25: Logistic Regression

Lisa Yan November 18, 2019



Model:

Observe:

Multinomial with m outcomes: p_i probability of outcome i

 $n_i = #$ of trials with outcome iTotal of $\sum_{i=1}^m n_i$ trials

> MAP with Laplace smoothing (Laplace estimate)

$$p_i = \frac{n_i + 1}{\sum_{i=1}^m n_i + m}$$

$$p_i = \frac{n_i}{\sum_{i=1}^m n_i}$$

Classification problem

Review



Training data: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(n)}, y^{(n)})$ *n* datapoints

Notation consistent with lecture notes (last lecture has been updated): *i*-th observation: $x^{(i)} = (x_1^{(i)}, x_2^{(i)}, \dots, x_m^{(i)})$

j-th feature of *i*-th observation:

$$\boldsymbol{x}^{(i)} = \left(x_1^{(i)}, x_2^{(i)}, \dots, x_m^{(i)} \right)$$
$$x_i^{(i)}$$

 $\widehat{Y} = \arg \max_{\substack{y \in \{0,1\}}} \widehat{P}(Y \mid \boldsymbol{X})$ $= \arg \max_{\substack{y \in \{0,1\}}} \frac{\widehat{P}(\boldsymbol{X}|Y)\widehat{P}(Y)}{\widehat{P}(\boldsymbol{X})}$

(Predict the Y that is most likely given our observation X)

(Bayes' Theorem)

(eliminate normalization constant $\hat{P}(\mathbf{X})$)

$$= \arg \max_{y=\{0,1\}} \widehat{P}(X|Y) \widehat{P}(Y)$$
$$\widehat{P}(X_1, X_2, \dots, X_m|Y)$$

Use MLE or Laplace estimates to find $\hat{P}(X_1, X_2, ..., X_m | Y)$ and Y

- $\hat{P}(X_1, X_2, \dots, X_m | Y = 1)$: Multinomial, 2^m outcomes
- $\hat{P}(X_1, X_2, \dots, X_m | Y = 0)$: Multinomial, 2^m outcomes
- $\hat{P}(Y)$: Multinomial, 2 outcomes

parameters:

Total #

 $O(2^{m})$

The problem with our Brute force Bayes classifier

 $\widehat{Y} = \arg \max_{\substack{y \in \{0,1\}}} \widehat{P}(Y \mid X)$ $= \arg \max_{\substack{y \in \{0,1\}}} \frac{\widehat{P}(X|Y)\widehat{P}(Y)}{\widehat{P}(X)}$

 $= \underset{y=\{0,1\}}{\operatorname{arg\,max}} \widehat{P}(\boldsymbol{X}|\boldsymbol{Y}) \widehat{P}(\boldsymbol{Y})$ $\widehat{P}(X_1, X_2, \dots, X_m|\boldsymbol{Y})$

(Predict the Y that is most likely given our observation X)

(Bayes' Theorem)

(eliminate normalization constant $\hat{P}(X)$)

too many parameters to estimate

What if we could make a simplifying (but naïve) assumption – that X_1, \ldots, X_m are **conditionally independent** given Y?

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Review

The Naïve Bayes assumption

$$\widehat{Y} = \underset{y=\{0,1\}}{\arg \max} \frac{\widehat{P}(Y \mid X)}{\widehat{P}(X)}$$
$$= \underset{y=\{0,1\}}{\arg \max} \frac{\widehat{P}(X \mid Y) \widehat{P}(Y)}{\widehat{P}(X)}$$

$$= \underset{y=\{0,1\}}{\operatorname{arg\,max}} \widehat{P}(\boldsymbol{X}|Y)\widehat{P}(Y)$$
$$= \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1}^{m} \widehat{P}(X_i|Y)\right)\widehat{P}(Y)$$

(Predict the Y that is most likely given our observation X)

(Bayes' Theorem)

(eliminate normalization constant $\hat{P}(X)$)

Naïve Bayes Assumption

 X_1, \ldots, X_m are conditionally independent given Y.





Logistic Regression

Naïve Bayes Classifier

$$\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1}^{m} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$$

Training
Laplace (MAP)
$$\hat{P}(X_i|Y=0), \hat{P}(X_i|Y=1), \forall i$$

Laplace (MAP) $\hat{P}(Y=0), \hat{P}(Y=1)$
Total # params: $O(m)$

Testing
$$\hat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\log \hat{P}(Y) + \sum_{i=1}^{m} \log \hat{P}(X_i | Y) \right)$$
 (for numeric stability)



and Learn

Will a user like the Pokémon TV series?

Input indicator variables $X = (X_1, X_2)$:



 $X_1 = 1$: "likes Star Wars"



 $X_2 = 1$: "likes Harry Potter"

Output *Y* indicator:



Y = 1: "likes Pokémon"

Observe indicator vars. $X = (X_1, X_2)$:

- X₁: "likes Star Wars"
- X₂: "likes Harry Potter"

Predict *Y*: "likes Pokémon"

- 1. How many datapoints (*n*) are in our train data?
- 2. How many parameters do we need to estimate?
- 3. Compute MLE estimates for $\hat{P}(X_1|Y)$:



 $\hat{Y} = \arg\max_{y=\{0,1\}} \left($

Training data counts



 $\widehat{P}(X_i|Y) \widehat{P}(Y)$

Observe indicator vars. $X = (X_1, X_2)$:

- X₁: "likes Star Wars"
- X₂: "likes Harry Potter"

Predict *Y*: "likes Pokémon"

- 1. How many datapoints (*n*) are in our train data?
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- 3. Compute MLE estimates for $\hat{P}(X_1|Y)$:



 $\widehat{Y} = \arg\max_{y=\{0,1\}} \left(\prod_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=$

Training data counts

$$n = 30$$

- $\hat{P}(X_1|Y=0), \hat{P}(X_1|Y=1)$: 4 params
- $\hat{P}(X_2|Y=0), \hat{P}(X_2|Y=1)$: 4 params
- $\hat{P}(Y)$: 2 params



 $\widehat{P}(X_i|Y) \hat{P}(Y)$

Observe indicator vars. $X = (X_1, X_2)$:

- X₁: "likes Star Wars"
- X₂: "likes Harry Potter"

Predict Y: "likes Pokémon"

- 1. How many datapoints (*n*) are in our train data?
- 2. How many parameters do we need to estimate?
- 3. Compute MLE estimates for $\hat{P}(X_1|Y)$:

Y	0	1	Y Y	0	1
0	3	10	0	5	8
1	4	13	1	7	10

 $\hat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1} \hat{P}(X_i | Y) \right) \hat{P}(Y)$

Training data counts

$$n = 30$$
• $\hat{P}(X_1|Y = 0), \hat{P}(X_1|Y = 1)$: 4 params
• $\hat{P}(X_2|Y = 0), \hat{P}(X_2|Y = 1)$: 4 params
• $\hat{P}(Y)$: 2 params
• $\hat{P}(Y)$: 2 params
• $\hat{P}(Y)$: 2 params
• $\hat{P}(X_1 = 0), \hat{P}(X_2|Y = 1)$: 4 params
• $\hat{P}(Y)$: 2 params
• $\hat{P}($





Now that we've trained and found parameters, It's time to classify new users!

 $\hat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1} \hat{P}(X_i | Y) \right) \hat{P}(Y)$

Observe indicator vars. $X = (X_1, X_2)$: $\setminus X_1$ 0 0 • *X*₁: "likes Star Wars" Y X_2 : "likes Harry Potter" 0 0.23 0.77 0 0.38 0.62 0 0.43 Predict *Y*: "likes Pokémon" 1 0.24 0.76 0.41 0.59 0.57 1

Suppose a **new person** "likes Star Wars" ($X_1 = 1$) but "dislikes Harry Potter" ($X_2 = 0$). Will they like Pokemon? Need to predict *Y*:

$$\hat{Y} = \arg \max_{y \in \{0,1\}} \hat{P}(X|Y)\hat{P}(Y) = \arg \max_{y \in \{0,1\}} \hat{P}(X_1|Y)\hat{P}(X_2|Y)\hat{P}(Y)$$

If Y = 0: $\hat{P}(X_1 = 1 | Y = 0) \hat{P}(X_2 = 0 | Y = 0) \hat{P}(Y = 0) = 0.77 \cdot 0.38 \cdot 0.43 = 0.126$

If Y = 1: $\hat{P}(X_1 = 1 | Y = 1)\hat{P}(X_2 = 0 | Y = 1)\hat{P}(Y = 1) = 0.76 \cdot 0.41 \cdot 0.57 = 0.178$

Since term is greatest when Y = 1, predict $\hat{Y} = 1$

 $\hat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1} \hat{P}(X_i | Y) \right) \hat{P}(Y)$

Naïve Bayes Classifier

$$\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1}^{m} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$$

We can use MLE or MAP to estimate our parameters.

Let's try using MAP with Laplace smoothing.

Observe indicator vars. $X = (X_1, X_2)$:

- X₁: "likes Star Wars"
- X₂: "likes Harry Potter"

Predict Y: "likes Pokémon"

YX1 Y	0	1	Y Y	0	1	
0	3	10	0	5	8	
1	4	13	1	7	10	

 $\widehat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$

Training data counts

What are our MAP estimates using Laplace smoothing for $\hat{P}(X_i|Y)$ and $\hat{P}(Y)$?

$$\hat{P}(X_{i} = x | Y = y): \qquad \hat{P}(Y = y): \\
A. \frac{\#(X_{i} = x, Y = y)}{\#(Y = y)} \qquad A. \frac{\#(Y = y)}{\#(Y = y) + 2} \\
B. \frac{\#(X_{i} = x, Y = y) + 1}{\#(Y = y) + 2} \qquad B. \frac{\#(Y = y) + 1}{n} \\
C. \frac{\#(X_{i} = x, Y = y) + 1}{\#(Y = y) + 4} \qquad C. \frac{\#(Y = y) + 1}{n + 2}$$

Observe indicator vars. $X = (X_1, X_2)$:

- X₁: "likes Star Wars"
- X₂: "likes Harry Potter"

Predict Y: "likes Pokémon"

YX1 Y	0	1	X_2 Y	0	1	
0	3	10	0	5	8	-
1	4	13	1	7	10	

 $\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1}^{n} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$

Training data counts

What are our MAP estimates using Laplace smoothing for $\hat{P}(X_i|Y)$ and $\hat{P}(Y)$?

$$\hat{P}(X_{i} = x | Y = y): \qquad \hat{P}(Y = y): \\
A. \frac{\#(X_{i} = x, Y = y)}{\#(Y = y)} \qquad A. \frac{\#(Y = y)}{\#(Y = y) + 2} \\
B. \frac{\#(X_{i} = x, Y = y) + 1}{\#(Y = y) + 2} \qquad B. \frac{\#(Y = y) + 1}{n} \\
C. \frac{\#(X_{i} = x, Y = y) + 1}{\#(Y = y) + 4} \qquad C. \frac{\#(Y = y) + 1}{\#(Y = y) + 4} \\
\end{array}$$



Naïve Bayes Classifier

$$\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1}^{m} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$$

What is the intuition behind the Naïve Bayes assumption?

Naïve Bayes Model is a Bayesian Network $\hat{Y} = \underset{y=\{0,1\}}{\operatorname{arg max}} \left(\prod_{i=1}^{\hat{P}(X_i|Y)} \hat{P}^{(Y)} \right)$

Naïve Bayes
Assumption
$$P(X|Y) = \prod_{i=1}^{m} P(X_i|Y) \implies P(X,Y) = P(Y) \prod_{i=1}^{m} P(X_i|Y)$$

Which Bayesian Network encodes this conditional independence?



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Naïve Bayes Model is a Bayesian Network

Naïve Bayes
Assumption
$$P(X|Y) = \prod_{i=1}^{m} P(X_i|Y) \implies P(X,Y) = P(Y) \prod_{i=1}^{m} P(X_i|Y)$$

Which Bayesian Network encodes this conditional independence?



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 $\widehat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} \left(\prod_{i=1} \widehat{P}(X_i | Y) \right) \widehat{P}(Y)$

Break for jokes/ announcements

Wednesday 12/4
(after break) Up to end of this week

Late day reminder: No late days permitted past last day of the quarter, 12/6 (Friday)

<u>CS109 Cc</u>	ontest
Due:	Monday 12/2 11:59pm
Note:	All serious submissions will
	get some extra credit

Naïve Bayes

Logistic Regression

- Chapter 0: Background
- Chapter 1: Big Picture
- Chapter 2: Details
- Chapter 3: Philosophy

If
$$X = (X_1, X_2, ..., X_m)$$
:
 $z = \theta^T X = \sum_{j=1}^m \theta_j X_j$ Weighted sum
(aka dot product)
 $= \theta_1 X_1 + \theta_2 X_2 + \dots + \theta_m X_m$

Weighted sum with an intercept term:

$$z = \theta_0 + \sum_{j=1}^m \theta_j X_j$$

= $\theta_0 X_0 + \theta_1 X_1 + \theta_2 X_2 + \dots + \theta_m X_m$ Define $X_0 = 1$
= $\theta^T X$ New $X = (1, X_1, X_2, \dots, X_m)$

Background: Sigmoid function $\sigma(z)$

• The sigmoid function:

 $\sigma(z) = \frac{1}{1 + e^{-z}}$

 Sigmoid squashes z to a number between 0 and 1.



 Recall definition of probability: A number between 0 and 1



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 $\frac{\partial f(x)}{\partial x} = \frac{\partial f(z)}{\partial z} \frac{\partial z}{\partial x}$

Calculus Chain Rule

f(x) = f(z(x))

aka decomposition of composed functions Naïve Bayes

Logistic Regression

- Chapter O: Background
- Chapter 1: Big Picture
- Chapter 2: Details
- Chapter 3: Philosophy

From Naïve Bayes to Logistic Regression

Classification goal: Model $P(Y \mid X)$

$$\widehat{Y} = \arg \max_{y \in \{0,1\}} P(Y \mid X)$$

Predict the *Y* that is most likely given our observation *X*

Naïve Bayes Classifier:

- Estimate P(X | Y) and P(Y) because $\underset{y=\{0,1\}}{\arg \max P(Y | X)} = \underset{y=\{0,1\}}{\arg \max P(X | Y)P(Y)}$
- Actually modeling P(X, Y)
- Assume $P(X|Y) = P(X_1, X_2, ..., X_n|Y) = \prod_{i=1}^m P(X_i|Y)$

Can we model $P(Y \mid X)$ directly?

• Welcome our friend: Logistic Regression!

Logistic Regression

 $\widehat{Y} = \arg \max_{y \in \{0,1\}} P(Y \mid X)$

Predict the *Y* that is most likely given our observation *X*

Logistic Regression Model

$$P(Y = 1 | \mathbf{X} = \mathbf{x}) = \sigma \left(\theta_0 + \sum_{j=1}^m \theta_j x_j \right)$$

models $P(Y \mid X)$ directly

Logistic Regression



Logistic Regression Cartoon



θ parameter

Logistic Regression cartoon


Logistic Regression input/output





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Different predictions for different inputs



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Different predictions for different inputs



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Parameters affect prediction



Parameters affect prediction



 $\widehat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} P(Y \mid X)$ where

$$P(Y = 1 | \mathbf{X} = \mathbf{x}) = \sigma \left(\theta_0 + \sum_{j=1}^m \theta_j x_j \right)$$

Predict the Y that is most likely given our observation X

models $P(Y \mid X)$ directly

- $\sigma(z) = \frac{1}{1+e^{-z}}$, the sigmoid function
- For simplicity, define $x_0 = 1$: $P(Y = 1 | X = x) = \sigma(\theta^T x)$
- Since P(Y = 1 | X = x) + P(Y = 0 | X = x) = 1:

 $P(Y = 0 | \mathbf{X} = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$

Classifying using the sigmoid function





Classifying using the sigmoid function

Logistic Regression Model

$$\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} P(Y \mid \boldsymbol{X}) \quad \text{where} \quad P(Y=1 \mid \boldsymbol{X}=\boldsymbol{x}) = \sigma \left(\theta_0 + \sum_{j=1}^m \theta_j x_j \right)$$



When do we predict $\hat{Y} = 1$?

- A. If $\sigma(\theta^T x) > 1 \sigma(\theta^T x)$
- B. If $\sigma(\theta^T x) > 0.5$
- C. If $\theta^T x > 0$
- D. All are valid, but C is easiest
- E. None/Other



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Classifying using the sigmoid function

Logistic Regression Model

$$\widehat{Y} = \underset{y=\{0,1\}}{\operatorname{arg\,max}} P(Y \mid \boldsymbol{X}) \quad \text{where} \quad P(Y=1 \mid \boldsymbol{X}=\boldsymbol{x}) = \sigma \left(\theta_0 + \sum_{j=1}^m \theta_j x_j \right)$$



When do we predict $\hat{Y} = 1$? A. If $\sigma(\theta^T x) > 1 - \sigma(\theta^T x)$ B. If $\sigma(\theta^T x) > 0.5$ C. If $\theta^T x > 0$ D. All are valid, but C is easiest E. None/Other



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Naming algorithms

Regression Algorithms

Linear Regression



Classification Algorithms







If Lisa could rename it, she would call it: Sigmoidal Classification

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Training: Learning the parameters

Logistic regression gets its **intelligence** from its parameters $\theta = (\theta_0, \theta_1, \dots, \theta_m)$.

- Logistic Regression Model:
- Want to predict training data as correctly as possible:
- Therefore, choose θ that maximizes the conditional likelihood of observing i.i.d. training data:

$$P(Y = 1 | \mathbf{X} = \mathbf{x}) = \sigma(\theta^T \mathbf{x})$$

$$\underset{y=\{0,1\}}{\arg \max P(Y|X = x^{(i)}) = y^{(i)}} \text{ as often}$$

$$L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)} | \mathbf{X} = \mathbf{x}^{(i)}, \theta)$$

During training, find the θ that maximizes log-conditional likelihood of the training data. Use MLE!

Training: Learning the parameters via MLE

- 0. Add $x_0^{(i)} = 1$ to each $x^{(i)}$
- **1.** Logistic Regression model:

$$P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma(\theta^T \boldsymbol{x})$$

- 2. Compute log-likelihood $LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T x^{(i)}) + (1 y^{(i)}) \log (1 \sigma(\theta^T x^{(i)}))$ of training data:
- 3. Compute derivative of log-likelihood with respect to each θ_j , j = 0, 1, ..., m:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)}$$

Review

Walk uphill and you will find a local maxima (if your step is small enough).





Logistic regression $LL(\theta)$ is convex

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Training: Gradient ascent step

4. Optimize.
$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma(\theta^T x^{(i)}) \right] x_j^{(i)}$$

Repeat many times:

For

all thetas:

$$\theta_{j}^{\text{new}} = \theta_{j}^{\text{old}} + \eta \cdot \frac{\partial LL(\theta^{\text{old}})}{\partial \theta_{j}^{\text{old}}}$$

$$= \theta_{j}^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma \left(\theta^{\text{old}^{T}} \boldsymbol{x}^{(i)} \right) \right] x_{j}^{(i)}$$

What does this look like in code?

Gradient
Ascent Step
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

initialize $\theta_j = 0$ for $0 \le j \le m$ repeat many times:

gradient[j] = 0 for $0 \le j \le m$

// compute all gradient[j]'s
// based on n training examples

 $\theta_j += \eta * gradient[j] \text{ for all } 0 \leq j \leq m$

Gradient
Ascent Step
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:

gradient[j] = 0 for 0 ≤ j ≤ m
for each training example (x, y):
 for each 0 ≤ j ≤ m:

// update gradient[j] for
// current (x,y) example

 $\theta_j += \eta * \text{gradient[j] for all } 0 \leq j \leq m$

Gradient
Ascent Step
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

Initialize
$$\theta_j = 0$$
 for $0 \le j \le m$
Prepeat many times:
$$gradient[j] = 0 \text{ for } 0 \le j \le m$$
for each training example (x, y):
for each $0 \le j \le m$:
$$gradient[j] += \left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j$$

$$\theta_j += \eta * \text{ gradient[j] for all } 0 \le j \le m$$

What are important implementation details?

m

Gradient
Ascent Step
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

initialize $\theta_i = 0$ for $0 \le j \le m$ repeat many times: gradient[j] = 0 for $0 \le j \le m$ for each training example (x, y): for each $0 \leq j \leq m$: gradient[j] += $\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j$ $\theta_i += \eta * \text{gradient}[j] \text{ for all } 0 \leq j \leq m$

• x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$

Initialize
$$\theta_j = 0$$
 for $0 \le j \le m$
repeat many times:

gradient[j] = 0 for $0 \le j \le m$
for each training example (x, y):
 for each $0 \le j \le m$:

gradient[j] += $\left[y - \frac{1}{1 + e^{-\theta^T x}}x_j\right]$

 θ_j += η * gradient[j] for all $0 \le j \le j$

• x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$

• Insert $x_0 = 1$ before training

m

initialize $\theta_i = 0$ for $0 \le j \le m$ repeat many times: gradient[j] = 0 for $0 \le j \le m$ for each training example (x, y): for each $0 \leq j \leq m$: gradient[j] += $\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j$ $\theta_i += \eta * \text{ gradient}[j] \text{ for all } 0 \leq j \leq m$

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training
- Finish computing gradient before updating any part of θ

initialize $\theta_i = 0$ for $0 \le j \le m$ repeat many times: gradient[j] = 0 for $0 \le j \le m$ for each training example (x, y): for each $0 \le j \le m$: gradient[j] += $\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j$ $\theta_i += \eta$ gradient[j] for all $0 \le j \le m$ • x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$

• Insert $x_0 = 1$ before training

- Finish computing gradient before updating any part of θ
- Learning rate η is a constant you set before training

initialize
$$\theta_j = 0$$
 for $0 \le j \le m$
repeat many times:
gradient[j] = 0 for $0 \le j \le m$
for each training example (x, y):
for each $0 \le j \le m$:

gradient[j] +=
$$\left[y - \frac{1}{1 + e^{-\theta^T x}}\right] x_j$$

 $\theta_j += \eta * \text{gradient[j] for all } 0 \leq j \leq m$

- x_j is *j*-th feature of input var $x = (x_1, ..., x_m)$
- Insert $x_0 = 1$ before training
- Finish computing gradient before updating any part of θ
- Learning rate η is a constant you set before training

Testing: Classification with Logistic Regression

Training

Learn parameters
$$\theta = (\theta_0, \theta_1, \dots, \theta_m)$$

via gradient ascent: $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^n \left[y^{(i)} - \sigma \left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$

- Compute $\hat{y} = P(Y = 1 | X = x) = \sigma(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$
- Classify instance as:

Testing

 $\begin{cases} 1 \quad \hat{y} > 0.5, \text{ equivalently } \theta^T x > 0 \\ 0 \qquad \text{otherwise} \end{cases}$

A Parameters θ_i are <u>not</u> updated during testing phase

Naïve Bayes

Logistic Regression

- Chapter O: Background
- Chapter 1: Big Picture
- Chapter 2: Details
- Chapter 3: Philosophy

Introducing notation \hat{y}

Logistic Regression model:

$$\hat{y} = P(Y = 1 | X = x) = \sigma(\theta^T x)$$

$$P(Y = y | \mathbf{X} = \mathbf{x}) = \begin{cases} \hat{y} & \text{if } y = 1\\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$

Prediction:

$$\hat{Y} = \underset{y \in \{0,1\}}{\operatorname{arg\,max}} P(Y | \mathbf{X} = \mathbf{x}) = \begin{cases} 1 & \text{if } \hat{y} > 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Training: Learning the parameters via MLE

- 0. Add $x_0^{(i)} = 1$ to each $x^{(i)}$
- **1.** Logistic Regression model:

$$P(Y = 1 | \mathbf{X} = \mathbf{x}) = \hat{y}$$
$$\hat{y} = \sigma(\theta^T \mathbf{x})$$

- 2. Compute log-likelihood of training data: $LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^T x^{(i)}) + (1 y^{(i)}) \log (1 \sigma(\theta^T x^{(i)}))$
- 3. Compute derivative of log-likelihood with respect to each θ_j , j = 0, 1, ..., m:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)}$$

Training: Learning the parameters via MLE

- 0. Add $x_0^{(i)} = 1$ to each $x^{(i)}$
- 1. Logistic Regression model:

$$p(Y = 1 | \mathbf{X} = \mathbf{x}) = \hat{y}$$
$$\hat{y} = \sigma(\theta^T \mathbf{x})$$

- 2. Compute $LL(\theta) = \sum_{i=1}^{T} y^{(i)} \log \sigma \left(\theta^T \boldsymbol{x}^{(i)} \right) + \left(1 - y^{(i)} \right) \log \left(1 - \sigma \left(\theta^T \boldsymbol{x}^{(i)} \right) \right)$ log-likelihood of training data:
- 3. Compute derivative How did we get this likelihood function? log-likelihood with respect to each θ_i , j = 0, 1, ..., m:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)}$$

Log-likelihood of data

Logistic
Regression
model:
$$P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$
where $\hat{y} = \sigma(\theta^T x)$ $= (\hat{y})^y (1 - \hat{y})^{1-y}$ (see Bernoulli
MLE PMF)

$$L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)} | \mathbf{X} = \mathbf{x}^{(i)}, \theta)$$

- Actually conditional likelihood
- Still correctly gets correct θ_{MLE} since X, θ independent
- See lecture notes

Log-likelihood of data

Logistic
Regression
model:
$$P(Y = y | X = x) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$
where $\hat{y} = \sigma(\theta^T x)$ $= (\hat{y})^y (1 - \hat{y})^{1-y}$ (see Bernoulli
MLE PMF)

Likelihood
of training data:
$$L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)} | X = x^{(i)}, \theta) = \prod_{i=1}^{n} (\hat{y}^{(i)})^{y^{(i)}} (1 - \hat{y}^{(i)})^{1-y^{(i)}}$$

Log-likelihood:
$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})$$

$$= \sum_{i=1}^{n} y^{(i)} \log \sigma(\theta^{T} \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log(1 - \sigma(\theta^{T} \mathbf{x}^{(i)}))$$

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Training: Learning the parameters via MLE

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$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)}$$



Aside: Sigmoid has a beautiful derivative

Sigmoid function:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{d}{dz}\sigma(z) = \sigma(z)[1 - \sigma(z)]$$

What is
$$\frac{\partial}{\partial \theta_j} \sigma(\theta^T x)$$
?
A. $\sigma(x_j) [1 - \sigma(x_j)] x_j$
B. $\sigma(\theta^T x) [1 - \sigma(\theta^T x)] x$
C. $\sigma(\theta^T x) [1 - \sigma(\theta^T x)] x_j$
D. $\sigma(\theta^T x) x_j [1 - \sigma(\theta^T x) x_j]$
E. None/other



Derivative:

Aside: Sigmoid has a beautiful derivative


Compute gradient of log-conditional likelihood



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Compute gradient of log-likelihood

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \frac{\partial}{\partial \theta_j} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \qquad \text{Let } \hat{y}^{(i)} = \sigma(\theta^T \boldsymbol{x}^{(i)})$$

$$= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{y}^{(i)}} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \cdot \frac{\partial \hat{y}^{(i)}}{\partial \theta_{j}}$$

(Chain Rule)

$$= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} + (1 - y^{(i)}) \frac{1}{1 - \hat{y}^{(i)}} \right] \cdot \hat{y}^{(i)} (1 - \hat{y}^{(i)}) x_j^{(i)} \qquad \text{(calculus)}$$
$$= \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)} \right] x_j^{(i)} \qquad = \sum_{i=1}^{n} \left[y^{(i)} - \sigma(\theta^T \boldsymbol{x}^{(i)}) \right] x_j^{(i)} \qquad \text{(simplify)}$$

Compute gradient of log-likelihood

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^n \frac{\partial}{\partial \theta_j} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \qquad \text{Let } \hat{y}^{(i)} = \sigma(\theta^T \boldsymbol{x}^{(i)})$$

$$= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{y}^{(i)}} \left[y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}) \right] \cdot \frac{\partial \hat{y}^{(i)}}{\partial \theta_j}$$
(Chain Rule)

$$= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} + (1 - y^{(i)}) \frac{1}{1 - \hat{y}^{(i)}} \right] \cdot \hat{y}^{(i)} (1 - \hat{y}^{(i)}) x_j^{(i)}$$
(calculus)



Naïve Bayes

Logistic Regression

- Chapter O: Background
- Chapter 1: Big Picture
- Chapter 2: Details
- Chapter 3: Philosophy

Logistic Regression Model

$$P(Y = 1 | X = x) = \sigma(\theta^T x)$$
 where $\theta^T x = \sum_{j=0}^{m} \theta_j x_j$

Logistic Regression is trying to fit a <u>line</u> that separates data instances where y = 1 from those where y = 0:



m

- We call such data (or functions generating the data <u>linearly separable</u>.
- Naïve Bayes is linear too, because there is no interaction between different features.

Data is often not linearly separable





- Not possible to draw a line that successfully separates all the y = 1 points (green) from the y = 0 points (red)
- Despite this fact, Logistic Regression and Naive Bayes still often work well in practice

Many tradeoffs in choosing an algorithm

Modeling goal

Generative or discriminative?

Continuous input features

Discrete input features

Generative: could use joint distribution to generate new points (!but you might not need this extra effort)

Naïve Bayes

 $P(\boldsymbol{X},\boldsymbol{Y})$

Needs parametric form (e.g., Gaussian) or discretized buckets (for multinomial features)

Yes, multi-value discrete data = multinomial $P(X_i|Y)$

Lisa Yan, CS109, 2019

Logistic Regression P(Y|X)

Discriminative: just tries to discriminate y = 0 vs y = 1(cannot generate new points b/c no P(X, Y))

🗹 Yes, easily