CS 188: Artificial Intelligence Machine Learning: Naïve Bayes



University of California, Berkeley

[These slides were created by Dan Klein and Pieter Abbeel, Anca Dragan, Sergey Levine, with some materials from A. Farhadi. All CS188 materials are at http://ai.berkeley.edu.]

Machine Learning

- Up until now: how use a model to make optimal decisions
- Machine learning: how to acquire a model from data / experience
 - Learning parameters (e.g. probabilities)
 - Learning structure (e.g. BN graphs)
 - Learning features or hidden concepts (e.g. neural nets, clustering)
- What's our roadmap?

Our Machine Learning Roadmap

Define the problem

- Type of problem, domain (i.e. spam filtering, digit recognition)
- Look at several learning approaches / models
 - Naïve Bayes (today), Perceptrons, Logistic Regression, Neural Networks (next week)
- How to find model parameters: Maximum Likelihood
 - Special cases: solve analytically (today)
 - In general: numerical optimization (next week)

Themes throughout

- Working with data
- Preventing overfitting
- Evaluating performance

Multiple Types of Learning Problems

- Supervised learning: correct answers for each training example
 - Classification: learning predictor with *discrete* outputs
 - Regression: learning predictor with *real-valued* outputs

Reinforcement learning: reward function, no correct answers

 Unsupervised learning: no correct answers, just find good representations / features of the data

Classification



Classification and Machine Learning

- Dataset: each data point, x, is associated with some label (aka class), y
- Goal of classification: given inputs x, write an algorithm to predict labels y
- Workflow of classification process:
 - Input is provided to you
 - Extract features from the input: attributes of the input that characterize each x and hopefully help with classification
 - Run some machine learning algorithm on the features: today, *Naïve Bayes*
 - Output a predicted label y



Training and Machine Learning

- Big idea: ML algorithms learn patterns between features and labels from *data*
 - You don't have to reason about the data yourself
 - You're given training data: lots of example datapoints and their actual labels





Training: Learn patterns from labeled data, and periodically test how well you're doing

Eventually, use your algorithm to predict labels for unlabeled data

Example: Spam Filter

- Input: an email
- Output: spam/ham
- Setup:

...

- Get a large collection of example emails, each labeled "spam" or "ham"
- Note: someone has to hand label all this data!
- Want to learn to predict labels of new, future emails
- Features: The attributes used to make the ham / spam decision
 - Words: FREE!
 - Text Patterns: \$dd, CAPS
 - Non-text: SenderInContacts, WidelyBroadcast



First, I must solicit your confidence in this transaction, this is by virture of its nature as being utterly confidencial and top secret. ...

TO BE REMOVED FROM FUTURE MAILINGS, SIMPLY REPLY TO THIS MESSAGE AND PUT "REMOVE" IN THE SUBJECT.

99 MILLION EMAIL ADDRESSES FOR ONLY \$99

Ok, Iknow this is blatantly OT but I'm beginning to go insane. Had an old Dell Dimension XPS sitting in the corner and decided to put it to use, I know it was working pre being stuck in the corner, but when I plugged it in, hit the power nothing happened.

Example: Digit Recognition

- Input: images / pixel grids
- Output: a digit 0-9



0

1

2

1

??

Setup:

...

- Get a large collection of example images, each labeled with a digit
- Note: someone has to hand label all this data!
- Want to learn to predict labels of new, future digit images
- Features: The attributes used to make the digit decision
 - Pixels: (6,8)=ON
 - Shape Patterns: NumComponents, AspectRatio, NumLoops

Other Classification Tasks

- Classification: given inputs x, predict labels (classes) y
- Examples:
 - Object recognition
 - Input: images; classes: object type
 - Medical diagnosis input: symptoms; classes: diseases
 - Automatic essay grading input: document; classes: grades
 - Fraud detection input: account activity; classes: fraud / no fraud
 - Customer service email routing
 - ... many more



Classification is an important commercial technology!

Model-Based Classification



Model-Based Classification

- Model-based approach
 - Build a model (e.g. Bayes' net) where both the label and features are random variables
 - Instantiate any observed features
 - Query for the distribution of the label conditioned on the features
- Challenges
 - What structure should the BN have?
 - How should we learn its parameters?



Naïve Bayes Model

- Naïve Bayes: Assume all features are independent effects of the label
- Random variables in this Bayes' net:
 - Y = The label
 - $F_1, F_2, ..., F_n$ = The n features
- Probability tables in this Bayes' net:
 - P(Y) = Probability of each label, given no information about the features.
 - Sometimes called the *prior*.
 - $P(F_i|Y)$ = One table per feature. Probability of feature, given the label.



Naïve Bayes for Digits

- Simple digit recognition version:
 - One feature (variable) F_{ij} for each grid position <i,j>
 - Feature values are on / off, based on whether intensity is more or less than 0.5 in underlying image
 - Each input maps to a feature vector, e.g.

- Here: lots of features, each is binary valued
- What are the parameters of this model?





Naïve Bayes for Digits: Parameters



Naïve Bayes for Text

how many features are there?

how many values?

- Bag-of-words Naïve Bayes:
 - Features: W_i is the word at positon i
 - As before: predict label conditioned on feature variables (spam vs. ham)
 - As before: assume features are conditionally independent given label
 - New: each W_i is identically distributed, so P(W₁|Y) = P(W₂|Y) = ...
- "Tied" distributions and bag-of-words
 - Usually, each variable gets its own conditional probability distribution P(F|Y)
 - In a bag-of-words model
 - Each position is identically distributed
 - All positions share the same conditional probs P(W|Y)
 - Why make this assumption?
 - Called "bag-of-words" because model is insensitive to word order or reordering

free our offer try please

please try our free offer



Naïve Bayes for Text: Parameters

• What are the parameters?

P(Y)			
ham :	0.66		
spam:	0.33		

 $D(T_{7})$

P(W|spam)

the	:	0.0156
to	:	0.0153
and	:	0.0115
of	:	0.0095
you	:	0.0093
а	:	0.0086
with	1:	0.0080
from	1:	0.0075
•••		

P(W|ham)

the :	0.0210
to :	0.0133
of :	0.0119
2002:	0.0110
with:	0.0108
from:	0.0107
and :	0.0105
a :	0.0100
•••	

Naïve Bayes Model

In general, the joint probability in Naïve Bayes model is:

|Y| parameters

$$P(\mathbf{Y}, \mathbf{F}_{1} \dots \mathbf{F}_{n}) = P(\mathbf{Y}) \prod_{i} P(\mathbf{F}_{i} | \mathbf{Y})$$

$$|\mathbf{Y}| \ge |\mathbf{F}|^{n} \text{ values} \qquad n \ge |\mathbf{F}| \ge |\mathbf{Y}|$$
parameters



- We only have to specify how each feature depends on the class
- Total number of parameters is *linear* in n
- Model is very simplistic, but often works anyway

Inference for Naïve Bayes

- Goal: compute posterior distribution over label variable Y
 - Step 1: get joint probability of label and evidence for each label

$$P(Y, f_1 \dots f_n) = \begin{bmatrix} P(y_1, f_1 \dots f_n) \\ P(y_2, f_1 \dots f_n) \\ \vdots \\ P(y_k, f_1 \dots f_n) \end{bmatrix} \longrightarrow \begin{bmatrix} P(y_1) \prod_i P(f_i | y_1) \\ P(y_2) \prod_i P(f_i | y_2) \\ \vdots \\ P(y_k) \prod_i P(f_i | y_k) \end{bmatrix} \end{pmatrix}$$

$$P(f_1 \dots f_n) + Step 2 \qquad P(Y | f_1 \dots f_n)$$

Example: Spam Filtering

- Model: $P(Y, W_1 \dots W_n) = P(Y) \prod_i P(W_i | Y)$
- Parameters:

P(Y)			
	ham	:	0.66
	spam	:	0.33

P(W|spam)

the :	•	0.0156
to	•	0.0153
and a	:	0.0115
of :	:	0.0095
you :		0.0093
a	:	0.0086
with		0.0080
from	:	0.0075
•••		

P(W|ham)

the :	0.0210
to :	0.0133
of :	0.0119
2002:	0.0110
with:	0.0108
from:	0.0107
and :	0.0105
a :	0.0100
•••	

Example: Spam Filtering

	Word	P(w spam)	P(w ham)	Tot Spam	Tot Ham
P(Y)	(prior)	0.33333	0.66666	-1.1	-0.4
$P(W_1 Y)$					
$P(W_2 Y)$					
:					
:					
-					

General Naïve Bayes

What do we need in order to use Naïve Bayes?

- Inference method (we just saw this part)
 - Start with a bunch of probabilities: P(Y) and the P(F_i|Y) tables
 - Use standard inference to compute P(Y|F₁...F_n)
 - Nothing new here
- Estimates of local conditional probability tables
 - P(Y), the prior over labels
 - P(F_i|Y) for each feature (evidence variable)
 - These probabilities are collectively called the *parameters* of the model and denoted by *\theta*
 - Up until now, we assumed these appeared by magic, but they typically come from training data counts

Parameter Estimation



Parameter Estimation

- Estimating the distribution of a random variable
- Elicitation: ask a human (why is this hard?)
- Empirically: use training data (learning!)
 - Example: The parameter θ is the true fraction of red beans in the jar.
 You don't know θ but would like to estimate it.
 - Collecting training data: You randomly pull out 3 beans:



- Estimating θ using counts, you guess 2/3 of beans in the jar are red.
- Can we mathematically show that using counts is the "right" way to estimate θ?



- θ is the true fraction of red beans in the jar (i.e. P(red | θ) = θ)
- Can we mathematically show that using counts is the "right" way to estimate θ?
- Maximum likelihood estimation: Choose the θ value that maximizes the probability of the observation
 - In other words, choose the θ value that maximizes P(observation | θ)
 - For our problem:

```
P(observation \mid \theta)
```

= P(randomly selected 2 red and 1 blue | θ of beans are red)

```
= P(red | \theta) * P(red | \theta) * P(blue | \theta)
```

```
= \theta^2 (1 - \theta)
```

• We want to compute:

```
\operatorname{argmax}_{\theta} \theta^2 (1 - \theta)
```

• We want to compute:



- Set derivative to 0, and solve!
 - Common issue: The likelihood (expression we're maxing) is the product of a lot of probabilities. This can lead to complicated derivatives.
 - Solution: Maximize the log-likelihood instead. Useful fact:

```
\underset{\theta}{\operatorname{argmax}} f(\theta) = \underset{\theta}{\operatorname{argmax}} \ln f(\theta)
```

 $\operatorname*{argmax}_{\theta} \theta^2 (1-\theta)$ $= \operatorname{argmax}_{\theta} \ln \left(\theta^2 (1 - \theta) \right)$ $\frac{d}{d\theta}\ln\left(\theta^2(1-\theta)\right) = 0$ $\frac{d}{d\theta} \left[\ln(\theta^2) + \ln(1-\theta) \right] = 0$ $\frac{d}{d\theta}2\ln(\theta) + \frac{d}{d\theta}\ln(1-\theta) = 0$ $\frac{2}{\theta} - \frac{1}{1-\theta} = 0$ $\theta = \frac{2}{3}$

Find θ that maximizes likelihood

Find θ that maximizes log-likelihood (will be the same θ)

Set derivative to 0

Logarithm rule: products become sums

 $\frac{d}{d\theta} \left[2\ln(\theta) + \ln(1-\theta)\right] = 0$ Logarithm rule: exponentiation becomes multiplication

Now we can derive each term of the original product separately

Reminder: Derivative of $ln(\theta)$ is $1/\theta$

Use algebra to solve for θ . If we used arbitrary red and blue counts r and b instead of r=2 and b=1, we'd get θ = r / (r+b), the count estimate.

Parameter Estimation with Maximum Likelihood (General Case)

• Model:
$$\begin{array}{c|c} X & \text{red} & \text{blue} \\ P(X|\theta) & \theta & 1-\theta \end{array}$$

- Data: draw N balls, N_r come up red and N_b come up blue
 - Dataset $D = \{x_1, \dots, x_N\}$ of N ball draws

$$P(D|\theta) = \prod_{i} P(x_i|\theta) = \theta^{N_r} \cdot (1-\theta)^{N_b}$$



• Maximum Likelihood Estimation: find θ that maximizes $P(D|\theta)$:

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} P(D|\theta) = \underset{\theta}{\operatorname{argmax}} \log P(D|\theta) \leftarrow N_r \log(\theta) + N_b \log(1-\theta)$$

Take derivative and set to 0:

$$\frac{\partial \log P(D|\theta)}{\partial \theta} = \frac{N_r}{\theta} - \frac{N_b}{1-\theta} = 0 \qquad \qquad \rightarrow \hat{\theta} = \frac{N_r}{N_r + N_b} = \frac{\text{\# of red balls}}{\text{total \# of balls}}$$

Parameter Estimation with Maximum Likelihood (General Case)

• Maximum Likelihood Estimation: find θ that maximizes $P(D|\theta)$: $\hat{\theta} = \underset{\theta}{\operatorname{argmax}} P(D|\theta) = \underset{\theta}{\operatorname{argmax}} \log P(D|\theta) \leftarrow N_r \log(\theta) + N_b \log(1-\theta)$

Take derivative and set to 0:

$$\frac{\partial}{\partial \theta} \log P(D|\theta) = \frac{\partial}{\partial \theta} [N_r \log(\theta) + N_b \log(1-\theta)]$$

$$= N_r \frac{\partial}{\partial \theta} [\log(\theta)] + N_b \frac{\partial}{\partial \theta} [\log(1 - \theta)]$$
$$= N_r \frac{1}{\theta} + N_b \frac{1}{1 - \theta} \cdot -1$$
$$= N_r (1 - \theta) - N_b \theta$$
$$= N_r - \theta (N_r + N_b) = 0$$
$$\rightarrow \hat{\theta} = \frac{N_r}{N_r + N_b}$$

- Collectively name all model parameters (i.e. probability tables) as θ
- Maximum Likelihood Estimation: find θ that maximizes P(Data $|\theta$)
 - In practice, maximize log P instead because computation is easier
 - To solve, either take derivative and set to 0, or use numerical optimization (next lectures)
- For Naïve Bayes maximum likelihood estimates of prob. tables are:

 $P(y) = \frac{\text{\# of occurrences of class } y}{\text{total \# of observations}} \qquad P(f \mid y) = \frac{\text{\# of occurrences of feature } f \text{ and class } y}{\text{total \# of occurrences of class } y}$

Need to be careful though ... let's see what can go wrong..

What is the best way to fit this data?



Empirical Risk Minimization

- How should we evaluate the quality of our model?
- Empirical risk minimization
 - Basic principle of machine learning
 - We want the model (classifier, etc) that does best on the true test distribution
 - Don't know the true distribution so pick the best model on our actual training set
 - Finding "the best" model on the training set is phrased as an optimization problem
- Main worry: overfitting to the training set
 - Better with more training data (less sampling variance, training more like test)
 - Better if we limit the complexity of our hypotheses (regularization and/or small hypothesis spaces)
- Another worry: our training distribution doesn't match true distribution

Underfitting and Overfitting



Example: Overfitting



2 wins!!

Generalization and Overfitting

- Relative frequency parameters will overfit the training data!
 - Just because we never saw a 3 with pixel (15,15) on during training doesn't mean we won't see it at test time
 - Unlikely that every occurrence of "minute" is 100% spam
 - Unlikely that every occurrence of "seriously" is 100% ham
 - What about all the words that don't occur in the training set at all?
 - In general, we can't go around giving unseen events zero probability
- As an extreme case, imagine using the entire email as the only feature
 - Would get the training data perfect (if deterministic labeling)
 - Wouldn't *generalize* at all
 - Just making the bag-of-words assumption gives us some generalization, but isn't enough
- To generalize better: we need to smooth or regularize the estimates

Smoothing


Unseen Events





Laplace Smoothing

- Laplace's estimate:
 - Pretend you saw every outcome once more than you actually did

$$P_{LAP}(x) = \frac{c(x) + 1}{\sum_{x} [c(x) + 1]}$$
$$= \frac{c(x) + 1}{N + |X|}$$

$$P_{ML}(X) =$$

$$P_{LAP}(X) =$$

 Can derive this estimate with Dirichlet priors (see cs281a)

Laplace Smoothing

- Laplace's estimate (extended):
 - Pretend you saw every outcome k extra times

$$P_{LAP,k}(x) = \frac{c(x) + k}{N + k|X|}$$

- What's Laplace with k = 0?
- k is the strength of the prior
- Laplace for conditionals:
 - Smooth each condition independently:

$$P_{LAP,k}(x|y) = \frac{c(x,y) + k}{c(y) + k|X|}$$

r r b

 $P_{LAP,0}(X) =$

 $P_{LAP,1}(X) =$

 $P_{LAP,100}(X) =$

Naïve Bayes: No Smoothing (Overfitting)

Relative probabilities (odds ratios):

 $\frac{P(W|\mathsf{ham})}{P(W|\mathsf{spam})}$

south-west	:	inf
nation	:	inf
morally	:	inf
nicely	:	inf
extent	:	inf
seriously	•	inf
•••		

P(W ha)	m))
screens	:	inf
minute	:	inf

P(W|spam)

guaranteed : inf
\$205.00 : inf
delivery : inf
signature : inf



What went wrong here?

Naïve Bayes: With Smoothing

- For real classification problems, smoothing is critical
- New odds ratios:

 $\frac{P(W|\text{ham})}{P(W|\text{spam})} \qquad \frac{P(W|\text{spam})}{P(W|\text{ham})}$

helvetica	:	11.4
seems	:	10.8
group	:	10.2
ago	:	8.4
areas	:	8.3
•••		

verdana	: 28.8
Credit	: 28.4
ORDER	: 27.2
	: 26.9
money	: 26.5
• • •	



Do these make more sense?

What we did today

- Discussed various learning problems
 - Supervised (classification or regression), reinforcement, unsupervised
- Saw our first machine learning algorithm: Naïve Bayes
 - Model is a Bayes Net where features are independent given class label
 - Classification is just inference in Bayes Nets
 - Learning is just counting feature occurrences in training data
- Saw Maximum Likelihood as a principled way to estimate parameters
 - Maximize probability of the data given model parameters
 - For Naïve Bayes, we solved maximization problem analytically
- Saw that fitting training data too well can cause issues (Overfitting)

Next: Perceptrons



- Step 1: Select a ML algorithm. We choose to model the problem with Naïve Bayes.
- Step 2: Choose features to use.



Y: The label (spam or ham)		
Y P(Y)		
ham	?	
spam	?	

F ₁ : A feature (do I know the sender?)		
F_1 Y $P(F_1 Y)$		
yes	ham	?
no	ham	?
yes	spam	?
no	spam	?

F ₂ : Another feature (# of occurrences of FREE)		
F ₂	Y	$P(F_2 Y)$
0	ham	?
1	ham	?
2	ham	?
0	spam	?
1	spam	?
2	spam	?

Step 3: Training: Use training data to fill in the probability tables.

F ₂ : # of occurrences of FREE		
F ₂	Y	P(F ₂ Y)
0	ham	0.5
1	ham	0.5
2	ham	0.0
0	spam	0.25
1	spam	0.50
2	spam	0.25

	Training Data		
#	Email Text	Label	
1	Attached is my portfolio.	ham	
2	Are you free for a meeting tomorrow?	ham	
3	Free unlimited credit cards!!!!	spam	
4	Mail \$10,000 check to this address	spam	
5	Sign up now for 1 free Bitcoin	spam	
6	Free money free money	spam	

Row 4: $P(F_2=0 | Y=spam) = 0.25$ because 1 out of 4 spam emails contains "free" 0 times. Row 5: $P(F_2=1 | Y=spam) = 0.50$ because 2 out of 4 spam emails contains "free" 1 time. Row 6: $P(F_2=2 | Y=spam) = 0.25$ because 1 out of 4 spam emails contains "free" 2 times.

Model trained on a larger dataset:



Y: The label (spam or ham)		
Y P(Y)		
ham	0.6	
spam	0.4	

F ₁ : A feature (do I know the sender?)		
F_1 Y $P(F_1 Y)$		
yes	ham	0.7
no	ham	0.3
yes	spam	0.1
no	spam	0.9

F ₂ : Another feature (# of occurrences of FREE)		
F ₂	Y	$P(F_2 Y)$
0	ham	0.85
1	ham	0.07
2	ham	0.08
0	spam	0.75
1	spam	0.12
2	spam	0.13

- Step 4: Classification
- Suppose you want to label this email from a known sender: "Free food in Soda 430 today"
- Step 4.1: Feature extraction:
 - F_1 = yes, known sender
 - F₂ = 1 occurrence of "free"



- Step 4.2: Inference
- Instantiate features (evidence):
 - $F_1 = yes$
 - F₂ = 1
- Compute joint probabilities:
 - P(Y = spam, F₁ = yes, F₂ = 1) = P(Y = spam) P(F₁ = yes | spam) P(F₂ = 1 | spam) = 0.4 * 0.1 * 0.12 = 0.0048
 - P(Y = ham, F₁ = yes, F₂ = 1) = P(Y = ham) P(F₁ = yes | ham) P(F₂ = 1 | ham) = 0.6 * 0.7 * 0.07 = 0.0294
- Normalize:
 - $P(Y = spam | F_1 = yes, F_2 = 1) = 0.0048 / (0.0048+0.0294) = 0.14$
 - $P(Y = ham | F_1 = yes, F_2 = 1) = 0.0294 / (0.0048+0.0294) = 0.86$
- Classification result:
 - 14% chance the email is spam. 86% chance it's ham.
 - Or, if you don't need probabilities, note that 0.0294 > 0.0048 and guess ham.



 F_2

Y: The label (spam or ham)		
Y	P(Y)	
ham	0.6	
spam	0.4	

F ₁ : do I know the sender?		
F_1	Y	$P(F_1 Y)$
yes	ham	0.7
no	ham	0.3
yes	spam	0.1
no	spam	0.9
	F ₁ yes no yes	F ₁ Y yes ham no ham yes spam

F ₂ : # of occurrences of FREE		
F ₂	Y	$P(F_2 Y)$
0	ham	0.85
1	ham	0.07
2	ham	0.08
0	spam	0.75
1	spam	0.12
2	spam	0.13