Machine Learning 10-601

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

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Today:
- MLE and MAP
- Bayes Classifiers
- Naïve Bayes

Readings:
Mitchell:
"Naïve Bayes and Logistic Regression"
(available on class website)

Summary: Maximum Likelihood Estimate

- Data:
  - We observed N ***iid*** coin tossing: D={1, 0, 1, …, 0}
- Representation:

  Binary r.v: $x_n = \{0,1\}$

- Model:

Bernoulli distribution

$$P(x) = \begin{cases} 1-\theta & \text{for } x = 0 \\ \theta & \text{for } x = 1 \end{cases} \quad \Rightarrow \quad P(x) = \theta^x (1-\theta)^{1-x}$$

- The likelihood of dataset $D=\{x_1, \ldots, x_N\}$:

$$P(x_1, x_2, \ldots, x_N \mid \theta) = \prod_{i=1}^{N} P(x_i \mid \theta) = \prod_{i=1}^{N} \left(\theta^{x_i}(1-\theta)^{1-x_i}\right) = \theta^{\sum_{i=1}^{N} x_i} (1-\theta)^{\sum_{i=1}^{N} 1-x_i} = \theta^{\#\text{head}} (1-\theta)^{\#\text{tails}}$$

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$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(x_1, x_2 \ldots x_n | \theta) = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

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what does all this have to do with function approximation?

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

Consider Y=Wealth, X=<Gender, HoursWorked>

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

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 must we estimate?

Gender	HrsWorked	P(rich | G,HW)	P(poor | G,HW)
F	<40.5	.09	.91
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Suppose X =<X_1,… X_n>
where X_i and Y are boolean RV's

To estimate P(Y| X_1, X_2, … X_n)

If we have 30 X_i's instead of 2?

Bayes Rule

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

Which is shorthand for:

$$(\forall i,j) P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{P(X = x_j)}$$

Equivalently:

$$(\forall i,j) P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{\sum_k P(X = x_j | Y = y_k) P(Y = y_k)}$$

Can we reduce params using Bayes Rule?

Suppose X =<X_1,… X_n>
where X_i and Y are boolean RV's

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

How many parameters to define P(X_1,… X_n | Y)?

How many parameters to define P(Y)?

Naïve Bayes

Naïve Bayes assumes

$$P(X_1 \ldots X_n|Y) = \prod_i P(X_i|Y)$$

i.e., that X_i and X_j are conditionally independent given Y, for all i≠j

Conditional Independence

Definition: X is conditionally independent of Y given Z, if the probability of X is independent of the value of Y, given the value of Z

$$(\forall i, j, k) P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k)$$

Which we often write

$$P(X|Y, Z) = P(X|Z)$$

E.g.,

$$P(Thunder|Rain, Lightning) = P(Thunder|Lightning)$$

Naïve Bayes uses assumption that the X_i are conditionally independent, given Y

Given this assumption, then:

$$P(X_1, X_2|Y) = P(X_1|X_2, Y)P(X_2|Y)$$
$$= P(X_1|Y)P(X_2|Y)$$

in general: $P(X_1 ... X_n|Y) = \prod_i P(X_i|Y)$

How many parameters to describe $P(X_1 ... X_n|Y)$? $P(Y)$?

- Without conditional indep assumption?
- With conditional indep assumption?

Naïve Bayes in a Nutshell

Bayes rule:

$$P(Y = y_k|X_1 \dots X_n) = \frac{P(Y = y_k)P(X_1 \dots X_n|Y = y_k)}{\sum_j P(Y = y_j)P(X_1 \dots X_n|Y = y_j)}$$

Assuming conditional independence among X_i's:

$$P(Y = y_k|X_1 \dots X_n) = \frac{P(Y = y_k) \prod_i P(X_i|Y = y_k)}{\sum_j P(Y = y_j) \prod_i P(X_i|Y = y_j)}$$

So, classification rule for $X^{new} = \langle X_1, \dots, X_n \rangle$ is:

$$Y^{new} \leftarrow \arg\max_{y_k} \; P(Y = y_k) \prod_i P(X_i^{new}|Y = y_k)$$

Naïve Bayes Algorithm – discrete X_i

- Train Naïve Bayes (examples)
  for each* value y_k
  estimate $\pi_k \equiv P(Y = y_k)$
  for each* value x_{ij} of each attribute X_i
  estimate $\theta_{ijk} \equiv P(X_i = x_{ij} | Y = y_k)$

- Classify (X^{new})

$$Y^{new} \leftarrow \arg\max_{y_k} \; P(Y = y_k) \prod_i P(X_i^{new} | Y = y_k)$$

$$Y^{new} \leftarrow \arg\max_{y_k} \; \pi_k \prod_i \theta_{ijk}$$

* probabilities must sum to 1, so need estimate only n-1 of these...

Estimating Parameters: Y, X_i discrete-valued

Maximum likelihood estimates (MLE's):

$$\widehat{\pi}_k = \widehat{P}(Y = y_k) = \frac{\#D\{Y = y_k\}}{|D|}$$

$$\widehat{\theta}_{ijk} = \widehat{P}(X_i = x_{ij} | Y = y_k) = \frac{\#D\{X_i = x_{ij} \wedge Y = y_k\}}{\#D\{Y = y_k\}}$$

Number of items in dataset D for which $Y=y_k$

Example: Live in Sq Hill? P(S|G,D,E)

- S=1 iff live in Squirrel Hill
- G=1 iff shop at SH Giant Eagle
- D=1 iff Drive to CMU
- E=1 iff even # of letters in last name

What probability parameters must we estimate?

Example: Live in Sq Hill? P(S|G,D,E)

- S=1 iff live in Squirrel Hill
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P(S=1) :	P(S=0) :
P(D=1 | S=1) :	P(D=0 | S=1) :
P(D=1 | S=0) :	P(D=0 | S=0) :
P(G=1 | S=1) :	P(G=0 | S=1) :
P(G=1 | S=0) :	P(G=0 | S=0) :
P(E=1 | S=1) :	P(E=0 | S=1) :
P(E=1 | S=0) :	P(E=0 | S=0) :

Naïve Bayes: Subtlety #1

Often the X_i are not really conditionally independent

- We use Naïve Bayes in many cases anyway, and it often works pretty well
  - often the right classification, even when not the right probability (see [Domingos&Pazzani, 1996])
- What is effect on estimated P(Y|X)?
  - Special case: what if we add two copies: $X_i = X_k$

Naïve Bayes: Subtlety #2

If unlucky, our MLE estimate for $P(X_i \mid Y)$ might be zero. (e.g., X_i = Birthday_Is_February_29)

- Why worry about just one parameter out of many?

- What can be done to avoid this?

Estimating Parameters

- Maximum Likelihood Estimate (MLE): choose θ that maximizes probability of observed data $\mathcal{D}$

$$\widehat{\theta} = \arg\max_{\theta} \; P(\mathcal{D} \mid \theta)$$

- Maximum a Posteriori (MAP) estimate: choose θ that is most probable given prior probability and the data

$$\widehat{\theta} = \arg\max_{\theta} \; P(\theta \mid \mathcal{D})$$

$$= \arg\max_{\theta} \; = \frac{P(\mathcal{D} \mid \theta) P(\theta)}{P(\mathcal{D})}$$

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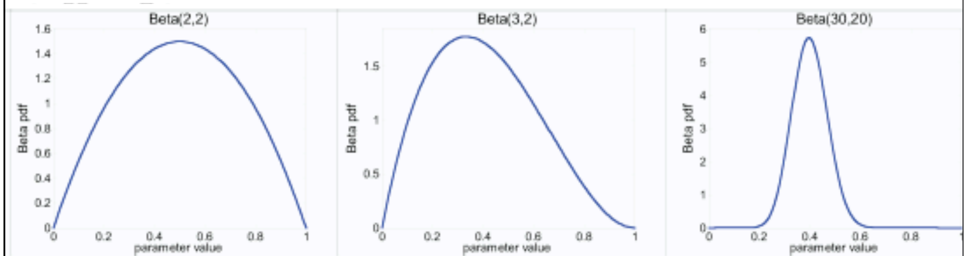
$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(x_1, x_2 \ldots x_n | \theta) = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

Beta prior distribution – P(θ)

- $$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$



[C. Guestrin]

Beta prior distribution – P(θ)

- $$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$

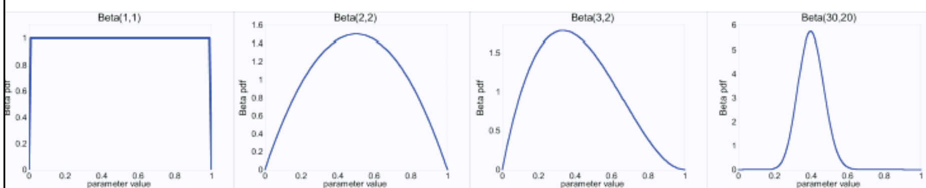
- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

[C. Guestrin]

Posterior distribution

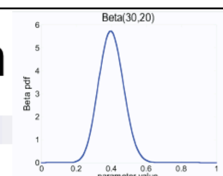
- Prior: $Beta(\beta_H, \beta_T)$
- Data: α_H heads and α_T tails
- Posterior distribution:

$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



[C. Guestrin]

MAP for Beta distribution



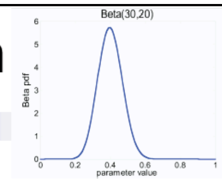
$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H, \beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H, \beta_T+\alpha_T)$$

- MAP: use most likely parameter:

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D}) =$$

[C. Guestrin]

MAP for Beta distribution



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- MAP: use most likely parameter:

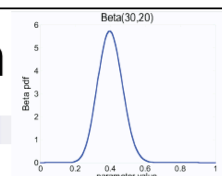
$$\hat{\theta}_{MAP} = \arg\max_\theta P(\theta|D) = \frac{\beta_H+\alpha_H-1}{(\beta_H+\alpha_H-1)+(\beta_H+\alpha_T-1)}$$

versus

$$\hat{\theta}_{MLE} = \arg\max_\theta P(D|\theta) = \frac{\alpha_H}{\alpha_H+\alpha_T}$$

[C. Guestrin]

MAP for Beta distribution



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versus

$$\hat{\theta}_{MLE} = \arg\max_\theta P(D|\theta) = \frac{\alpha_H}{\alpha_H+\alpha_T}$$

- Beta prior equivalent to extra thumbtack flips
- As $N \rightarrow \infty$, prior is "forgotten"
- **But, for small sample size, prior is important!**

[C. Guestrin]

Conjugate priors

- P(θ) and P(θ|D) have the same form

Eg. 1 Coin flip problem

Likelihood is ~ Binomial

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

If prior is Beta distribution,

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$

Then posterior is Beta distribution

$$P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

For Binomial, conjugate prior is Beta distribution.

[A. Singh]

Conjugate priors

- P(θ) and P(θ|D) have the same form

Eg. 2 Dice roll problem (6 outcomes instead of 2)

Likelihood is ~ Multinomial($\theta = \{\theta_1, \theta_2, \ldots, \theta_k\}$)

$$P(\mathcal{D} \mid \theta) = \theta_1^{\alpha_1}\theta_2^{\alpha_2}\ldots\theta_k^{\alpha_k}$$

If prior is Dirichlet distribution,

$$P(\theta) = \frac{\prod_{i=1}^{k}\theta_i^{\beta_i - 1}}{B(\beta_1, \ldots, \beta_k)} \sim \text{Dirichlet}(\beta_1, \ldots, \beta_k)$$

Then posterior is Dirichlet distribution

$$P(\theta|D) \sim \text{Dirichlet}(\beta_1 + \alpha_1, \ldots, \beta_k + \alpha_k)$$

For Multinomial, conjugate prior is Dirichlet distribution.

[A. Singh]

Dirichlet distribution

- number of heads in N flips of a two-sided coin
  - follows a binomial distribution
  - Beta is a good prior (conjugate prior for binomial)

- what if it's not two-sided, but k-sided?
  - follows a *multinomial* distribution
  - *Dirichlet* distribution is the conjugate prior

$$P(\theta_1, \theta_2, \ldots \theta_K) = \frac{1}{B(\alpha)} \prod_i^K \theta_i^{(\alpha_1 - 1)}$$

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Probability & Stats: You should know

- Probability basics
  - random variables, events, sample space, conditional probs, …
  - independence of random variables
  - Bayes rule
  - Joint probability distributions
  - calculating probabilities from the joint distribution
- Estimating parameters from data
  - maximum likelihood estimates (MLE)
  - maximum a posteriori estimates (MAP)
  - distributions – binomial, Beta, Dirichlet, …
  - conjugate priors

Naïve Bayes Classifier: What you should know:

- Training and using classifiers based on Bayes rule
- Conditional independence
  - What it is
  - Why it's important
- Naïve Bayes
  - What it is
  - Why we use it so much
  - Training using MLE, MAP estimates
  - Next: Discrete variables and continuous (Gaussian)

Questions to consider:

- What error will the classifier achieve if Naïve Bayes assumption is satisfied and we have infinite training data?
- Can you use Naïve Bayes for a combination of discrete and real-valued X_i?
- How can we extend Naïve Bayes if just 2 of the n X_i are <u>dependent</u>?
- What does the decision surface of a Naïve Bayes classifier look like?