LECTURE 22

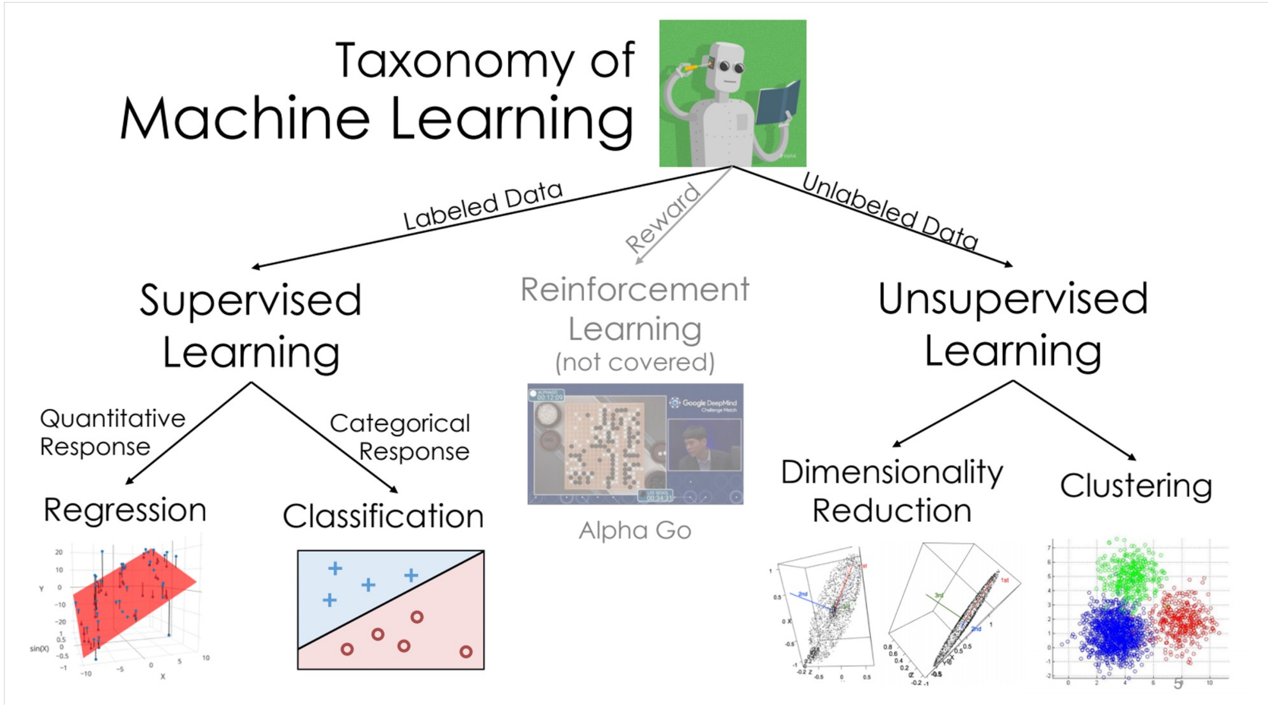
Logistic Regression

Moving from regression to classification.

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.



Regression vs Classification

Regression vs Classification

Logistic regression model derivation

- logistic function (sigmoid)
- Parameter interpretation

Loss function

- Pitfalls of Squared Loss
- Cross Entropy

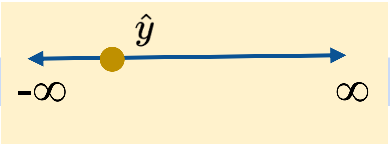
Maximum likelihood estimation

So Far: Regression

In regression, we use unbounded numeric features to predict an *unbounded numeric output.*

GAME_ID	TEAM_NAME	MATCHUP	REB	FTM	TOV	GOAL_DIFF	WON
21700001	Boston Celtics	BOS @ CLE	46	19	12	-0.049	0
21700002	Golden State Warriors	GSW vs. HOU	41	19	17	0.053	0
21700003	Charlotte Hornets	CHA @ DET	47	23	17	-0.030	0
21700004	Indiana Pacers	IND vs. BKN	47	25	14	0.041	1
21700005	Orlando Magic	ORL vs. MIA	50	22	15	0.042	1

$$x^\top \theta$$



Input: numeric features

Model: linear combination

Output: numeric prediction

Examples:

- Predict goal difference from turnover %
- Predict tip from total bill
- Predict mpg from hp

Now: Classification

In **classification**, we use unbounded numeric features to predict a *categorical class*.

Examples:

- Predict *which team won* from turnover %
- Predict *day of week* from total bill
- Predict *model of car* from hp

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$$p = \sigma(x^\top \theta)$$

Win?
If p > 0.5: predict a win
Other: predict a loss

Input: numeric features

Model: linear combination transformed by non-linear **sigmoid**

Decision rule

Output: **class**

An aside: we will use logistic “regression” to perform a *classification* task. Here, “regression” refers to the type of model, not the task being performed.

Kinds of Classification

We are interested in predicting some **categorical variable**, or **response**, y.

Binary classification

- Two classes
- **Responses** y are either 0 or 1

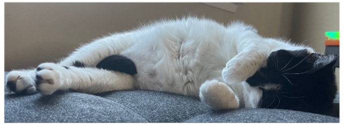
win or lose

disease or no disease

spam or ham

Multiclass classification

- Many classes
- Examples: Image labeling (Pishi, Thor, Hera), next word in a sentence, etc.



Structured prediction tasks

- Multiple related classification predictions
- Examples: Translation, voice recognition, etc.

Our new goal: predict a **binary** output (y_hat = 0 or y_hat = 1) given inputted numeric features

The Modeling Process

	Regression ($y \in \mathbb{R}$)	**Classification** ($y \in \{0, 1\}$)
1. Choose a model	Linear Regression $\hat{y} = f_\theta(x) = x^T\theta$	??
2. Choose a loss function	Squared Loss or Absolute Loss	??
3. Fit the model	Regularization Sklearn/Gradient descent	Regularization Sklearn/Gradient descent
4. Evaluate model performance	R^2, Residuals, etc.	?? (next lecture)

Logistic Regression model derivation

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.

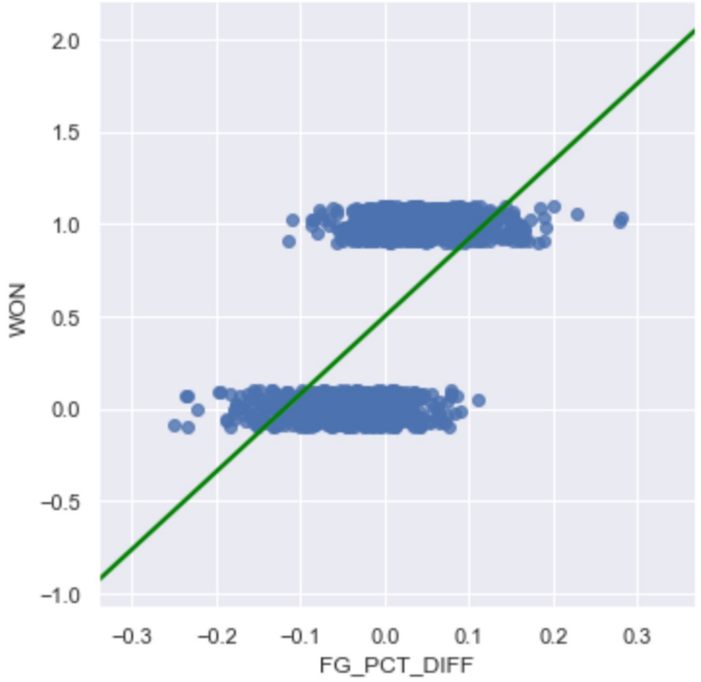
TEAM_NAME	MATCHUP	WON	FG_PCT_DIFF
Boston Celtics	BOS @ CLE	0	-0.049
Golden State Warriors	GSW vs. HOU	0	0.053
Charlotte Hornets	CHA @ DET	0	-0.030
Indiana Pacers	IND vs. BKN	1	0.041
Orlando Magic	ORL vs. MIA	1	0.042

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/ imbalanced data.
- Many other statistical reasons.

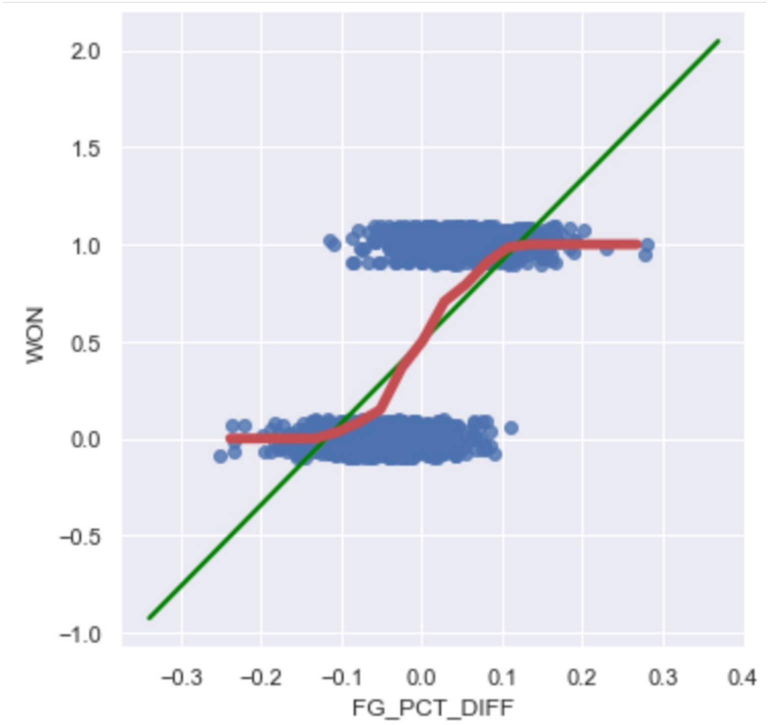


Graph of averages

If we **bin the x-axis**, and take 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").

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

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

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.

1. Choose a model

2. Choose a loss function

3. Fit the model

4. Evaluate model performance

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

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!

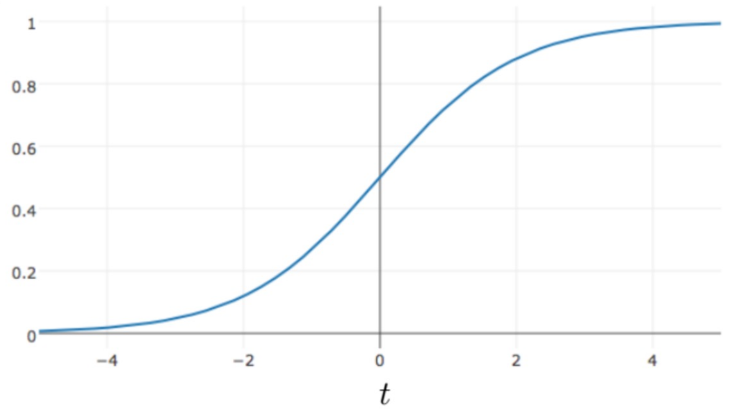
$$\hat{y} = f_\theta(x) = P(Y = 1|x) = \sigma(x^T\theta)$$

Logistic Function

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

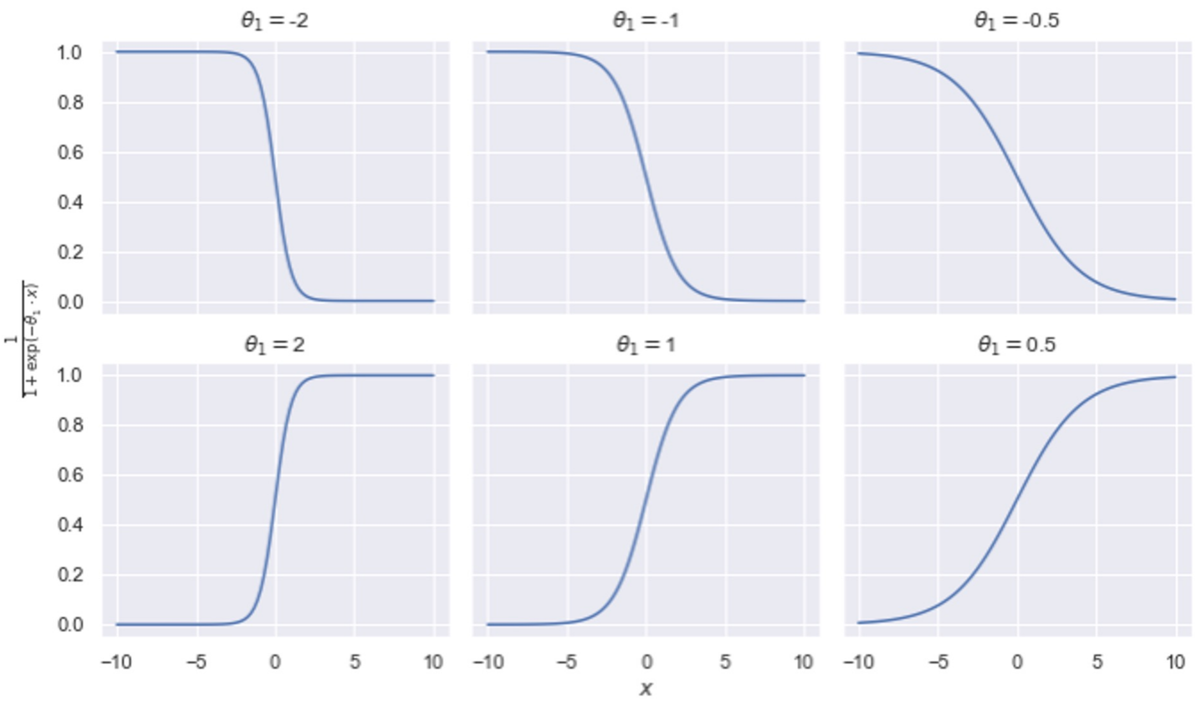
$$\frac{d}{dt}\sigma(t) = \sigma(t)(1-\sigma(t)) = \sigma(t)\sigma(-t)$$

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

Parameter interpretation

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

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

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."

Loss Function

Logistic Regression with squared loss?

1. Choose a model

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

2. Choose a loss function

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

?

3. Fit the model

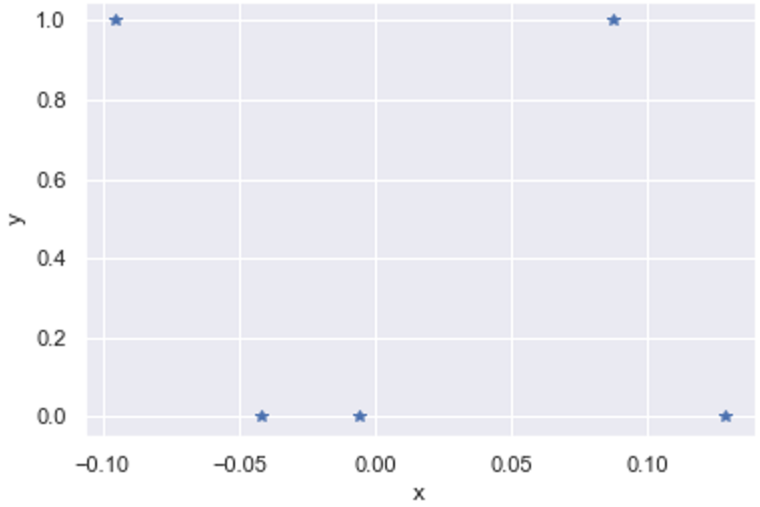
4. Evaluate model performance

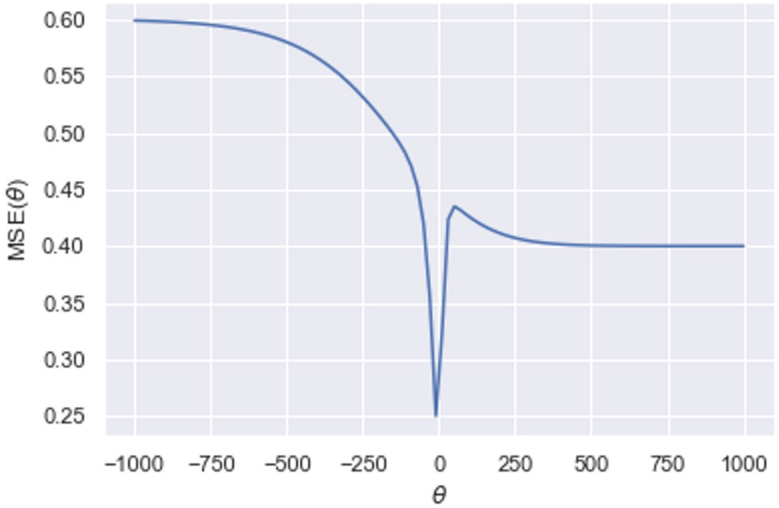
Pitfalls of squared loss with logistic regression

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 of θ (i.e. the loss surface).

What is the issue?

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





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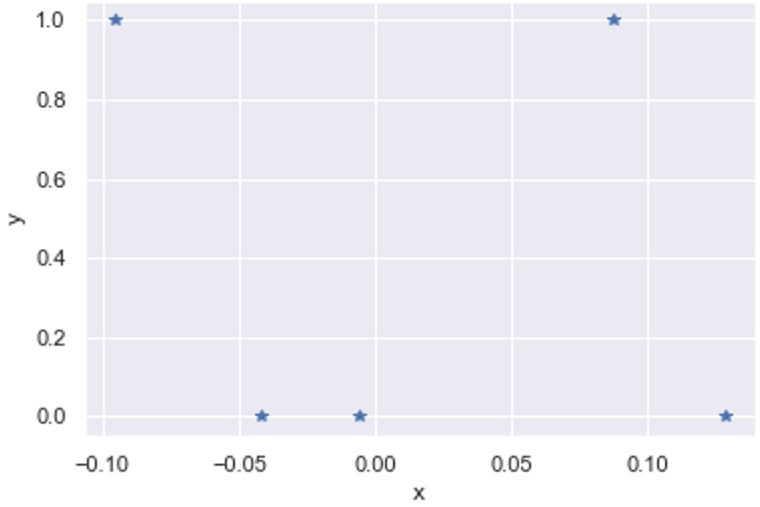
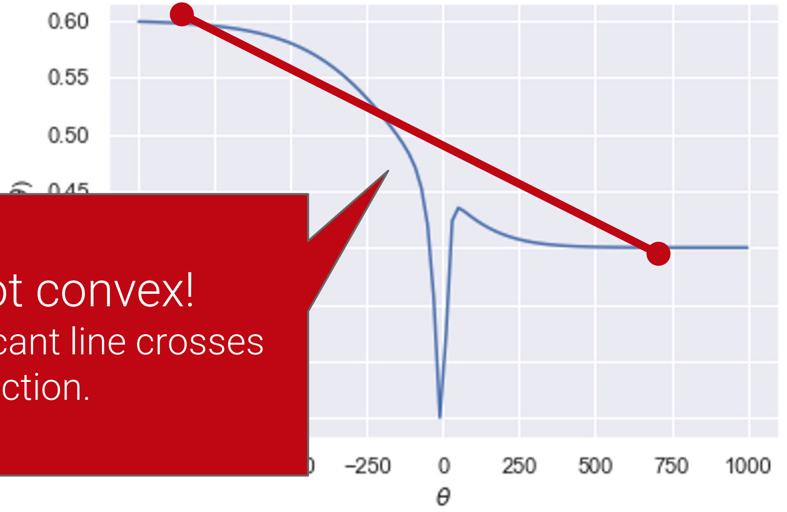




Not convex!
Secant line crosses function.

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:

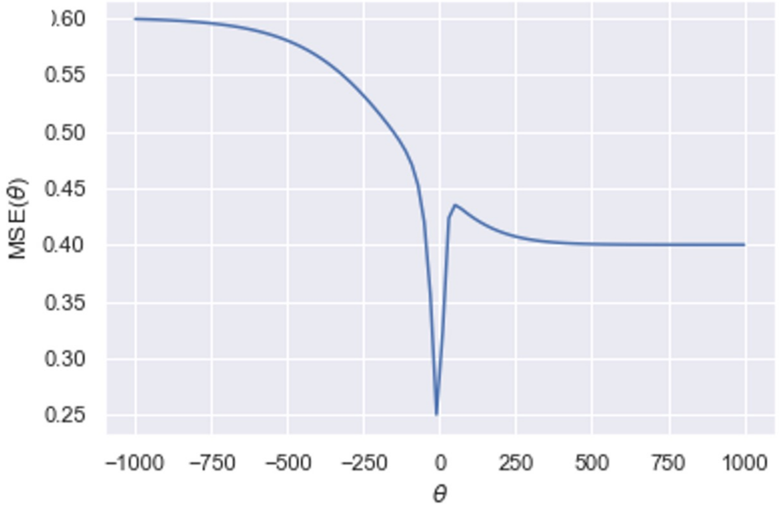
```
minimize(mse_loss_single_arg_toy, x0 = 0)["x"][0]
```

```
-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.



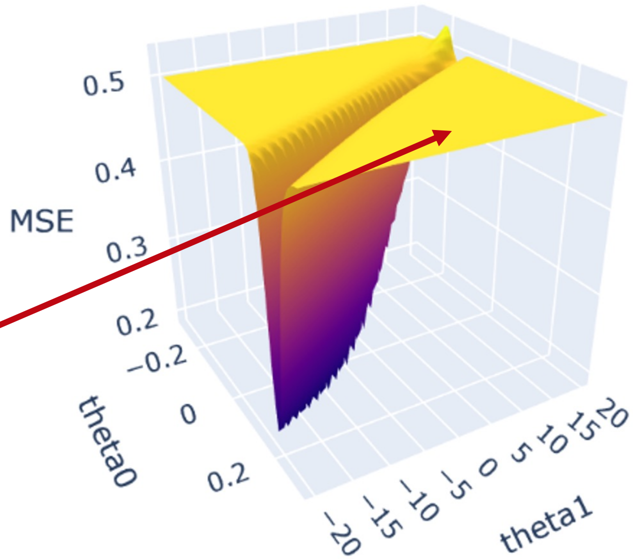
Pitfalls of squared loss with logistic regression

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

If your initial guess for $\hat{\theta}$ is way out in the flat yellow region, routine can get stuck. The model gets stuck in local minima

If the gradient is 0, your update rule will stop changing.

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \boxed{\nabla_\theta R(\theta, \mathbb{X}, \mathbb{Y})}$$



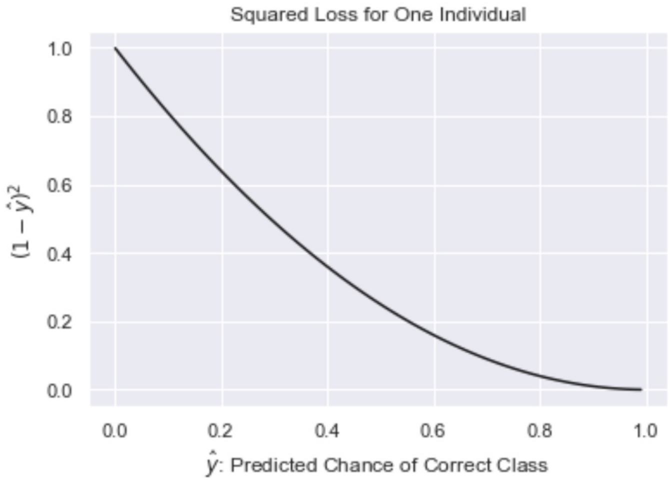
Pitfalls of squared loss with logistic regression

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

Suppose the observation we're trying to predict is actually in **class 1**.

On the right, we have a plot of $(1 - \hat{y})^2$ vs $\hat{y}$.
This is the squared loss for a single prediction.



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 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.

Loss in Classification

Let y be a binary label {0, 1}, and p be the model's predicted probability of the label being 1.

In a classification task, how do we want our loss function to behave?

- When the true y is 1, we should incur *low* loss when the model predicts large p.
- When the true y is 0, we should incur *high* loss when the model predicts large p.

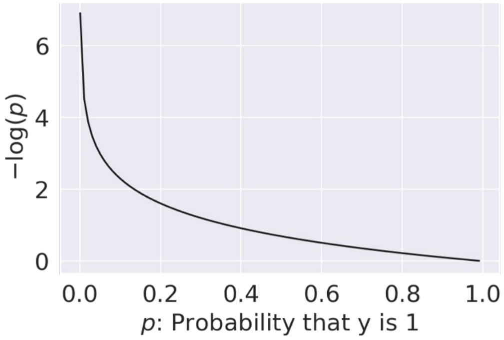
In other words, the behavior we need from our loss function depends on the value of the true class, y.

Cross-Entropy Loss

Let y be a binary label {0, 1}, and p be the probability of the label being 1.

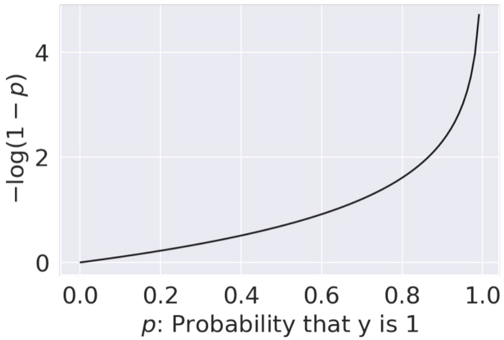
The **cross-entropy loss** is defined as:

$$\text{CE loss} = \begin{cases} -\log(p), & \text{if } \; y = 1 \\ -\log(1-p), & \text{if } \; y = 0 \end{cases}$$



For y = 1,

- p → 0: ∞ loss
- p → 1: zero loss



For y = 0,

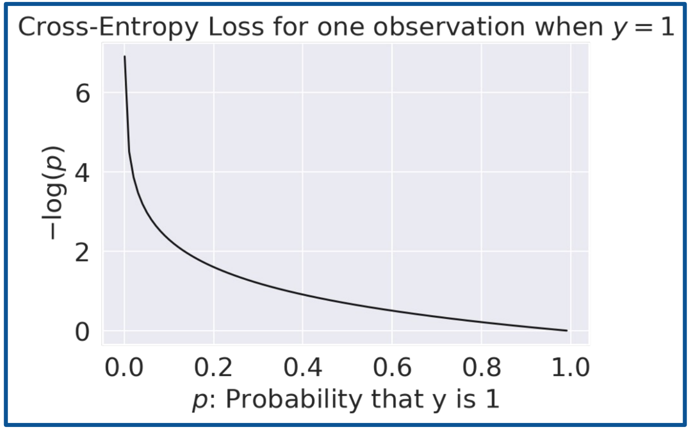
- p → 0: zero loss
- p → 1: ∞ loss

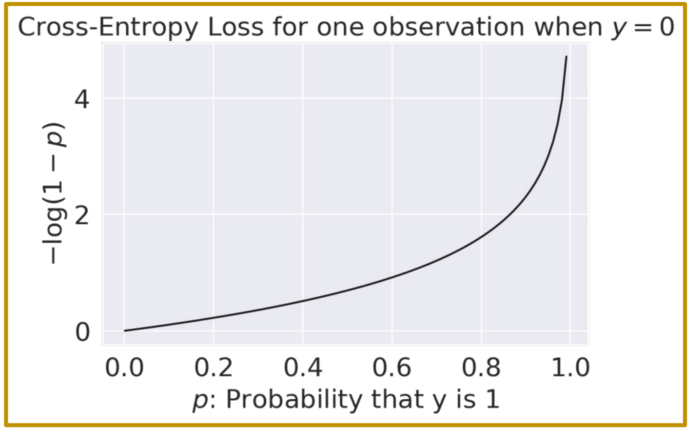
Cross-Entropy Loss: Two Loss Functions In One!

The piecewise loss function we introduced just then is difficult to optimize – we don't want to check "which" loss to use at each step of optimizing theta.

Cross-entropy loss can be equivalently expressed as:

$$\text{CE loss} = \begin{cases} -\log(p), & \text{if } \ y = 1 \\ -\log(1-p), & \text{if } \ y = 0 \end{cases} \;\rightarrow\; \underbrace{\boxed{-}}_{\text{makes loss positive}}\big(\underbrace{y\log(p)}_{\text{for } y = 1\text{, only this term stays}} + \underbrace{(1-y)\log(1-p)}_{\text{for } y = 0\text{, only this term stays}}\big)$$





Empirical Risk: Average Cross-Entropy Loss

For a single datapoint, the cross-entropy curve is convex. It has a global minimum.

$$-\left(y\log(p)+(1-y)\log(1-p)\right)$$

What about average cross-entropy loss, i.e., empirical risk?

For logistic regression, the empirical risk over a sample of size n is:

$$R(\theta) = -\frac{1}{n}\sum_{i=1}^{n}\left(y_i\log(p_i)+(1-y_i)\log(1-p_i)\right)$$

$$= -\frac{1}{n}\sum_{i=1}^{n}\left(y_i\log\left(\sigma\left(X_i^T\theta\right)\right)-(1-y_i)\log\left(1-\sigma\left(X_i^T\theta\right)\right)\right)$$

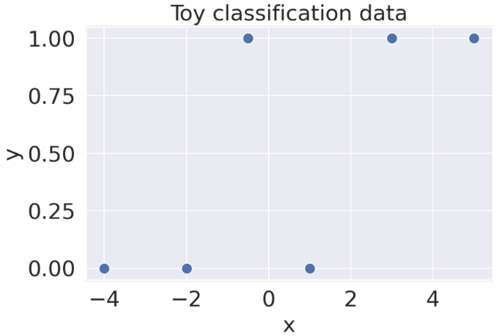
[Recall our model is $\hat{y}_i = p_i = \sigma\left(X_i^T\theta\right)$]

The optimization problem is therefore to find the estimate $\hat{\theta}$ that minimizes R(θ):

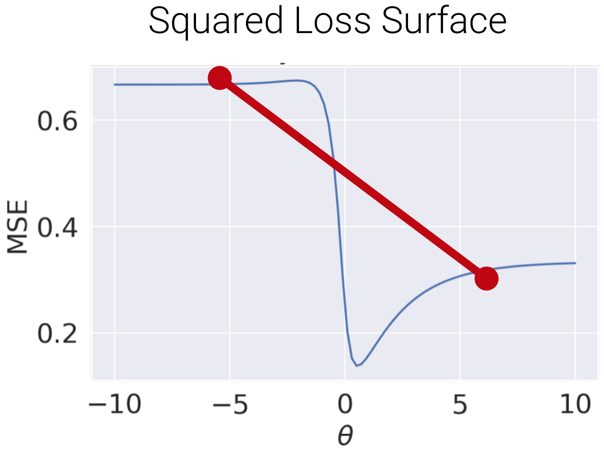
$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \; -\frac{1}{n}\sum_{i=1}^{n}\left(y_i\log\left(\sigma\left(X_i^T\theta\right)\right)-(1-y_i)\log\left(1-\sigma\left(X_i^T\theta\right)\right)\right)$$

Convexity Proof By Picture

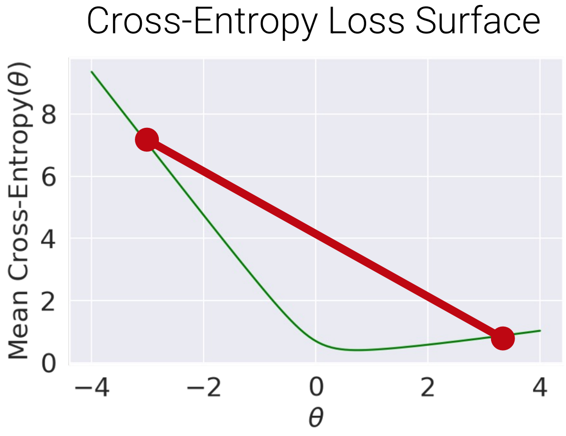
$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} \; -\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log\left(\sigma(X_i^T\theta)\right) - (1-y_i)\log\left(1-\sigma(X_i^T\theta)\right)\right)$$



	x	y
0	-4.0	0
1	-2.0	0
2	-0.5	1
3	1.0	0
4	3.0	1
5	5.0	1



A straight line crosses the curve
Non-convex



Convex!

Logistic Regression with cross entropy

1. Choose a model

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

2. Choose a loss function

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

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

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

3. Fit the model

4. Evaluate model performance

Logistic Regression with cross entropy

1. Choose a model

2. Choose a loss function

3. Fit the model

4. Evaluate model performance

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

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

For logistic regression, we can use squared loss if we want to!

- Using squared loss and using cross-entropy loss will usually result in different $\hat{\theta}$
  - **Different optimization problems, different solutions**.
- **Cross-entropy loss is strictly better than squared loss for logistic regression.**
  - Convex, so easier to minimize using numerical techniques.
  - Better suited for modeling probabilities.

Maximum Likelihood Estimation

PMF of the Bernoulli distribution

If Y is the result of one toss of a coin that lands heads with chance p,

$$P(Y = y) = \begin{cases} p & \text{if } y = 1 \\ 1 - p & \text{if } y = 0 \end{cases}$$

$$= p^y (1-p)^{1-y}$$

Then, if Y_1 and Y_2 are the results of tosses of two coins:

$$P(Y_1 = y_1, Y_2 = y_2) = \left(p_1^{y_1}(1-p_1)^{1-y_1}\right)\left(p_2^{y_2}(1-p_2)^{1-y_2}\right)$$

Estimating the two probabilities

- Suppose we want to estimate the values of p_1 and p_2.
- We know what the likelihood is.

$$P(Y_1 = y_1, Y_2 = y_2) = \left(p_1^{y_1}(1-p_1)^{1-y_1}\right)\left(p_2^{y_2}(1-p_2)^{1-y_2}\right)$$

- Our goal is to find the p_1 and p_2 that **maximize** the above function, over all p_1 and p_2.
  - Maximize, because we are looking for the p_1 and p_2 that are “most likely” to have generated the data that we observed.
- As before, this involves differentiating, setting equal to 0, and solving.

Log likelihoods

- Maximizing $P(Y_1 = y_1, Y_2 = y_2) = \left(p_1^{y_1}(1-p_1)^{1-y_1}\right)\left(p_2^{y_2}(1-p_2)^{1-y_2}\right)$ is annoying.
  - Products -> chain rule.
- log(x) is a **strictly increasing** function.
  - If a > b, then log(a) > log(b).
- This means, the values of p_1 and p_2 that maximize $P(Y_1 = y_1, Y_2 = y_2)$ are the same values that maximize

$$
\begin{aligned}
&\log\left(\left(p_1^{y_1}(1-p_1)^{1-y_1}\right)\left(p_2^{y_2}(1-p_2)^{1-y_2}\right)\right) \\
&= y_1\log(p_1) + (1-y_1)\log(1-p_1) + y_2\log(p_2) + (1-y_2)\log(1-p_2) \\
&= \sum_{i=1}^{2}\left(y_i\log(p_i) + (1-y_i)\log(1-p_i)\right)
\end{aligned}
$$

Starting to look familiar!

Estimating n probabilities

- For $i = 1, 2, \ldots, n$, let Y_i be Bernoulli(p_i).
  - Each Y_i is independent of each other.
- To estimate $p_1, p_2, \ldots, p_n$:

$$\text{Find } \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n \text{ that maximize } \sum_{i=1}^{n} \left(y_i \log(p_i) + (1 - y_i)\log(1 - p_i)\right)$$

Equivalently:

$$\text{Find } \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n \text{ that } \textit{minimize } -\frac{1}{n}\sum_{i=1}^{n} \left(y_i \log(p_i) + (1 - y_i)\log(1 - p_i)\right)$$

We choose this equivalent form because we are more used to minimizing loss.

Cross-entropy loss

$$\text{Find } \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n \text{ that } \textit{minimize } -\frac{1}{n}\sum_{i=1}^{n}\left(y_i \log(p_i) + (1-y_i)\log(1-p_i)\right)$$

What does this have to do with logistic regression?

- We have n observations ($y_1, y_2, \ldots, y_n$). Each is either 1 or 0.
  - Assume that each is independent of one another.
- Can think of observation y_i as the result of a coin toss with probability p_i.
  - The output of our logistic regression model is our estimate for the probability that $y_i = 1$.
- Thus, we can use the above average loss, with $p_i = \sigma(\mathbb{X}_i^T\theta)$.
- This gives us the exact same expression for cross-entropy loss that we saw before!

Maximum likelihood estimation

Minimizing cross-entropy loss is equivalent to maximizing the likelihood of the data.

- We are choosing the model parameters that are “most likely”, given this data.
- Another perspective of fitting our model to the data.

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

This technique is called **maximum likelihood estimation (MLE)**.

- It turns out, many of the model + loss combinations we’ve seen in this class can be motivated using MLE.
  - OLS, Ridge Regression.
- You will study this further in probability and ML classes. But now you know it exists.

Solving Maximum Likelihood Estimation (Not required)

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

- Approach 1: Gradient Descent (take larger – more certain – steps opposite the gradient)
- Approach 2: Stochastic Gradient Descent (SGD) (take many small steps opposite the gradient)
- Approach 3: Newton’s Method (use second derivatives to better follow curvature)

1. Choose a model

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

2. Choose a loss function

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

3. Fit the model

✅

4. Evaluate model performance

Next time!