Bayes and Naïve Bayes

Concepts:

Discriminative and Generative model

Bayes Classifier

Modeling joint distribution of discrete variables

Naïve Bayes assumption

Naïve Bayes classifier

Bernoulli and Multi-nomial Naïve Bayes

MLE and MAP estimation, smoothing

Two main approaches for learning probabilistic classifiers

- **Discriminative:**
  - Learn $P(y|\mathbf{x})$ directly
  - Logistic regression is one of such techniques

- **Generative:**
  - Learn $P(y)$ and $P(\mathbf{x}|y)$
  - Compute $P(y|\mathbf{x})$ using <u>Bayes rule</u>

$$P(y|\mathbf{x}) = \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})} = \frac{P(\mathbf{x}|y)P(y)}{\sum_y P(\mathbf{x}, y)}$$

Generative models

- A generative model specifies a generative story regarding how the data was created
  - E.g. by flipping a coin (with p_h for head)
- Given parameters (p_h) for the model, new data can be generated
  - E.g. flipping the coin again
- Maximum likelihood estimation is typically used for estimation the model parameters

A simple generative model

- Here is a simple generative story:

1. Flip a coin to decide the gender of the individual: head = male, tail = female
2. If male, sample the weight and height from Gaussian distribution $N(\mu_m, \Sigma_m)$
3. If female, sample the weight and height from Gaussian distribution $N(\mu_f, \Sigma_f)$

Repeating this process, we get a population of females and males with weights and heights

- Let's try to define a generative model for emails of two classes (spam vs. non-spam)
- How to represent an email of M words as a feature vector? --- popular options: bag of words

Option 1: binary vector

With a dictionary of size V, $\mathbf{x} = [x_1, x_2, \ldots, x_V]$ where $x_i \in \{0,1\}$

- $x_i = 1$ if email contains the ith dictionary word
- $x_i = 0$ otherwise

Option 2: integer vector

With a dictionary of size V, $\mathbf{x} = [x_1, x_2, \ldots, x_V]$ where $x_i \in N_0$

- x_i: nonnegative integer count of the ith dictionary word

Generative model for emails

1. Flip a weighted coin (y)
2. If head (y=1, aka spam), generate an email $\mathbf{x} = [x_1, x_2, \ldots, x_V]$ from the spam distribution
3. If tail (y=0, non-spam), generate an email $\mathbf{x} = [x_1, x_2, \ldots, x_V]$ from the non-spam distribution

$$P(\mathbf{x}, y) = P(\mathbf{x}|y)P(y)$$

Classification with a generative model

- Generative model learns $P(y)$ and $P(\mathbf{x}|y)$
- Prediction is made by

$$P(y|\mathbf{x}) = \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})} = \frac{P(\mathbf{x}|y)P(y)}{\sum_y P(\mathbf{x}, y)}$$

- Often referred to as the Bayes Classifier due to using the Bayes rule

Estimating $p(y)$ and $p(\mathbf{x}|y)$

- $P(y)$: prior distribution of y
  - $P(y = 1)$: portion of spams
  - $P(y = 0)$: portion of non-spams

- $P(\mathbf{x}|y)$: the distribution of $\mathbf{x}$ given y
  - $P(\mathbf{x}|y = 1)$: distribution of $\mathbf{x}$ given $y = 1$ (spam)
  - $P(\mathbf{x}|y = 0)$: distribution of $\mathbf{x}$ given $y = 0$ (non-spam)

- Learning $P(\mathbf{x}|y = 1)$ or $P(\mathbf{x}|y = 0)$ is a (joint) density estimation problem

Joint Distribution of Boolean Variables

Recipe for making a joint distribution of M variables:

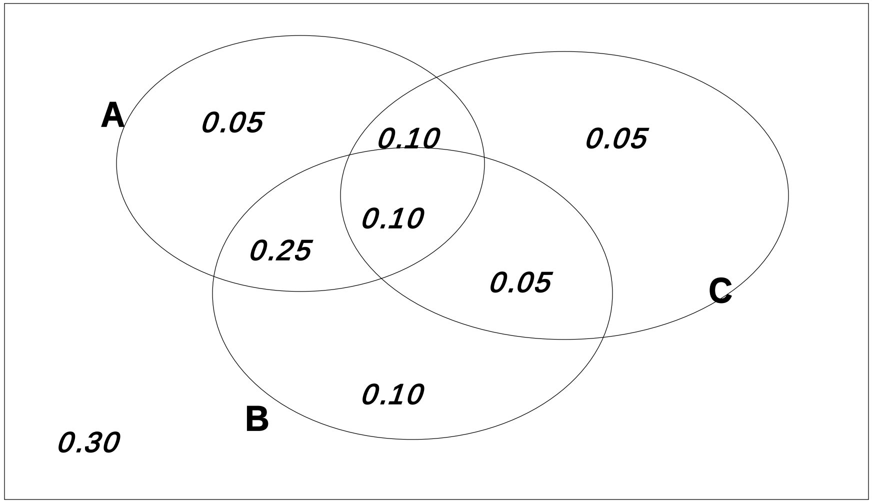
1. Make a table listing all value combinations of the variables (M Boolean variables $\Rightarrow 2^M$ rows).

2. For each value combination, say how probable it is.

3. Due to the axioms of probability, those numbers must sum to 1.

Example: Boolean variables A, B, C

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



Learning a joint distribution

Build a JD table in which the probabilities are unspecified

A	B	C	Prob
0	0	0	?
0	0	1	?
0	1	0	?
0	1	1	?
1	0	0	?
1	0	1	?
1	1	0	?
1	1	1	?

The fill in each row with

$$\hat{P}(\text{row}) = \frac{\text{examples matching row}}{\text{total number of examples}}$$

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	**0.25**
1	1	1	0.10

Fraction of all training examples in which A and B are True but C is False

Example of Learning a Joint

- This Joint was obtained by learning from three attributes in the UCI "Adult" Census Database [Kohavi 1995]

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

UCI machine learning repository: http://www.ics.uci.edu/~mlearn/MLRepository.html

A basic classifier

Given training data

- Learn $P(y)$
- Learn $P(\mathbf{x}|y=1), P(\mathbf{x}|y=2), \ldots, P(\mathbf{x}|y=k)$ each as a large joint distribution table
- Compute

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

- Predict with decision theory or use:

$$\arg\max_y P(y|\mathbf{x})$$

Joint distribution overfits

- Let $\mathbf{x}$ be a d-dim binary vector, and $y \in \{1,2,\ldots,k\}$
- Learning the joint distribution $\mathrm{P}(\mathbf{x}|y=i)$ for $i=1,\ldots,k$ involves estimating $k \times \left(2^d - 1\right)$ parameters
- For large d, this number is prohibitively large and we have not enough data to estimate them accurately
- A common situation: no training examples have the exact $\mathbf{x} = [u_1,\ldots,u_d]^T$ value combination
  - $P(\mathbf{x} = [u_1,\ldots,u_d]^T | y = i) = 0$ for all values of i
  - Overfitting

Naïve Bayes Assumption

- Assume $p(x_1, x_2, \ldots, x_d|y) = p(x_1|y)p(x_2|y)\ldots p(x_d|y)$

i.e., the features are independent from one another <u>given the class label</u>

- **Conditional independence:** x is **(conditionally) independent** of y given z, if

$$\forall\, i, j, k\; P(x = i|y = j, z = k) = P(x = i|z = k)$$

Or equivalently

$$\forall i, j, k\; P(x = i, y = j|z = k) = P(x = i|z = k)P(y = j|z = k)$$

Often denoted as

$$p(x|y, z) = p(x|z)$$

or $p(x, y|z) = p(x|z)p(y|z)$

Example

$$p(thunder|raining, lightening)$$
$$= p(thunder|lightening)$$

- Note that the events thunder and raining are not independent from one another
- However, once we observe lightening, they become independent
- They are conditionally independent given lightening

Conditional independence vs. independence

- Conditional independence (x and y are conditionally independent given z):

$$p(x, y|z) = p(x|z)p(y|z)$$

or equivalently: $p(x|y, z) = p(x|z)$

- Independence (x and y are independent):

$$p(x, y) = p(x)(y)$$

or equivalently: $p(x|y) = p(x)$

Conditional independence ≠ Independence

Conditional Independence

Independence

Thunder and rain given lightening

Thunder and rain?

Let A and B be two random variables representing rock paper scissor for two opponents, and C represents the outcome of the game

A and B given C ?

A and B

Naive Bayes Classifier

Given training data

- Learn $P(y = j)$ for $j = 1, \ldots, k$
- Learn $P(x_i | y = j)$ for $i = 1, \ldots, d$ and $j = 1, \ldots, k$
- Compute

$$P(y|\mathbf{x}) = \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})} = \frac{\prod_i P(x_i|y)P(y)}{\sum_j \left(\prod_i P(x_i|y=j)P(y=j)\right)}$$

- Predict with decision theory or use:

$$\arg\max_y P(y|\mathbf{x})$$

# of parameters? see concept warehouse question

Generative story for Bernoulli Naïve Bayes

Flip weighted coin

y	x_1	x_2	x_3	…	x_V
0	1	0	1	…	1
1	0	1	0	…	1
1	1	1	1	…	1
0	0	0	1	…	1
0	1	0	1	…	0
1	1	0	1	…	0

If head, flip each of V spam coins. One per word.

If head, flip each of V non-spam coins. One per word.

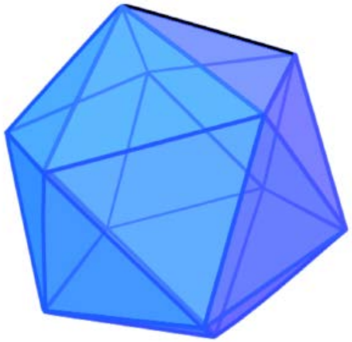
We do not really generate emails this way --- but this is what we assume to be the process how emails are generated

Generative story for Multi-nomial Naïve Bayes

Flip weighted coin

If head, roll the spam die M times and record the count for each of the V sides

y	x_1	x_2	x_3	…	x_V
0	2	0	7	…	1
1	0	1	0	…	5
1	10	1	0	…	1
0	0	0	15	…	3
0	11	0	0	…	0
1	7	0	1	…	0



If head, roll the non-spam die M times and record the count for each of the V sides

We do not really generate emails this way --- but this is what we assume to be the process how emails are generated

Multinomial model vs Bernoulli model

- The likelihood of observing one email E :

Bernoulli model:

$$x_i \in \{0,1\}$$

$$P(\mathbf{x}|y) = \prod_{i=1}^{V} P(x_i|y)$$

Single occurrence is equivalent to Multiple occurrences

Multinomial model:

$$x_i \in N_0$$

$$P(\mathbf{x}|y) = p(y) \prod_{i=1}^{V} P(w_i|y)^{x_i}$$

Multiple occurrences make a difference. Allow us to take counts into consideration

MLE for Naïve Bayes with Bernoulli Model

For Spam Filter

Given a set of N training emails, MLE of the parameters are:

$$P(y=1) = \frac{N_1}{N}, \text{ where } N_1 \text{ is the number of spam emails}$$

- For each feature i, learn a Bernoulli model for each class:

$$P(x_i = 1 \mid y=1) = \frac{N_{i|1}}{N_1},$$

# of spam emails the i-th word appeared

i.e., the fraction of spam emails where x_i appeared

$$P(x_i = 1 \mid y=0) = \frac{N_{i|0}}{N_0}$$

# of non-spam emails the i-th word appeared

i.e., the fraction of the nonspam emails where x_i appeared

Total number of parameters for k classes? $(k-1) + k * V$

MLE for Naïve Bayes with Multinomial model

- MLE estimate for the i-th word in the dictionary:

$$p(w_i|y) = \frac{\text{total \# of word } i \text{ in class } y \text{ emails}}{\text{total \# of words in class } y \text{ emails}}$$

- Total number of parameters?
  - $k(V-1) + (k-1)$

Discrete and Continuous Features

- Naïve Bayes can be easily extended to handle features that are not binary-valued
- Discrete: $x_i \in \{1,2,\dots,k_i\}$
  - $P(x_i = j|y)$ for $j \in \{1,2,\dots,k_i\}$ - categorical distribution in place of Bernoulli
- Continuous: $x_i \in R$
  - Learn a continuous distribution for each $p(x_i|y)$, e.g., Gaussian
  - Alternatively, we can discretize the feature, then build categorical distribution for each feature. When the feature does not follow Gaussian, this can result in a better classifier

Problem with MLE

- Suppose you picked up a new word “Mahalanobis” in your class and started using it in your email $\mathbf{x}$
- Because “Mahalanobis” (the $n+1$ th word in the vocabulary) has never appeared in the training emails
$$P(x_{n+1}=1|y=1)=P(x_{n+1}=1|y=0)=0$$
- Now $P(\mathbf{x}|y)=\prod_i P(x_i|y)=0$ for both $y=0$ and $y=1$
- Given limited training data, MLE can results in prob. of 0 or 1 which are “too strong” and cause problems
- To solve this problem, we can use Maximum A Posterior (MAP) estimate

Bayesian Parameter Estimation

- Parameters are random variables
- Prior distribution captures our prior believe about the parameter before seeing any data
- When the observed data is sparse, we fall back to the prior and avoid the issues faced by MLE

Example: Bernoulli

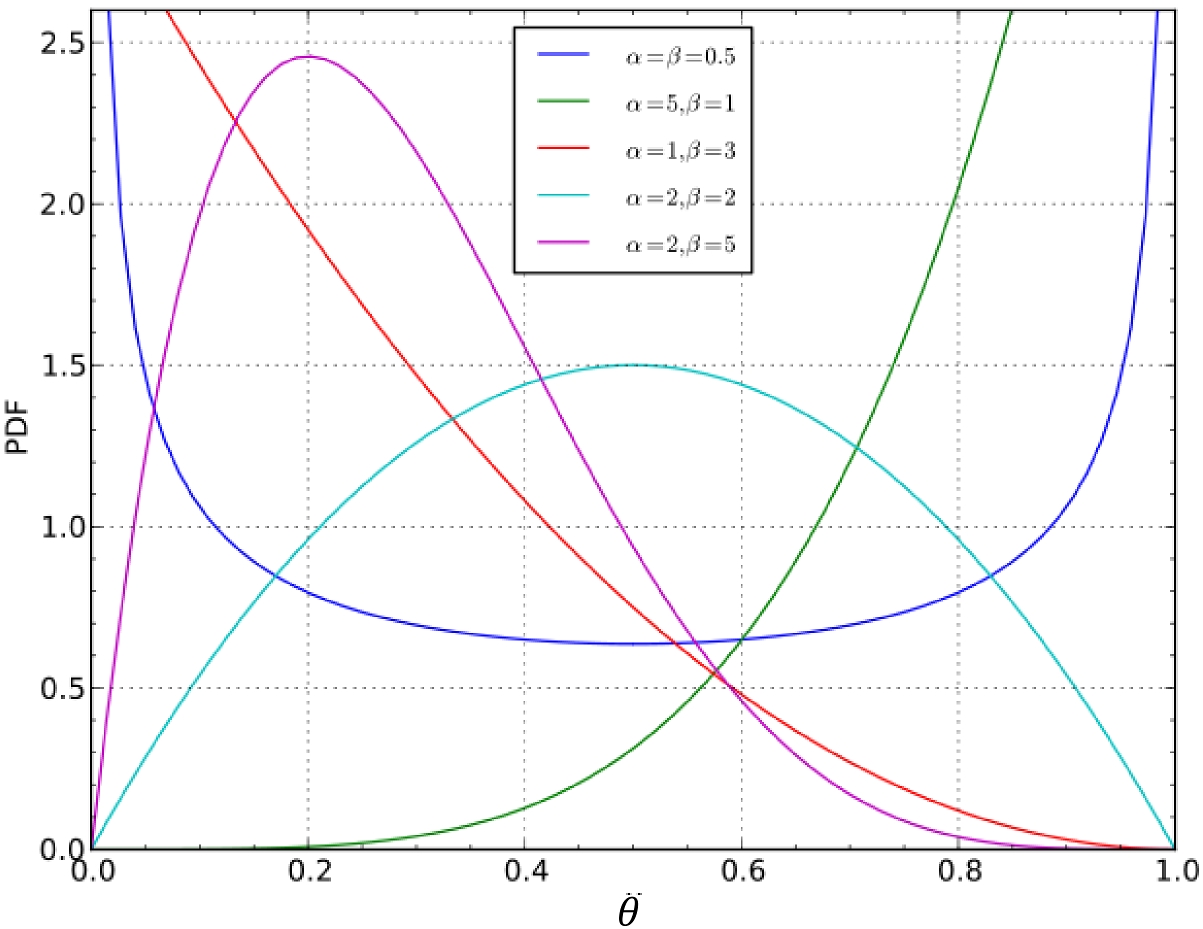
- Given a unfair coin, we want to estimate θ - the probability of head
- We toss the coin n times, and observe n_1 heads
- MLE estimate: $\theta = \frac{n_1}{n}$
- Now assume that θ is a random variable and has a prior
- For reasons that will become clear later, we assume the following prior for θ:

$$\theta \sim Beta(\alpha, \beta)$$

$$p(\theta; \alpha, \beta) = \frac{1}{B(\alpha, \beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1}$$

Beta distribution

$$p(\theta; \alpha, \beta) = \frac{1}{B(\alpha, \beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1}$$



- $\alpha = \beta = 1$: uniform
- $\alpha, \beta < 1$: U-shape
- $\alpha, \beta > 1$: uni-model
- $\alpha = \beta$: symmetric
- Mode ($\alpha, \beta > 1$): $\frac{\alpha - 1}{\alpha + \beta - 2}$

What parameter should you choose if you strongly believe your parameter is approximately 2/3?

Posterior distribution of θ

$$p(\theta|\mathrm{D}) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

$$p(\theta|\mathrm{D}) \propto p(D|\theta)p(\theta)$$

$$p(\theta|\mathrm{D}) \propto \theta^{n_1}(1-\theta)^{n_0}\frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$

$$p(\theta|\mathrm{D}) \propto \frac{1}{B(\alpha,\beta)}\theta^{n_1+\alpha-1}(1-\theta)^{n_0+\beta-1}$$

$$p(\theta|\mathrm{D}) = \frac{1}{B(n_1+\alpha, n_0+\beta)}\theta^{n_1+\alpha-1}(1-\theta)^{n_0+\beta-1}$$

Noting that the posterior has exactly the same form as the prior. This is not a coincidence, it is due to careful selection of the prior distribution – **conjugate prior**

Maximum *a-Posterior* (MAP)

- A full Bayesian treatment will not care about estimating the parameters

- Instead, it will use the posterior distribution to make predictions for the target variable by marginalizing θ

$$p(y|\mathbf{x}) = \int p(y|\mathbf{x}, \theta) p(\theta|D) d\theta$$

- This can be computationally expensive or intractable

- Frequently, we use Maximum A Posterior estimation:

$$\theta_{map} = \arg\max_{\theta} p(\theta|D)$$

MAP for Bernoulli

$$p(\theta|\mathrm{D}) = \frac{1}{B(n_1 + \alpha, n_0 + \beta)} \theta^{n_1 + \alpha - 1} (1 - \theta)^{n_0 + \beta - 1}$$

- Mode: the maximum point for $Beta(a, b)$ (for $a, b > 1$) is
$$\frac{a - 1}{a + b - 2}$$
- In this case $a = n_1 + \alpha, b = n_0 + \beta$, we have:
$$\theta_{MAP} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2}$$
- Let $\alpha = 2, \beta = 2$, we have $\theta_{MAP} = \frac{n_1 + 1}{n + 2}$
  - Comparing to MLE, it is like adding two fake coin tosses (one head, one tail) into the observed data – this is also called Laplace smoothing

MAP for Naïve Bayes Spam Filter

- When estimating $p(x_i|y=1)$ and $p(x_i|y=0)$
  - Bernoulli case:

$$P(x_i = 1 \mid y = 0) = \frac{N_{i|0}}{N_0} \qquad \text{MLE}$$

$$P(x_i = 1 \mid y = 0) = \frac{N_{i|0} + 1}{N_0 + 2}$$

MAP ($\alpha = \beta = 2$), or
Laplace smoothing

- When encounter a new word not appeared in training set, now the probabilities do not go to zero

MAP estimation for Multi-nomial

- The conjugate prior for multinomial is called Dirichlet distribution
- For K outcomes, a Dirichlet distribution has K parameters, each serves a similar purpose as Beta distribution's parameters
  - Acting as fake observation(s) for the corresponding output, the count depends on the value of the parameter
- Laplace smoothing for this case:

$$P(z=k)=\frac{n_k+1}{n+K}$$

Laplace Smoothing for Multi-nomial case

MLE: $$p(w_i|y=1) = \frac{\text{total \# of word } i \text{ in spam emails}}{\text{total \# of words in spam emails}}$$

With Laplace smoothing:

$$p(w_i|y=1) = \frac{\text{total \# of word } i \text{ in spam emails} + 1}{\text{total \# of words in spam emails} + v}$$

where V is the size of the dictionary

Summary

- Generative classifier
  - learn P($\mathbf{x}|y$) and P(y)
  - Use Bayes rule to compute P($y|\mathbf{x}$) for classification
  - Predict with $\arg\max_y P(y|\mathbf{x})$ or use decision thoery
- Naïve Bayes assumes conditional independence between features <u>given class labels</u>
  - Greatly reduces the numbers of parameters to learn
- Bernoulli and Muti-nomial Naïve Bayes for text classification
- MAP estimation (or smoothing) is necessary to avoid overfitting and extreme probability values