Yale NUS College

YSC2239 Lecture 19-20

Today’s class

- Logistic regression – Part 1

Regression vs. Classification

Linear Regression

In a **linear regression** model, our goal is to predict a **quantitative** variable (i.e., some real number) from a set of features.

- Our output, or **response**, y, could be any real number.
- We determined optimal model parameters by minimizing some average loss, and (sometimes) an added regularization penalty.

$$\hat{y} = f_\theta(x) = x^T\theta$$

Remember, $x^T\theta = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_p x_p$.

Classification

When performing classification, we are instead interested in predicting some **categorical** variable.

spam or ham

win or lose

disease or no disease

Classification

- **Binary** classification: two classes.
  - Examples: spam / not spam.
  - Our **responses** are either 0 or 1.
  - Our focus today.
- **Multiclass** classification: many classes.
  - Examples: Image labeling (cat, dog, car), next word in a sentence, etc.

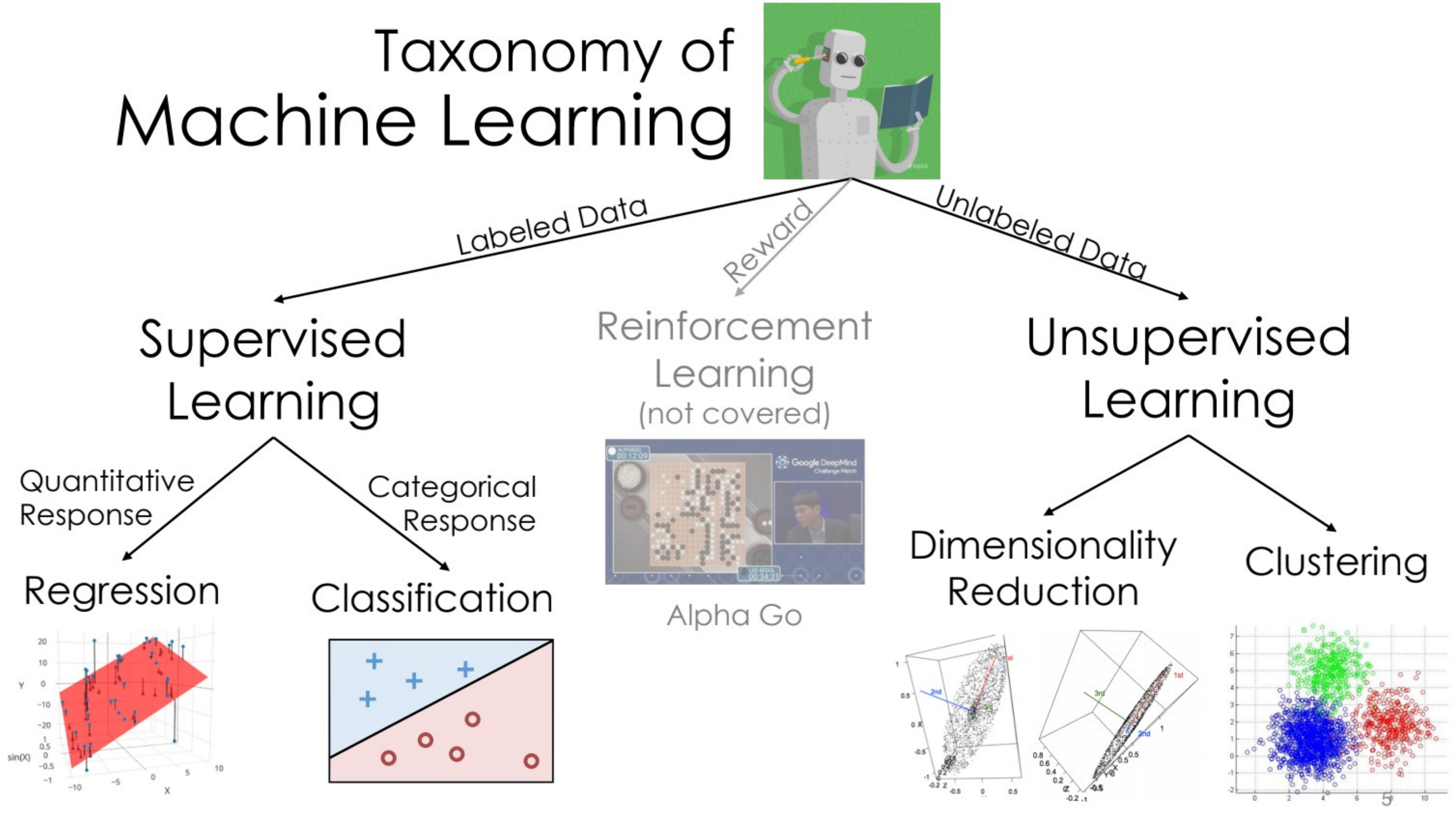
This is not the first time you are seeing classification!

- k-Nearest Neighbors was a classification technique we have learned earlier.

Machine learning taxonomy

Regression and Classification are both forms of **supervised learning**.

Logistic regression, the topic of this lecture, is mostly used for **classification**, even though it has “regression” in the name.



from Joseph Gonzalez

Deriving the logistic regression model

In this section, we will mostly work out of the lecture notebook.

Example dataset

In this lecture, we will primarily use data from the 2017-18 NBA season.

Goal: Predict whether or not a team will win, given their FG_PCT_DIFF.

- This is the difference in field goal percentage between the two teams.
- Positive FG_PCT_DIFF: team made more shots than the opposing team.

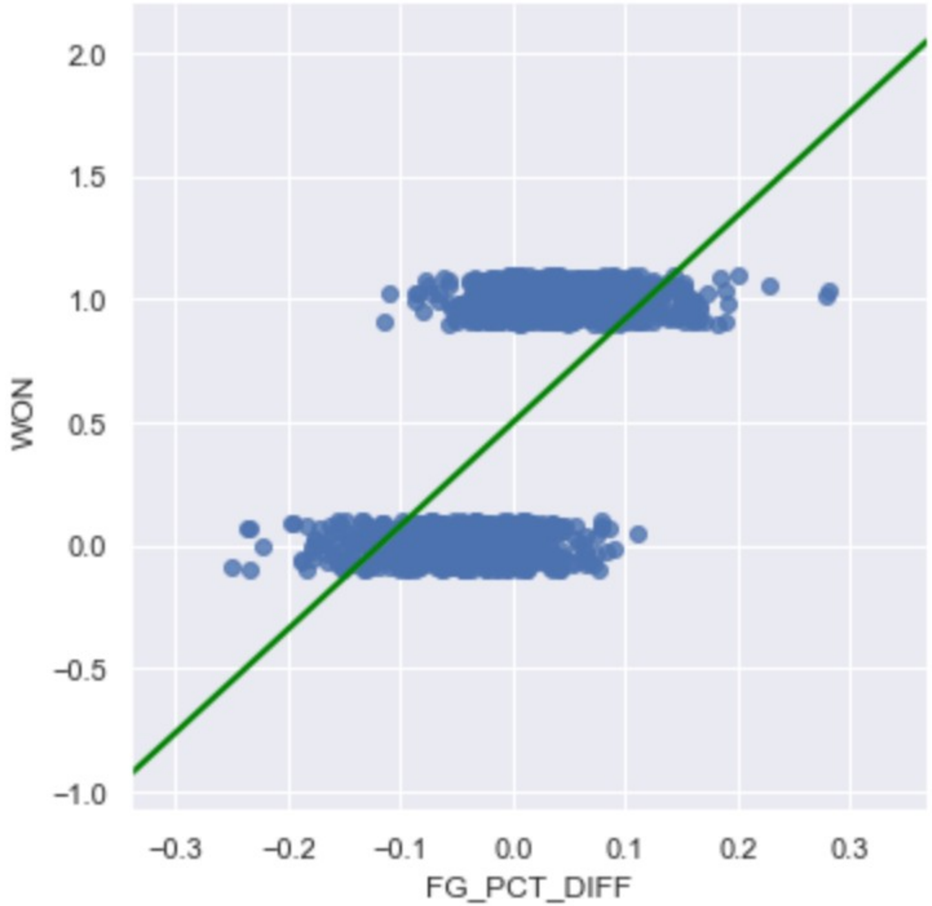
TEAM_NAME	MATCHUP	WON	FG_PCT_DIFF
Boston Celtics	BOS @ CLE	0	-0.049
Golden State Warriors	GSW vs. HOU	0	0.053
Charlotte Hornets	CHA @ DET	0	-0.030
Indiana Pacers	IND vs. BKN	1	0.041
Orlando Magic	ORL vs. MIA	1	0.042

1s represent wins, 0s represent losses.

Why not use Ordinary Least Squares?

We already have a model that can predict any quantitative response. Why not use it here?

- The output can be outside of the range [0, 1]. What does a predicted WON value of -2 mean?
- Very sensitive to outliers.
- Many other statistical reasons.
    - Not the point of our class.

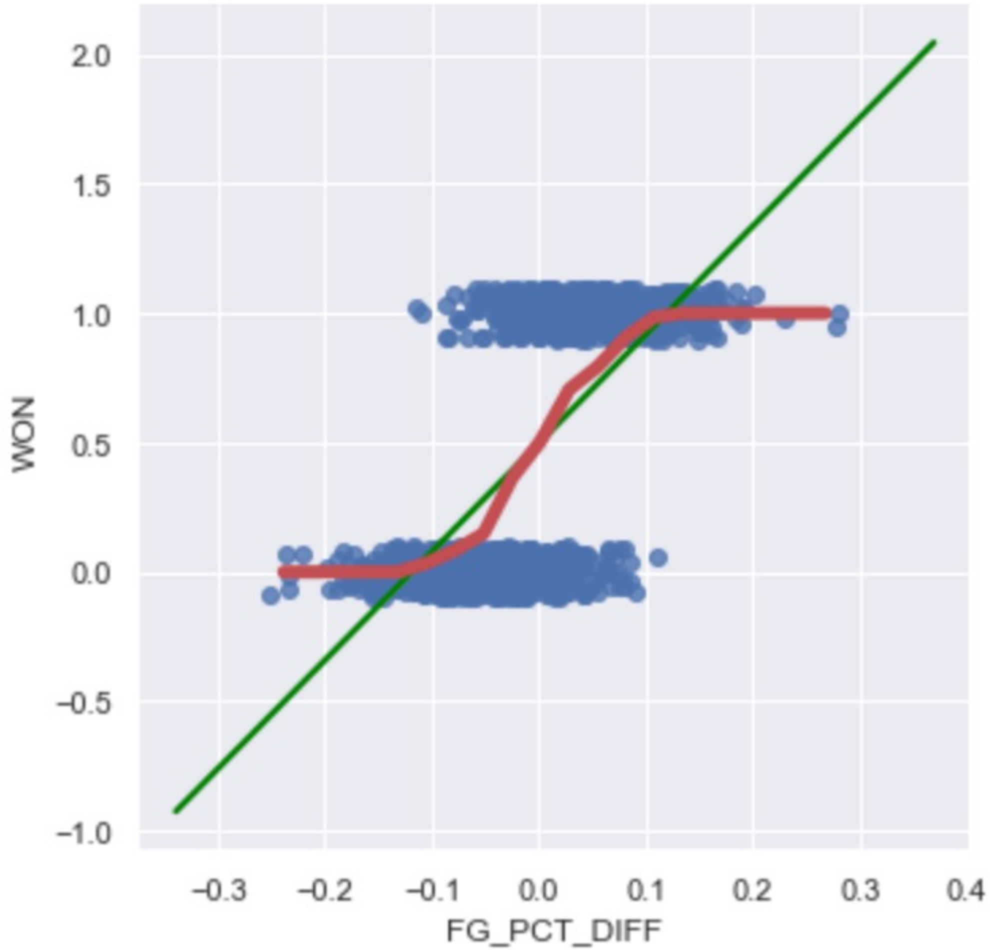


Graph of averages

When defining the simple linear regression model, we binned the x-axis, and took the average y-value for each bin, and tried to model that.

Doing so here yields a curve that resembles an s.

- Since our true y is either 0 or 1, this curve models the **probability that WON = 1**, given FG_PCT_DIFF.
    - WON = 1 means “belong to class 1”.
- **Our goal is to model this red curve as best as possible**.



Log-odds of probability is roughly linear

In the demo, we noticed that the **log-odds of the probability of belonging to class 1 was linear**. **This is the assumption that logistic regression is based on**

$$\text{odds}(p) = \frac{p}{1-p} \qquad \text{log-odds}(p) = \log\left(\frac{p}{1-p}\right)$$

For now, let's let t denote our linear function (since log-odds is linear). Solving for p:

$$t = \log\left(\frac{p}{1-p}\right)$$

$$e^t = \frac{p}{1-p}$$

$$e^t - pe^t = p$$

$$p = \frac{e^t}{1+e^t} = \frac{1}{1+e^{-t}}$$

With logistic regression, we are always referring to log base e ("ln").

This is called the **logistic function**, σ(t).

Arriving at the logistic regression model

We know how to model linear functions quite well.

- We can substitute $t = x^T\theta$, since t was just a placeholder.

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

p represents the probability of belonging to class 1.

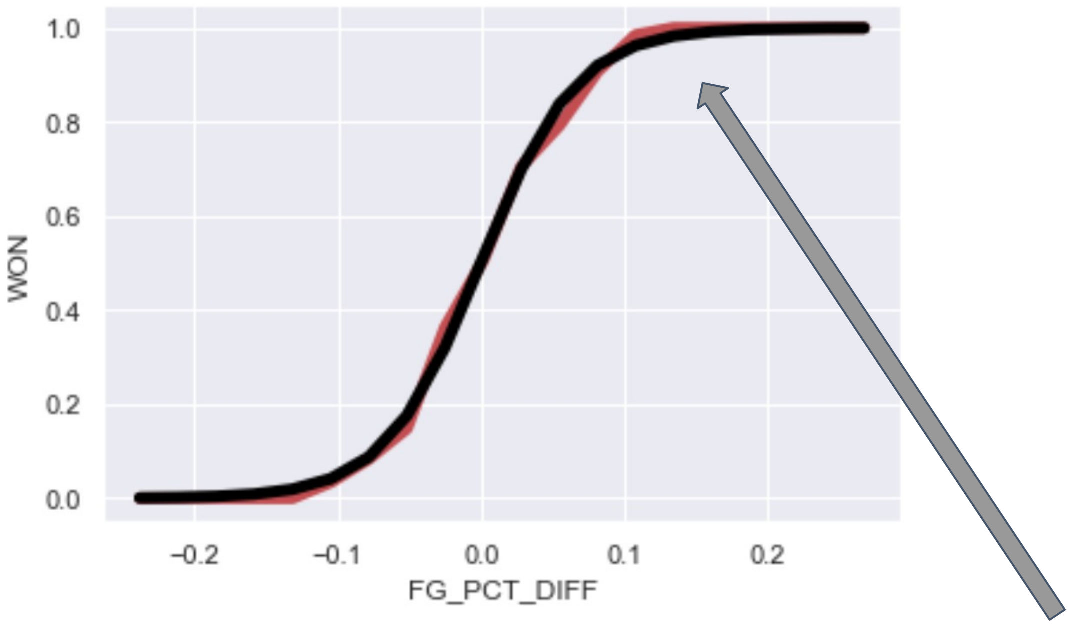
- We are modeling $P(Y=1|x)$.

Putting this all together:

$$P(Y=1|x) = \frac{1}{1+e^{-x^T\theta}} = \sigma(x^T\theta)$$

Looks just like the linear regression model, with a $\boldsymbol{\sigma}(\ )$ wrapped around it.
We call logistic regression a **generalized linear model**, since it is a non-linear transformation of a linear model.

Arriving at the logistic regression model



In red:
Empirical graph of averages

In black:
$\hat{y} = \sigma(30 \cdot \mathrm{FG\ PCT\ DIFF})$

Logistic regression

Linear vs. logistic regression

In a **linear regression** model, we predict a **quantitative** variable (i.e., some real number) as a linear function of features.

- Our output, or **response**, y, could be any real number.

$$\hat{y} = f_\theta(x) = x^T\theta$$

In a **logistic regression** model, our goal is to predict a binary **categorical** variable (class 0 or class 1) as a linear function of features, passed through the logistic function.

- Our **response** is the probability that our observation belongs to class 1.
- Haven't yet done classification!

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

Example calculation

Suppose I want to predict the probability that LeBron's shot goes in, given **shot distance** (first feature) and **# of seconds left on the shot clock** (second feature).

I fit a logistic regression model using my training data, and somehow compute

$$\hat{\theta}^T = [0.1 \quad -0.5]$$

Under the logistic model, compute the probability his shot goes in, given that

- He shoots it from 15 feet.
- There is 1 second left on the shot clock.

Example calculation (solution)

$$x^T = [\,15 \qquad 1\,] \qquad\qquad \hat{\theta}^T = [\,0.1 \qquad -0.5\,]$$

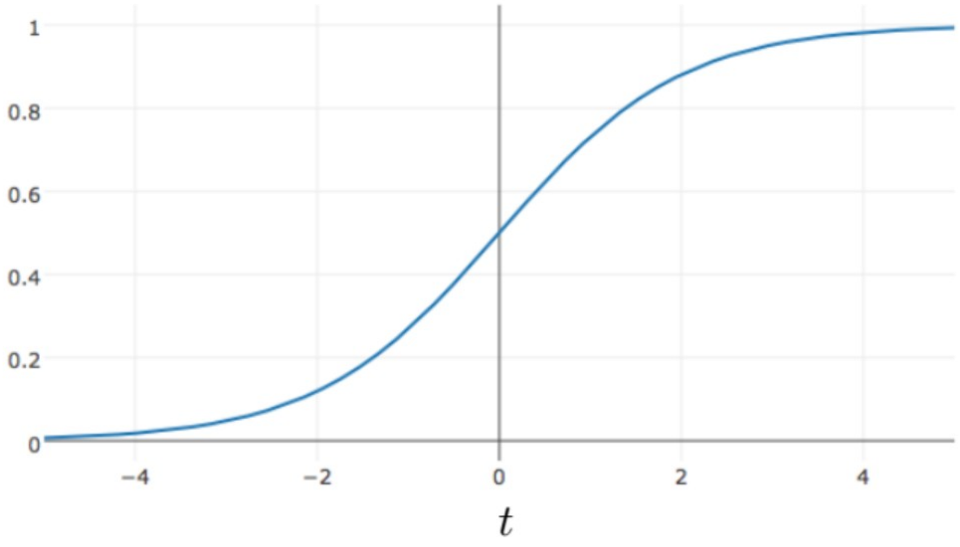
$$\begin{aligned} P(Y=1|x) &= \sigma(x^T\hat{\theta}) \\ &= \sigma(\hat{\theta}_1 \cdot \textbf{SHOT DISTANCE} + \hat{\theta}_2 \cdot \textbf{SECONDS LEFT}) \\ &= \sigma(0.1 \cdot 15 + (-0.5) \cdot 1) \\ &= \sigma(1) \\ &= \frac{1}{1+e^{-1}} \\ &\approx 0.7311 \end{aligned}$$

An explicit expression representing our model.

Properties of the logistic function

The logistic function is a type of **sigmoid**, a class of functions that share certain properties.

$$\sigma(t) = \frac{1}{1 + e^{-t}} \qquad -\infty < t < \infty$$



- Its output is bounded between 0 and 1, no matter how large t is.
  - Fixes an issue with using linear regression to predict probabilities.
- We can interpret it as mapping real numbers to probabilities.

Properties of the logistic function

Definition

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

Range

$$0 < \sigma(t) < 1$$

Inverse

$$t = \sigma^{-1}(p) = \log\left(\frac{p}{1-p}\right)$$

Reflection and Symmetry

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

Derivative

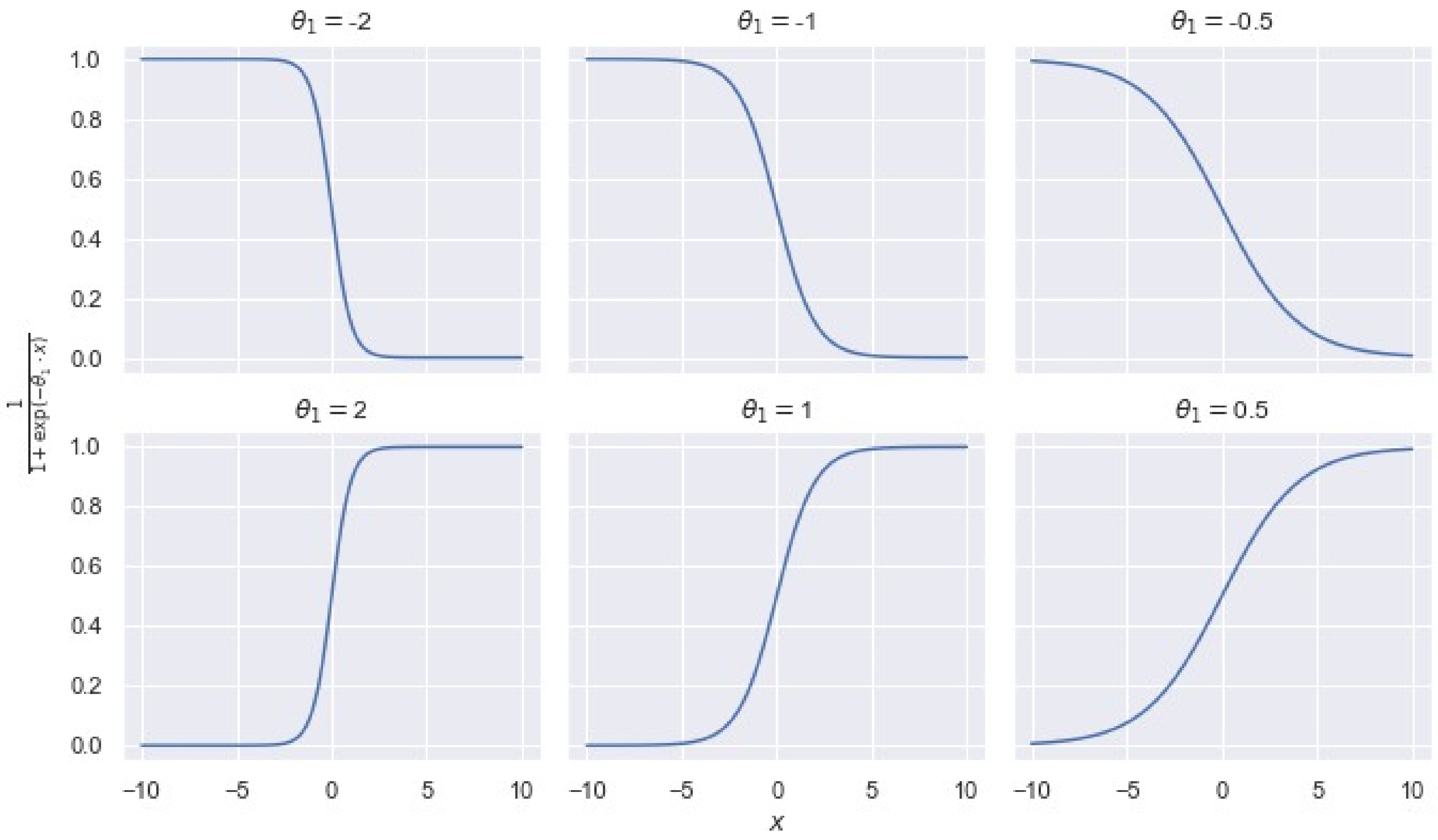
$$\frac{d}{dt}\sigma(t) = \sigma(t)(1-\sigma(t)) = \sigma(t)\sigma(-t)$$

Shape of the logistic function

Consider the plot of $\sigma(\theta_1 x)$, for several different values of θ_1.

- If θ_1 is positive, the curve increases to the right.
- The further θ_1 is from 0, the steeper the curve.

In the notebook, we explore more sophisticated logistic curves.



Parameter interpretation

Recall, we arrived at the model by assuming that the log-odds of the probability of belonging to class 1 was linear.

$$P(Y=1|x) = \sigma(x^T\theta) \quad \Leftarrow \quad \log\left(\frac{P(Y=1|x)}{P(Y=0|x)}\right) = x^T\theta \quad \Leftarrow \quad \frac{P(Y=1|x)}{P(Y=0|x)} = e^{x^T\theta}$$

This is the same as $\frac{p}{1-p}$, because

$$P(Y=1|x) + P(Y=0|x) = 1$$

(Remember, we are dealing with binary classification – we are predicting 1 or 0.)

Parameter interpretation

Let's suppose our linear component has just a single feature, along with an intercept term.

$$\frac{P(Y=1|x)}{P(Y=0|x)} = e^{\theta_0+\theta_1 x}$$

What happens if you increase x by one unit?

- Odds is multiplied by e^{θ_1}.
- If $\theta_1 > 0$, the odds increase.
- If $\theta_1 < 0$, the odds decrease.

What happens if $x^T\theta = \theta_0 + \theta_1 x = 0$?

- This means class 1 and class 0 are equally likely.
- $e^0 = 1 \implies \frac{P(Y=1|x)}{P(Y=0|x)} = 1 \implies P(Y=1|x) = P(Y=0|x)$.

The odds ratio can be interpreted as the "number of successes for each failure."

Today’s class

- Logistic regression – Part 2

Logistic regression with squared loss

Logistic regression with squared loss

To find $\hat{\theta}$ so that we can make predictions, we need to choose a loss function.

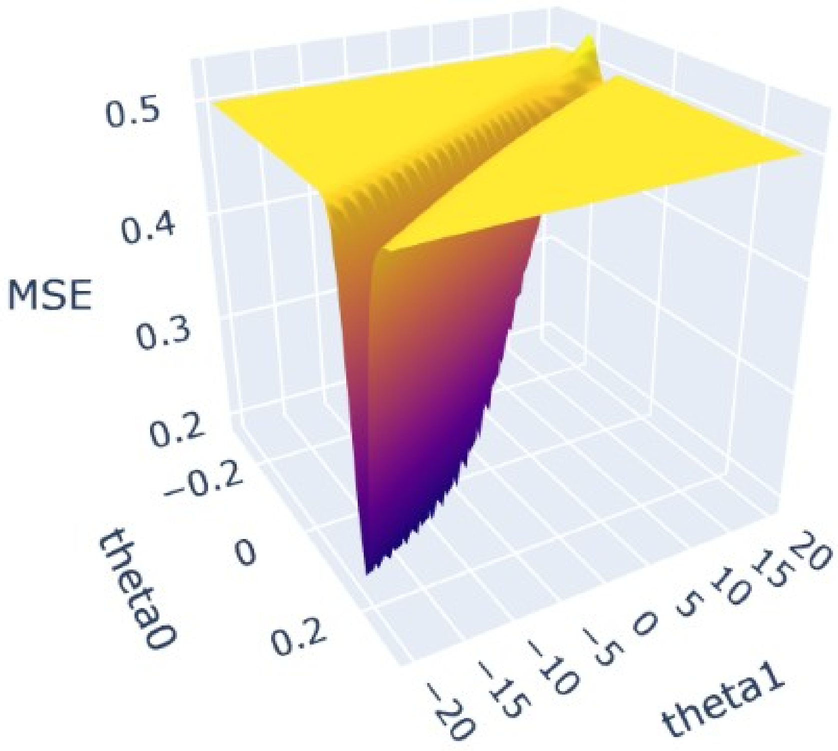
- We can start with our old friend, squared loss.
- Doing so yields the following MSE:

$$R(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \sigma(\mathbb{X}_i^T\theta))^2$$

Sometimes, this works fine (and it is actually still used in some applications). Other times...

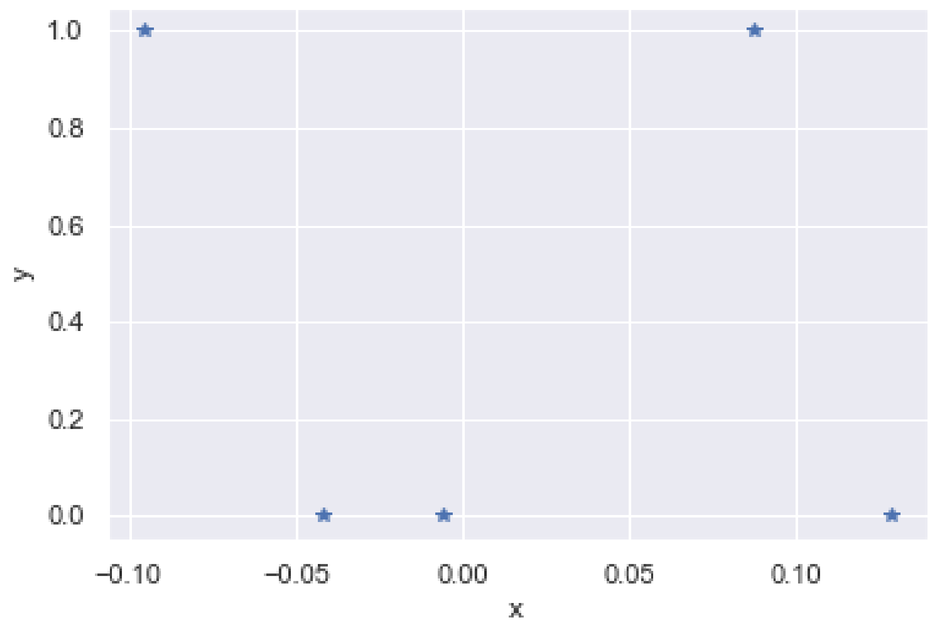
Pitfalls of squared loss with logistic regression

The loss surface of MSE for a logistic regression model with a single slope plus an intercept often looks something like this.

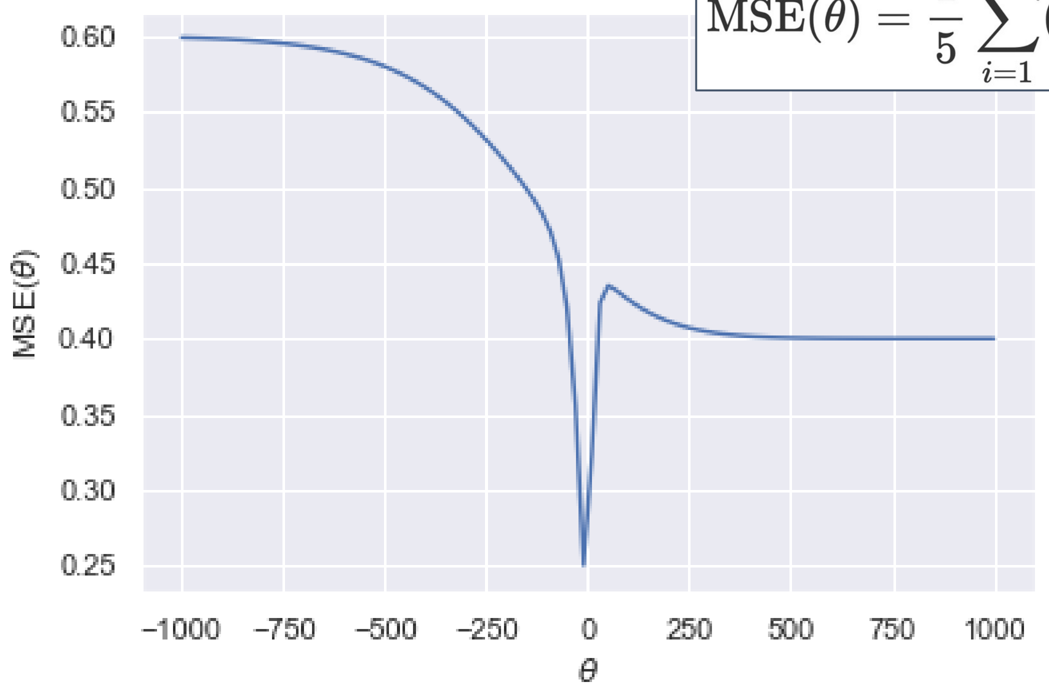


Pitfalls of squared loss with logistic regression

On the left, we have a toy dataset (i.e. we've plotted the original data, y vs. x).
On the right, we have a plot of the mean squared error of this dataset when fitting a single-feature logistic regression model, for different values θ (i.e. the loss surface).



$$\mathrm{MSE}(\theta) = \frac{1}{5}\sum_{i=1}^{5}(y_i - \sigma(\theta x_i))^2$$



Pitfalls of squared loss with logistic regression

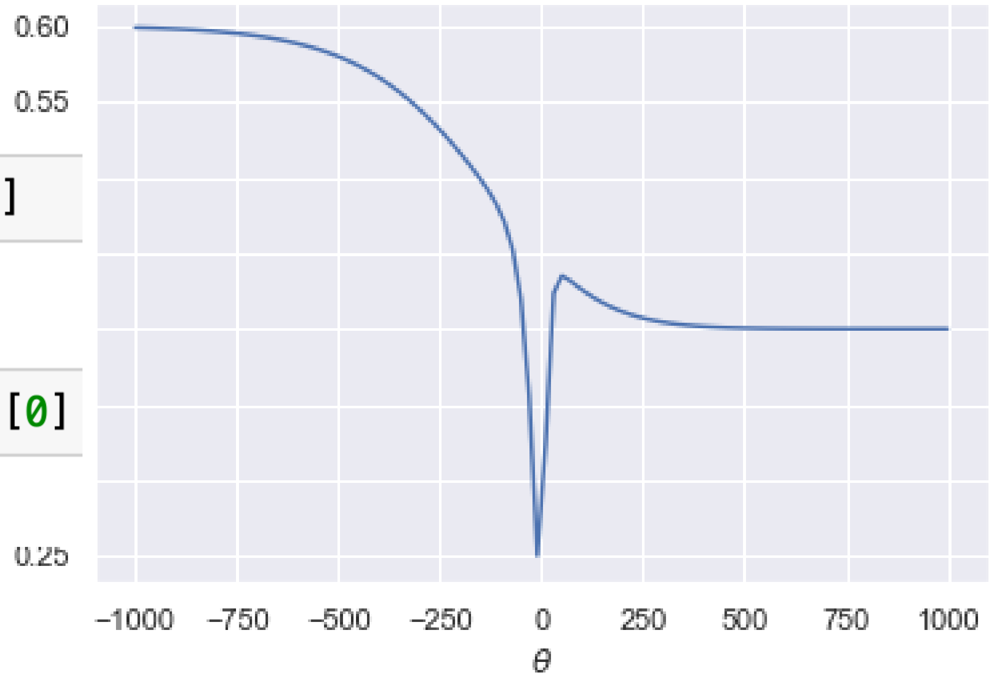
For this particular loss surface, different initial guesses for thetahat yield different "optimal values", as per scipy.optimize.minimize:

```
minimize(mse_loss_single_arg_toy, x0 = 0)["x"][0]
```

```
-4.801981341432673
```

```
minimize(mse_loss_single_arg_toy, x0 = 500)["x"][0]
```

```
500.0
```



This loss surface is not convex.
We'd like it to be convex.

Pitfalls of squared loss with logistic regression

Another issue: since y_i is either 0 or 1, and $\hat{y}_i$ is between 0 and $(y_i - \hat{y}_i)^2$ is also bounded between 0 and 1.

- Even if our probability is nowhere close, the loss isn't that large in magnitude.
  - If we say the probability is 10^-6, but it happens anyway, error should be large.
- We want to penalize wrong answers significantly.

Summary of issues with squared loss and logistic regression

While it can work, squared loss is not the best choice of loss function for logistic regression.

- Average squared loss is not nice (non-convex).
  - Numerical methods will struggle to find a solution.
- Wrong predictions aren't penalized significantly enough.
  - Squared loss (and hence, average squared loss) are bounded between 0 and 1.

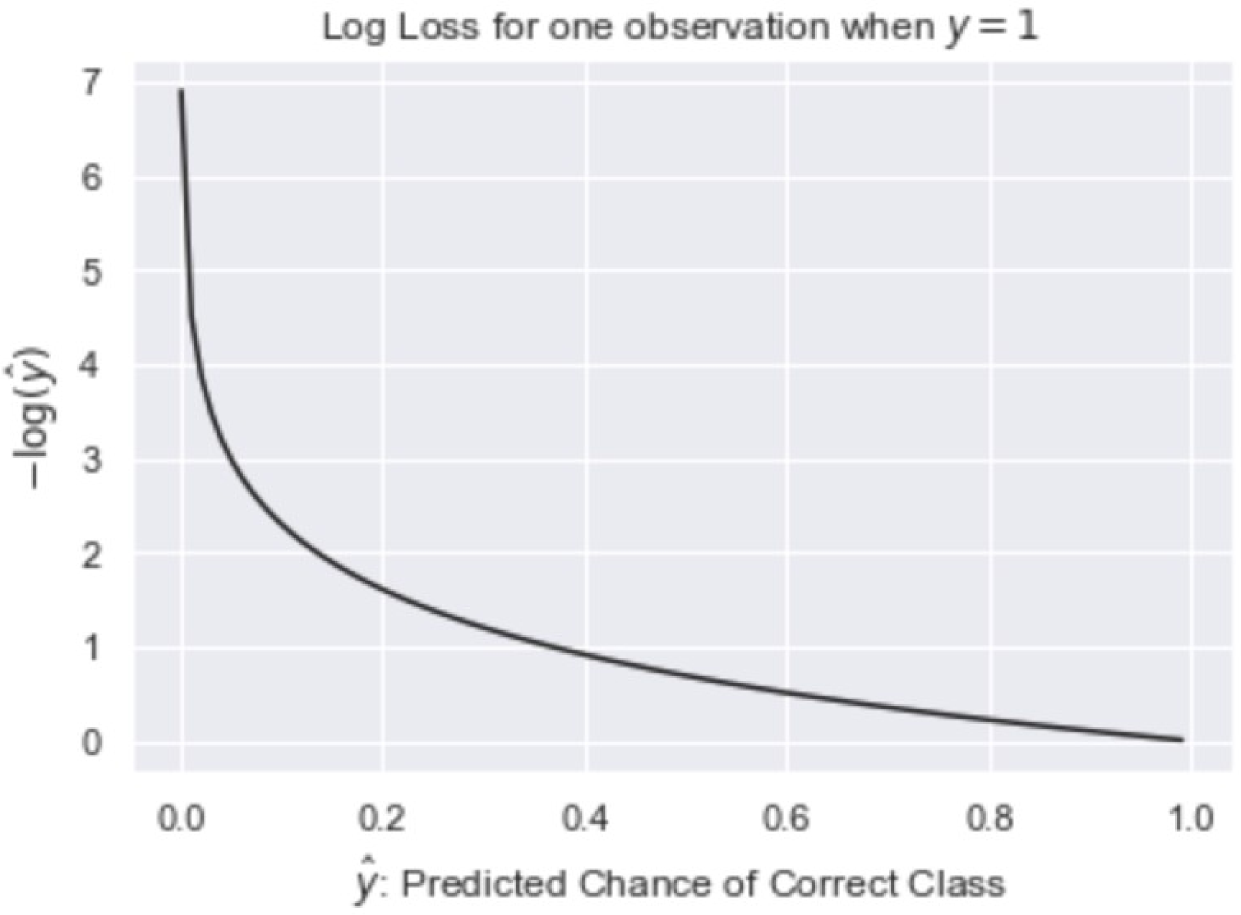
Fortunately, there's a solution.

Cross-entropy loss

Log loss

Consider this new loss, called the (negative) **log loss**, for a single observation when the true y is equal to 1.

We can see that as our prediction gets further and further from 1, the loss approaches infinity (unlike squared loss, which maxed out at 1).

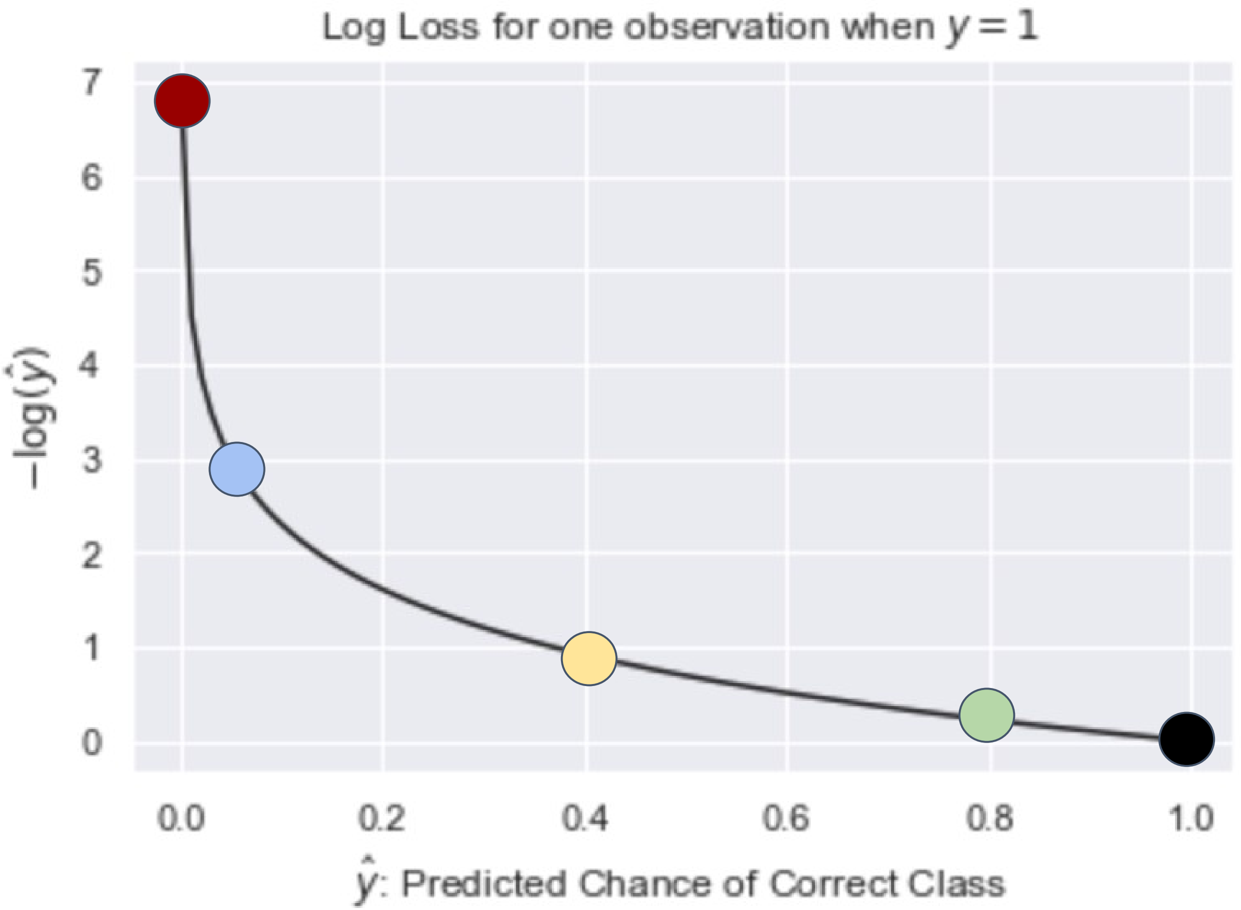


Log loss

Let's look at some losses in particular:

$\hat{y}$	$-\log(\hat{y})$
1	0
0.8	0.25
0.4	1
0.05	3
0	infinity!

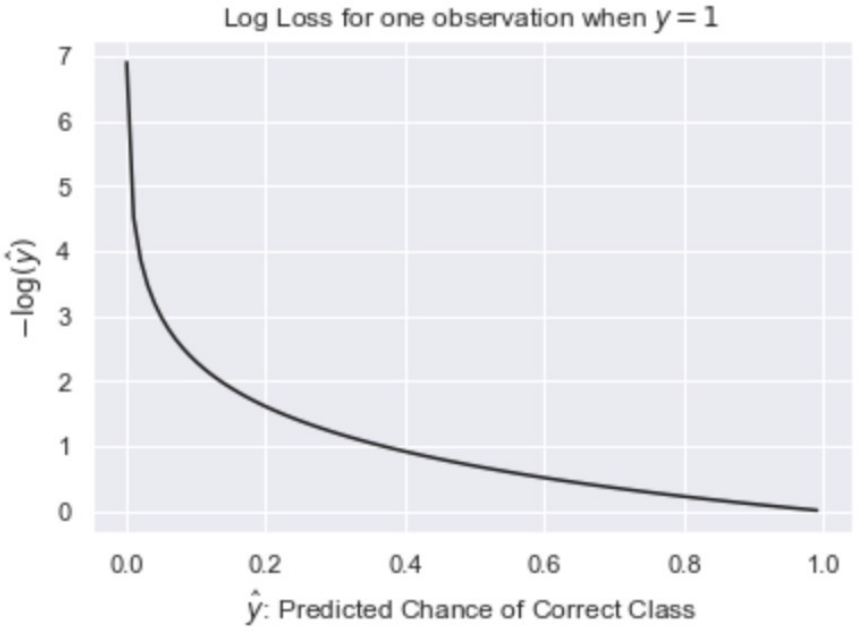
Note: The logistic function never outputs 0 or 1 exactly, so there's never actually 0 loss or infinite loss.

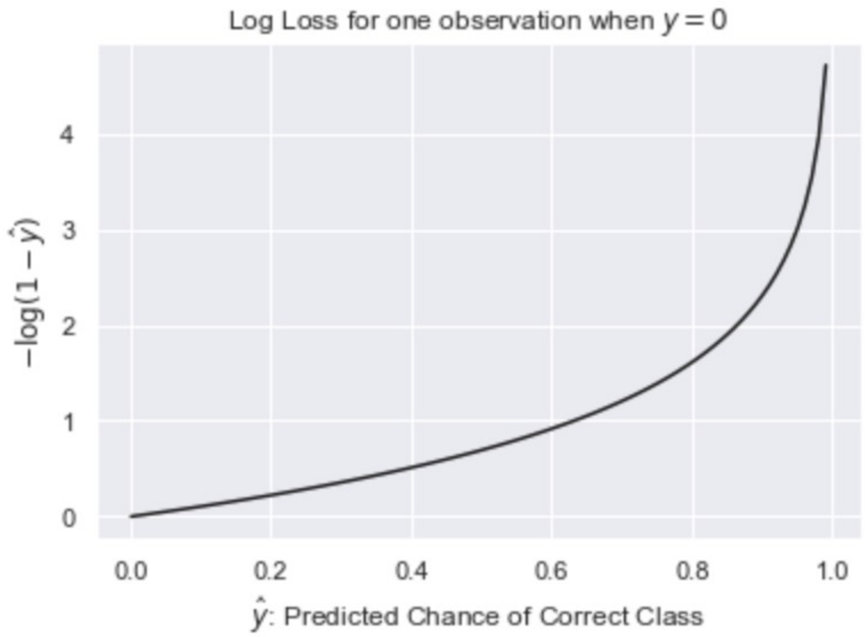


Log loss

So far, we've only looked at log loss when the correct class was 1.

What if our correct class is 0?





If the correct class is 0, we want to have low loss for values of $\hat{y}$ close to 0, and high loss for values of $\hat{y}$ close to 1. This is achieved by just "flipping" the plot on the left!

Cross-entropy loss

We can combine the two cases from the previous slide into a single loss function:

$$\text{loss} = \begin{cases} -\log(1-\hat{y}) & y = 0 \\ -\log(\hat{y}) & y = 1 \end{cases}$$

This is often written unconditionally as:

$$\boxed{\text{loss} = -y\log(\hat{y}) - (1-y)\log(1-\hat{y})}$$

Note: Since y = 0 or 1, one of these two terms is always equal to 0, which reduces this equation to the piecewise one above.

We call this loss function **cross-entropy** loss (or “log loss”).

Mean cross-entropy loss

The empirical risk for the logistic regression model when using cross-entropy loss is then

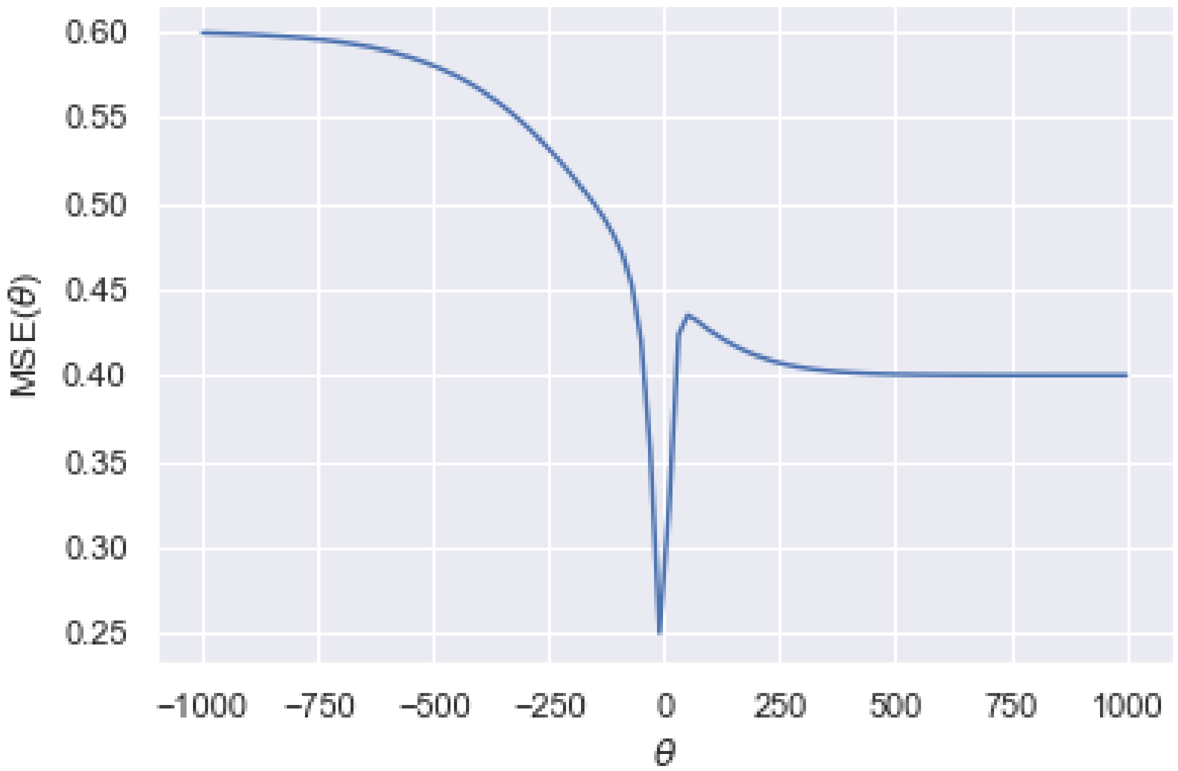
$$R(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \left(y_i \log(\sigma(\mathbb{X}_i^T \theta)) + (1 - y_i) \log(1 - \sigma(\mathbb{X}_i^T \theta)) \right)$$

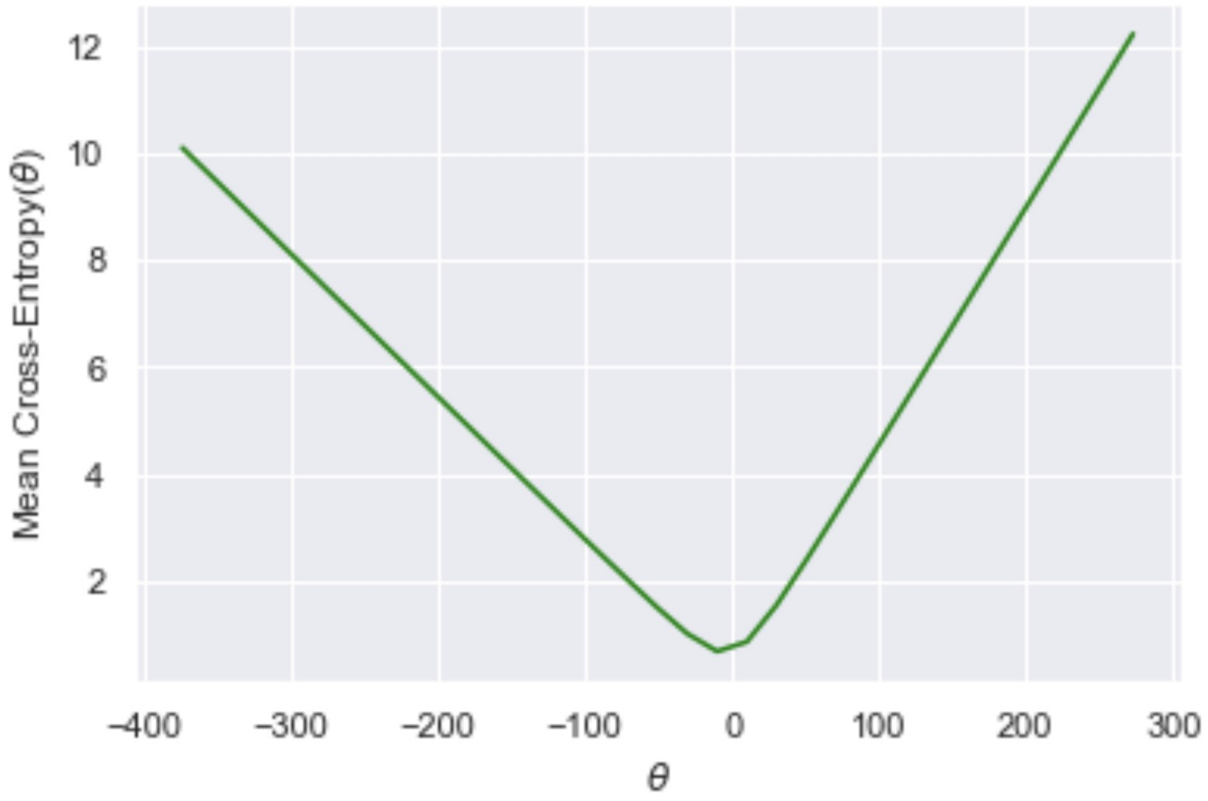
Benefits over mean squared error for logistic regression:

- Loss surface is guaranteed to be nice (convex).
- More strongly penalizes bad predictions.
- Has roots in probability and information theory

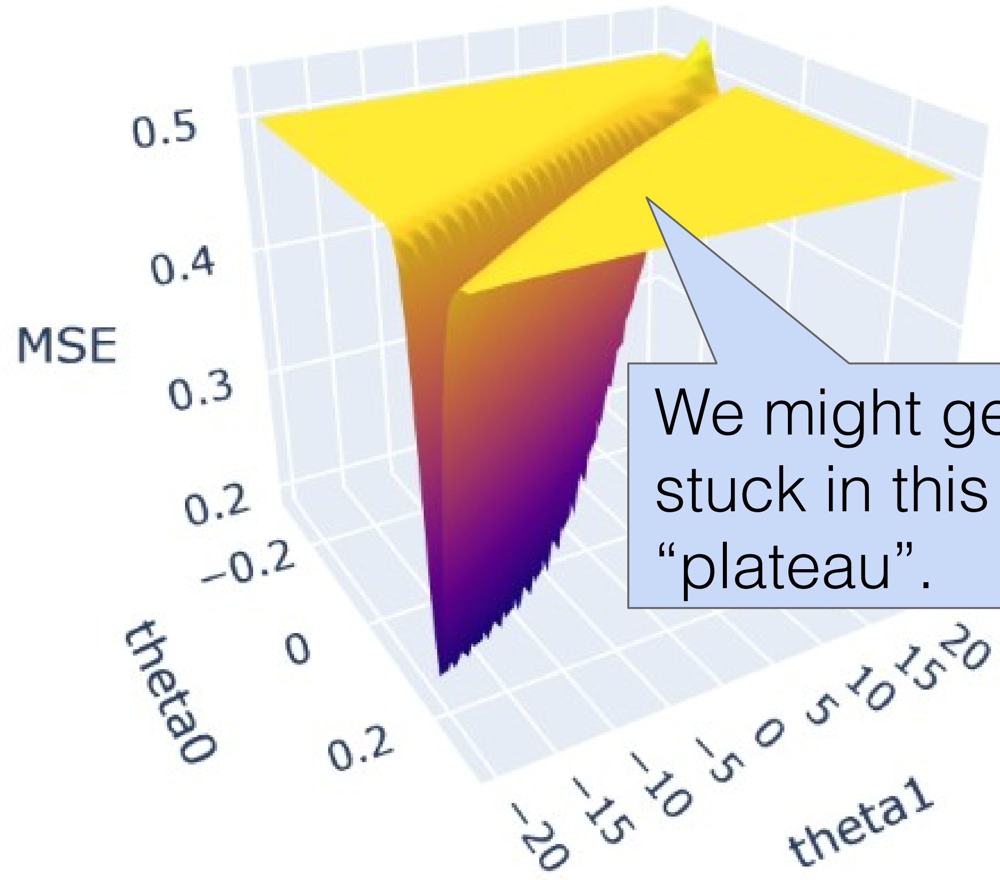
Comparing loss surfaces

On the left, we have a plot of the MSE loss surface on our toy dataset from before. On the right, we have a plot of the mean cross-entropy loss surface on the same dataset.

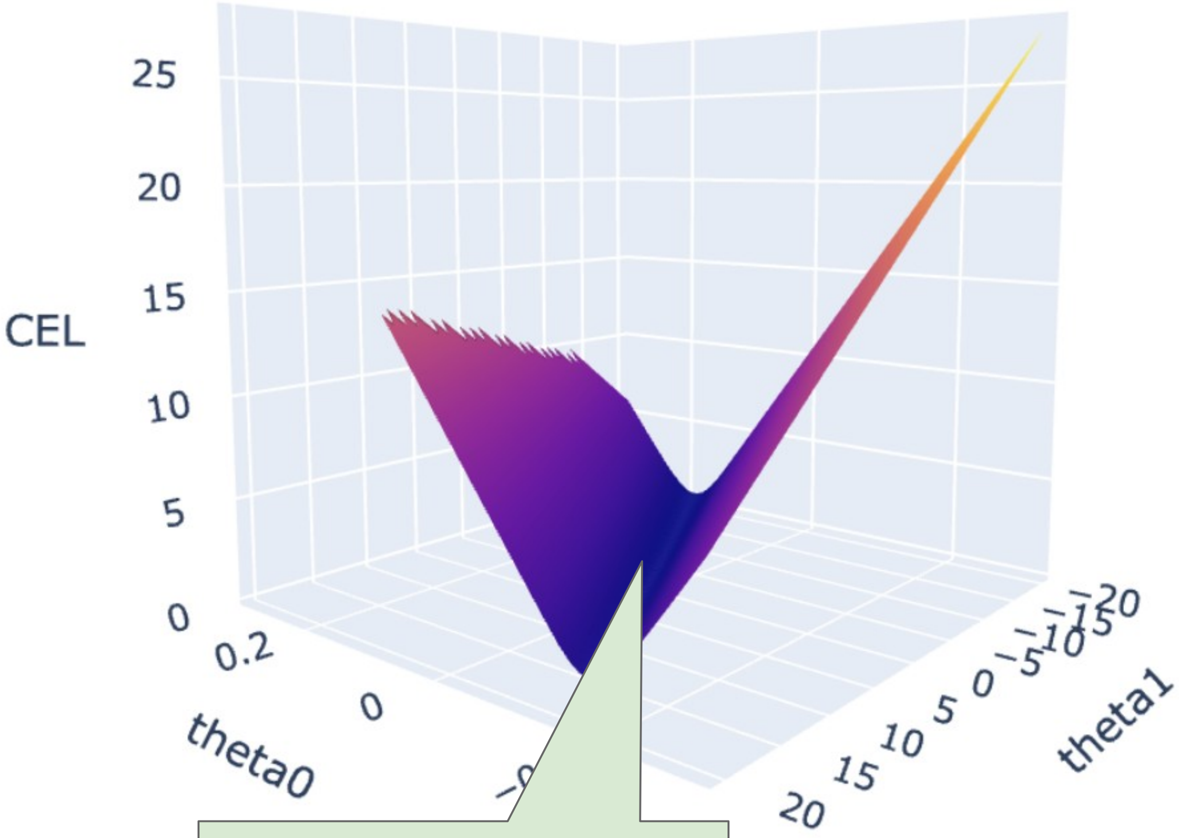




Comparing loss surfaces



We might get stuck in this "plateau".



We will always end up in this "valley".

Summary

Logistic regression

- In a **logistic regression** model, our goal is to predict a binary **categorical** variable (class 0 or class 1) as a linear function of features, passed through the logistic function.
    - Our **response** is the probability that our observation belongs to class 1.

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

- We arrived at this model by assuming that the **log-odds of the probability of belonging to class 1 is linear.**
- To find $\hat{\theta}$, we can choose squared loss or cross-entropy loss.
    - Squared loss works, but is generally not a good idea.
    - Cross-entropy loss is much better (convex, better suited for modeling probabilities).