CSE/STAT 416

Logistic Regression

Amal Nanavati University of Washington July 13, 2022

Adapted from Hunter Schafer's slides



Administrivia

- Week 5: Other ML models for classification
- Week 6: Deep Learning
- Homework 2 due yesterday
 Up to Thurs 11:59PM with late days
- HW3 Released today, due Tues 7/19 11:59PM
- Next week's homework, <u>HW4, will allow groups of up to 2</u> for the programming part!
 - See Ed for information about group formation!
- LR4 Due Fri 11:59PM

HW3 Walkthrough

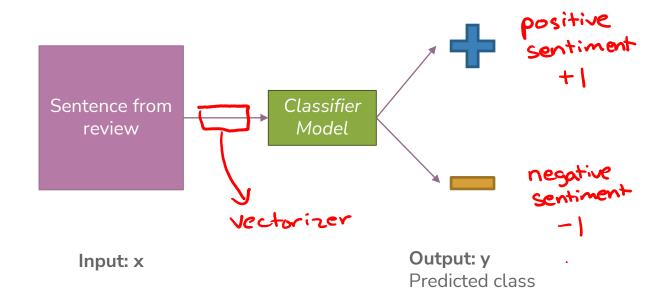
Recap: Intro to Classification

Continuing from Lec5

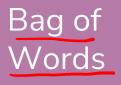
Sentiment Classifier



In our example, we want to classify a restaurant review as positive or negative.



Converting Text to Numbers (Vectorizing):





Idea: One feature per word!

Example: "Sushi was great, the food was awesome, but the service was terrible"

h. (x) h_2(x)

sushi	was	great	the	food	awesome	but	service	terrible
	3		2		l	1		1

This has to be too simple, right?

Stay tuned (today and V)(d) for issues that arise and how to address them
 week 7

Attempt 3: Linear Classifier

(Another View) Idea: Only predict the sign of the output!

Predicted Sentiment = $\hat{y} = sign(Score(x))$

Linear Classifier

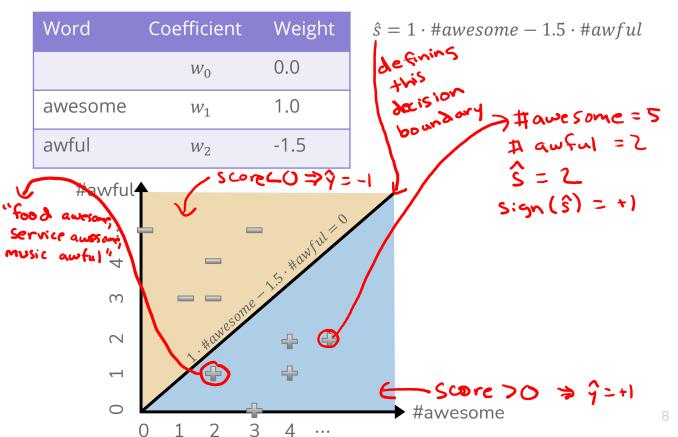
Input *x*: Sentence from review

- Compute Score(x)
- If Score(x) > 0: ← Threshold - $\hat{y} = +1$
- Else: - $\hat{v} = -1$

Earlier Example: Score (x) = 2 $\hat{y} = +1$

Decision Boundary

Consider if only two words had non-zero coefficients



Classification Error



Ratio of examples where there was a mistaken prediction

What's a mistake?

- If the true label was positive (y = +1), but we predicted negative $(\hat{y} = -1)$ -> False Negative
- If the true label was negative (y = -1), but we predicted positive $(\hat{y} = +1)$ \rightarrow False Positive

Classification Error <u><u><u></u></u><u>mistakes</u> <u><u></u><u>t</u><u>e</u><u>w</u>amples</u></u>

n 1 2 4 7

Classification Accuracy $\underbrace{\underbrace{\xi 1}_{\xi} \underbrace{\xi}_{Y_i} = \widehat{y_i}}_{\sharp examples} = 1 - error$

Confusion Matrix

For binary classification, there are only two types of mistakes

$$\hat{y} = +1, \ y = -1$$

$$\hat{y} = -1, y = +1$$

Generally we make a confusion matrix to understand mistakes.

C	- omplete the sev	itence: "my predic Predicte	tion was a " ed Label
		÷	
Frue Label	÷	True Positive (TP)	False Negative (FN)
Tru		False Positive (FP)	True Negative (TN)



Binary Classification Measures



Notation • $C_{TP} = \#TP$, $C_{FP} = \#FP$, $C_{TN} = \#TN$, $C_{FN} = \#FN$ $N = C_{TP} + C_{FP} + C_{TN} + C_{FN}$ $N_P = C_{TP} + C_{FN}, \quad N_N = C_{FP} + C_{TN}$ н. **Error Rate True Positive Rate or** Recall $C_{FP} + C_{FN}$ $\frac{C_{TP}}{N_P}$ Ν **Accuracy Rate** $C_{TP} + C_{TN}$ Precision Ν C_{TP} False Positive rate (FPR) $C_{TP} + C_{FP}$ $\frac{C_{FP}}{N_N}$ F1-Score $2\frac{Precision \cdot Recall}{2}$ False Negative Rate (FNR) Precison + Recall C_{FN} N_P See more!

Precision & Recall



Two particularly important metrics in binary classification are:

Precision: Of the ones I predicted positive, how many of them were actually positive?

- How precise is my model in its predictions?
- TP/(TP + FP) > num you predicted to be positive

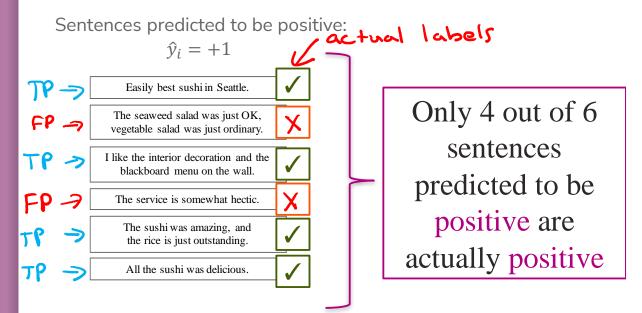
Recall: Of all the things that are truly positive, how many of them did I correctly predict as positive?

I num datapoints that are actually

- How good is your model at recalling the patterns in the training data?
- TP / (TP + FN)

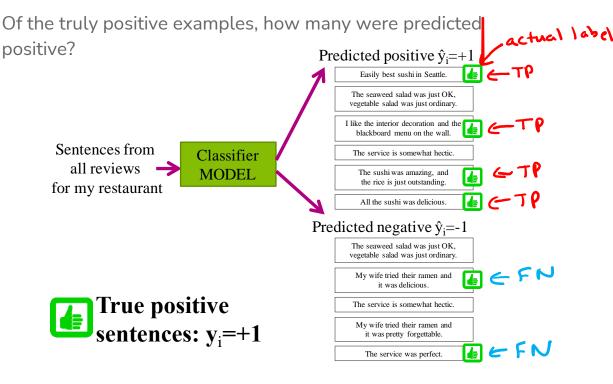
Precision

What fraction of the examples I predicted positive were correct?



 $precision = \frac{C_{TP}}{C_{TP} + C_{FP}} = \frac{4}{4 + 2} = \frac{4}{6}$

Recall



$$recall = \frac{C_{TP}}{N_P} = \frac{C_{TP}}{C_{TP} + C_{FN}} = \frac{4}{4 + 2} = \frac{4}{6}$$

Precision & Recall



There is a tradeoff between precision and recall!

An optimistic model will predict almost everything as positiveHigh recall, low precision

A pessimistic model will predict almost everything as negative

High precision, low recall



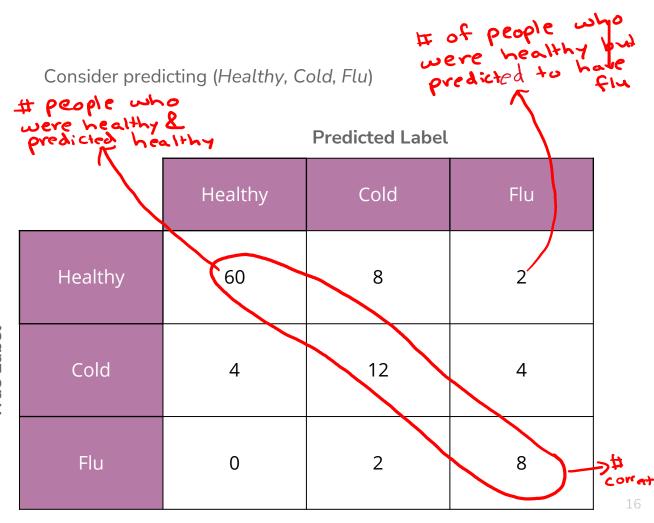
Finds few positive sentences, but includes no false positives Finds all positive sentences, but includes many false positives



..

Multiclass Confusion Matrix





I Poll Everywhere

1 min



Suppose we trained a classifier and computed its confusion matrix on the training dataset. Is there a class imbalance in the dataset and if so, which class has the highest representation?

Predicted Label

	Pupper	Doggo	Woofer
Pupper	2	27	4
Doggo	4	25	4
Woofer	1	30	2





2 min

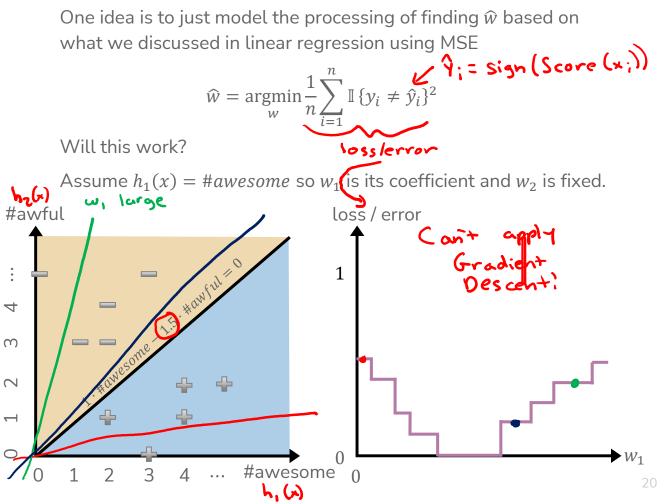


Suppose we trained a classifier and computed its confusion matrix on the training dataset. Is there a class imbalance in the dataset and if so, which class has the highest representation?

		Pr	redicted Lab	7395 a 0998 27% no imbolore	
		Pupper	Doggo	Woofer	Pair 55% doggo 45% no imbalorr
le	Pupper	2	27	4	333 use no imbalore
True Label	Doggo	4	25	4	333 Total # in dataset
Tr	Woofer	1	30	2	333 label
	Total # model predicted to be that class	7	82	10	2:00

Logistic Regression Can we use MSE for classification task?





Quality Metric for Classification

The MSE loss function doesn't work because of different reasons:

- The outputs are discrete values with no ordered nature, so we need a different way to frame how close a prediction is to a certain correct category
- The MSE loss function for classification task is not continuous, differentiable or convex, so we can't use optimization algorithm like Gradient Descent to find an optimal set of weights

Note: Convexity is an important concept in Machine Learning. By minimizing error, we want to find where that global minimum is, and that's ideal in a convex function.

Let's frame this problem in term of probabilities instead.

Probabilities

$$P(y|x) = \begin{cases} P(y=+1|x) \\ if y = 1 \\ P(y=-1|x) \\ if y = -1 \end{cases}$$

P(y=1 1x) probability that the true label is positive for x

Assume that there is some randomness in the world, and instead will try to model the probability of a positive/negative label.

Examples:

P(y=+1|x)+P(y=-1|x) = 1

"The sushi & everything else were awesome!"

- Definite positive (+1)
- P(y = +1 | x = "The sushi & everything else were awesome!") = 0.99

"The sushi was alright, the service was OK"

- Not as sure
- P $\left(y = -1 \mid x = "The sushi alright, the service was okay!"\right) = 0.5$

Use probability as the measurement of certainty P(y|x)

Probability Classifier



Idea: Estimate probabilities $\hat{P}(y|x)$ and use those for prediction

Probability Classifier

Input *x*: Sentence from review

- Estimate class probability $\hat{P}(y = +1|x)$
- If $\hat{P}(y = +1|x) > 0.5$: threshold - $\hat{y} = +1$
- Else: - $\hat{y} = -1$

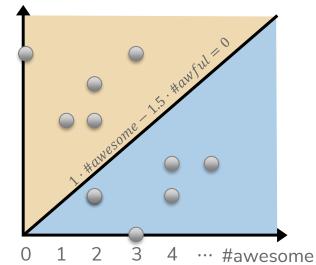
Notes:

- Estimating the probability improves interpretability.
 - Unclear how much better a score of 5 is from a score of 3. Clear how much better a probability of 0.75 is than a probability of 0.5

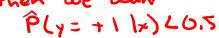
Connecting Score & Probability

Idea: Let's try to relate the value of Score(x) to $\hat{P}(y = +1|x)$

#awful



What if Score(x) is positive? If $Score(x) \ge 0$, then we want $\hat{P}(y = +1 | x) \ge 0.5$ What if Score(x) is negative? If $Score(x) \le 0$, then we want

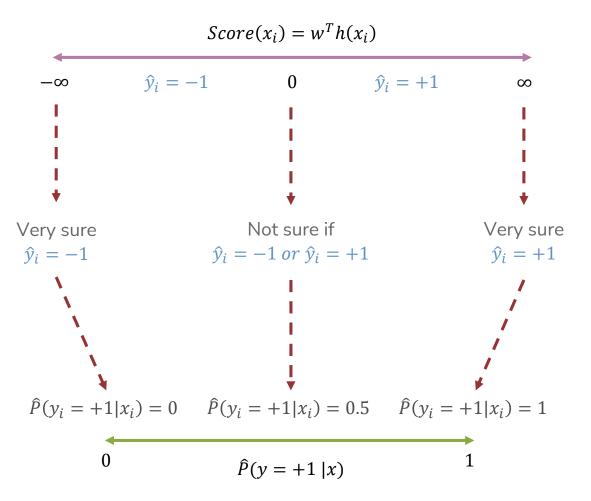


What if Score(x) is 0?

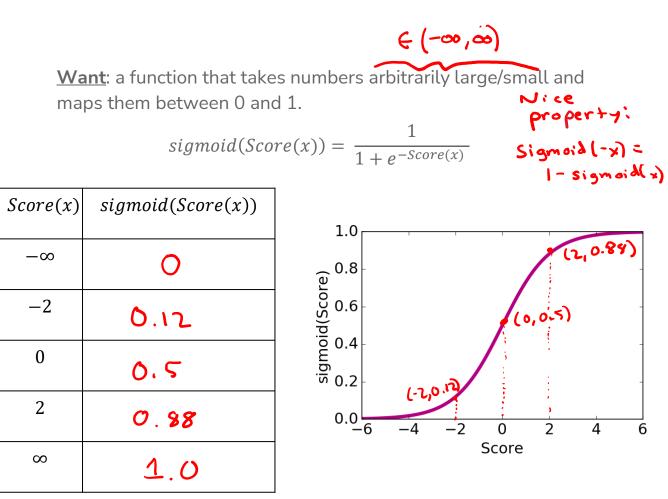
we want +1 12)=0.5

Connecting Score & Probability

 $\nabla 0$



Logistic Function



Logistic Regression Model

 $P(y_i = +1|x_i, w) = sigmoid(Score(x_i)) = \frac{1}{1 + e^{-w^T h(x_i)}}$

Logistic Regression Classifier

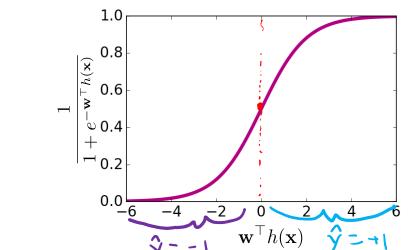
Input *x*: Sentence from review

Estimate class probability $\hat{P}(y = +1|x, \hat{w}) = sigmoid(\hat{w}^T h(x_i))$

If
$$\hat{P}(y = +1|x, \hat{w}) > 0.5$$

 $\hat{y} = +1$

 $\hat{y} = -1$



Poll Everywhere

Think &

1 min

P(y=+1 |x,w) = sigmoid (score(x))

What would the Logistic Regression model predict for P(y = -1 | x, w)?

- "Sushi was great, the food was awesome, but the service was terrible"
- a) ≈ 0
- b) sigmoid(-2) ≈ 0.12
- c) ≈ 0.5
- d) sigmoid(2) ≈ 0.88

e) ≈ 1

	$h_1(x)$	$h_2(x)$	$h_3(x)$	$h_4(x)$	$h_5(x)$	$h_6(x)$	$h_7(x)$	$h_8(x)$	$h_9(x)$
	sushi	was	great	the	food	awesome	but	service	terrible
ł	1	3	1	2	1	1	1	1	1

Word	Weight
sushi	0
was	0
great	1
the	0
food	0
awesome	2
but	0
service	0
terrible	-1

Doll Everywhere
Group 22
2 min

P(y=+1|x,w) = sigmoid(score(x))

Score = wTh(x)

= 1 + 2 + 1 +

-1.1

2

What would the Logistic Regression model predict for P(y = -1 | x, w)?

- "Sushi was great, the food was awesome, but the service was terrible"
- a) ≈ 0
- b) sigmoid(-2) ≈ 0.12
- c) ≈ 0.5
- d) sigmoid(2) ≈ 0.88

e) ≈ 1

$h_1(x)$	$h_2(x)$	$h_3(x)$	$h_4(x)$	$h_5(x)$	$h_6(x)$	$h_7(x)$	$h_8(x)$	$h_9(x)$
sushi	was	great	the	food	awesome	but	service	terrible
1	3	1	2	1	1	1	1	1

Word	Weight
sushi	0
was	0
great	1
the	0
food	0
awesome	2
but	0
service	0
terrible	-1

Group 오울오
2 min
$ \begin{array}{c} & & \\ & & $

Poll Everywhere

P(y=+1 | x, w) = sigmoid(score(x))

Score = wTh(x)

-1.1

What would the Logistic Regression model predict for P(y = -1 | x, w)?

"Sushi was great, the food was awesome, but the service was terrible"

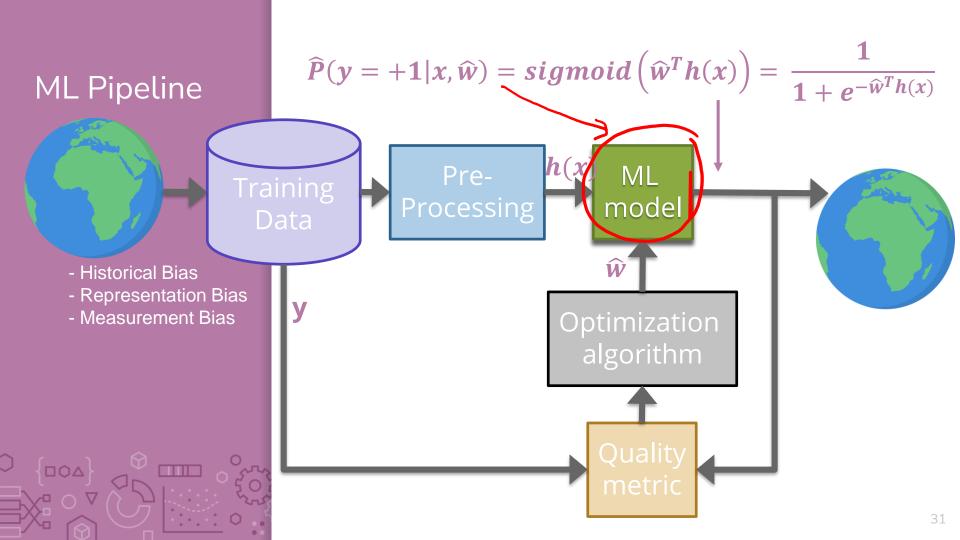
 ≈ 0

- b) $sigmoid(-2) \approx 0.12$ = |-|+2.1+
 - c) ≈ 0.5
- d) sigmoid(2) ≈ 0.88

e)
$$\approx 1$$

 $P(y=+1|x,w) = sigmoid(2)$
 $P(y=-1|x,w) = 1 - P(y=+1|x,w)$
 $= 1 - sigmoid(2)$
 $= sigmoid(-2)$

Word	Weight
sushi	0
was	0
great	1
the	0
food	0
awesome	2
but	0
service	0
terrible	-1



Demo



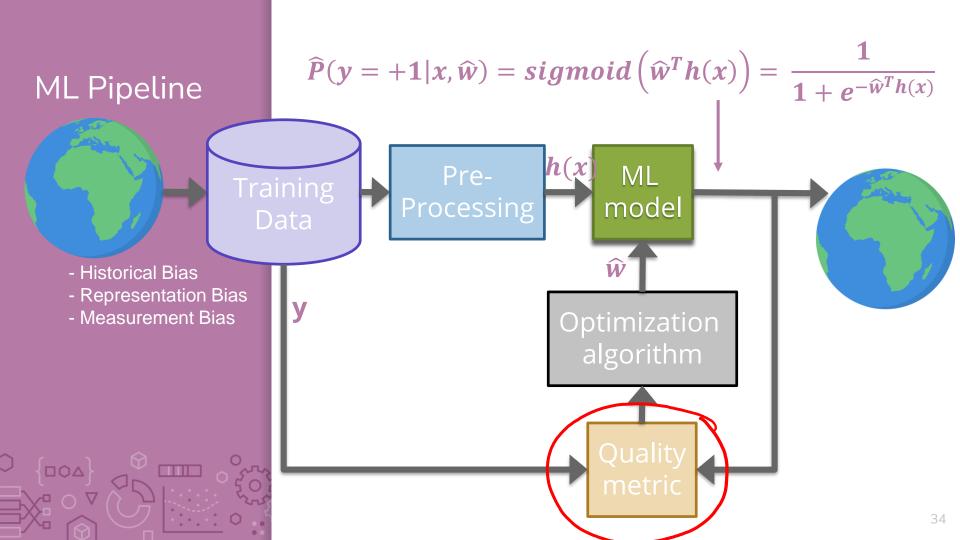
Show logistic demo (see course website)





3:33





Quality Metric = Maximum Likelihood Estimate

Quality Metric = Likelihood

$$P(y_{i} = + | | x_{i} \omega) = \frac{1}{1 + e^{-\omega^{T}h(x_{i})}} P(y_{i} = -1 | x_{i} \omega) = \frac{e^{-\omega^{T}h(x_{i})}}{1 + e^{-\omega^{T}h(x_{i})}}$$

Want to compute the probability of seeing our dataset for every possible setting for w. Find w that makes data most likely!

	\sim		~~~	
Data Point	$h_1(x)$	$h_2(x)$	У	Choose <i>w</i> to maximize
$x^{(1)}, y^{(1)}$	2	1	+1	$P(y^{(1)} = +1 x^{(1)}, w)$
$x^{(2)}, y^{(2)}$	0	2	-1	$P(y^{(2)} = -1 x^{(2)}, w)$
$x^{(3)}$, $y^{(3)}$	3	3	-1	$P(y^{(3)} = -1 x^{(3)}, w)$
x ⁽⁴⁾ , y ⁽⁴⁾	4	1	+1	$P(y^{(4)} = +1 x^{(4)}, w)$
01.2 -			P1~ 1	$\mathbf{x} \mapsto \mathbf{P}(\mathbf{y}) \times \mathbf{P}(\mathbf{y})$

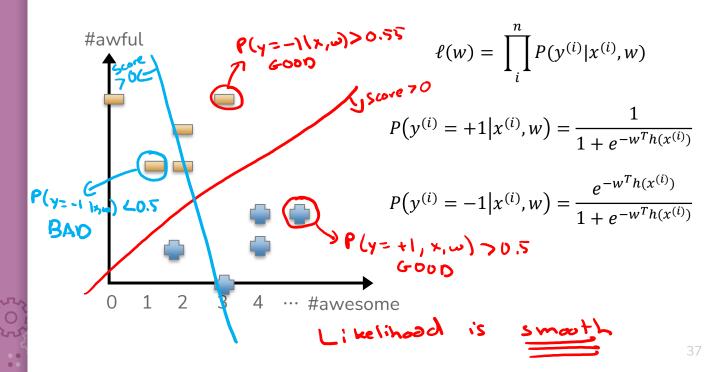
$$\mathcal{L}(\omega) = \mathcal{P}(y_1 | x_1, \omega) \cdot \mathcal{P}(y_2 | x_2, \omega) \cdot \mathcal{P}(y_3 | x_3, \omega) \cdot \mathcal{P}(y_4 | x_4, \omega)$$
$$= \prod_{i=1}^{\infty} \mathcal{P}(y_i | x_i, \omega)$$

Learn \widehat{w}

likelihood of seeing data given the predictor is high likelihood of seeing data given predictor is <u>low</u>

Now that we have our new model, we will talk about how to choose \widehat{w} to be the "best fit".

The choice of w affects how likely seeing our dataset is



Maximum Likelihood Estimate (MLE)

Find the *w* that maximizes the likelihood

$$\widehat{w} = \underset{w}{\operatorname{argmax}} \ell(w) = \underset{w}{\operatorname{argmax}} \prod_{i=1}^{n} P(y_i | x_i, w)$$

Generally, we maximize the log-likelihood which looks like

$$\widehat{w} = \underset{w}{\operatorname{argmax}} \ell(w) = \underset{w}{\operatorname{argmax}} \log(\ell(w)) = \underset{w}{\operatorname{argmax}} \sum_{i=1}^{n} \log(P(y_i|x_i, w))$$

Also commonly written by separating out positive/negative terms

$$\widehat{w} = \underset{w}{\operatorname{argmax}} \sum_{i=1:y_i=+1}^{n} \ln\left(\frac{1}{1+e^{-w^{T}h(x)}}\right) + \sum_{i=1:y_i=-1}^{n} \ln\left(1-\frac{1}{1+e^{-w^{T}h(x)}}\right)$$

$$\underset{for \ pos \ terms}{\overset{og \ P(y_i=+1 \ x_iw)}{\overset{og \ P(y_i=-1 \ x_iw)}{$$

Likelihood vs Error/Loss

- In understanding how to measure error for the classification problem, we want to understand how close a prediction is to the correct class, which means we want to assign a high probability for a correct prediction, and low probability for an incorrect prediction
- Likelihood and error are the inverse of each other:
 Maximizing likelihood = Minimizing Error



I Poll Everywhere

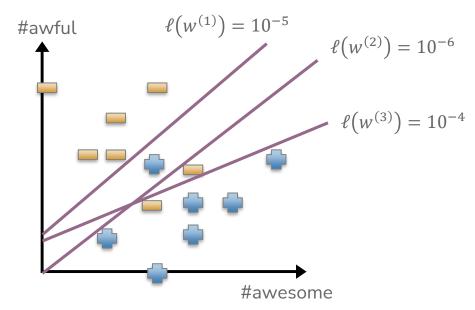
Think &

1 min



SKIPPED

Which setting of w should we use?

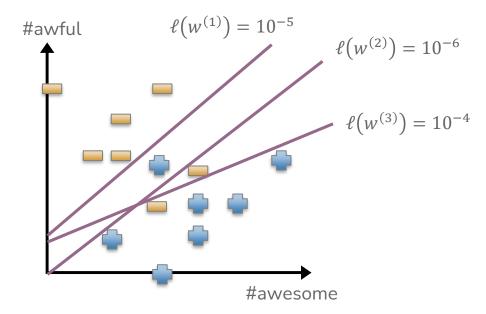


Poll Everywhere Group နိုန္နီ

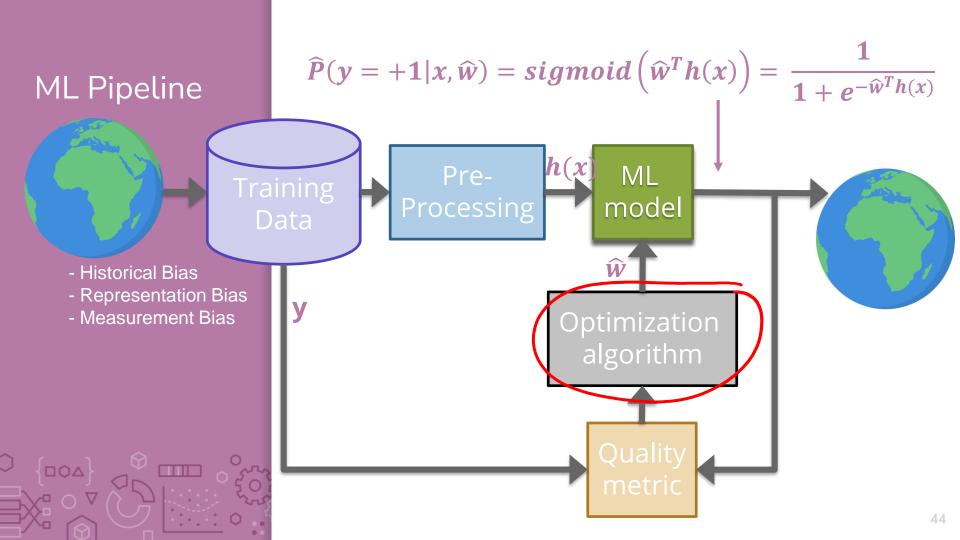


SKIPPED

Which setting of w should we use?



Revisiting Gradient Descent / Ascent



Is Gradient Descent <u>Really</u> Used in Linear Regression?



- No!
- It can be, but isn't in practice.
- Linear regression has a closed form solution. The best weights are:

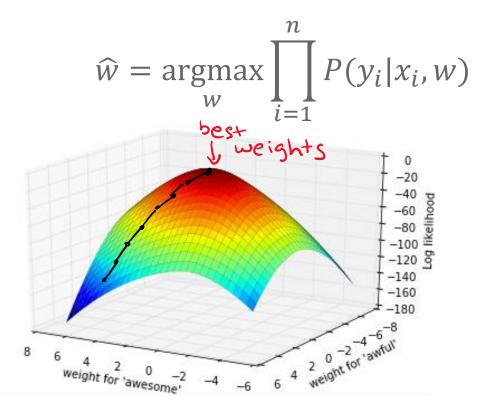
$$\widehat{w} = (XX^T)^{-1}X^T y$$

- You don't need to know the formula. What you need to know is that for Linear Regression a closed-form solution, or a solution we can write out with simple mathematical expressions, exists.
- This is not the case with Logistic Regression.
 We <u>must</u> use Gradient Ascent/Descent!

Finding MLE

No closed-form solution, have to use an iterative method.

Since we are **maximizing** likelihood, we use gradient **ascent**.



Gradient Ascent



Gradient ascent is the same as gradient descent, but we go "up the hill".

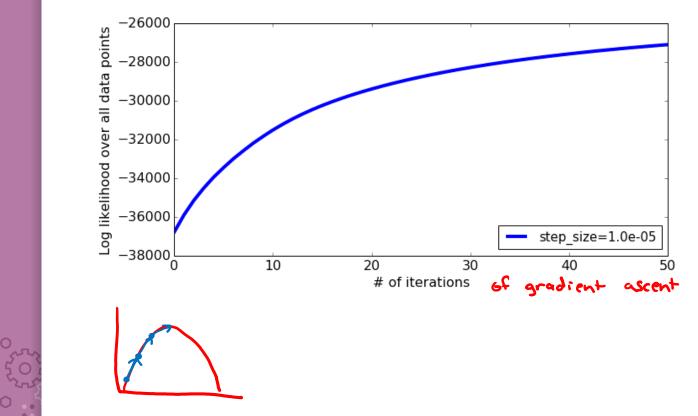
start at some (random) point
$$w^{(0)}$$
 when $t = 0$
while we haven't converged
 $w^{(t+1)} \leftarrow w^{(t)} + \eta \nabla \ell(w^{(t)})$
 $t \leftarrow t+1$ Gradient of like libood
learning rate

This is just describing going up the hill step by step.

 η controls how big of steps we take, and picking it is crucial for how well the model you learn does!

Learning Curve

 ∇

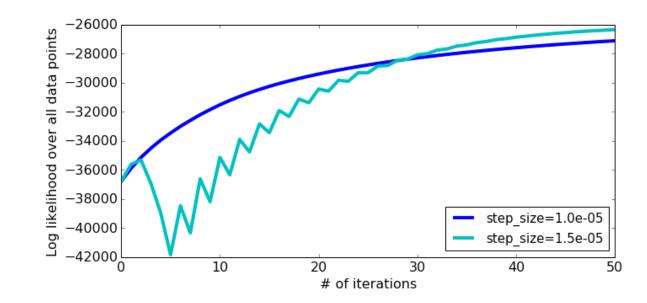


-26000 Log likelihood over all data points -28000 -30000 -32000 -34000 -36000 step_size=1.0e-06 step_size=1.0e-05 –38000∟ 0 10 20 30 40 50 # of iterations

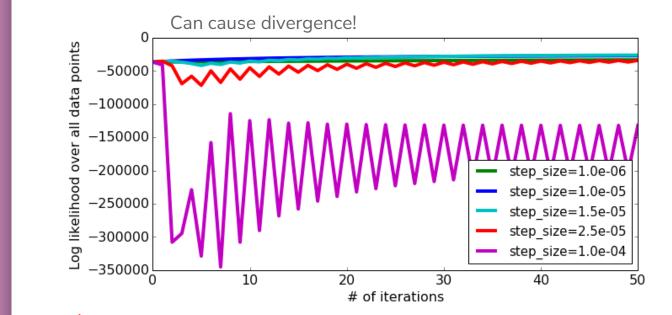
Step-size too small



What about a larger step-size?







What about a larger step-size?



Unfortunately, you have to do a lot of trial and error \otimes

Try several values (generally exponentially spaced)

Find one that is too small and one that is too large to narrow search range. Try values in between!

Advanced: Divergence with large step sizes tends to happen at the end, close to the optimal point. You can use a decreasing step size to avoid this

$$\eta_t = \frac{\eta_0}{t} \qquad \text{annealing}$$

Grid Search

We have introduced yet another hyperparameter that you have to choose, that will affect which predictor is ultimately learned.

If you want to tune multiple hyperparameters at once (e.g., both a Ridge penalty and a learning rate), you will need to try all pairs of settings!

- For example, suppose you wanted to try using a validation set to select the right settings out of:
 - $\lambda \in [0.01, 0.1, 1, 10, 100] = 5$
 - $\eta_t \in \left[0.001, 0.01, 0.1, 1, \frac{1}{t}, \frac{10}{t}\right] \to 6$
- You will need to train 30 different models and evaluate each one!

Train 5.6=30 models

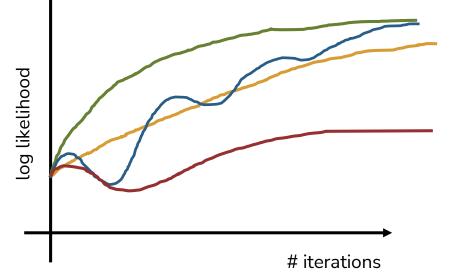
I Poll Everywhere

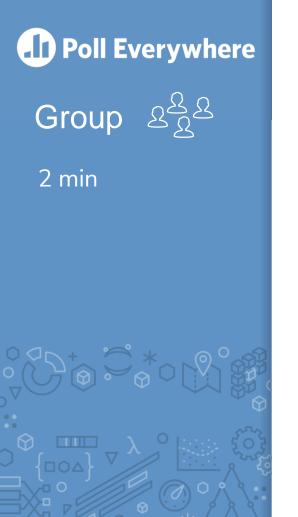
1 min



SKIPPED

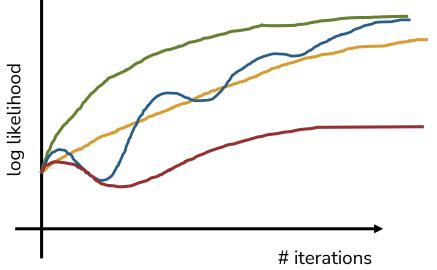
- Match the below lines to the following labels:
 - "Very High Learning Rate"
 - "High Learning Rate"
 - "Good Learning Rate"
 - "Low Learning Rate"





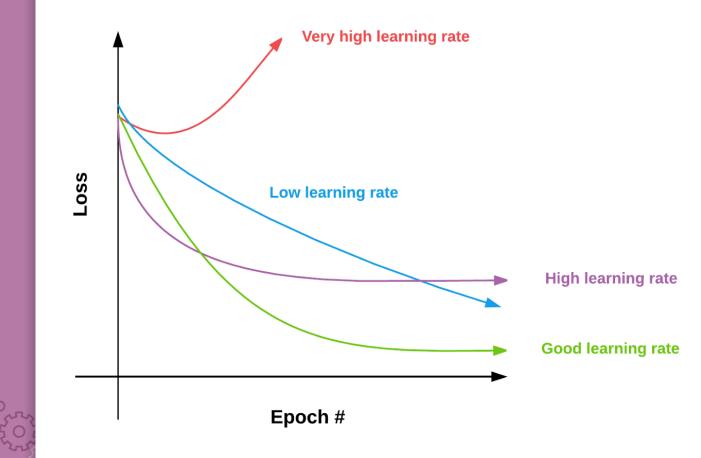
SKIPPED

- Match the below lines to the following labels:
 - "Very High Learning Rate"
 - "High Learning Rate"
 - "Good Learning Rate"
 - "Low Learning Rate"



Likelihood vs. Loss

 $\bigcirc \nabla$



Overfitting -Classification

More Features



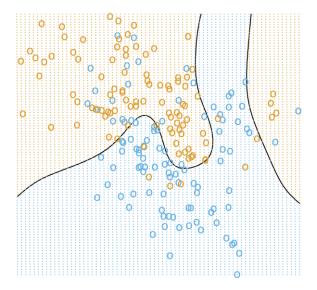
Linear

Like with regression, we can learn more complicated models by including more features or by including more complex features.

Instead of just using $h_1(x) = \#awesome$ $h_2(x) = \#awful$

We could use $h_1(x) = \#awesome$ $h_2(x) = \#awful$ $h_3(x) = \#awesome^2$ $h_4(x) = \#awful^2$

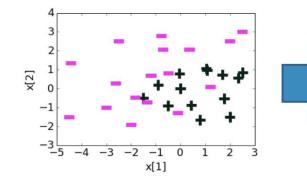
. . .

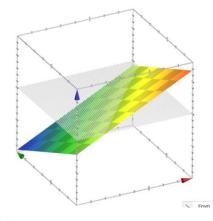


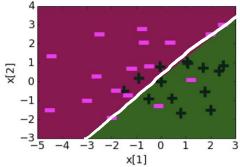


$w^{T}h(x) = 0.23 + 1.12x[1] - 1.07x[2]$

Feature	Value	Coefficient learned
h ₀ (x)	1	0.23
h ₁ (x)	x[1]	1.12
h ₂ (x)	x[2]	-1.07

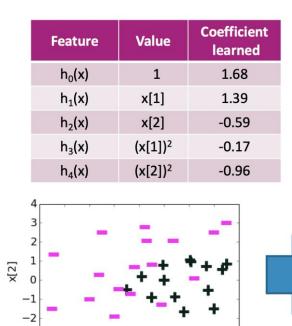








$w^{T}h(x) = 1.68 + 1.39x[1] - 0.59x[2] - 0.17x[1]^{2} - 0.96x[2]^{2}$



x[1]

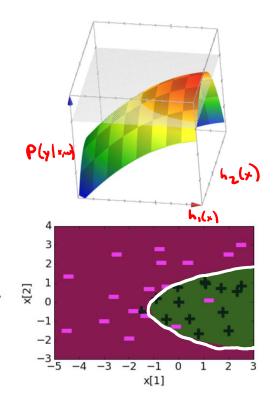
2 3

1

-3∟ -5

-4

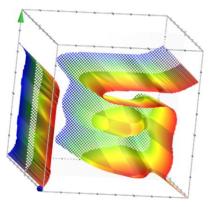
-3 -2 -1 0

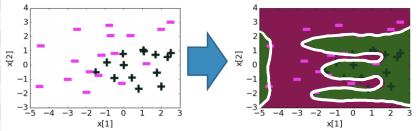




Feature	Value	Coefficient learned
h _o (x)	1	21.6
h1(x)	x[1]	5.3
h ₂ (x)	x[2]	-42.7
h₃(x)	(x[1]) ²	-15.9
h ₄ (x)	(x[2]) ²	-48.6
h₅(x)	(x[1]) ³	-11.0
h ₆ (x)	(x[2]) ³	67.0
h ₇ (x)	(x[1]) ⁴	1.5
h ₈ (x)	(x[2]) ⁴	48.0
h ₉ (x)	(x[1]) ⁵	4.4
h ₁₀ (x)	(x[2])⁵	-14.2
h ₁₁ (x)	(x[1]) ⁶	0.8
h ₁₂ (x)	(x[2]) ⁶	-8.6

$$w^T h(x) = \cdots$$





 $\bigcirc \nabla$

Feature
 Value
 Coefficient
learned

$$h_0(x)$$
 1
 8.7

 $h_1(x)$
 x[1]
 5.1

 $h_2(x)$
 x[2]
 78.7

 ...
 ...
 ...

 $h_{11}(x)$
 (x[1])⁶
 -7.5

 $h_{12}(x)$
 (x[2])⁶
 3803

 $h_{13}(x)$
 (x[1])⁷
 21.1

 $h_{14}(x)$
 (x[2])⁷
 -2406

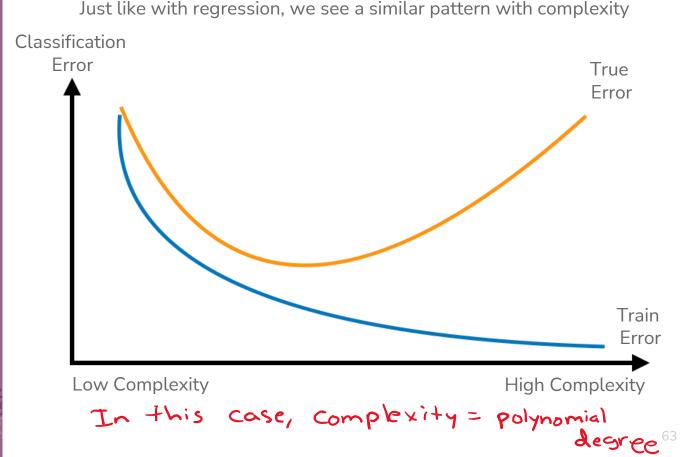
 ...
 ...
 ...

 $h_{37}(x)$
 (x[1])¹⁹
 -2*10⁻⁶
 $h_{38}(x)$
 (x[2])¹⁹
 -0.15

 $h_{39}(x)$
 (x[1])²⁰
 -2*10⁻⁸
 $h_{40}(x)$
 (x[2])²⁰
 0.03

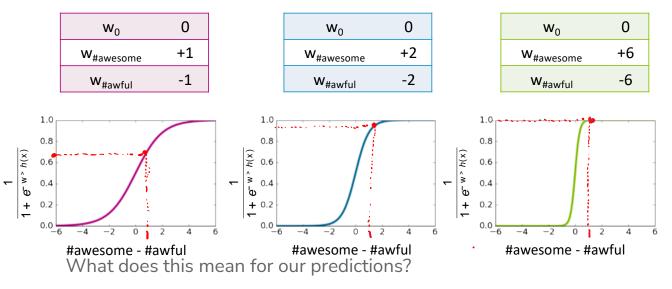
$$w^T h(x) = \cdots$$

Overfitting



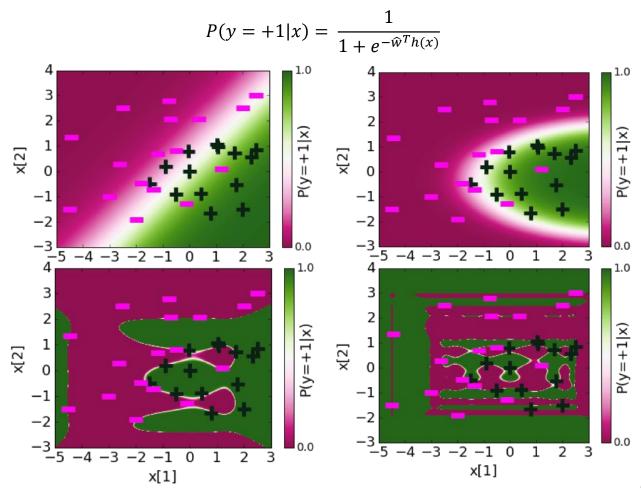
Effects of Overfitting

The logistic function become "sharper" with larger coefficients.



Because the Score(x) is getting larger in magnitude, the probabilities are closer to 0 or 1!

Plotting Probabilities



I Poll Everywhere

0.5 mins



SKIPPED

- What ideas do you have for preventing overfitting in Logistic Regression?
 - (Many possible answers)



- What ideas do you have for preventing overfitting in Logistic Regression?
 - (Many possible answers)

Regression Some as in

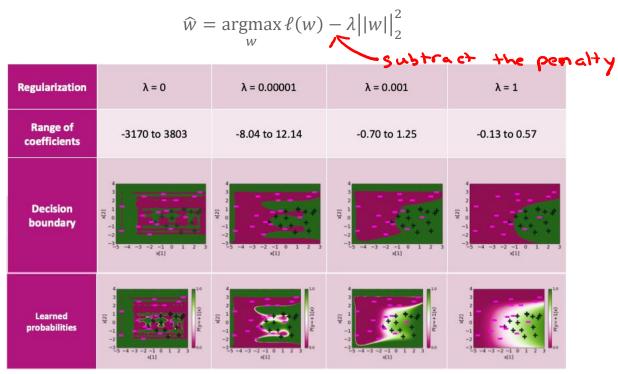


Regularization



L2 Regularized Logistic Regression

Just like in regression, can change our quality metric **<u>during</u> <u>training</u>** to lower the likelihood of learning an overfit model





Some Details

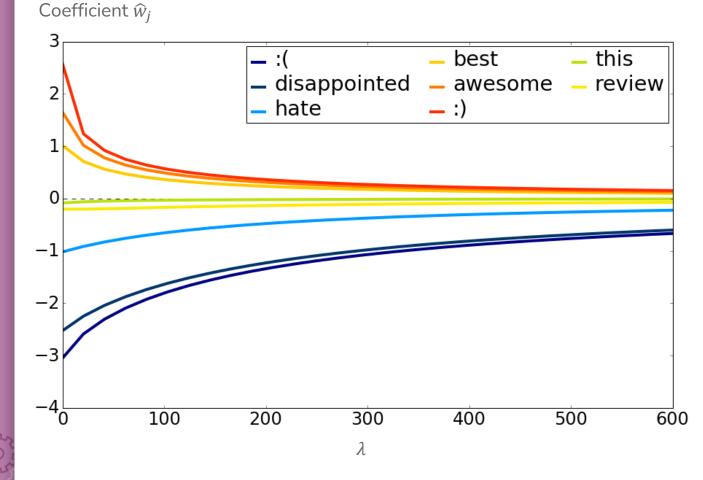
Why do we subtract the L2 Norm?

$$\widehat{w} = \underset{w}{\operatorname{argmax}} \ell(w) - \lambda \big| |w| \big|_{2}^{2}$$

How does λ impact the complexity of the model?

How do we pick λ ?

Coefficient Path: L2 Penalty



Other Regularization Penalties?

Could you use the L1 penalty instead? Absolutely!

 $\widehat{w} = \operatorname*{argmax}_{w} \ell(w) - \lambda \big| |w| \big|_{1}$

This is **L1 regularized logistic regression**

It has the same properties as the LASSO

- Increasing λ decreases $||\widehat{w}||_{1}$
- The L1 penalty favors sparse solutions

I Poll Everywhere

1 min



- Max wants to find the best Logistic Regression model for a sentiment analysis dataset by tuning the regularization parameter $\lambda \in [0, 10^{-2}, 10^{-1}, 1, 10]$ and the learning rate $\eta \in [10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}]$. He does the following:
 - Runs cross-validation on λ to get the best value for the regularization parameter.
 - For that value of λ , run cross-validation on η to get the best value for the learning rate.
- After running this procedure, he is convinced he has the best Logistic Regression model for his dataset, given the hyper-parameter values he wanted to test.
- What did Max do wrong?

Poll Everywhere

2 min

Group



- Max wants to find the best Logistic Regression model for a sentiment analysis dataset by tuning the regularization parameter $\lambda \in [0, 10^{-2}, 10^{-1}, 1, 10]$ and the learning rate $\eta \in [10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}]$. He does the following:
 - Runs cross-validation on λ to get the best value for the regularization parameter.
 - For that value of λ , run cross-validation on η to get the best value for the learning rate.
- After running this procedure, he is convinced he has the best Logistic Regression model for his dataset, given the hyper-parameter values he wanted to test.
- What did Max do wrong?

Recap

Theme: Details of logistic classification and how to train it Ideas:

- Predict with probabilities
- Using the logistic function to turn Score to probability
- Logistic Regression
- Minimizing error vs maximizing likelihood
- Gradient Ascent
- Effects of learning rate
- Overfitting with logistic regression
 - Over-confident (probabilities close to 0 or 1)
 - Regularization