CSE/STAT 416

Logistic Regression

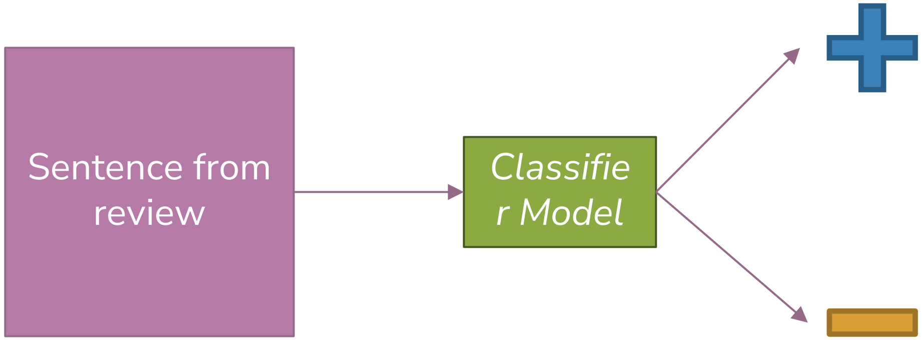
Pre-Class Videos

Tanmay Shah
University of Washington

July 3, 2024

Sentiment Classifier

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



Features

#awesome

#awful

⋮

Input: x

"sentence"

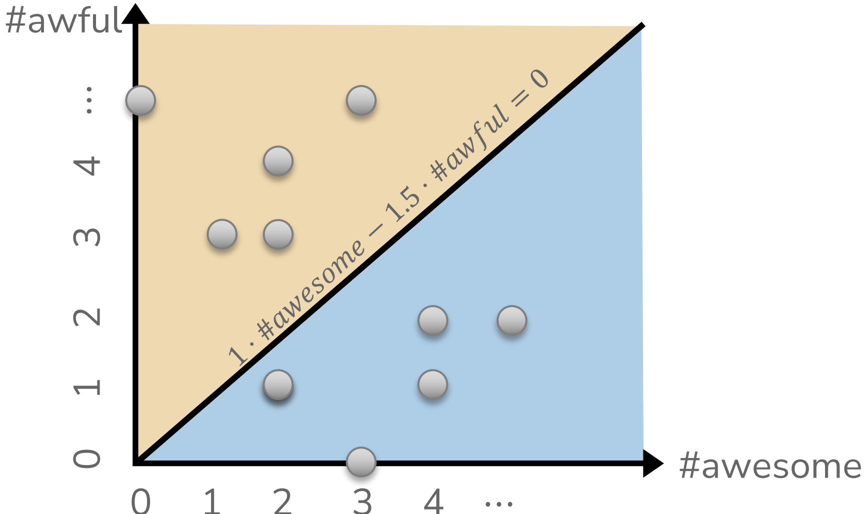
Output: y
Predicted class

Decision Boundary

Consider if only two words had non-zero coefficients

Word	*Coefficient*	*Weight*
	w_0	*0.0*
awesome	w_1	*1.0*
awful	w_2	*-1.5*

$$\hat{s} = 1 \cdot \#awesome - 1.5 \cdot \#awful$$



Learning $\hat{w}$

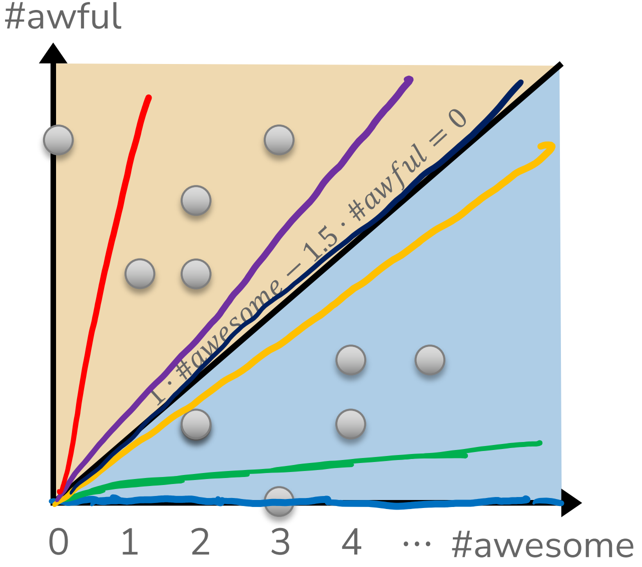
All the Same?

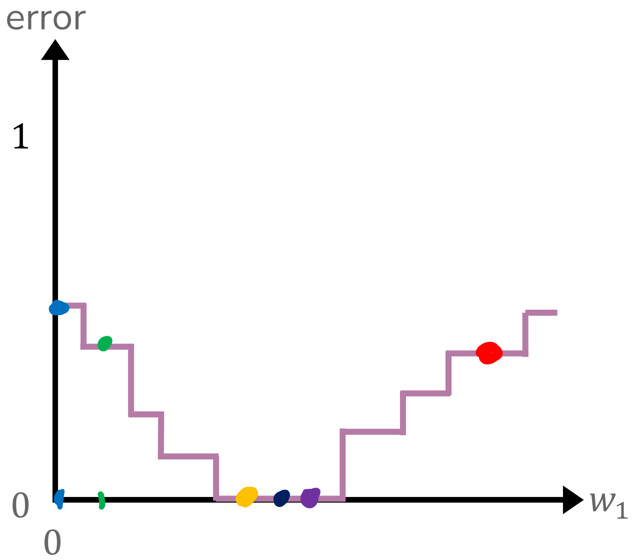
One idea is to just model the processing of finding $\hat{w}$ based on what we discussed in linear regression

$$\hat{w} = \underset{w}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{y_i \neq \hat{y}_i\}$$

Will this work?

Assume $h_1(x) = \#awesome$ so w_1 is its coefficient and w_2 is fixed.





Minimizing Error

Minimizing classification error is probably the most intuitive thing to do given all we have learned from regression. However, it just doesn't work in this case with classification.

We aren't able to use a method like gradient descent here because the function isn't "nice" (it's not continuous, it's not differentiable, etc.).

We will use a stand-in for classification error that will allow us to use an optimization algorithm. But first, we have to change the problem we care about a bit.

Instead of caring about the classifications, let's look at some probabilities

Probabilities

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

$$P(y=+1 \mid x) + P(y=-1 \mid x) = 1$$

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

Examples:

"The sushi & everything else were awesome!"

Definite positive (+1)

$$P\left(y = +1 \mid x = \text{“The sushi \& everything else were awesome!”}\right) = 0.99$$

$$P(y=+1 \mid x = \text{“...”}) \in [0,1]$$

"The sushi was alright, the service was OK"

Not as sure

$$P\left(y = -1 \mid x = \text{“The sushi alright, the service was okay!”}\right) = 0.5$$

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

- $\hat{y} = +1$

Else:

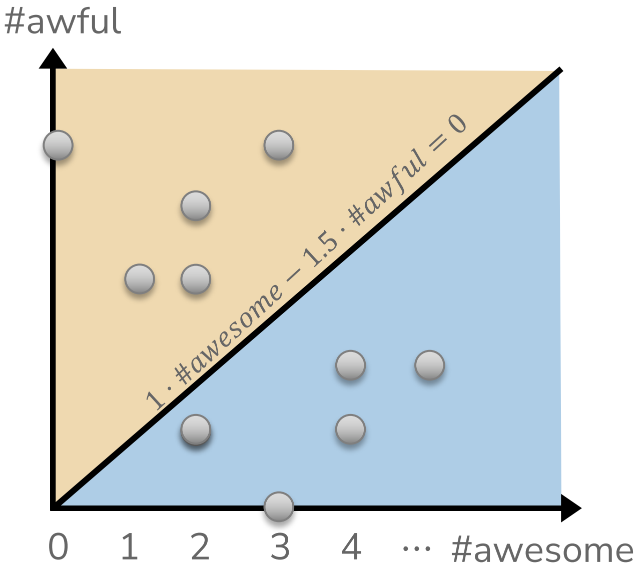
- $\hat{y} = -1$

Notes:

Estimating the probability improves **interpretability**

Score Probabilities?

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



What if $Score(x)$ is positive?

$P(y=+1 \mid x) > 1/2$

What if $Score(x)$ is negative?

$P(y=-1 \mid x) > 1/2$

equiv

$P(y=+1 \mid x) < 1/2$

What if $Score(x)$ is 0?

$P(y=+1 \mid x) = 1/2$

Interpreting Score

$$Score(x_i) = w^T h(x_i)$$

$-\infty$ $\quad \hat{y}_i = -1 \quad$ 0 $\quad \hat{y}_i = +1 \quad$ ∞

Very sure
$\hat{y}_i = -1$

Not sure if
$\hat{y}_i = -1 \; or \; \hat{y}_i = +1$

Very sure
$\hat{y}_i = +1$

$\hat{P}(y_i = +1|x_i) = 0$ $\quad \hat{P}(y_i = +1|x_i) = 0.5$ $\quad \hat{P}(y_i = +1|x_i) = 1$

0 $\quad \hat{P}(y = +1\,|x) \quad$ 1

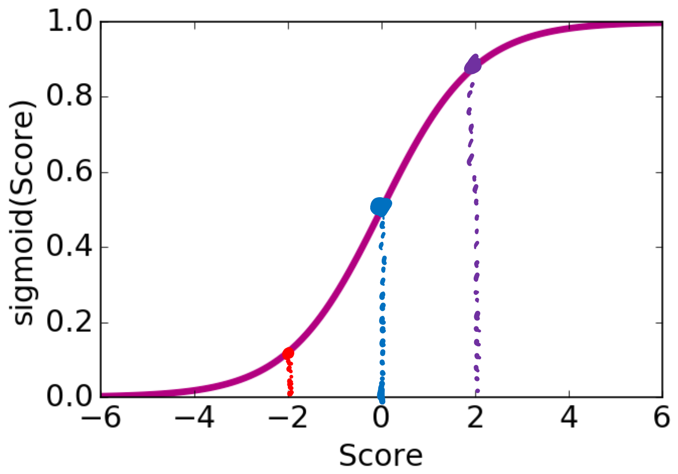
Logistic Function

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

Use a function that takes numbers arbitrarily large/small and maps them between 0 and 1.

$$sigmoid(Score(x)) = \frac{1}{1 + e^{-Score(x)}}$$

$Score(x)$	$sigmoid(Score(x))$
$-\infty$	$\frac{1}{1+e^{--\infty}} = \frac{1}{1+e^{\infty}} = 0$
-2	≈ 0.12
0	$\frac{1}{1+e^{-0}} = \frac{1}{1+1} = \frac{1}{2}$
2	≈ 0.88
∞	$\frac{1}{1+e^{-\infty}} = \frac{1}{1+1/e^{\infty}} = \frac{1}{1}$



Logistic Regression Model

$Score(x) = w^T h(x)$

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

Logistic Regression Classifier

Input x: Sentence from review

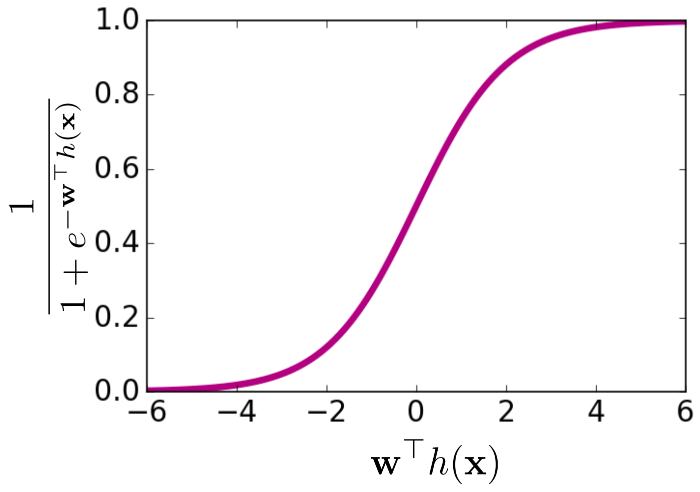
Estimate class probability $\hat{P}(y = +1 | x, \hat{w}) = sigmoid(\hat{w}^T h(x_i))$

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

- $\hat{y} = +1$

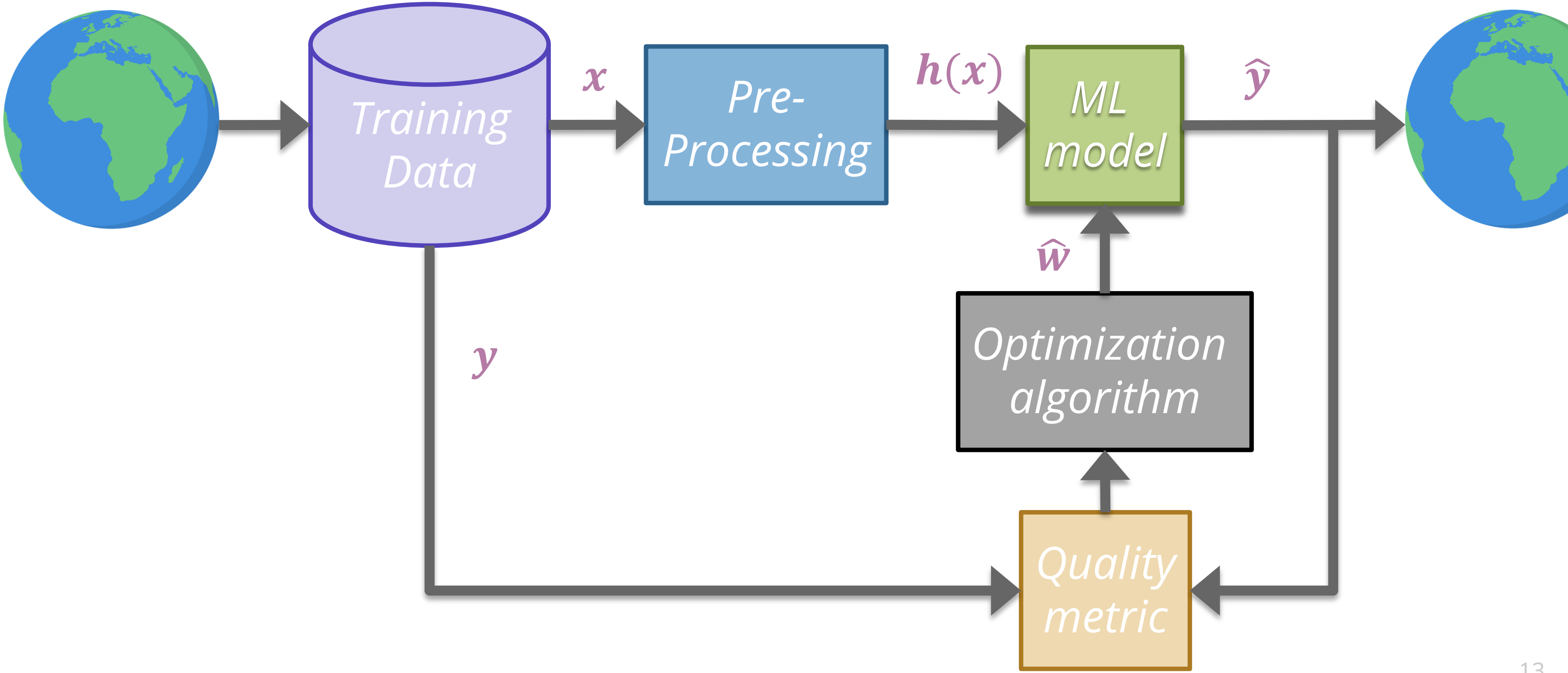
Else:

- $\hat{y} = -1$



ML Pipeline

$$\hat{P}(y=+1|x,\hat{w}) = sigmoid\left(\hat{w}^T h(x)\right) = \frac{1}{1+e^{-\hat{w}^T h(x)}}$$



CSE/STAT 416

Logistic Regression

Tanmay Shah
University of Washington
June 3, 2024

❓ **Questions?** Raise hand or **sli.do #cs416**
💬 **Before Class:** Does a straw have two holes or one?
🎵 **Listening to:** New Jeans

Administrivia

Coming up

- Week 3: Societal Impacts of ML (Fairness and Bias)
- Week 4: Other ML models for classification
- Week 5: Deep Learning

HW3 released today, due next Tuesday

Midterm

- Released Friday 4/21 at 8:30 am. Due Monday 4/24 at 11:59 pm.
  - Untimed, but would be good to time yourself as practice for the final
  - Should take ~1 hour if you know the material
- Format: Think longer conceptual assignment from HW
- Covers everything from Module 0 (Regression) to Module 3 (Societal Impact, Bias, Fairness)
- Should follow our normal collaboration policy
  - Think of it as a trial run for the final exam

Confusion Matrix

For binary classification, there are only two types of mistakes

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

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

Generally we make a **confusion matrix** to understand mistakes.

		Predicted Label	
		+	−
True Label	+	*True Positive (TP)*	*False Negative (FN)*
	−	*False Positive (FP)*	*True Negative (TN)*

Tip on remembering: complete the sentence “My prediction was a …”

Confusion Matrix Example

Predicted Label

True Label

	+	−
+	*True Positive (TP)*	*False Negative (FN)*
−	*False Positive (FP)*	*True Negative (TN)*

Which is Worse?

What's worse, a false negative or a false positive?

It entirely depends on your application!

Detecting Spam

False Negative: Annoying

False Positive: Email lost

Medical Diagnosis

False Negative: Disease not treated

False Positive: Wasteful treatment

In almost every case, how treat errors depends on your context.

Errors and Fairness

We mentioned on the first day how ML is being used in many contexts that impact crucial aspects of our lives.

Models making errors is a given, what we do about that is a choice:

- Are the errors consequential enough that we shouldn't use a model in the first place?
- Do different demographic groups experience errors at different rates?
  - If so, we would hopefully want to avoid that model!

Will talk more about how to define whether or a not a model is fair / discriminatory next week. Will use these notions of error as a starting point!

Binary Classification Measures

Notation

$$C_{TP} = \#\mathrm{TP},\quad \mathrm{C_{FP}} = \#\mathrm{FP},\quad \mathrm{C_{TN}} = \#\mathrm{TN},\quad \mathrm{C_{FN}} = \#\mathrm{FN}$$

$$N = C_{TP} + C_{FP} + C_{TN} + C_{FN}$$

$$N_P = C_{TP} + C_{FN},\quad N_N = C_{FP} + C_{TN}$$

Error Rate

$$\frac{C_{FP} + C_{FN}}{N}$$

Accuracy Rate

$$\frac{C_{TP} + C_{TN}}{N}$$

False Positive rate (FPR)

$$\frac{C_{FP}}{N_N}$$

False Negative Rate (FNR)

$$\frac{C_{FN}}{N_P}$$

True Positive Rate or Recall

$$\frac{C_{TP}}{N_P}$$

Precision

$$\frac{C_{TP}}{C_{TP} + C_{FP}}$$

F1-Score

$$2\,\frac{Precision \cdot Recall}{Precison + Recall}$$

[See more!]

Multiclass Confusion Matrix

Consider predicting (*Healthy, Cold, Flu*)

Predicted Label

True Label	*Healthy*	*Cold*	*Flu*
Healthy	*60*	*8*	*2*
Cold	*4*	*12*	*4*
Flu	*0*	*2*	*8*

Poll Everywhere

Think

1 min

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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

True Label	*Pupper*	*Doggo*	*Woofer*
Pupper	2	27	4
Doggo	4	25	4
Woofer	1	30	2

Poll Everywhere

Think

2 min

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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

True Label	*Pupper*	*Doggo*	*Woofer*
Pupper	2	27	4
Doggo	4	25	4
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Learning Theory

How much data?

The more the merrier

- But data quality is also an extremely important factor

Theoretical techniques can bound how much data is needed

- Typically too loose for practical applications
- But does provide some theoretical guarantee

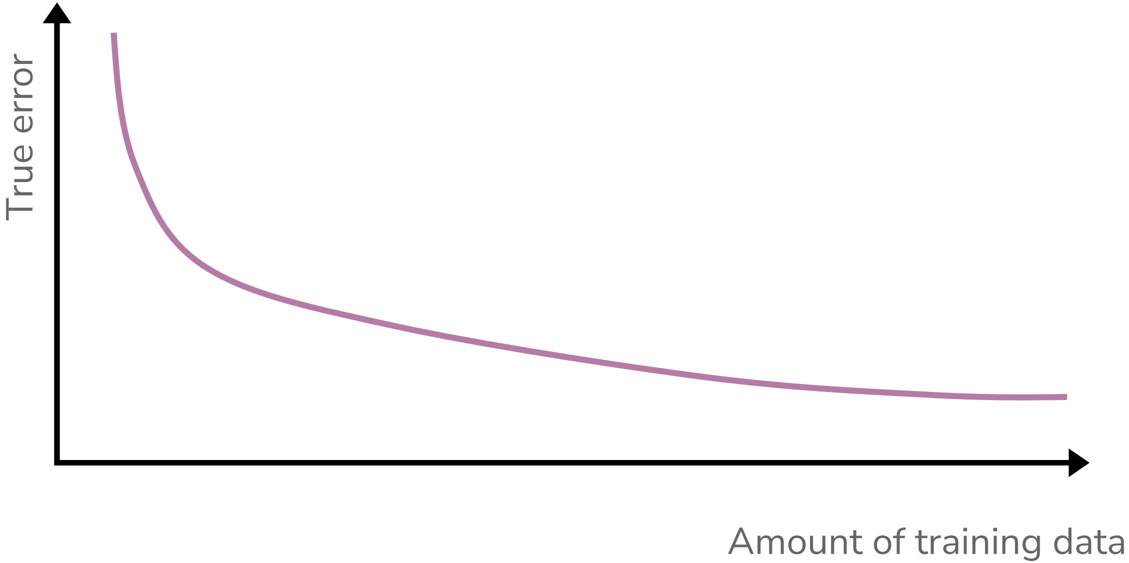
In practice

- More complex models need more data

Learning Curve

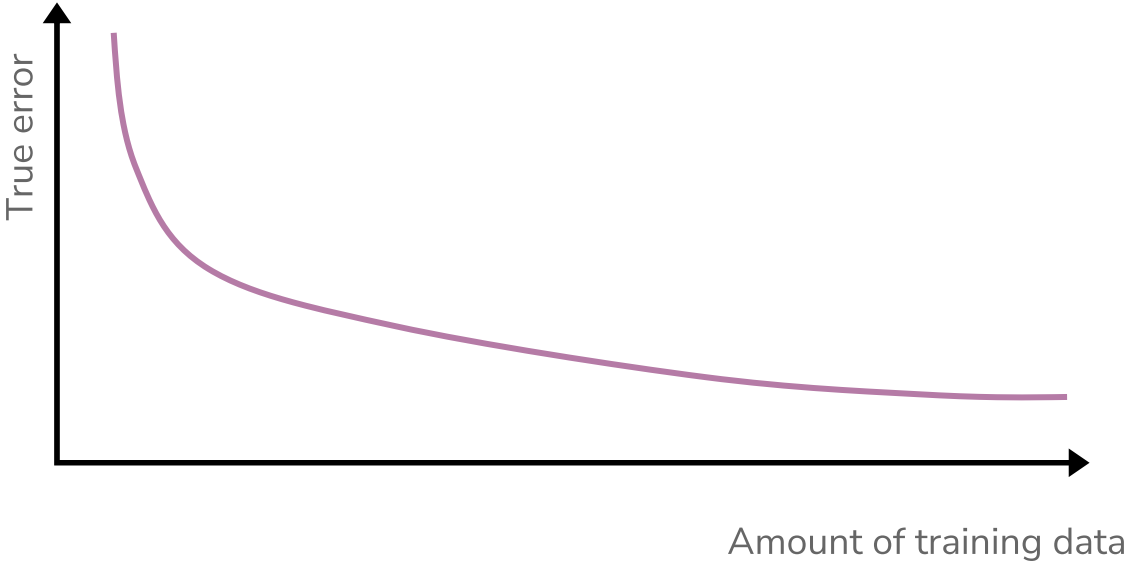
How does the true error of a model relate to the amount of training data we give it?

Hint: We've seen this picture before



Learning Curve

What if we use a more complex model?



Recap of classification so far

Theme: Describe high level idea and metrics for classification

Ideas:

- Applications of classification
- Linear classifier
- Decision boundaries
- Classification error / Classification accuracy
- Class imbalance
- Confusion matrix
- Learning theory

All the Same?

One idea is to just model the processing of finding $\hat{w}$ based on what we discussed in linear regression

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Will this work?

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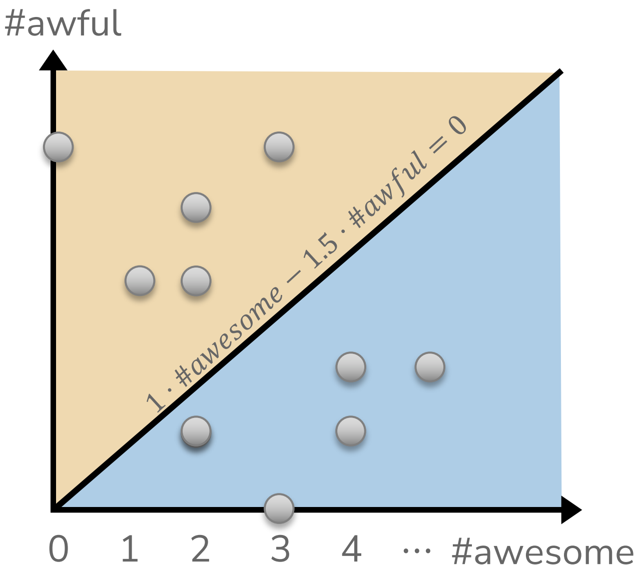

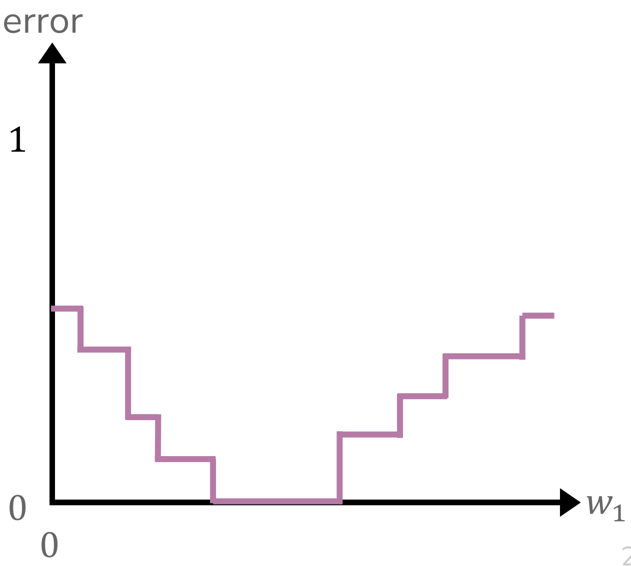

Logistic Regression Model

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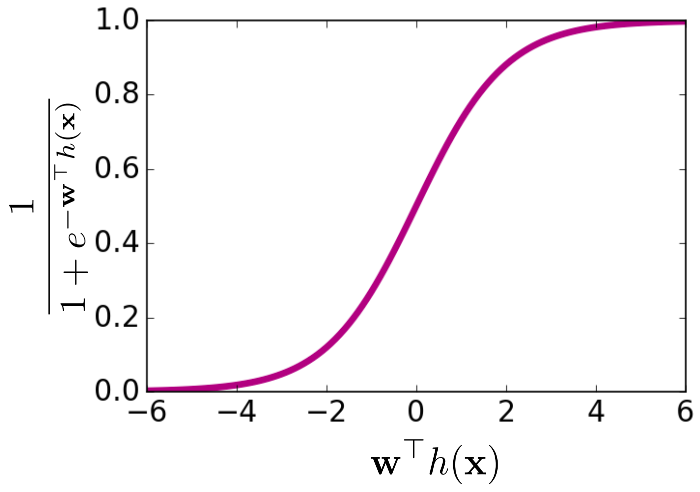

Demo

Show logistic demo (see course website)

slido

Think

1 min

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

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

$h_1(x)$	$h_2(x)$	$h_3(x)$	$h_4(x)$	$h_5(x)$	$h_6(x)$	$h_7(x)$	$h_8(x)$	$h_9(x)$
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

slido

Group

2 min

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

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

$h_1(x)$	$h_2(x)$	$h_3(x)$	$h_4(x)$	$h_5(x)$	$h_6(x)$	$h_7(x)$	$h_8(x)$	$h_9(x)$
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

Quality Metric = Likelihood

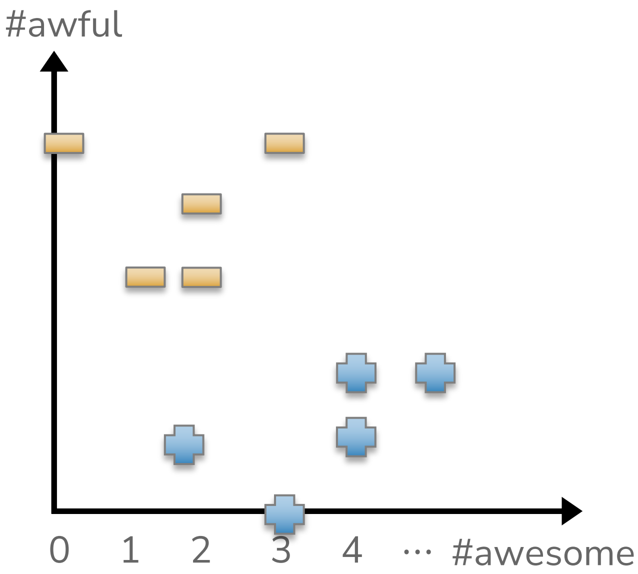
Want to compute the probability of seeing our dataset for every possible setting for w. Find w that makes data most likely! (e.g., *maximize* this likelihood metric)

Data Point	$h_1(x)$	$h_2(x)$	y	Choose w to maximize
x_1, y_1	2	1	$+1$	$P(y_1 = +1 \mid x_1, w)$
x_2, y_2	0	2	-1	$P(y_2 = -1 \mid x_2, w)$
x_3, y_3	3	3	-1	$P(y_3 = -1 \mid x_3, w)$
x_4, y_4	4	1	$+1$	$P(y_4 = +1 \mid x_4, w)$

Learn $\hat{w}$

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

The choice of w affects how likely seeing our dataset is



$$\ell(w) = \prod_{i}^{n} P(y_i | x_i, w)$$

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

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

Maximum Likelihood Estimate (MLE)

Find the w that maximizes the likelihood

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

Generally, we maximize the log-likelihood which looks like

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

Also commonly written by separating out positive/negative terms

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

slido

Group

1 min

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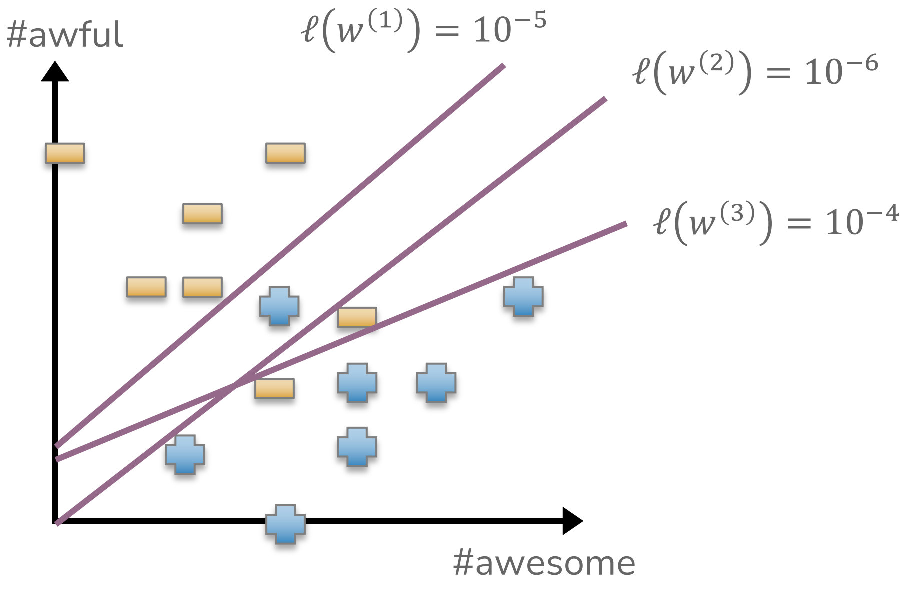
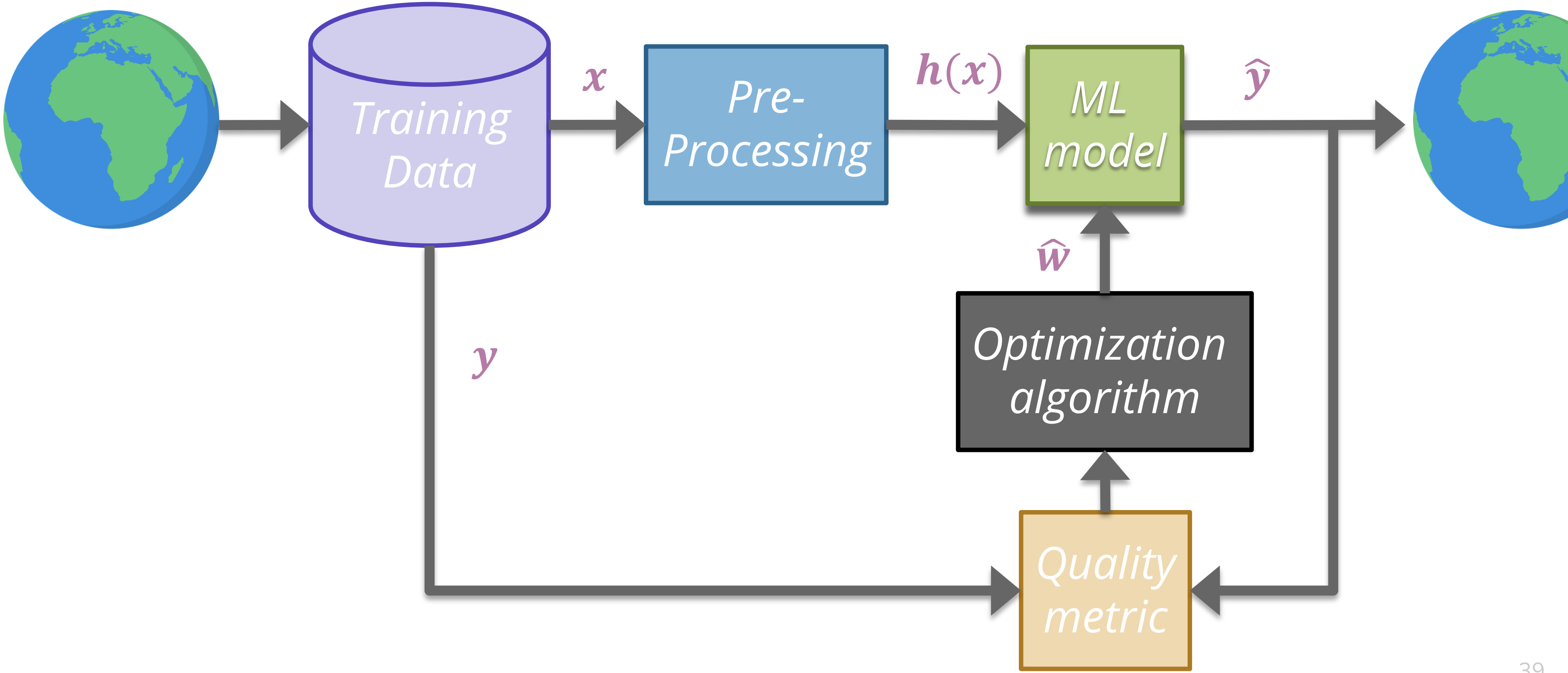
Which setting of w should we use?



Brain Break

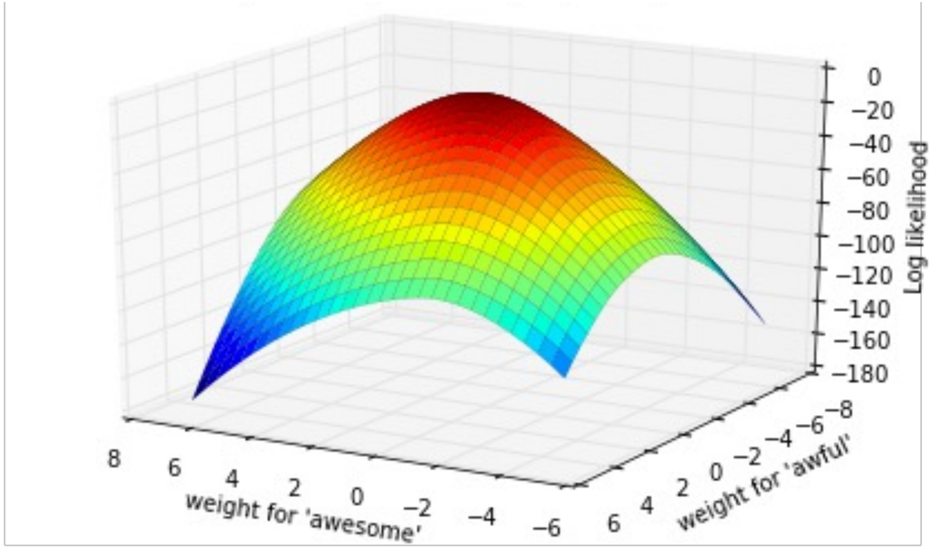

Training Data
x
Pre-Processing
$h(x)$
ML model
$\hat{y}$
$\hat{w}$
y
Optimization algorithm
Quality metric

Finding MLE

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

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

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



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

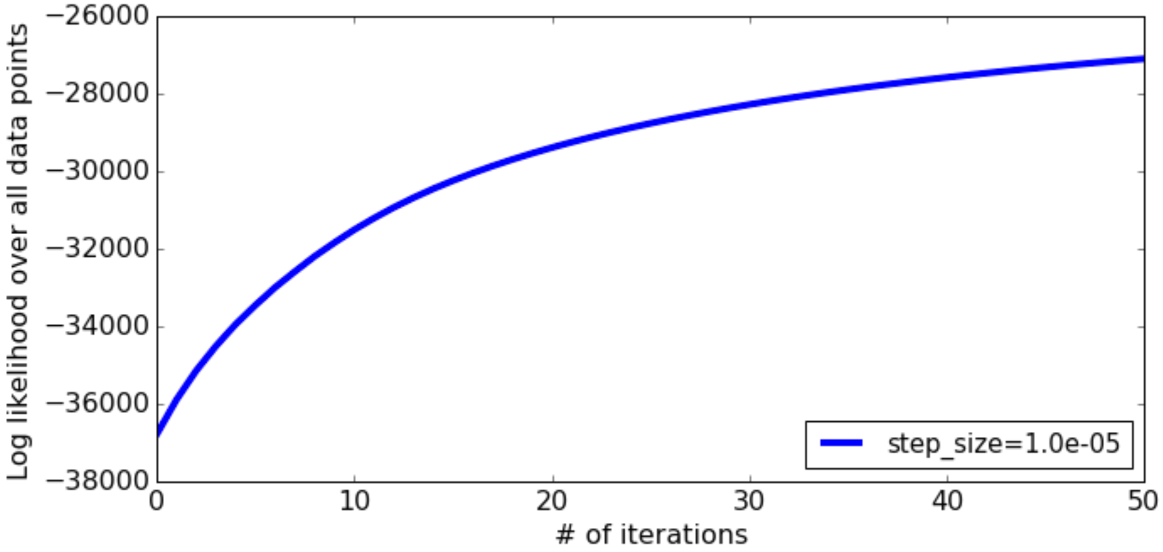
$$w^{(t+1)} \leftarrow w^{(t)} + \eta \nabla \log(\ell(w^{(t)}))$$

$$t \leftarrow t + 1$$

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

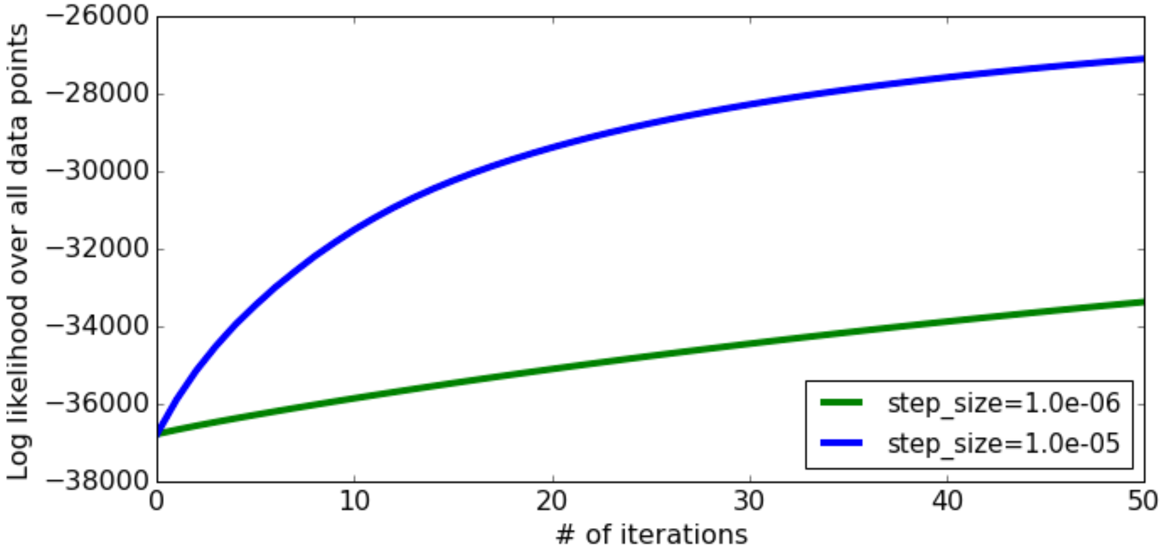
η controls how big of steps we take, and picking it is crucial for how well the model you learn does!

Learning Curve



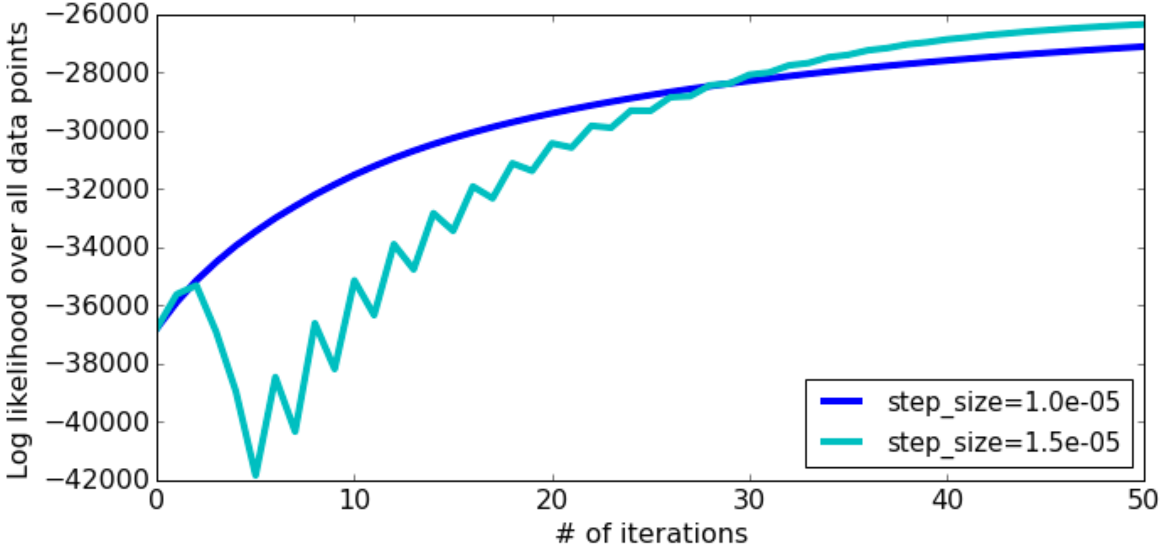
Choosing η

Step-size too small



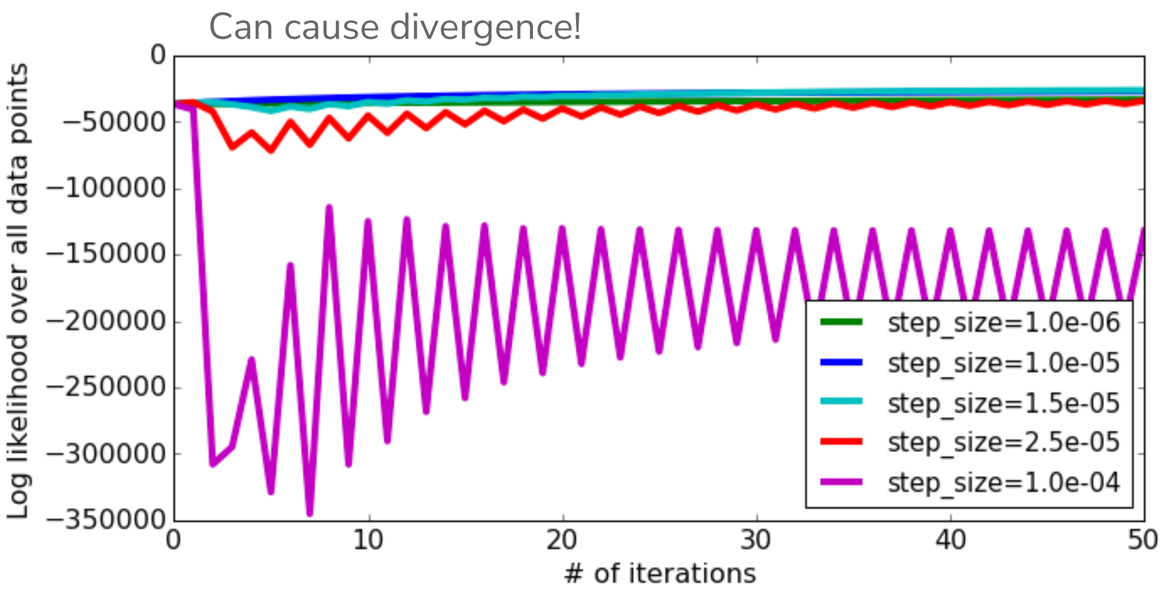
Choosing η

What about a larger step-size?



Choosing η

What about a larger step-size?



Choosing η

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

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

$$\eta_t = \frac{\eta_0}{t}$$

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 both a Ridge penalty and a learning rate (step size for gradient descent), 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:

- $\lambda \in [0.01, 0.1, 1, 10, 100]$
- $\eta_t \in \left[0.001, 0.01, 0.1, 1, \frac{1}{t}, \frac{10}{t}\right]$

You will need to train 30 different models and evaluate each one!

Brain Break

Overfitting - Classification

More Features

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

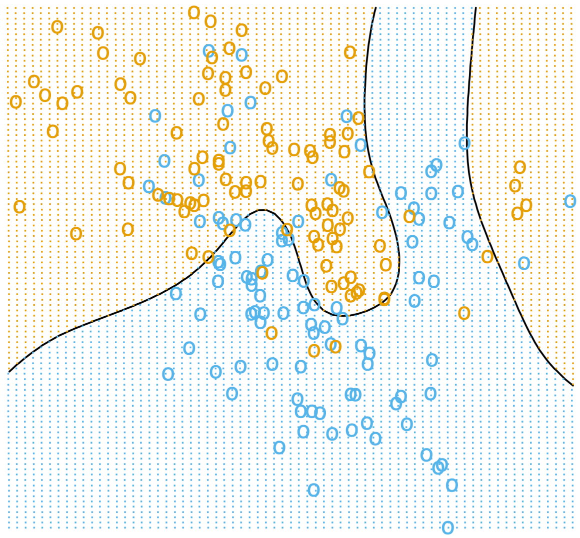
$h_1(x) = \#awesome$

$h_2(x) = \#awful$

$h_3(x) = \#awesome^2$

$h_4(x) = \#awful^2$

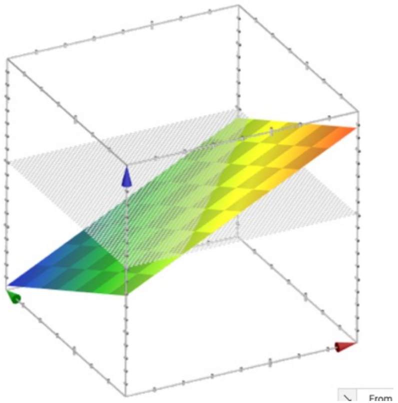
…

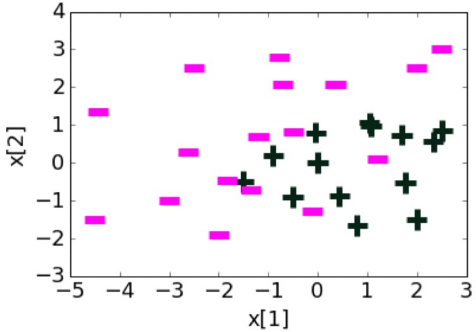


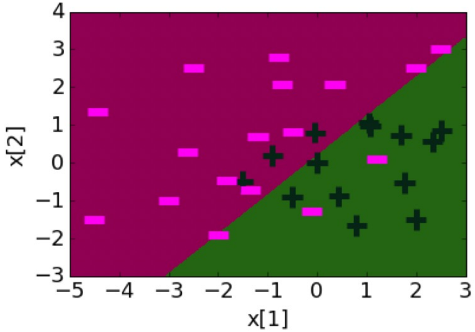
Decision Boundary

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

Feature	Value	Coefficient learned
$h_0(x)$	1	0.23
$h_1(x)$	x[1]	1.12
$h_2(x)$	x[2]	-1.07



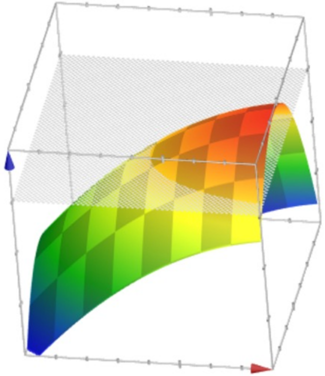


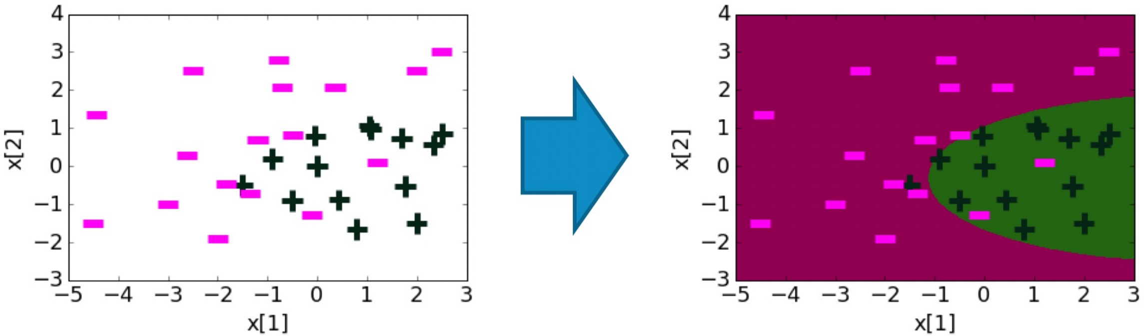


Decision Boundary

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

Feature	Value	Coefficient learned
$h_0(x)$	1	1.68
$h_1(x)$	x[1]	1.39
$h_2(x)$	x[2]	-0.59
$h_3(x)$	$(x[1])^2$	-0.17
$h_4(x)$	$(x[2])^2$	-0.96

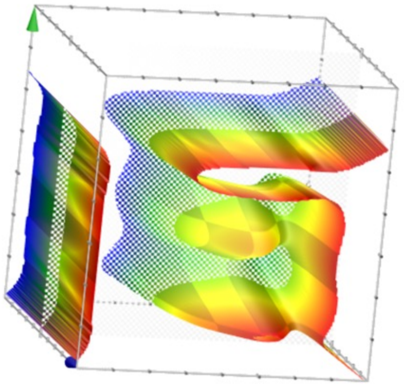


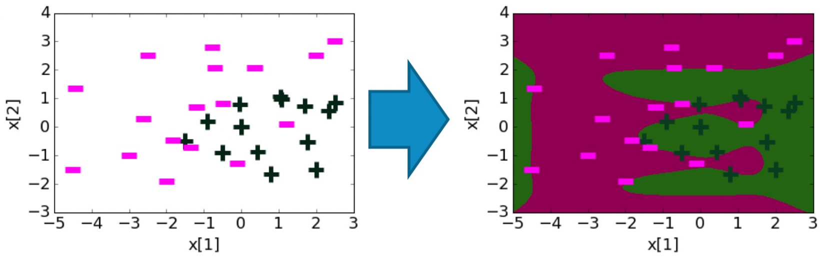


Decision Boundary

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

Feature	Value	Coefficient learned
$h_0(x)$	1	21.6
$h_1(x)$	x[1]	5.3
$h_2(x)$	x[2]	-42.7
$h_3(x)$	$(x[1])^2$	-15.9
$h_4(x)$	$(x[2])^2$	-48.6
$h_5(x)$	$(x[1])^3$	-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

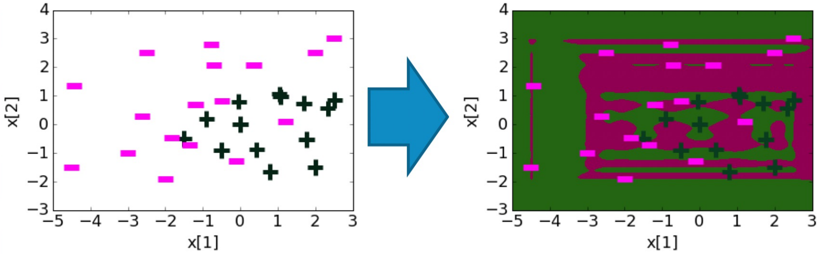




Decision Boundary

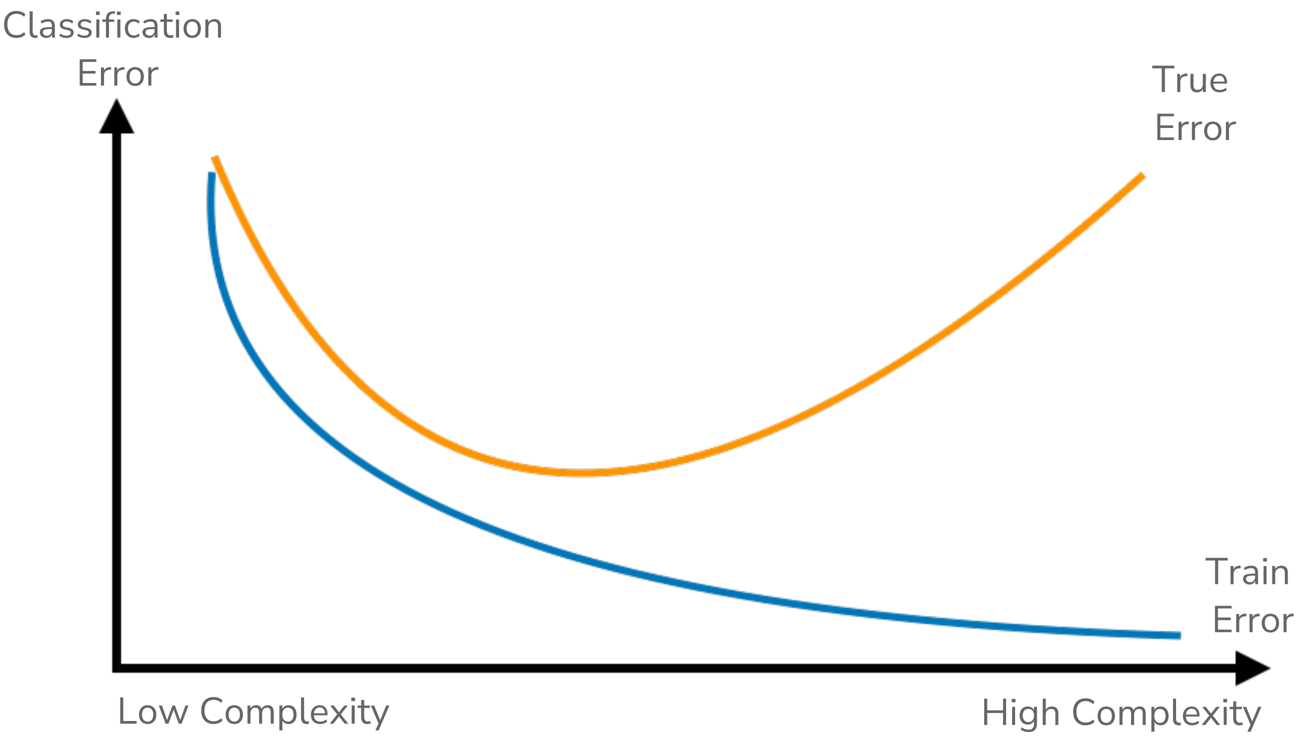
$$w^T h(x) = \cdots$$

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



Overfitting

Just like with regression, we see a similar pattern with complexity



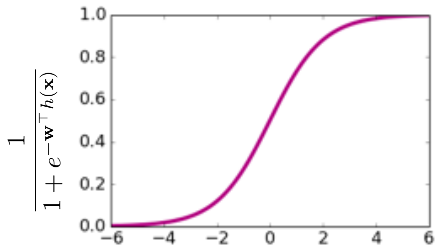
Effects of Overfitting

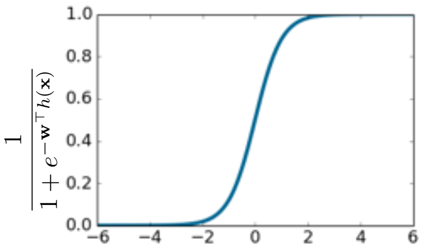
Remember, we say the logistic function become "sharper" with larger coefficients.

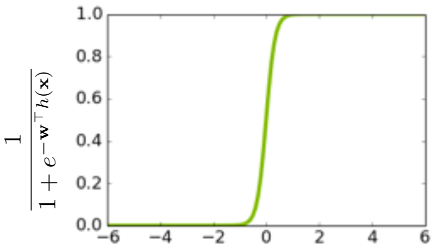
w_0	0
$w_{\#awesome}$	+1
$w_{\#awful}$	-1

w_0	0
$w_{\#awesome}$	+2
$w_{\#awful}$	-2

w_0	0
$w_{\#awesome}$	+6
$w_{\#awful}$	-6





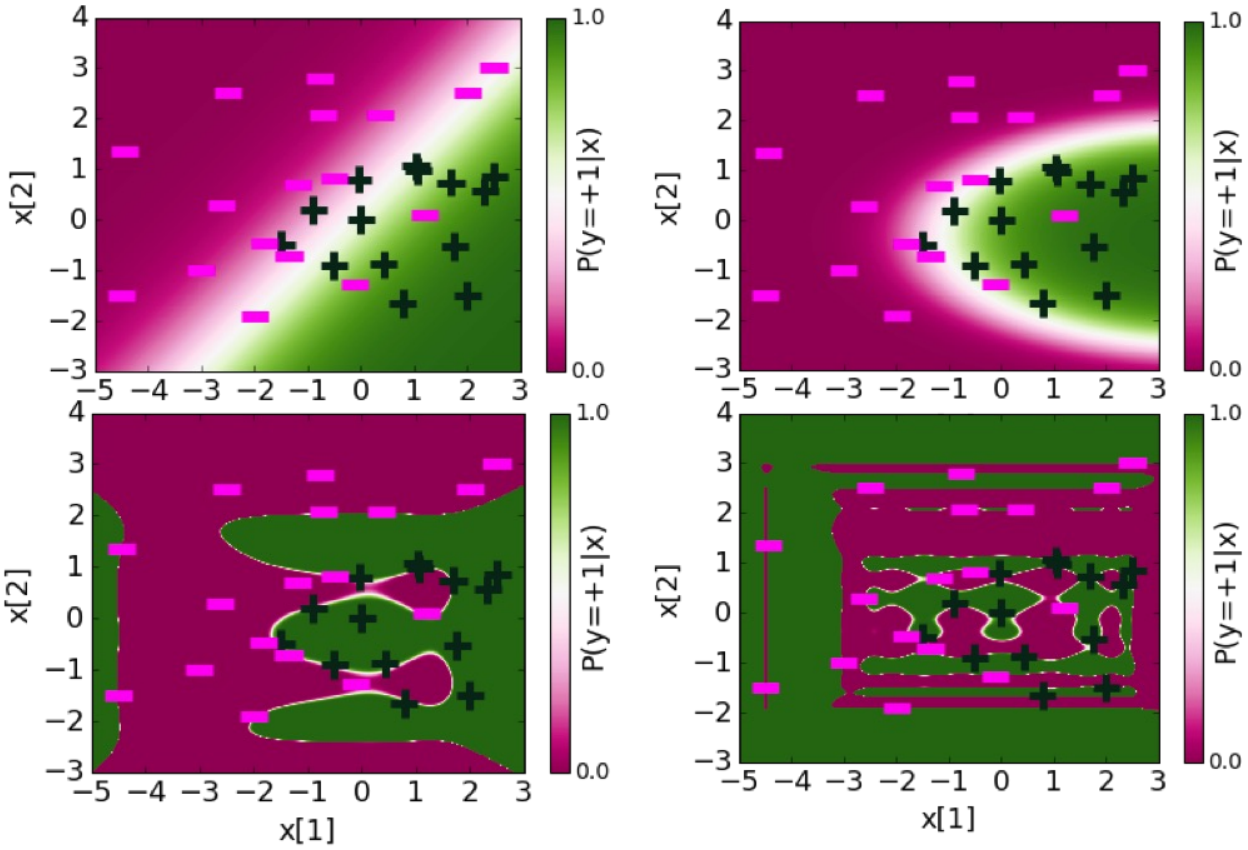


What does this mean for our predictions?

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

Plotting Probabilities

$$P(y=+1|x) = \frac{1}{1+e^{-\hat{w}^T h(x)}}$$

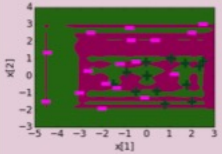
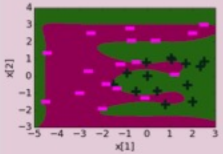
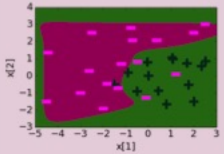
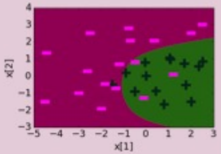
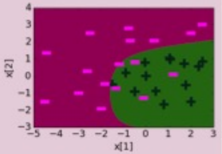
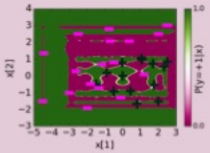
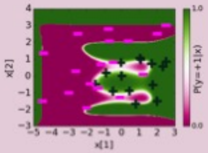
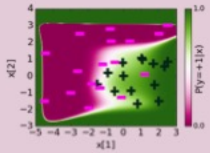
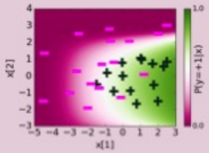


Regularization

L2 Regularized Logistic Regression

Just like in regression, can change our quality metric to avoid overfitting when training a model

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log(\ell(w)) - \lambda ||w||_2^2$$

Regularization	λ = 0	λ = 0.00001	λ = 0.001	λ = 1	λ = 10
Range of coefficients	-3170 to 3803	-8.04 to 12.14	-0.70 to 1.25	-0.13 to 0.57	-0.05 to 0.22
Decision boundary					
Learned probabilities					

Some Details

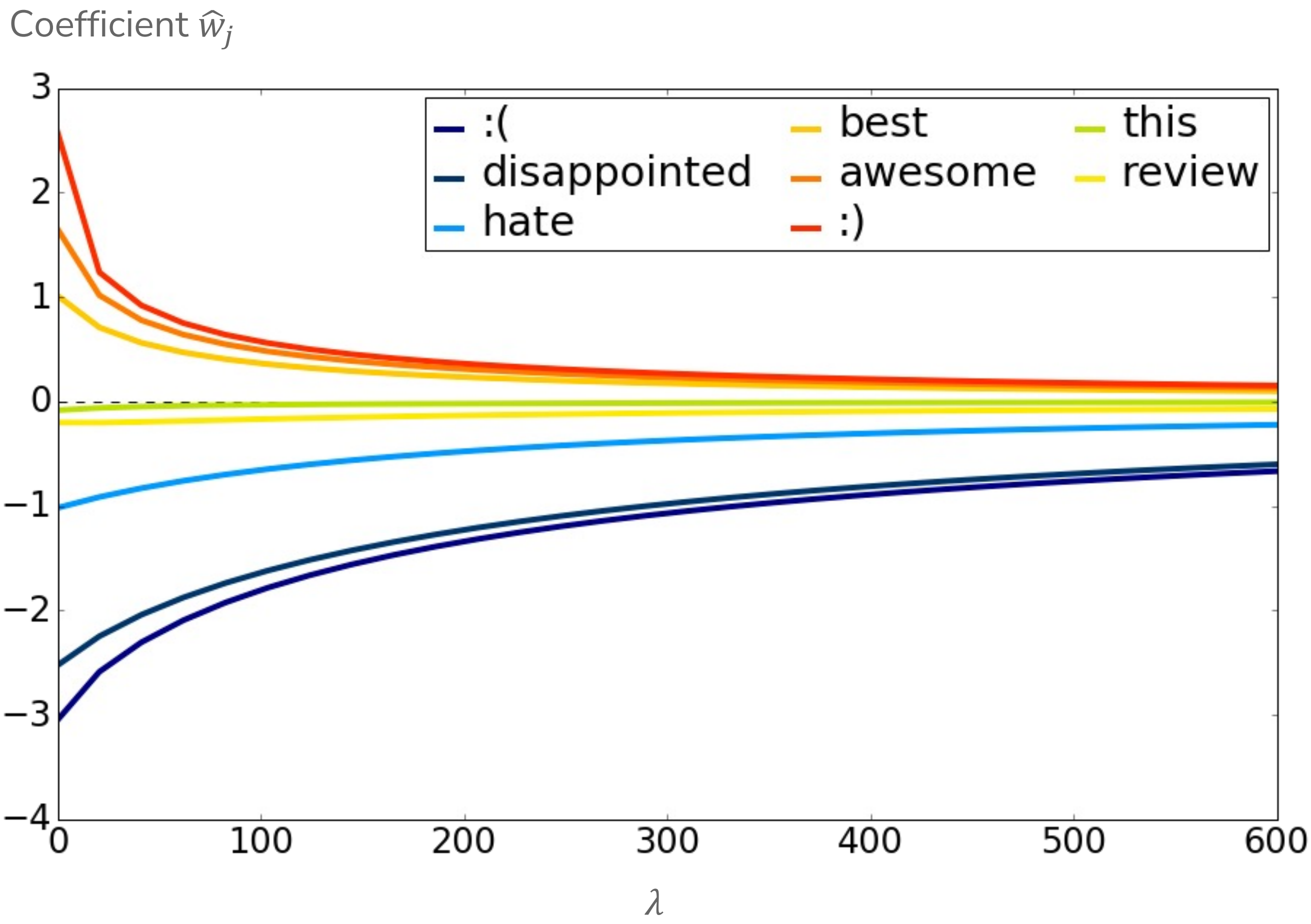
Why do we subtract the L2 Norm?

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log\big(\ell(w)\big) - \lambda||w||_2^2$$

How does λ impact the complexity of the model?

How do we pick λ?

Coefficient Path: L2 Penalty



slido

Group

2 min

Jake 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 Jake 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