A Probabilistic View of Machine Learning, Naïve Bayes

CMSC 422

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Slides adapted from MARINE CARPUAT

Today's topics

- Bayes rule review
- A probabilistic view of machine learning
  - Joint Distributions
  - Bayes optimal classifier
- Statistical Estimation
  - Maximum likelihood estimates
  - Derive relative frequency as the solution to a constrained optimization problem

Bayes Rule

$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)}$$ Bayes' rule

we call P(A) the "prior"

and P(A|B) the "posterior"

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London,* **53:370-418**

…by no means merely a curious speculation in the doctrine of chances, but necessary to be solved in order to a sure foundation for all our reasonings concerning past facts, and what is likely to be hereafter…. necessary to be considered by any that would give a clear account of the strength of *analogical* or *inductive reasoning…*

Exercise: Applying Bayes Rule

- Consider the 2 random variables

  A = You have covid

  B = You just coughed

- Assume

  $P(A) = 0.05$

  $P(B|A) = 0.8$

  $P(B|\text{not } A) = 0.2$

- What is $P(A|B)$?

Using a Joint Distribution

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

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- Given the joint distribution, we can find the probability of any logical expression E involving these variables

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

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Given the joint distribution, we can make inferences

- E.g., P(Male|Poor)?
- Or P(Wealth | Gender, Hours)?

Recall: Machine Learning as Function Approximation

Problem setting

- Set of possible instances X
- Unknown target function $f: X \rightarrow Y$
- Set of function hypotheses $H = \{h \mid h: X \rightarrow Y\}$

Input

- Training examples $\{(x^{(1)}, y^{(1)}), \ldots (x^{(N)}, y^{(N)})\}$ of unknown target function f

Output

- Hypothesis $h \in H$ that best approximates target function f

Recall: Formal Definition of Binary Classification (from CIML)

TASK: BINARY CLASSIFICATION

Given:

1. An input space $\mathcal{X}$
2. An unknown distribution $\mathcal{D}$ over $\mathcal{X} \times \{-1, +1\}$

Compute: A function f minimizing: $\mathbb{E}_{(x,y)\sim\mathcal{D}}\left[f(\boldsymbol{x}) \neq y\right]$

The Bayes Optimal Classifier

- Assume we know the data generating distribution $\mathcal{D}$
- We define the **Bayes Optimal classifier** as

$$f^{(\mathrm{BO})}(\hat{x}) = \arg\max \mathcal{D}(\hat{x}, \hat{y})$$

- **Th**
  cl
- **B**
  –
  – Best error rate we can ever hope to achieve under zero/one loss

If we had access to $\mathcal{D}$,
Finding an optimal classifier would be trivial!

we don't have access to $\mathcal{D}$
So let's try to estimate it instead!

What does “training” mean in probabilistic settings?

- Training = estimating $\mathcal{D}$ from a finite training set
  - We typically assume that $\mathcal{D}$ comes from a specific family of probability distributions

    e.g., Bernouilli, Gaussian, etc
  - Learning means inferring parameters of that distributions

    e.g., mean and covariance of the Gaussian

Training assumption: training examples are iid

- **Independently and Identically distributed**
  - i.e. as we draw a sequence of examples from $\mathcal{D}$, the n-th draw is independent from the previous n-1 sample
- This assumption is usually false!
  - But sufficiently close to true to be useful

How can we estimate the joint probability distribution from data?

What are the challenges?

Maximum Likelihood Estimation

- Find the parameters that maximize the probability of the data

- Example: how to model a biased coin?

Maximum Likelihood Estimates

X=1 X=0

P(X=1) = θ

P(X=0) = 1-θ

(Bernoulli)

Each coin flip yields a Boolean value for X

X ~ Bernouilli: $P(X) = \theta^{X}(1 - \theta)^{X}$

Given a data set D of iid flips, which contains α_1 ones and α_0 zeros

$$P_\theta(D) = \theta^{\alpha_1}(1 - \theta)^{\alpha_0}$$

$$\hat{\theta}_{MLE} = argmax_\theta \; P_\theta(D) = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

Let's learn a classifier by learning P(Y|X)

- Goal: learn a classifier P(Y|X)

- Prediction:
  - Given an example x
  - Predict $\hat{y} = argmax_y \, P(Y = y \,|X = x)$

Parameters for P(X,Y) vs. P(Y|X)

Y = Wealth
X = <Gender, Hours_worked>

Joint probability distribution P(X,Y)

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
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Conditional probability distribution P(Y|X)

Gender	HrsWorked	P(rich | G,HW)	P(poor | G,HW)
F	<40.5	.09	.91
F	>40.5	.21	.79
M	<40.5	.23	.77
M	>40.5	.38	.62

How many parameters do we need to learn?

Suppose $X = < X_1, X_2, \ldots X_d >$
where X_i and Y are Boolean random variables

Q: How many parameters do we need to estimate $P(Y|X_1, X_2, \ldots X_d)$?

A: Too many to estimate P(Y|X) directly from data!

Naïve Bayes Assumption

Naïve Bayes assumes

$$P(X_1, X_2, \dots X_d | Y) = \prod_{i=1}^{d} P(X_i | Y)$$

i.e., that X_i and X_j are **conditionally independent** given Y, for all $i \neq j$

Conditional Independence

- Definition:
  X is conditionally independent of Y given Z
  if **P(X|Y,Z) = P(X|Z)**

- Recall that X is independent of Y if P(X|Y)=P(Y)

Naïve Bayes classifier

$$\hat{y} = argmax_y \, P(Y = y \,|X = x)$$

$$= argmax_y P(Y = y)P(X = x \,|Y = y)$$

$$= argmax_y P(Y = y) \prod_{i=1}^{d} P(X_i = x_i \,|Y = y)$$

Bayes rule

+ Conditional independence assumption

How many parameters do we need to learn?

- To describe P(Y)?

- To describe $P(X = < X_1, X_2, \ldots X_d > | Y)$
  - Without conditional independence assumption?

  - With conditional independence assumption?

(Suppose all random variables are Boolean)

Training a Naïve Bayes classifier

Let's assume discrete Xi and Y 

TrainNaïveBayes (Data)

for each value y_k of Y

estimate $\pi_k = P(Y = y_k)$

$$\frac{\#\ examples\ for\ which\ Y = y_k}{\#\ examples}$$

for each value x_{ij} of X_i

estimate $\theta_{ijk} = P(X_i = x_{ij} | Y = y_k)$

$$\frac{\#\ examples\ for\ which\ X_i = x_{ij}\ and\ Y = y_k}{\#\ examples\ for\ which\ Y = y_k}$$

Naïve Bayes Wrap-up

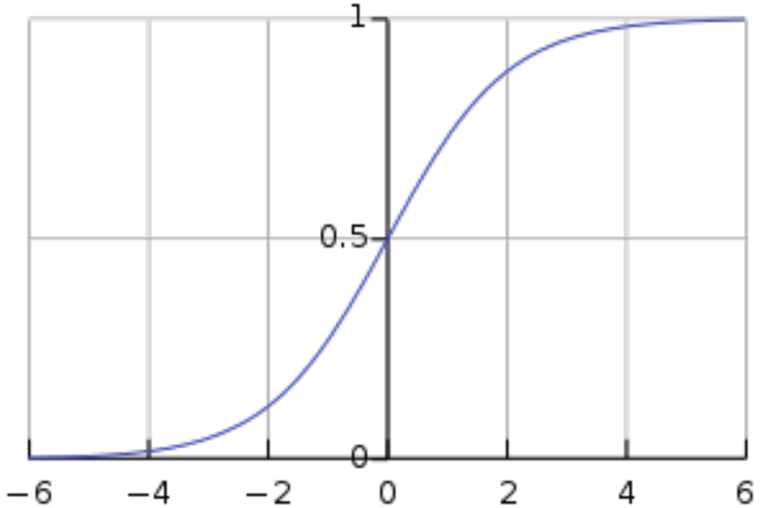
- An easy to implement classifier, that performs well in practice
- Subtleties
  - Often the Xi are not really conditionally independent
  - What if the Maximum Likelihood estimate for P(Xi|Y) is zero?

Logistic Regression

- Binary classification

$$P(Y^{(i)} = 1 | X^{(i)}, \theta) = g(< \theta, X^{(i)} >)$$

$$P(Y^{(i)} = 0 | X^{(i)}, \theta) = 1 - g(< \theta, X^{(i)} >)$$



Sigmoid function

$$g(z) = \frac{1}{1 + \exp(-z)}$$

Logistic Regression

- Maximum Likelihood

$$\max_{\theta} \quad \prod_{i=1}^{N} P(Y^{(i)} | X^{(i)}, \theta)$$

$$\max_{\theta} \quad \prod_{i=1}^{N} g(< \theta, X^{(i)} >)^{Y^{(i)}} (1 - g(< \theta, X^{(i)} >))^{1 - Y^{(i)}}$$

$$\max_{\theta} \quad \sum_{i=1}^{N} \underbrace{Y^{(i)} \log g(< \theta, X^{(i)} >) + (1 - Y^{(i)}) \log(1 - g(< \theta, X^{(i)} >))}$$

Cross-entropy loss function

How to solve it?

- Gradient Descent

- A good property of sigmoid:

$$\nabla_z g(z) = g(z)(1 - g(z))$$

- SGD: $\theta_{k+1} = \theta_k + \eta(Y^i - g(< \theta, X^i >))X^{(i)}$

- Why? Intuition behind the updates