pre>metrics.recall_score(y_true, y_pred, *[,])</pre>	Compute the recall.
	•

Naïve Bayes

Naïve Bayes Overview

Heads Up This section will return to some math as we go in depth. But, much of it is that you already know with a new application (Naïve Bayes Classification) – ask questions if you are lost

- Introduction to Naïve Bayes Classifier
- Maximum Likelihood Estimation

Math Prep

N RVs conditionally independent, given Z, if and only if:

$$p(X_1,\ldots,X_N\mid Z)=\prod_{i=1}^N p(X_i\mid Z)$$
 Probability 3, page 25

Bayes' rule

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}$$

Probability 2, page 24

Maximum likelihood estimation

Statistics 2

Bernoulli and Gaussian distribution

Probability 3, 4 Statistics 2

Intuition

Training Data:

Person	height (feet)
male	6
male	5.92 (5'11")
male	5.58 (5'7")
male	5.92 (5'11")
female	5
female	5.5 (5'6")
female	5.42 (5'5")
female	5.75 (5'9")



Task: observe feature x_n , predict label $y_n \in (0,1)$

Choose the class with higher probability:

$$P(Y_n = 1 | X_n = x_n)$$
 vs $P(Y_n = 0 | X_n = x_n)$

$$P(Y_n = 1|X_n = x_n) = \frac{P(Y_n = 1, X_n = x_n)}{P(X_n = x_n)}$$

$$P(Y_n = 0|X_n = x_n) = \frac{P(Y_n = 0, X_n = x_n)}{P(X_n = x_n)}$$

How to learn a joint probability model for P(Y, X)?

Probabilistic Approach to ML

Training Data:

Person	height (feet)	weight (lbs)	foot size(inches)
male	6	180	12
male	5.92 (5'11")	190	11
male	5.58 (5'7")	170	12
male	5.92 (5'11")	165	10
female	5	100	6
female	5.5 (5'6")	150	8
female	5.42 (5'5")	130	7
female	5.75 (5'9")	150	9



Task: Observe features $x_1, ..., x_D$ and predict class label $y \in \{1, ..., C\}$

Model: Assume that the feature x and its label y follows certain type of distribution \mathcal{D} with parameter θ .

 $(x,y) \stackrel{\text{i.i.d.}}{\sim} \mathcal{D}_{\theta}$

Training Algorithm: Estimate θ e.g., MLE $\hat{\theta}$

To classify: Compute

$$\hat{y} = \arg\max_{c \in \{1,\dots,C\}} p(y = c \mid x; \hat{\theta})$$

what comes after semicolon is the parameter of the distribution

Naïve Bayes is a Specific Probabilistic Approach

Training Data:

Person height (feet)		weight (lbs)	foot size(inches)	
male	6	180	12	
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Task: Observe features $x_1, ..., x_D$ and predict class label $y \in \{1, ..., C\}$

Naïve Bayes Model: Treat features as conditionally independent given class label,

$$p(x,y) = p(y)p(x|y) = p(y) \prod_{d=1}^{D} p(x_d \mid y)$$
build individual models for these

To classify a given instance x: Bayes rule!

$$p(y = c \mid x) = \frac{p(y = c)p(x \mid y = c)}{p(x)}$$

Key concept in Naïve Bayes

$$p(x,y) = p(y)p(x|y) = p(y) \prod_{d=1}^{D} p(x_d \mid y)$$
Class prior distribution Class conditional distribution

Given one data point, it has 4 features (input), and the label is 0 (output)

$$p(x_1, x_2, x_3, x_4, y = 0) = p(y = 0) \cdot p(x_1, x_2, x_3, x_4 | y = 0)$$
$$= p(y = 0) \cdot p(x_1 | y = 0) \cdot p(x_2 | y = 0) \cdot p(x_3 | y = 0) \cdot p(x_4 | y = 0)$$

Class prior distribution

$$p(x,y) = p(y)p(x|y) = p(y) \prod_{d=1}^{D} p(x_d \mid y)$$
Class prior distribution
Class conditional distribution

For the class prior distribution, take categorical distribution.

$$y \sim \text{Categorical}(\pi), \qquad \pi \in \mathbb{R}^C, \pi_c \ge 0, \sum_c \pi_c = 1$$

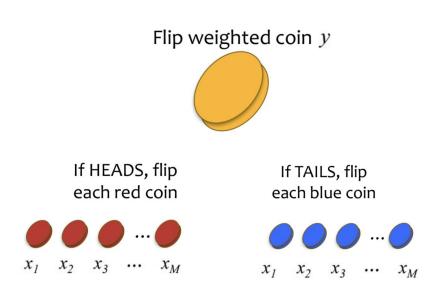
$$=> p(y = c) = \pi_c$$

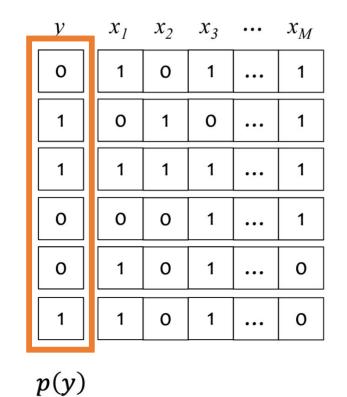
Example: biased 4-sided die Y, given:

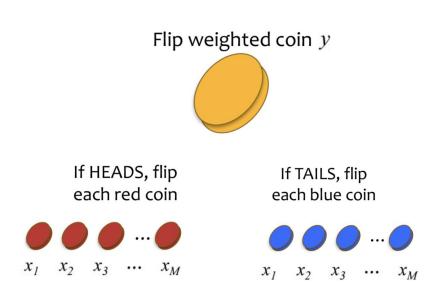
•
$$P(Y=1) = 0.2$$
, $P(Y=2) = 0.3$, $P(Y=3) = 0.1$, $P(Y=4) = 0.4$



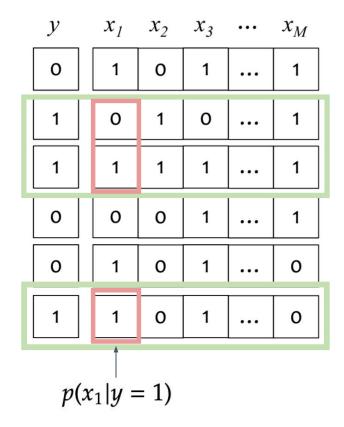
Class prior distribution

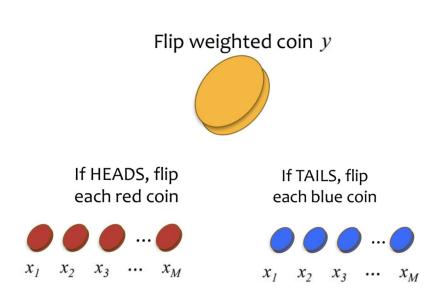




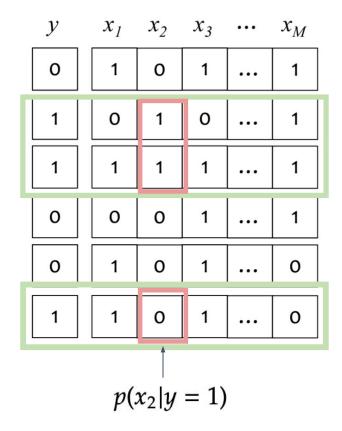


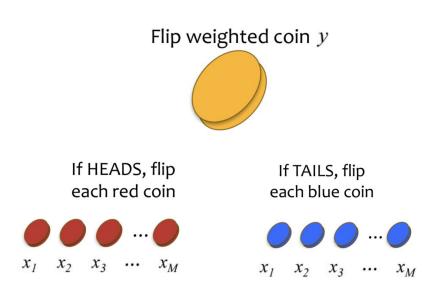
Each red / blue coin biases can be different.



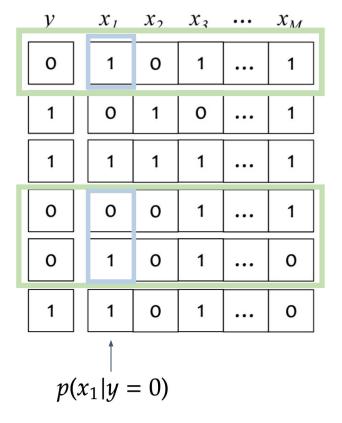


Each red / blue coin biases can be different.





Each red / blue coin biases can be different.



Simplifying Assumption: "Class conditional" distribution assumes features are conditionally independent given class

$$p(x \mid y) = \prod_{d=1}^{D} p(x_d \mid y)$$

- "Naïve" as in general features are likely to be dependent.
- Every feature can have a different class-conditional distribution

$$P(x_1|y)$$
 can be different from $P(x_2|y)$

Features are typically not independent!

Example 1 If a recent news article contains word "Donald" it is much more likely to contain the word "Trump".

Example 2 If flower <u>petal width</u> is very large then <u>petal length</u> is also likely to be high.





NEWS IN BRIEF August 18, 2016

VOL 52 ISSUE 32 - Politics - Politicians - Election 2016 - Donald Trump



Source: Matt Gormley

Simplifying Assumption: "Class conditional" distribution assumes features are conditionally independent given class

$$p(x \mid y) = \prod_{d=1}^{D} p(x_d \mid y)$$

- "Naïve" as in general features are likely to be dependent.
- Every feature can have a different class-conditional distribution

Doesn't capture correlation among features. But why would it be a good idea?

- Easy computation: For C classes and D features only O(CD) parameters
- Prevents overfitting
- Simplicity

For real-valued features we can use Normal distribution:

$$p(x \mid y = c) = \prod_{d=1}^{D} \mathcal{N}(x_d \mid \mu_{cd}, \sigma_{cd}^2)$$

quiz candidate

Q: how many parameters?

Parameters of featured for class c

For binary features $x_d \in \{0,1\}$ can use Bernoulli distributions:

$$p(x \mid y = c) = \prod_{d=1}^{D} \text{Bernoulli}(x_d \mid \theta_{cd})$$
 quiz candidate Q: how many parameters?

"Coin bias" for dth feature and class c

- K-valued discrete features: use Categorical.
- Can mix-and-match, e.g. some discrete, some continuous features

$$p(x \mid y = c) = \prod_{d=1}^{D'} \text{Bernoulli}(x_d \mid \theta_{cd}) \prod_{d=D'+1}^{D} \mathcal{N}(x_d \mid \mu_{cd}, \sigma_{cd}^2)$$

Naïve Bayes Model: Maximum Likelihood

Fitting the model requires learning all parameters...

$$p(x,y=c) = p(y=c;\pi) \prod_{d=1}^{D} p(x_d \mid \theta_{cd})$$
Class Prior Parameters
Likelihood Parameters

Given training data $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$ maximize the likelihood function,

$$\theta^{\text{MLE}} = \arg \max_{\pi, \theta} \, \log p(\mathcal{D}; \pi, \theta)$$

Naïve Bayes Model: Maximum Likelihood

$$\theta^{\text{MLE}} = \arg \max_{\pi, \theta} \log p(\mathcal{D}; \pi, \theta) \qquad (\mathcal{D} := \{(x^{(i)}, y^{(i)})\}_{i=1}^{m})$$

$$= \arg \max_{\pi, \theta} \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)}; \pi, \theta)$$

$$log(ab) = log a + log b$$

Since data are iid

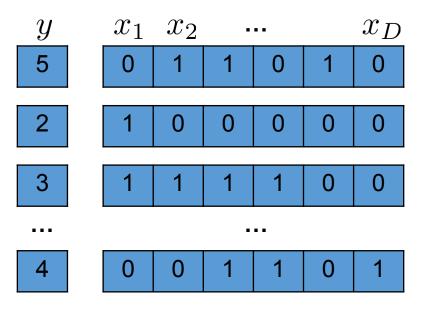
$$=\arg\max_{\pi,\theta}\sum_{i=1}^{m}\log p(x^{(i)},y^{(i)};\pi,\theta)$$

$$= \arg \max_{\pi,\theta} \sum_{i=1}^{m} \log p(y^{(i)};\pi) + \sum_{i=1}^{m} \sum_{d=1}^{D} \log p\left(x_d^{(i)} \middle| y^{(i)}; \theta_{y^{(i)}d}\right)$$

 θ_{cd} : parameter for feature d for class c

Find zero-gradient if concave, or gradient-based optimization otherwise

Analogy:



Let each feature follow a Bernoulli distribution then the model is...

$$y \sim \text{Categorical}(\pi)$$
 $x_d \mid y = c \sim \text{Bernoulli}(\theta_{cd})$

The Naïve Bayes joint distribution is then:

$$p(\mathcal{D}; \pi, \theta) = \prod_{i=1}^{m} \left(p(y^{(i)}; \pi) \prod_{d} p\left(x_d^{(i)}; \theta_{y^{(i)}d}\right) \right)$$
$$= \prod_{i=1}^{m} \left(\prod_{c} \left(\pi_c^{\mathbf{I}\{y_i = c\}} \prod_{j} p(x_{ij} | \theta_{jc})^{\mathbf{I}\{y_i = c\}} \right) \right)$$

Write down log-likelihood and optimize...

Bernoulli Naïve Bayes MLE

Let $m_c := \sum_{i=1}^m \mathbb{I}\{y^{(i)} = c\}$ be number of training examples in class c then,

$$\sum_{i=1}^{m} \log p(\mathcal{D}; \pi, \theta) = \sum_{c=1}^{C} m_c \log \pi_c + \sum_{c=1}^{C} \sum_{i: v^{(i)} = c} \sum_{d=1}^{D} \log p\left(x_d^{(i)}; \theta_{cd}\right)$$

Log-likelihood function is concave in all parameters so...

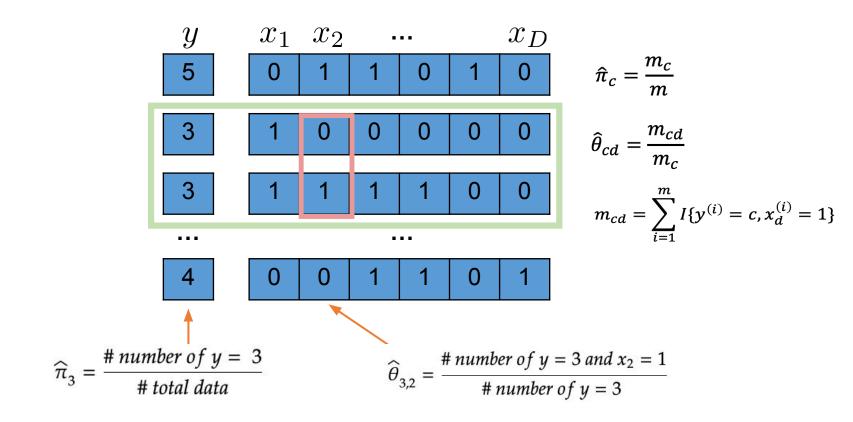
- 1. Take derivatives with respect to π and θ separately.
- Set derivatives to zero and solve

$$\hat{\pi}_c = \frac{m_c}{m}$$
 Fraction of training examples from class c

$$\widehat{ heta}_{cd} = rac{m_{cd}}{m_c}$$
 Number of "heads" in training set from class c

$$m_{cd} = \sum_{i=1}^{m} I\{y^{(i)} = c, x_d^{(i)} = 1\}$$

Analogy:



Bernoulli Naïve Bayes: making prediction

$$\hat{\pi}_c = \frac{m_c}{m}$$

$$\hat{\theta}_{cd} = \frac{m_{cd}}{m_c}$$

Given one data point, it has 4 features (input), compare the probabilities:
$$p(x_1, x_2, x_3, x_4, y = 0) = p(y = 0) \cdot p(x_1, x_2, x_3, x_4 | y = 0)$$
$$= p(y = 0) \cdot p(x_1 | y = 0) \cdot p(x_2 | y = 0) \cdot p(x_3 | y = 0) \cdot p(x_4 | y = 0)$$
$$p(x_1, x_2, x_3, x_4, y = 1) = p(y = 1) \cdot p(x_1, x_2, x_3, x_4 | y = 1)$$
$$= p(y = 1) \cdot p(x_1 | y = 1) \cdot p(x_2 | y = 1) \cdot p(x_3 | y = 1) \cdot p(x_4 | y = 1)$$

Bernoulli Naïve Bayes MLE: issue

$$p(y=2)=0$$

no data points in class 1 & 3 is 1:

$$p(x_1 = 0 | y = 3) = 0$$

$$p(x_1 = 0 | y = 1) = 0$$

$$egin{array}{c|c} y & x_1 & x_2 \ \hline 1 & 0 & 1 \ \hline \end{array}$$

Bernoulli Naïve Bayes MLE: issue

What if there are *no* examples of class c in the training set?

$$\hat{\pi}_c = 0$$
 Model will never learn to guess class c

What if all data points i in class c has $x_d^{(i)} = 0$ in the training set?

$$\hat{\theta}_{cd} = 0$$

Model will assign 0 likelihood for test data with $x_d = 1$ for class c (i.e., p(x|y=c)).

What does it imply on p(y = c|x)? 0!

Training data needs to see every possible outcome for each feature

Any ideas how we can fix this problem?

Fixing Bernoulli MLE

We could add a small constant to prevent zero probabilities...

$$\hat{\pi}_c \propto m_c + lpha$$
 $\hat{ heta}_{cj} \propto m_{cj} + eta$ $lpha, eta > 0$

Pseudocounts add- $lpha$ Smoothing Laplace smoothing typical choice: set $lpha = eta = 1$

Another smoothing method:

$$\hat{P}(w_i|c) \ = \ \frac{count(w_i,c)+1}{\sum_{w \in V} (count(w,c)+1)} = \frac{count(w_i,c)+1}{\left(\sum_{w \in V} count(w,c)\right)+|V|}$$
 Word count in category c Vocabulary size in whole corpus

Naïve Bayes in Sentiment Classification

	Cat	Documents
Training	-	just plain boring
	-	entirely predictable and lacks energy
	-	no surprises and very few laughs
	+	very powerful
	+	the most fun film of the summer
Test	?	predictable with no fun

$$\widehat{\pi}_c = \frac{m_c}{m}$$

$$\hat{\pi}_c = \frac{m_c}{m}$$
 $P(-) = \frac{3}{5}$ $P(+) = \frac{2}{5}$

Naïve Bayes in Sentiment Classification

$$\hat{P}(w_i|c) = \frac{count(w_i,c)}{\sum_{w \in V} count(w,c)}$$

smoothing
$$\frac{count(w_i,c) + 1}{(\sum_{w \in V} count(w,c)) + |V|}$$

	Cat	Documents
Training	-	just plain boring
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Test	?	predictable with no fun

Vocabulary size

$$20 = 14 + 9 - 3$$

3: the, and, very (duplicate)

$$P(\text{``predictable''}|-) = \frac{1+1}{14+20} \qquad P(\text{``predictable''}|+) = \frac{0+1}{9+20}$$

$$P(\text{``no''}|-) = \frac{1+1}{14+20} \qquad P(\text{``no''}|+) = \frac{0+1}{9+20}$$

$$P(\text{``fun''}|-) = \frac{0+1}{14+20} \qquad P(\text{``fun''}|+) = \frac{1+1}{9+20}$$

Naïve Bayes in Sentiment Classification

	Cat	Documents	
Training	-	just plain boring	
	-	entirely predictable and lacks energy	
	-	no surprises and very few laughs	
	+	very powerful	Jegnore unknown words
	+	the most fun film of the summer	
Test	?	predictable with no fun	

$$P(-)P(S|-) = \frac{3}{5} \times \frac{2 \times 2 \times 1}{34^3} = 6.1 \times 10^{-5}$$
$$P(+)P(S|+) = \frac{2}{5} \times \frac{1 \times 1 \times 2}{29^3} = 3.2 \times 10^{-5}$$

The model thus predicts the class *negative* for the test sentence.

Naïve Bayes in Scikit-learn

Scikit-learn has separate classes each feature type

```
sklearn.naive bayes.GaussianNB
```

Real-valued features

```
sklearn.naive bayes.MultinomialNB
```

Discrete K-valued feature counts (e.g. multiple die rolls)

```
sklearn.naive bayes.BernoulliNB
```

Binary features (e.g. coinflip)

```
sklearn.naive bayes.CategoricalNB
```

Discrete K-valued features (e.g. single die roll)

For large training data that don't fit in memory use Scikit-learn's out-of-core learning