CS 188: Artificial Intelligence Naïve Bayes and Perceptrons



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

Today's Topics

Naïve Bayes

- Review: making predictions / inference
- Learning parameters
- Machine Learning Workflow
- Perceptrons
 - Making predictions
 - Learning parameters

Last Time

Classification: given inputs x, predict labels (classes) y



- y liction)
- Convert input x into a collection of *features* f_1, \ldots, f_n

Last Time

- Naïve Bayes model: $P(Y, F_1, ..., F_n) = P(Y) \prod_i P(F_i|Y)$
 - Features and label are random variables
 - Input features F₁, ..., F_n are conditionally independent given label Y
 - Parameters θ : probability tables P(Y), $P(F_1|Y)$, ..., $P(F_n|Y)$
- Classification is inference in a Bayes Net:
 - Inference by enumeration
 - Given features f₁, ..., f_n probability over class labels is:

$$P(Y|f_1, \dots, f_n) \propto P(Y, f_1, \dots, f_n) = P(Y) \prod_i P(f_i|Y)$$

Enumerate over every label y:

$$\begin{bmatrix} P(y_1) \prod_i P(f_i|y_1) \\ P(y_2) \prod_i P(f_i|y_2) \\ \vdots \\ P(y_k) \prod_i P(f_i|y_k) \end{bmatrix} \xrightarrow{\text{Normalize}} \begin{bmatrix} P(y_1|f_1 \dots f_n) \\ P(y_2|f_1 \dots f_n) \\ \vdots \\ P(y_k|f_1 \dots f_n) \end{bmatrix}$$



Last Time

- *Naïve Bayes* model: $P(Y, F_1, ..., F_n) = P(Y) \prod_i P(F_i|Y)$
 - Features and label are random variables
 - Input features F_1, \ldots, F_n are conditionally independent given label Y
 - Parameters θ : probability tables P(Y), $P(F_1|Y)$, ..., $P(F_n|Y)$
- Learn parameters by counting:

•
$$P(\text{observing } x) = \frac{\# \text{ of times } x \text{ occured}}{\text{total } \# \text{ of events}}$$

For example:

- $P(\text{red}) = \frac{2}{2}$ (b (r)
- Comes from *Maximum Likelihood* estimation: find θ that maximizes P(observations| θ)
 - $= \operatorname{argmax} P(\operatorname{observations}|\theta)$
 - Take derivative and set to 0
 - In practice, maximize log P instead because derivatives are easier
- In general for Naïve Bayes maximum likelihood estimates of probability tables are:

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

Example: Naïve Bayes for Spam Filtering

- Predict if an email is spam or not
 - Features: W_i is the i'th word in the email (domain: words in the dictionary)
 - Labels: $Y \in \{spam, ham\}$

P(Y)

spam

2/6

Estimated parameters:

Y

P(Y)

		P(W Y)				
ham		W	"now"	"the"	"buy"	
4/6		P(W Y=spam)	2/6	1/6	3/6	
4/6		P(W Y=ham)	1/6	4/6	1/6	



- What is P(Y|"buy", "now")?
 - P(spam|"buy", "now") ∝ P(spam)P("buy"|spam)P("now"|spam) = ²/₆ ⋅ ³/₆ ⋅ ²/₆ = ¹²/_{6³}
 P(ham|"buy", "now") ∝ P(ham)P("buy"|ham)P("now"|ham) = ⁴/₆ ⋅ ¹/₆ ⋅ ¹/₆ = ⁴/_{6³}

 - Renormalize:

P(*Y*|*"buy"*, *"now"*)



Prediction: pick label with highest probability, so predict **spam** for text "buy now"

Example: Naïve Bayes for Spam Filtering

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- Predict if an email is spam or not
 - Features: W_i is the i'th word in the email (domain: words in the dictionary)
 - Labels: $Y \in \{spam, ham\}$
- Estimated parameters:

P(V)			P(W Y)				
V snam ham			W	"now"	"the"	"buy'	
P(V)	2/6	1/6		P(W Y=spam)	2/6	1/6	3/6
Γ(Ι)	2/0	4/0		P(W Y=ham)	1/6	4/6	1/6



How can we estimate these model parameters?

Parameter Estimation



Parameter Estimation with Maximum Likelihood

- Estimating the distribution of a random variable
- Use training data (learning!)
 - For each outcome x, look at the *empirical rate* of that value:

 $P_{\mathsf{ML}}(x) = \frac{\mathsf{count}(x)}{\mathsf{total samples}}$



- Example: probability of x=red given training data (r), (r), (b) $P_{ML}(r) = 2/3$
- This estimate maximizes the *likelihood of the data* for parametric model: $L(\theta) = P(red, red, blue \mid \theta) = P_{\theta}(red) \cdot P_{\theta}(red) \cdot P_{\theta}(blue) = \theta^{2} \cdot (1 - \theta)$
 - Why?

Take derivative and set to 0:

Parameter Estimation with Maximum Likelihood (General Case)



- Data: draw N balls, N_r come up red and N_b come up blue
 - Dataset $D = \{x_1, ..., x_N\}$
 - Ball draws are independent and identically distributed (i.i.d):

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



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

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

Take derivative and set to 0:

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

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

$$= N_r \frac{1}{\theta} + N_b \frac{1}{1-\theta} \cdot -1$$

$$= N_r (1-\theta) - N_b \theta$$

$$= N_r - \theta (N_r + N_b) = 0$$

$$\rightarrow \hat{\theta} = \frac{N_r}{N_r + N_b}$$

Example: Spam Filtering Parameter Estimation

- Predict if an email is spam or not
 - Features: W_i is the i'th word in the email (domain: words in the dictionary)
 - Labels: $Y \in \{spam, ham\}$
- Naïve Bayes model parameters:





- **Dataset:** M emails where k'th email contains words $\{w_1, \dots, w_{N_k}\}$ and label y_k
 - Emails are independent and identically distributed:

$$P(D|\theta) = \prod_{k}^{M} P(y_k, w_1, \dots, w_{N_k}) = \prod_{k}^{M} P(y_k) \prod_{i}^{N_k} P(w_i|y_k)$$

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

Example: Spam Filtering Parameter Estimation

- Predict if an email is spam or not
 - Features: W_i is the i'th word in the email (domain: words in the dictionary)
 - Labels: $Y \in \{spam, ham\}$
- Naïve Bayes model parameters:

 $P_{\theta}(W|Y)$



$P_{\alpha}(Y)$						
V	snam	ham	W	"now"	"the"	
Y)	Spann	Патт	P(W Y=spam)			
,			P(W Y=ham)			

Maximum Likelihood Estimation Result:

•
$$\theta_{spam} = \frac{\# \text{ of spam emails}}{\text{total } \# \text{ of emails}}$$

Ρ

More generally: parameters for model
$$P_{\theta}(F|Y)$$
 are:
 $\theta_{f,y} = \frac{\# \text{ of occurrences of feature } f \text{ and class } y}{\text{total } \# \text{ of occurrences of class } y}$

Parameter Estimation with Maximum Likelihood

- How do we estimate the conditional probability tables?
 - Maximum Likelihood, which corresponds to counting
- Need to be careful though ... let's see what can go wrong..

What is the best way to fit this data?



Underfitting and Overfitting



Example: Overfitting





2 wins!!

Example: Overfitting

relative probabilities (odds ratios):

P(W	ham)
$\overline{P(W)}$	spam)

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

P(W spam)
P(W ham)

saroons	•	inf
SCLEENS	•	
minute	:	inf
guaranteed	:	inf
\$205.00	:	inf
delivery	:	inf
signature	:	inf



What went wrong here?

Overfitting



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

 $P_{ML}(X) =$

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



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

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

r r b

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

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

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

Laplace Smoothing Can Be More Formally Derived

Relative frequencies are the maximum likelihood estimates

$$\theta_{ML} = \arg \max_{\theta} P(\mathbf{X}|\theta)$$

= $\arg \max_{\theta} \prod_{i} P_{\theta}(X_{i})$ $\longrightarrow P_{\mathsf{ML}}(x) = \frac{\mathsf{count}(x)}{\mathsf{total samples}}$

Another option is to consider the most likely parameter value given the data

$$\theta_{MAP} = \arg \max_{\theta} P(\theta | \mathbf{X})$$

$$= \arg \max_{\theta} P(\mathbf{X} | \theta) P(\theta) / P(\mathbf{X}) \qquad \qquad \text{``right'' choice of P(theta)}$$

$$= \arg \max_{\theta} P(\mathbf{X} | \theta) P(\theta)$$

Estimation: Linear Interpolation*

- In practice, Laplace can perform poorly for P(X|Y):
 - When |X| is very large
 - When |Y| is very large
- Another option: linear interpolation
 - Also get the empirical P(X) from the data
 - Make sure the estimate of P(X|Y) isn't too different from the empirical P(X)

$$P_{LIN}(x|y) = \alpha \hat{P}(x|y) + (1.0 - \alpha)\hat{P}(x)$$

- What if **α** is 0? 1?
- For even better ways to estimate parameters, as well as details of the math, see cs281a, cs288



Real NB: Smoothing

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

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

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?

Tuning



Tuning on Held-Out Data

Now we've got two kinds of unknowns

- Parameters: the probabilities P(X|Y), P(Y)
- Hyperparameters: e.g. the amount of smoothing k
- What should we learn where?
 - Learn parameters from training data
 - Tune hyperparameters on different data
 - Why?
 - For each value of the hyperparameters, train and test on the held-out data
 - Choose the best value and do a final test on the test data



Important Concepts

- Data: labeled instances, e.g. emails marked spam/ham
 - Training set
 - Held out set
 - Test set
- Features: attribute-value pairs which characterize each input
- Experimentation cycle
 - Learn parameters (e.g. model probabilities) on training set
 - (Tune hyperparameters on held-out set)
 - Compute accuracy on test set
 - Very important: never "peek" at the test set!
- Evaluation
 - Accuracy: fraction of instances predicted correctly
- Overfitting and generalization
 - Want a classifier which does well on *test* data
 - <u>Overfitting</u>: fitting the training data very closely, but not generalizing well
 - <u>Underfitting</u>: fits the training set poorly



Workflow

- Phase 1: Train model on Training Data. Choice points for "tuning"
 - Attributes / Features
 - Model types: Naïve Bayes vs. Perceptron vs. Logistic Regression vs. Neural Net etc..
 - Model hyperparameters
 - E.g. Naïve Bayes Laplace k
 - E.g. Logistic Regression weight regularization
 - E.g. Neural Net architecture, learning rate, ...
 - Make sure good performance on training data (why?)

Phase 2: Evaluate on Hold-Out Data

- If Hold-Out performance is close to Train performance
 - We achieved good generalization, onto Phase 3! 😌
- If Hold-Out performance is much worse than Train performance
 - We overfitted to the training data! 🙁
 - Take inspiration from the errors and:
 - Either: go back to Phase 1 for tuning (typically: make the model less expressive)
 - Or: if we are out of options for tuning while maintaining high train accuracy, collect more data (i.e., let the data drive generalization, rather than the tuning/regularization) and go to Phase 1
- Phase 3: Report performance on Test Data

Possible outer-loop: Collect more data



Practical Tip: Baselines

• First step: get a baseline

- Baselines are very simple "straw man" procedures
- Help determine how hard the task is
- Help know what a "good" accuracy is

Weak baseline: most frequent label classifier

- Gives all test instances whatever label was most common in the training set
- E.g. for spam filtering, might label everything as ham
- Accuracy might be very high if the problem is skewed
- E.g. calling everything "ham" gets 66%, so a classifier that gets 70% isn't very good...
- For real research, usually use previous work as a (strong) baseline

Perceptrons



Linear Classifiers



Feature Vectors



Some (Simplified) Biology

Very loose inspiration: human neurons



Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



activation_w(x) =
$$\sum_{i} w_i \cdot f_i(x) = w \cdot f(x)$$

If the activation is:

- Positive, output +1
- Negative, output -1



Weights

- Binary case: compare features to a weight vector
- Learning: figure out the weight vector from examples



Decision Rules



Binary Decision Rule

- In the space of feature vectors
 - Examples are points
 - Any weight vector is a hyperplane
 - One side corresponds to Y=+1
 - Other corresponds to Y=-1

free	:	4
money	:	2





Binary Decision Rule

- In the space of feature vectors
 - Examples are points
 - Any weight vector is a hyperplane
 - One side corresponds to Y=+1
 - Other corresponds to Y=-1

BIAS	:	-3
free	:	4
money	:	2
• • •		





Binary Decision Rule

- In the space of feature vectors
 - Examples are points
 - Any weight vector is a hyperplane
 - One side corresponds to Y=+1
 - Other corresponds to Y=-1





BIAS	:	-3
free	:	4
money	:	2
•••		

Weight Updates



Learning: Binary Perceptron

- Start with weights w = 0
- For each training instance f(x), y*:
 - Classify with current weights

If correct (i.e., y=y*), no change!

If wrong: adjust the weight vector



Learning: Binary Perceptron

- Start with weights w = 0
- For each training instance f(x), y*:
 - Classify with current weights

$$y = \begin{cases} +1 & \text{if } w \cdot f(x) \ge 0\\ -1 & \text{if } w \cdot f(x) < 0 \end{cases}$$

- If correct (i.e., y=y*), no change!
- If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if y* is -1.

$$w = w + y^* \cdot f$$



Learning: Binary Perceptron

- Start with weights w = 0
- For each training instance f(x), y*:
 - Classify with current weights

$$y = \begin{cases} +1 & \text{if } w \cdot f(x) \ge 0\\ -1 & \text{if } w \cdot f(x) < 0 \end{cases}$$

- If correct (i.e., y=y*), no change!
- If wrong: adjust the weight vector by adding or subtracting the feature vector. Subtract if y* is -1.

$$w = w + y^* \cdot f$$



Example: Perceptron

Iteration 0: x: "win the vote" f(x): [1 1 0 1 1] y*: -1
Iteration 1: x: "win the election" f(x): [1 1 0 0 1] y*: -1
Iteration 2: x: "win the game" f(x): [1 1 1 0 1] y*: +1
Iteration 3: x: "win the game" f(x): [1 1 1 0 1] y*: +1

$w \cdot f(x)$:	1	-2	-2	2
the	0	-1	-1	0
vote	0	-1	-1	-1
game	0	0	0	1
win	0	-1	-1	0
BIAS	1	0	0	1

Example: Perceptron

Separable Case



Multiclass Decision Rule

- If we have multiple classes:
 - A weight vector for each class:

 w_y

- Score (activation) of a class y:
 - $w_y \cdot f(x)$
- Prediction highest score wins

$$y = \underset{y}{\operatorname{arg\,max}} w_y \cdot f(x)$$





Binary = multiclass where the negative class has weight zero

Learning: Multiclass Perceptron

- Start with all weights = 0
- Pick up training examples f(x), y* one by one
- Predict with current weights

 $y = \arg \max_y w_y \cdot f(x)$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

$$w_y = w_y - f(x)$$
$$w_{y^*} = w_{y^*} + f(x)$$



Example: Multiclass Perceptron

Iteration 0: x: "win the vote" f(x): [1 1 0 1 1] y*: politics
Iteration 1: x: "win the election" f(x): [1 1 0 0 1] y*: politics
Iteration 2: x: "win the game" f(x): [1 1 1 0 1] y*: sports

w_{SPORTS}

BIAS	1	0	0	1
win	0	-1	-1	0
game	0	0	0	1
vote	0	-1	-1	-1
the	0	-1	-1	0
$w \cdot f(x)$:	1	-2	-2	

w_{POLITICS}

1

1

()

1

1

3

 \cap

3

 $\left(\right)$

 $\left(\right)$

-1

 $\left(\right)$

0

 $\left(\right)$

 $\left(\right)$

()

0

BIAS

win

game

vote

the

 $w \cdot f(x): 0$

w_{TECH}

BIAS	0	0	0	0	
win	0	0	0	0	
game	0	0	0	0	
vote	0	0	0	0	
the	0	0	0	0	

 $w \cdot f(x): 0 0 0$

Properties of Perceptrons

- Separability: true if some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)
- Mistake Bound: the maximum number of mistakes (binary case) related to the margin or degree of separability





Non-Separable



Problems with the Perceptron

- Noise: if the data isn't separable, weights might thrash
 - Averaging weight vectors over time can help (averaged perceptron)
- Mediocre generalization: finds a "barely" separating solution

- Overtraining: test / held-out accuracy usually rises, then falls
 - Overtraining is a kind of overfitting



iterations

Next Lecture: Improving Perceptron & Optimization

Improving the Perceptron



Non-Separable Case: Deterministic Decision



Non-Separable Case: Probabilistic Decision



How to get probabilistic decisions?

- Perceptron scoring: $z = w \cdot f(x)$
- If $z = w \cdot f(w)$ ry positive \Box want probability going to 1
- If $z = w \cdot f(w)$ ry negative \Box want probability going to 0



A 1D Example



The Soft Max



$$P(\operatorname{red}|x) = \frac{e^{w_{\operatorname{red}} \cdot x}}{e^{w_{\operatorname{red}} \cdot x} + e^{w_{\operatorname{blue}} \cdot x}}$$

Best w?

Maximum likelihood estimation:

$$\max_{w} \ ll(w) = \max_{w} \ \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$

with:
$$P(y^{(i)} = +1 | x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$
$$P(y^{(i)} = -1 | x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

= Logistic Regression

Separable Case: Deterministic Decision – Many Options





Separable Case: Probabilistic Decision – Clear Preference





Multiclass Logistic Regression

 w_y

 $w_{\mathcal{U}} \cdot f(x)$

- Recall Perceptron:
 - A weight vector for each class:
 - Score (activation) of a class y:
 - Prediction highest score wins

$$y = \arg \max_{y} w_{y} \cdot f(x)$$



How to make the scores into probabilities?

$$z_{1}, z_{2}, z_{3} \rightarrow \underbrace{\frac{e^{z_{1}}}{e^{z_{1}} + e^{z_{2}} + e^{z_{3}}}, \frac{e^{z_{2}}}{e^{z_{1}} + e^{z_{2}} + e^{z_{3}}}, \frac{e^{z_{3}}}{e^{z_{1}} + e^{z_{2}} + e^{z_{3}}}, \frac{e^{z_{3}}}{e^{z_{1}} + e^{z_{2}} + e^{z_{3}}}}$$

Best w?

Maximum likelihood estimation:

$$\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$
with:
$$P(y^{(i)} | x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_{y} e^{w_{y} \cdot f(x^{(i)})}}$$

= Multi-Class Logistic Regression

Next Lecture

- Optimization
 - i.e., how do we solve:

$$\max_{w} \ ll(w) = \max_{w} \ \sum_{i} \log P(y^{(i)} | x^{(i)}; w)$$