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- But how can we predict a categorical label?





- We've explored how to use Linear Regression and its many variations to predict a continuous label.
- But how can we predict a categorical label?
 - Logistic Regression





- Logistic Regression
 - Don't be confused by the use of the term "regression" in its name!
 - Logistic Regression is a classification algorithm designed to predict categorical target labels.





- Logistic Regression Section Overview
 - Transforming Linear Regression to Logistic Regression
 - Mathematical Theory behind Logistic Regression
 - Simple Implementation of Logistic Regression for Classification Problem





- Logistic Regression Section Overview
 - Interpreting Results
 - Odds Ratio and Coefficients
 - Classification Metrics
 - Accuracy
 - Precision
 - Recall
 - ROC Curves





- Logistic Regression Section Overview
 - Multiclass Classification with Logistic Regression
 - Logistic Regression Project
 - Logistic Regression Project Solutions





- Logistic Regression will allow us to predict a categorical label based on historical feature data.
- The categorical target column is two or more discrete class labels.





- Classification algorithms predict a class or category label:
 - Class 0: Car Image
 - Class 1: Street Image
 - Class 2: Bridge Image





 You may not have realized you are helping Google label class data!





- Keep in mind, any continuous target can be converted into categories through discretization.
 - Class 0: House Price \$0-100k
 - Class 1: House Price \$100k-200k
 - Class 2: House Price <\$200k



- Classification algorithms also often produce a **probability** prediction of belonging to a class:
 - Class 0: 10% Probability
 - Class 1: 85% Probability
 - Class 2: 5% Probability





- Classification algorithms also often produce a **probability** prediction of belonging to a class:
 - Class 0: 10% Probability Car Image
 - Class 1: 85% Probability Street Image
 - Class 2: 5% Probability Bridge Image
 - Model reports back prediction of Class 1, image is a street.





- Also note our prediction ŷ will be a category, meaning we won't be able to calculate a difference based on y-ŷ.
 - Car Image Street Image does not make sense.
- We will need to discover a completely different set of error metrics and performance evaluation!





Let's get started!





Logistic Regression Theory and Intuition

Part One: The Logistic Function





 Logistic Regression works by transforming a Linear Regression into a classification model through the use of the logistic function:

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



 Let's begin by understanding the history and motivation behind the logistic function (a.k.a the sigmoid function):

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





Note:

 For now, we're only referring to the logistic function itself, not the logistic regression model!

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



 1830-1850: Under guidance of Adolphe Quetelet, Pierre François Verhulst developed the logistic function:



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







• 1883: Logistic function was independently developed in chemistry as a model of autocatalysis by Wilhelm Ostwald.

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







 1830-1850: Under guidance of Adolphe Quetelet, Pierre François Verhulst developed the logistic function:



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

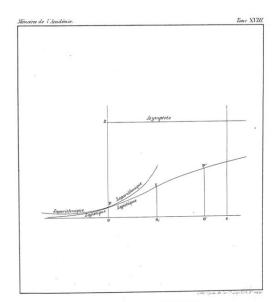






• 1830-1850: Developed for the purposes of modeling population growth.





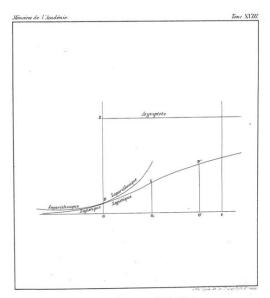






 Why the need for a logistic function versus a logarithmic function?



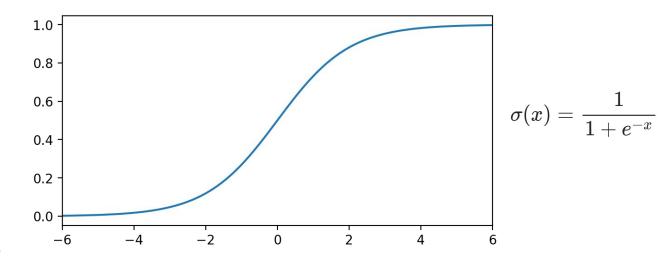








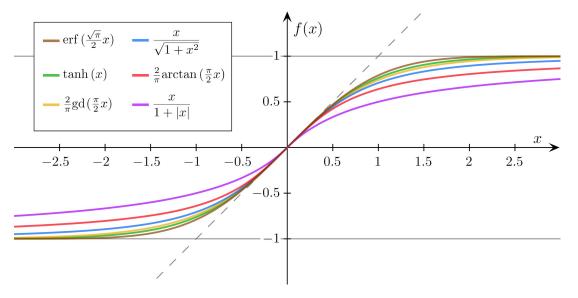
 Why the need for a logistic function versus a logarithmic function?







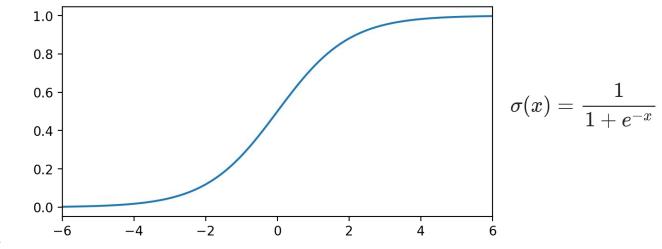
• Note: There is a "family" of logistic functions.







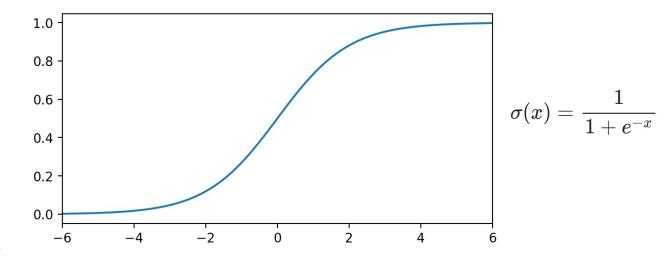
 Notice the "leveling off" behavior of the curve.







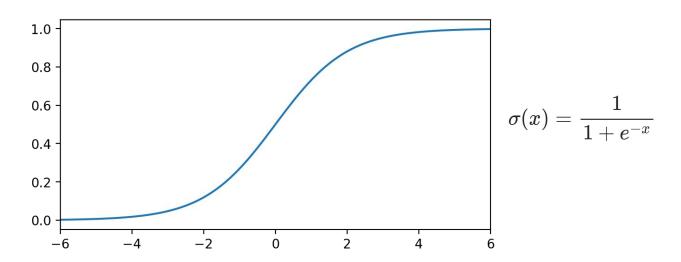
 Also notice any value of x will have an output range between 0 and 1.







 Many natural real world systems have a "carrying capacity" or a natural limiting factor.

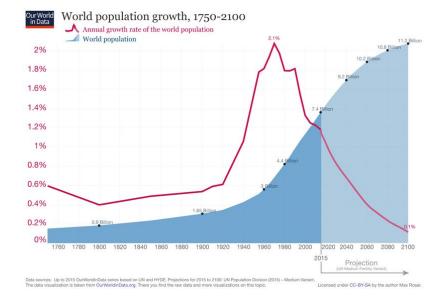






 Many natural real world systems have a "carrying capacity" or a natural limiting

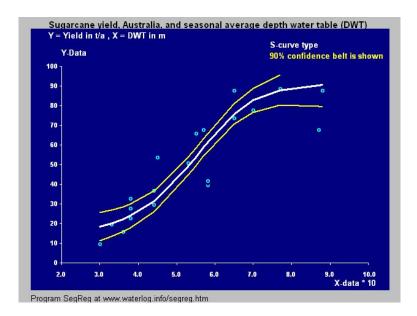
factor.





 Many natural real world systems have a "carrying capacity" or a natural limiting

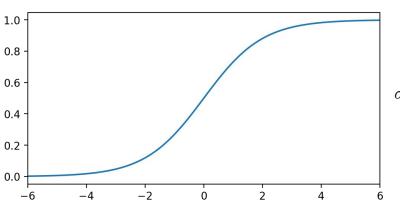
factor.







 1940s: Using the logistic function for statistical modeling was developed by Joseph Berkson.

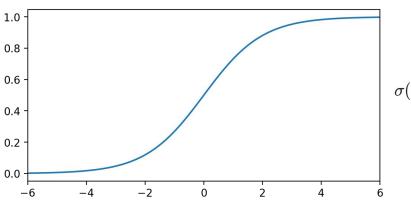


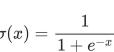
$$\sigma(x) = rac{1}{1+e^{-x}}$$





 1944: "Application of the logistic function to bio-assay" in the Journal of the American Statistical Association









 Quirky fact: Berkson was a prominent opponent of the idea that cigarette smoking causes cancer.









• Life magazine, Berkson: "...very doubtful that smoking causes cancer of the lung."

leaves another 'very doubtful'

though this has nover been or rectly demonstrated in any lab-cratory experiment. points in the same direction.

"The risk of developing lung cancer increases with duration of bronchitis," as well as from pul-monary emplyaers, destruction committee and narrevered to its of tiny air secs that perform the lungs hasic breathing function. I Hairz Disease: "Male cigaret smokers have a hipper death rate from coronary artary disease than nonamoking males, but it is not clear that the association has

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against cigarets.

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words mittee to its most serious charges these critics have persistently smoking and the number of ciga-rets smoked per day, and is dimin-ished by discontinuing emoking."

> Other Lung Diseases: "Cigaret up by conclusive laboratory proof smoking is the most important of the causes of chronic bronchitis in the United States, and increases the risk of dying from chronic transfer in the United States, and increases the risk of dying from chronic transfer in the state of the s bronchitis," as well as from pul- were carefully considered by the









- While we now know smoking is clearly bad for you, we still haven't learned how to convert a linear regression to a logistic regression!
- Let's continue on by seeing how a linear regression is unable to solve classification problems effectively and how the logistic function can fix this!





Logistic Regression Theory and Intuition

Part Two:

Linear to Logistic Intuition





- Let's explore how to convert a Linear
 Regression model used for a regression
 task into a Logistic Regression model used
 for a classification task.
- Imagine a dataset with a single feature (previous year's income) and a single target label (loan default)





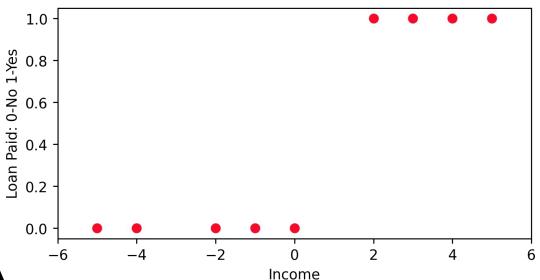
Our data set:

Income	Loan Paid
-5	0
-4	0
-2	0
-1	0
0	0
2	1
3	1
4	1
5	1





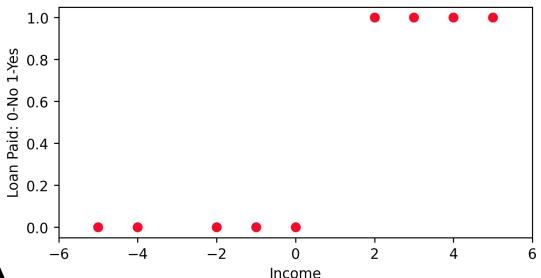
 Let's begin by plotting income versus default:







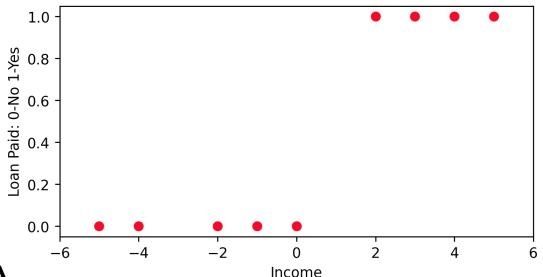
 Notice that people with negative income tend to default on their loans.







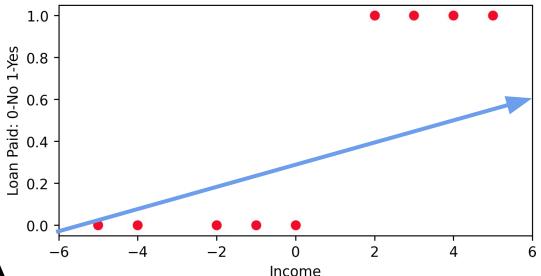
 What if we had to predict default status given someone's income?







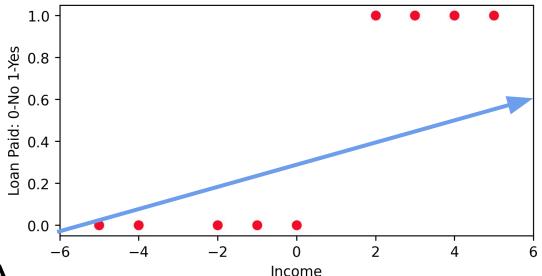
 Fitting a Linear Regression would not work (recall Anscombe's quartet):







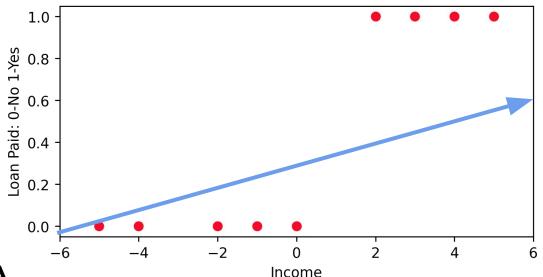
 Linear Regression easily distorted by only having 0 and 1 as possible y training values.







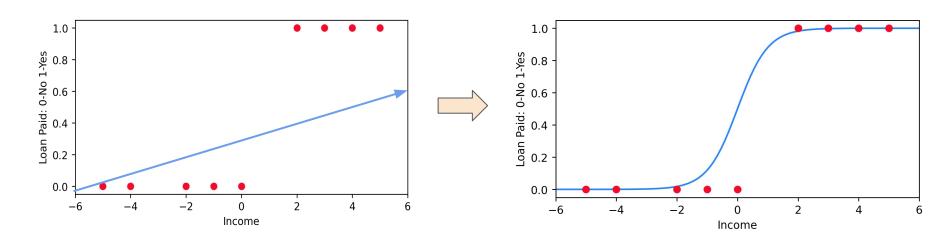
 Also would be unclear how to interpret predicted y values between 0 and 1.







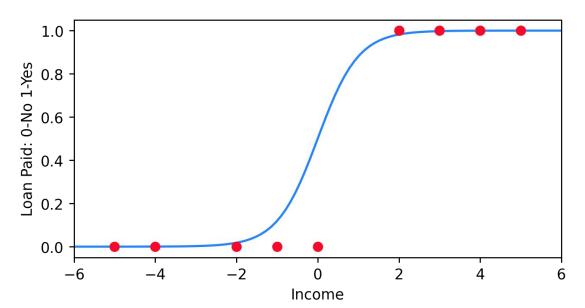
 We could make use of the Logistic Function for a conversion!







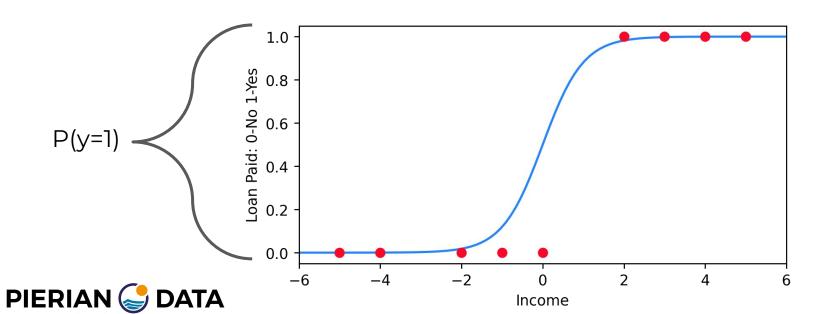
 Let's first focus on what this Logistic Regression would look like.





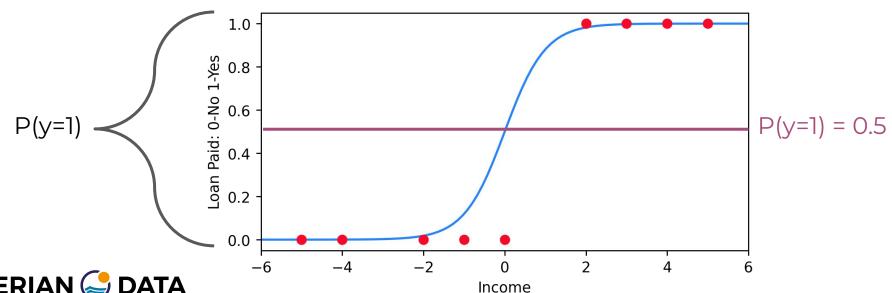


 Treat the y-axis as a probability of belonging to a class:





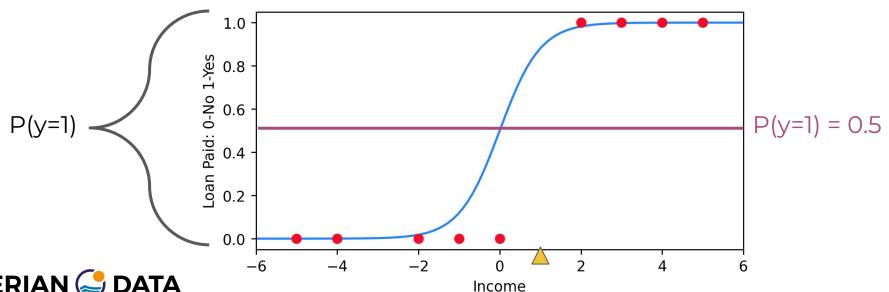
• Treating P(y=1) >= 0.5 as a cut-off for classification:







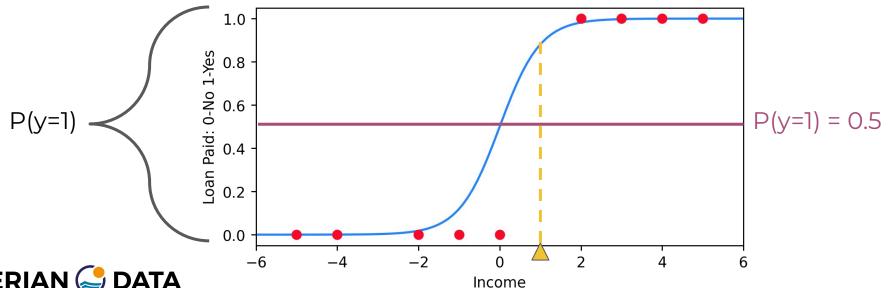
• For example, a new person with an income of 1:







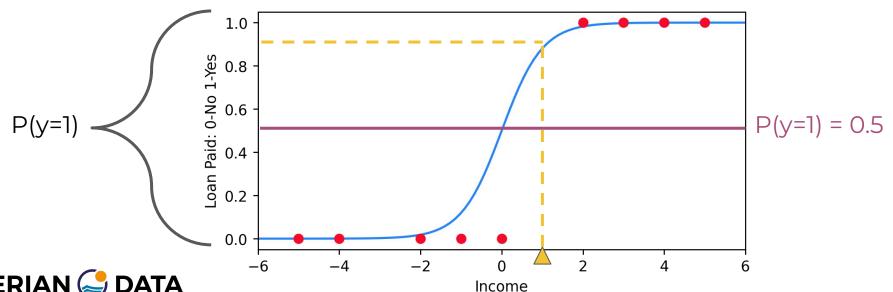
• For example, a new person with an income of 1:







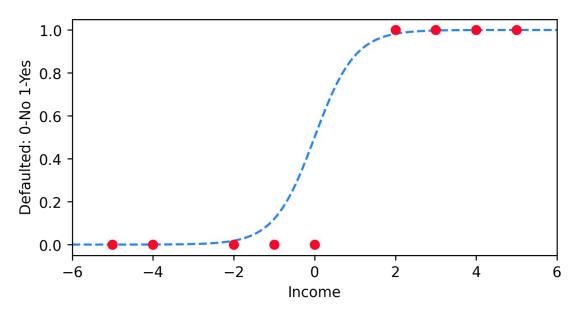
 Predict a 90% probability of paying off loan, return prediction of Loan Paid = 1.







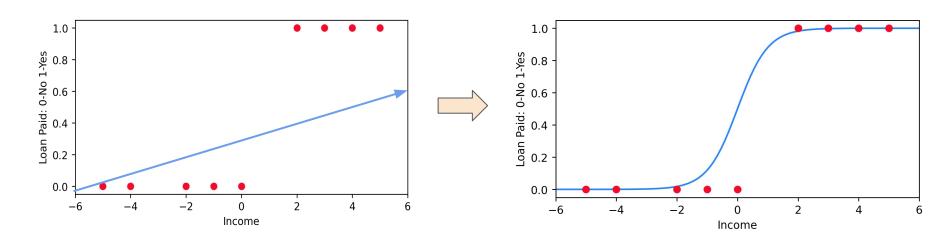
But how do we actually create this line?







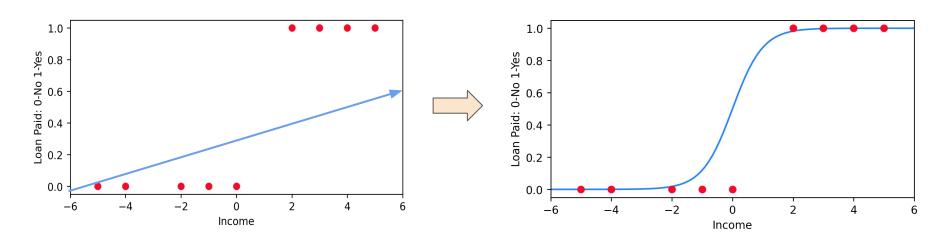
 Fortunately, the mathematics of the conversion are quite simple!







• In the next lecture we will go through the mathematical process of this conversion.







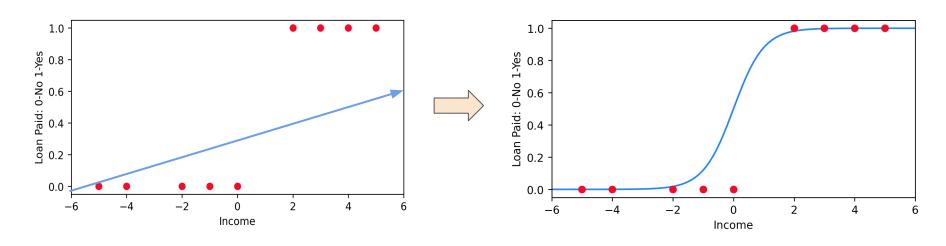
Logistic Regression Theory and Intuition

Part Two: Linear to Logistic Math





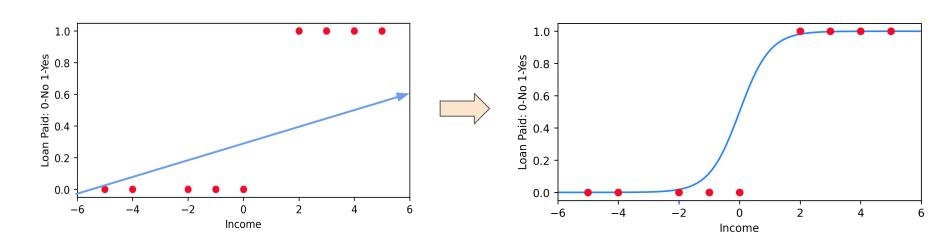
 Let's go through the math of converting Linear Regression to Logistic Regression.







- Relevant ISLR Reading:
 - Section 4.3 Logistic Regression







We already know the Linear Regression equation:

$$\hat{y} = eta_0 x_0 + \dots + eta_n x_n \ \hat{y} = \sum_{i=1}^n eta_i x_i$$



 We also know the Logistic function transforms any input to be between 0 and 1

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



 All we need to do is plug the Linear Regression equation into the Logistic function to create a Logistic Regression!

$$\hat{y}=eta_0x_0+\cdots+eta_nx_n \ \hat{y}=iggledel{\sum_{i=0}^neta_ix_i} \sigma(x)=rac{1}{1+e^{-x}}$$



• Simply put in terms of the logistic function:

$$\hat{y} = \sigma(eta_0 x_0 + \dots + eta_n x_n) \ \hat{y} = \sigmaigg(\sum_{i=0}^n eta_i x_iigg)$$



• Writing it out fully:

$$\hat{y} = rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i}}$$



• How do we interpret the coefficients and their relation to $\hat{\mathbf{y}}$?

$$\hat{y} = rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i}}$$



 First we need to understand the term odds.

A term you may be familiar with from

gambling odds.







- In gambling odds are often referred to in the sense of N to 1.
- But where does this actually come from?







 The odds of an event with probability p is defined as the chance of the event happening divided by the chance of the event not happening:

$$\frac{p}{1-p}$$



 Imagine an event with 50% probability of occurring. This is 0.5/1-0.5 which is 0.5/0.5, the same as 1/1 or 1 to 1 odds of occurring.

$$\frac{p}{1-p}$$



 Taking the formula below, we can rearrange it to show that it is equivalent to modelling the log of the odds as a linear combination of the features.

$$\hat{y} = rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i}}$$



 This will allow us to solve for the coefficients and feature x in terms of log odds.

$$\hat{y} = rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i}}$$



Solving for log odds:

$$\hat{y}=rac{1}{1+e^{-\sum_{i=0}^neta_ix_i}}$$



Solving for log odds:

$$\hat{y}=rac{1}{1+e^{-\sum_{i=0}^neta_ix_i}}$$

$$\hat{y}+\hat{y}e^{-\sum_{i=0}^neta_ix_i}=1$$



$$\hat{y}+\hat{y}e^{-\sum_{i=0}^neta_ix_i}=1$$



$$egin{aligned} \hat{y} + \hat{y}e^{-\sum_{i=0}^{n}eta_{i}x_{i}} &= 1 \ \hat{y}e^{-\sum_{i=0}^{n}eta_{i}x_{i}} &= 1 - \hat{y} \end{aligned}$$



$$egin{aligned} \hat{y} + \hat{y}e^{-\sum_{i=0}^{n}eta_{i}x_{i}} &= 1 \ \hat{y}e^{-\sum_{i=0}^{n}eta_{i}x_{i}} &= 1 - \hat{y} \ &rac{\hat{y}}{1-\hat{y}} &= e^{\sum_{i=0}^{n}eta_{i}x_{i}} \end{aligned}$$



$$rac{\hat{y}}{1-\hat{y}}=e^{\sum_{i=0}^neta_ix_i}$$



$$rac{\hat{y}}{1-\hat{y}}=e^{\sum_{i=0}^neta_ix_i}$$

$$\ln\left(rac{\hat{y}}{1-\hat{y}}
ight) = \sum_{i=0}^n eta_i x_i$$

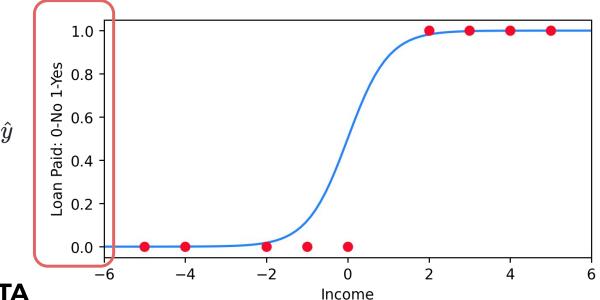


 What would the function curve look like in terms of log odds?

$$\ln\left(rac{\hat{y}}{1-\hat{y}}
ight) = \sum_{i=0}^n eta_i x_i$$



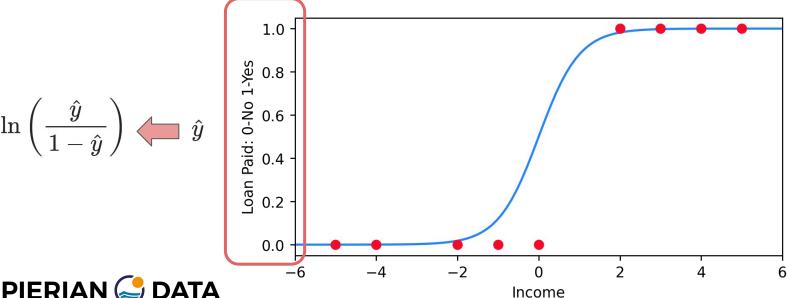
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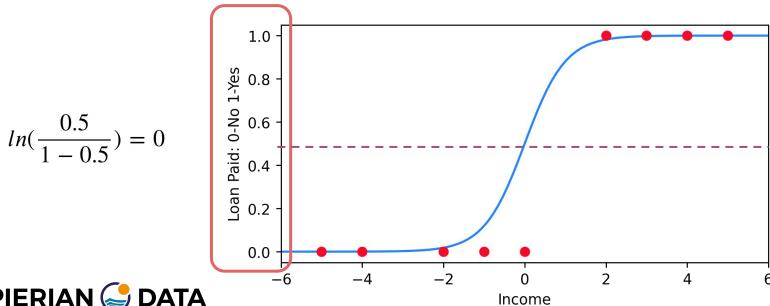
What would the function curve look like in terms of log odds?







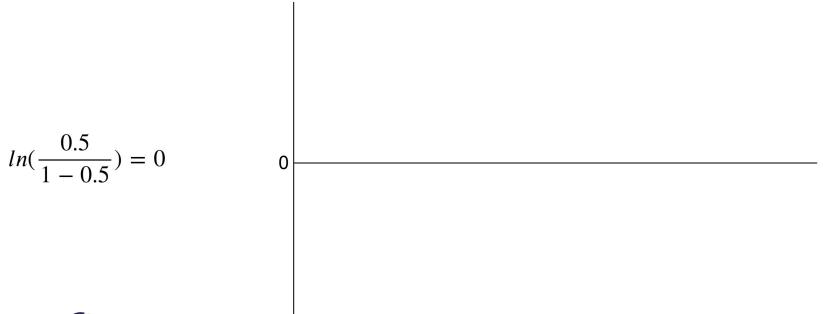
• Consider p=0.5







Consider p=0.5, halfway point now at 0.







As p goes to 1 then log odds becomes ∞

$$\lim_{p \to 1} \ln(\frac{p}{1-p}) = \infty$$

$$ln(\frac{0.5}{1-0.5}) = 0$$





PIERIAN 🈂 DATA

Logistic Regression

As p goes to 0 then log odds becomes -∞

$$\lim_{p \to 1} \ln(\frac{p}{1-p}) = \infty$$

$$\ln(\frac{0.5}{1-0.5}) = 0$$

$$\lim_{p \to 0} \ln(\frac{p}{1-p}) = -\infty$$



PIERIAN 🍪 DATA

Logistic Regression

Class points now at infinity

$$\lim_{p \to 1} \ln(\frac{p}{1-p}) = \infty$$

$$\ln(\frac{0.5}{1-0.5}) = 0$$

$$\lim_{p \to 0} \ln(\frac{p}{1-p}) = -\infty$$



On log scale logistic function is straight line

$$\lim_{p\to 1} ln(\frac{p}{1-p}) = \infty$$

$$ln(\frac{0.5}{1-0.5}) = 0$$

$$\lim_{p\to 0} ln(\frac{p}{1-p}) = -\infty$$
PIERIAN \bigcirc DATA



Coefficients in terms of change in log odds.

$$\lim_{p\to 1} ln(\frac{p}{1-p}) = \infty$$

$$ln(\frac{0.5}{1-0.5}) = 0$$

$$\lim_{p\to 0} ln(\frac{p}{1-p}) = -\infty$$
PIERIAN \bigcirc DATA



Is β simple to interpret? Not really...

 $\left|\ln\left(rac{\hat{y}}{1-\hat{y}}
ight) = \sum_{i=0}^n eta_i x_i \, .$

$$\lim_{p \to 1} ln(\frac{p}{1-p}) = \infty$$

$$ln(\frac{0.5}{1 - 0.5}) = 0$$

$$\lim_{p \to 0} \ln(\frac{p}{1-p}) = -\infty$$



• Since the log odds scale is nonlinear, a β value can not be directly linked to "one unit increase" as it could in Linear Regression.

$$\ln\left(rac{\hat{y}}{1-\hat{y}}
ight) = \sum_{i=0}^{m}eta_{i}x_{i}$$

• There are some straightforward insights we can gain however...

$$\ln\left(rac{\hat{y}}{1-\hat{y}}
ight) = \sum_{i=0}^n eta_i x_i$$



- Sign of Coefficient
 - \circ Positive β indicates an increase in likelihood of belonging to 1 class with increase in associated \mathbf{x} feature.
 - o Negative $\boldsymbol{\beta}$ indicates an decrease in likelihood of belonging to 1 class with increase in associated \boldsymbol{x} feature.





- Magnitude of Coefficient
 - Harder to directly interpret magnitude of β directly, especially when we could have discrete and continuous x feature values.
 - We can however begin to use **odds ratio**, essentially comparing magnitudes against each other.



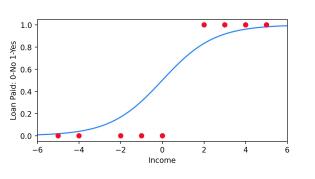


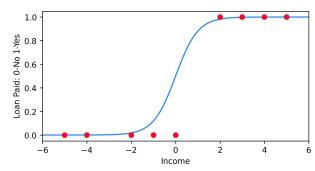
- Magnitude of Coefficient
 - Comparing magnitudes of coefficients against each other can lead to insight over which features have the strongest effect on prediction output.

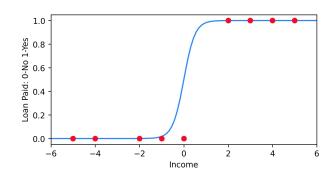




 The last mathematical topic we need to discuss concerning Logistic Regression is how we actually fit this curve!



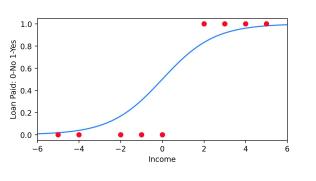


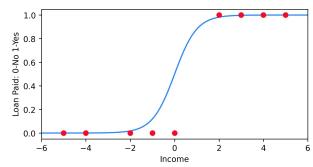


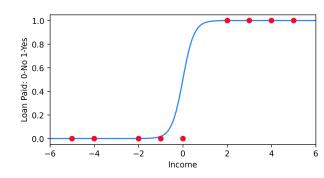




 We'll discuss the basics of fitting the best curve with maximum likelihood in the next lecture!











Logistic Regression Theory and Intuition

Part Three: Finding the Best Fit





- Logistic Regression uses Maximum
 Likelihood to find the best fitting model.
- This lecture will give you an intuition of how this method works.
- We'll also then display the cost function and gradient descent that is solved for by the computer.



Quick Note: ISLR Section 4.3.2

default status. In other words, we try to find $\hat{\beta}_0$ and $\hat{\beta}_1$ such that plugging these estimates into the model for p(X), given in (4.2), yields a number close to one for all individuals who defaulted, and a number close to zero for all individuals who did not. This intuition can be formalized using a mathematical equation called a *likelihood function*:

$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i':y_{i'}=0} (1 - p(x_{i'})). \tag{4.5}$$

The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to maximize this likelihood function.

Maximum likelihood is a very general approach that is used to fit many of the non-linear models that we examine throughout this book. In the linear regression setting, the least squares approach is in fact a special case of maximum likelihood. The mathematical details of maximum likelihood are beyond the scope of this book. However, in general, logistic regression



Quick Note: ISLR Section 4.3.2

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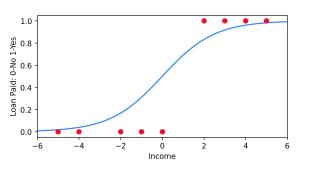
The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to maximize this likelihood function.

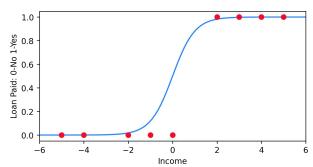
Maximum likelihood is a very general approach that is used to fit many of the non-linear models that we examine throughout this book. In the linear regression setting, the least squares approach is in fact a special case of maximum likelihood. The mathematical details of maximum likelihood are beyond the scope of this book. However, in general, logistic regression

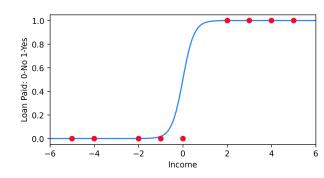




- Here we see three different Logistic
 Regression curves with different β values.
- How do we measure which is the best fit?



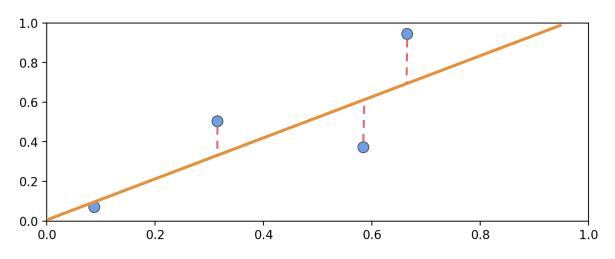








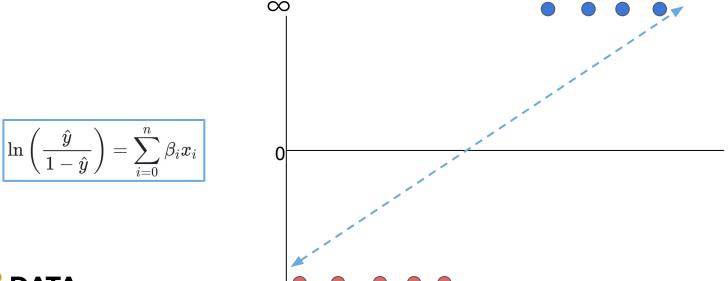
 Recall in Linear Regression we seek to minimize the Residual Sum of Squares (RSS).





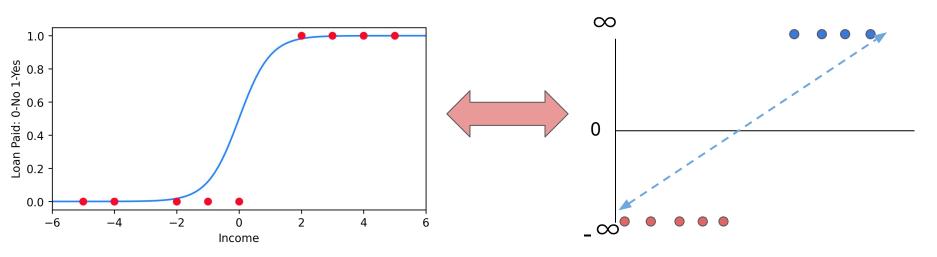


 Unfortunately, even in log odds targets are at infinity, making RSS unfeasible.













$$\ln(\frac{p}{1-p}) = \ln(odds)$$



$$\ln(\frac{p}{1-p}) = \ln(odds)$$

$$\frac{p}{1-p} = e^{\ln(odds)}$$

$$\ln(\frac{p}{1-n}) = \ln(odds)$$

$$\frac{p}{1-n} = e^{\ln(odds)}$$

$$p = (1 - p)e^{\ln(odds)}$$



$$p = (1 - p)e^{\ln(odds)}$$



$$p = (1 - p)e^{\ln(odds)}$$

$$p = e^{\ln(odds)} - pe^{\ln(odds)}$$

$$p = (1 - p)e^{\ln(odds)}$$

$$p = e^{\ln(odds)} - pe^{\ln(odds)}$$

$$p + pe^{\ln(odds)} = e^{\ln(odds)}$$



$$p = (1 - p)e^{\ln(odds)}$$

$$p = e^{\ln(odds)} - pe^{\ln(odds)}$$

$$p + pe^{\ln(odds)} = e^{\ln(odds)}$$

$$p(1 + e^{\ln(odds)}) = e^{\ln(odds)}$$





$$p = e^{\ln(odds)} - pe^{\ln(odds)}$$

$$p + pe^{\ln(odds)} = e^{\ln(odds)}$$

$$p(1 + e^{\ln(odds)}) = e^{\ln(odds)}$$

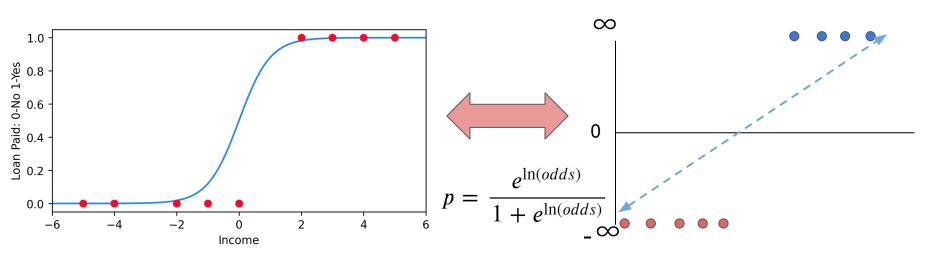




$$p = \frac{e^{\ln(odds)}}{1 + e^{\ln(odds)}}$$



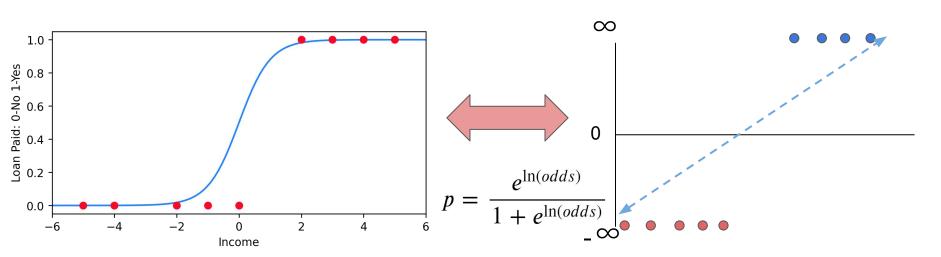
 We are now able to convert In(odds) into a probability.







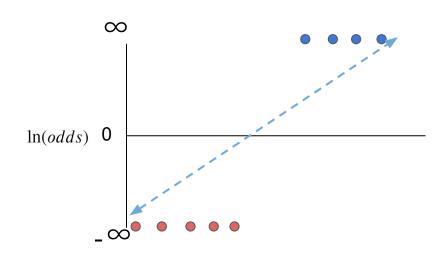
 Let's now explore the intuition behind maximum likelihood.







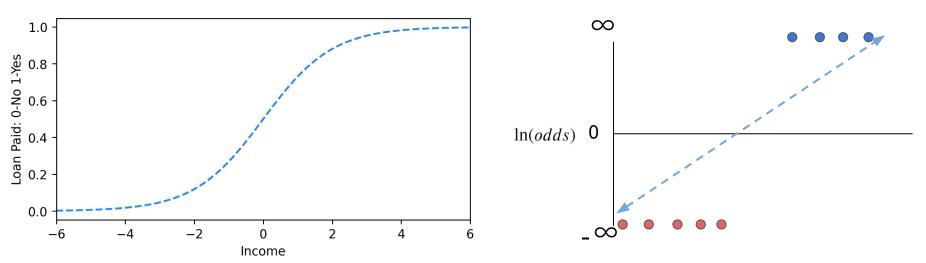
 We choose a line in the log(odds) axis and project the points on to the line:







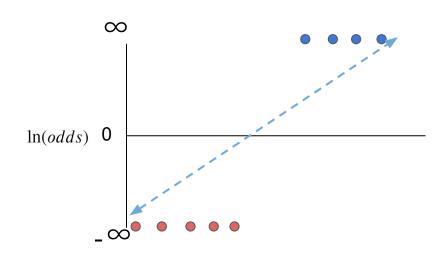
 We also know this line has a form on the probability y-axis.







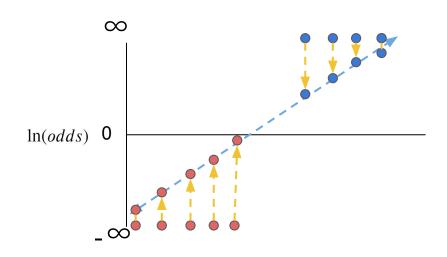
 We choose a line in the log(odds) axis and project the points on to the line:





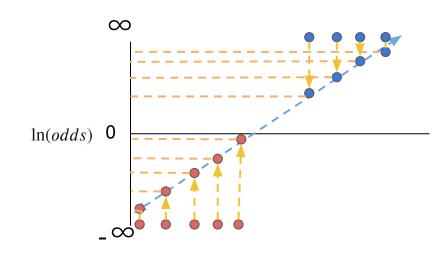


 We choose a line in the log(odds) axis and project the points on to the line:





 Calculate the log odds for the projected points on this line.





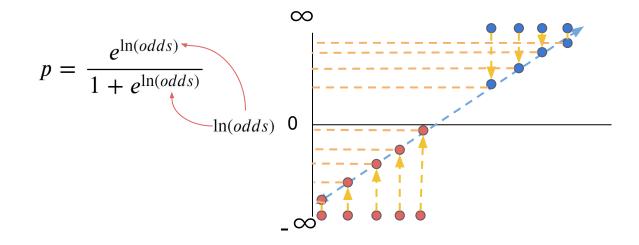


$$p = \frac{e^{\ln(odds)}}{1 + e^{\ln(odds)}}$$

$$\ln(odds) \quad 0$$

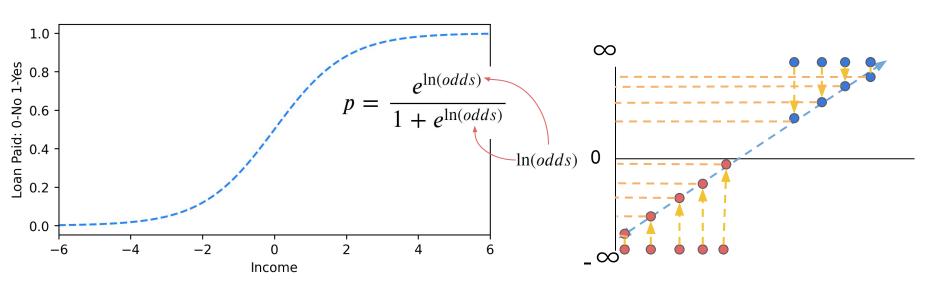






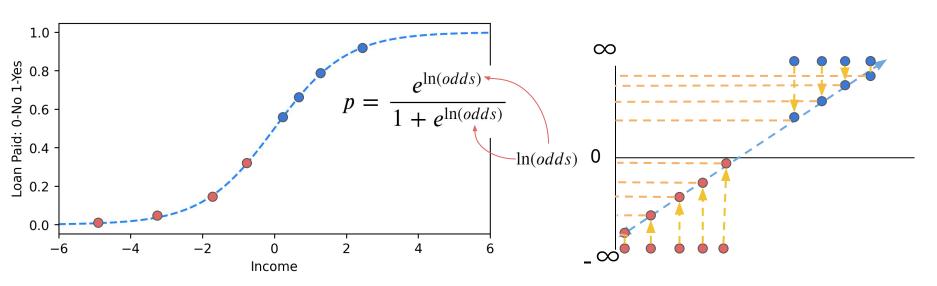








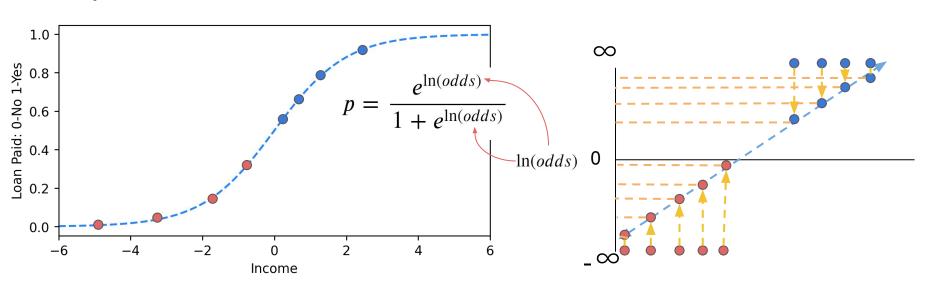








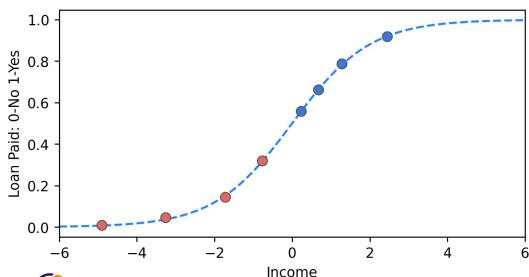
 We now measure the likelihood of these probabilities.







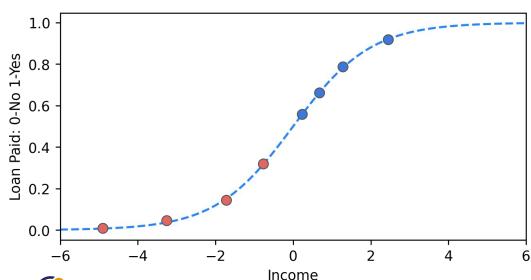
 We now measure the likelihood of these probabilities.







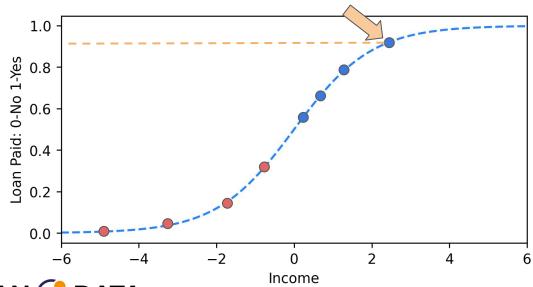
 Likelihood = Product of probabilities of belonging to class 1.







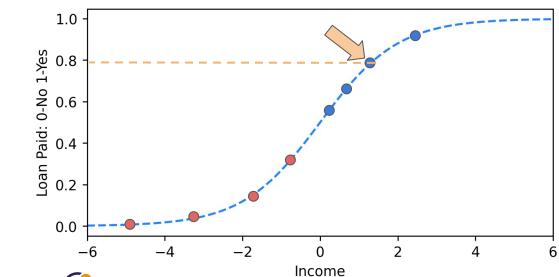
• Likelihood = 0.9 ...







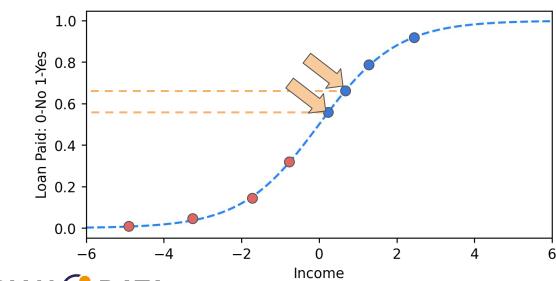
• Likelihood = 0.9 × 0.8 × ...







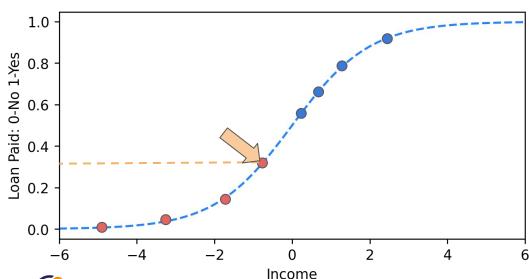
Likelihood = 0.9 × 0.8 × 0.65 × 0.55 × ...







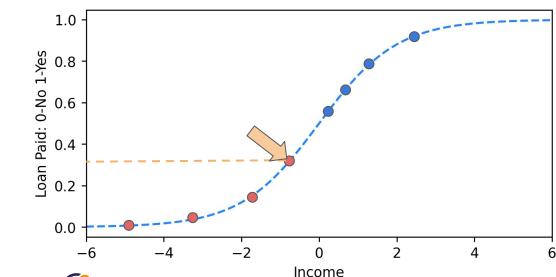
• Likelihood = $0.9 \times 0.8 \times 0.65 \times 0.55 \times (1-p) \times ...$







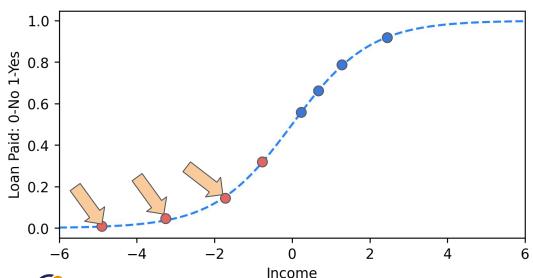
• Likelihood = $0.9 \times 0.8 \times 0.65 \times 0.55 \times (1-0.3) \times ...$







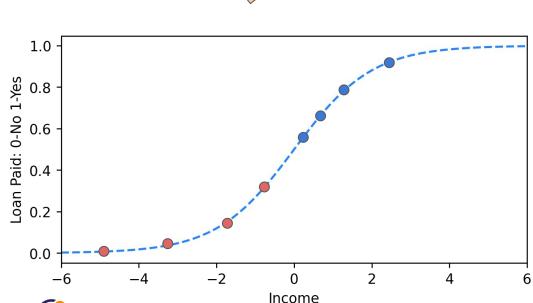
Likelihood = 0.9 × 0.8 × 0.65 × 0.55 × (1-0.3) × (1-0.2) × (1-0.08) × (1-0.02)







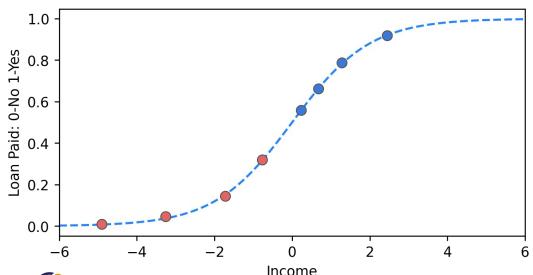
• Likelihood = 0.129







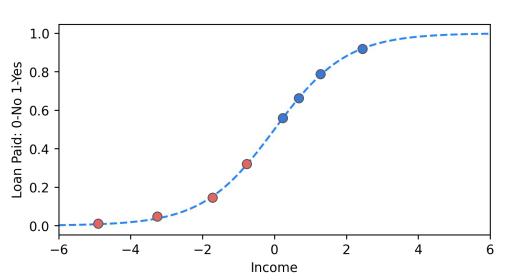
 Note in practice we actually maximize the log of the likelihoods. (e.g. In(0.9)×In(0.8)×...)

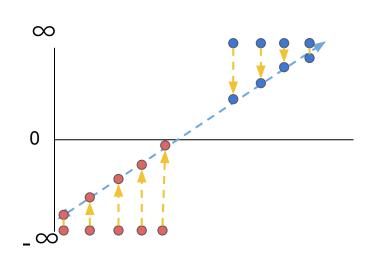






 There is some set of coefficients that will maximize these log likelihoods.

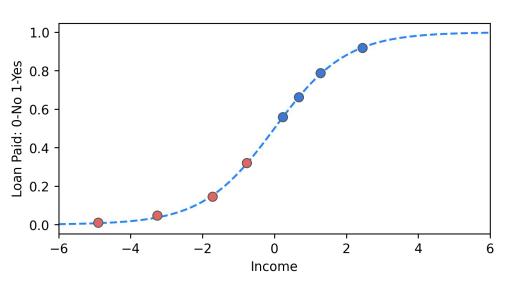


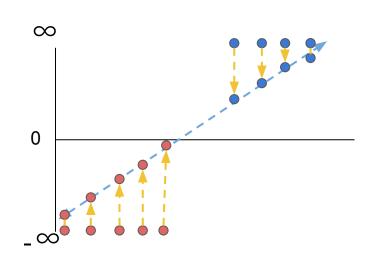






 Choose best coefficient values in log odds terms that creates maximum likelihood.

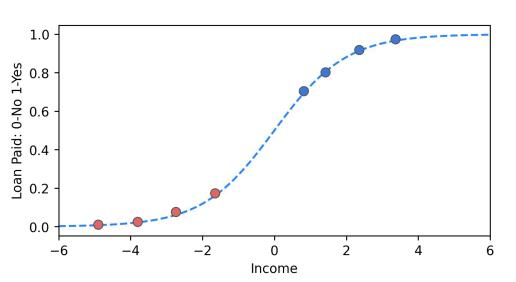


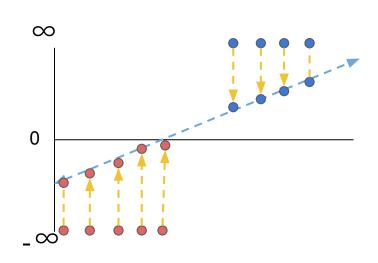






 Choose best coefficient values in log odds terms that creates maximum likelihood.









 While we are trying to maximize the likelihood, we still need something to minimize, since the computer's gradient descent methods can only search for minimums.



In terms of a cost function, we seek to minimize the following (log loss):

$$J(\mathbf{x}) = -rac{1}{m} \sum_{j=1}^m y^j \log\left(\hat{y}^j
ight) + (1-y^j) \log\left(1-\hat{y}^j
ight)$$

$$J(\mathbf{x}) = -rac{1}{m} \sum_{j=1}^m \left(y^j \log \left(rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i^j}}
ight) + (1-y^j) \log \left(1 - rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i^j}}
ight)
ight)$$



• Just as with Linear Regression, gradient descent can solve this for us!

$$J(\mathbf{x}) = -rac{1}{m} \sum_{j=1}^m y^j \log\left(\hat{y}^j
ight) + (1-y^j) \log\left(1-\hat{y}^j
ight)$$

$$J(\mathbf{x}) = -rac{1}{m} \sum_{j=1}^m \left(y^j \log \left(rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i^j}}
ight) + (1-y^j) \log \left(1 - rac{1}{1+e^{-\sum_{i=0}^n eta_i x_i^j}}
ight)
ight)$$



- Don't worry about fully understanding this gradient descent.
- In practice we never have to implement it ourselves.
- Main takeaway should be the relationship between log odds and probability.





 Now that we have an intuition of what happens "behind the scenes", let's explore Logistic Regression with Python!



Logistic Regression with Scikit-Learn

Part One: Exploratory Data Analysis





Logistic Regression with Scikit-Learn

Part Two: Creating and Training a Model





Logistic Regression Understanding Coefficients





Classification Performance Metrics

Part One: Confusion Matrix Basics





- You've probably heard of terms such as "false positive" or "false negative". As well as metrics like "accuracy".
- But what do these terms actually mean mathematically?





- Imagine we've developed a test or model to detect presence of a virus infection in a person based on some biological feature.
- We could treat this as a Logistic Regression, predicting:
 - O Not Infected (Tests Negative)
 - 1 Infected (Tests Positive)





- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - o Infected person tests positive.
 - o Healthy person tests negative.





- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - Infected person tests positive.
 - Healthy person tests negative.
 - Note, these are the outcomes we want! But it is unlikely our test is perfect...



- It is unlikely our model will perform perfectly. This means there 4 possible outcomes:
 - Infected person tests positive.
 - Healthy person tests negative.
 - o Infected person tests negative.
 - Healthy person tests positive.





- Based off these 4 possibilities, there are many error metrics we can calculate.
- First, let's start by visualizing these four possibilities as a matrix.





ACTUAL

INFECTED	HEALTHY



ACTUAL

	INFECTED	HEALTHY
INFECTED		
HEALTHY		





ACTUAL

	INFECTED	HEALTHY
INFECTED	TRUE POSITIVE	
HEALTHY		





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AC	LU	IΑI	L

	INFECTED	HEALTHY
INFECTED	TRUE POSITIVE	
HEALTHY		TRUE NEGATIVE





ΛC	Γυαί	ı
\neg		L

INFECTED HEALTHY

INFECTED TRUE FALSE POSITIVE

HEALTHY

TRUE NEGATIVE





		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	TRUE POSITIVE	FALSE POSITIVE
	HEALTHY	FALSE NEGATIVE	TRUE NEGATIVE





• Imagine a test group of 100 people:

ACTUAL

PREDICTED INFECTED HEALTHY

HEALTHY

PIERIAN 🈂 DATA



• 5 are infected. 95 are healthy.

ACTUAL

	INFECTED	HEALTHY
INFECTED		
HEALTHY		





We tested all of them with these results:

ACTUAL

INFECTED HEALTHY

PREDICTED

HEALTHY

1 93





What is accuracy?

ACTUAL

	INFECTED	HEALTHY
INFECTED	4	2
HEALTHY	1	93





What is accuracy?

		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

ACTUAL

- Accuracy:
 - How often is the model correct?



Calculating accuracy:

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

(4+93)/100 = 97% Accuracy

- Accuracy:
 - How often is the model correct?





Is this a good value for accuracy?

^ TII ^ I

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

(4+93)/100 = 97% Accuracy

- Accuracy:
 - How often is the model correct?





The accuracy paradox...

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

(4+93)/100 = 97% Accuracy

- Accuracy:
 - How often is the model correct?





Imagine we always report back "healthy"

ACTUAL

INFECTED **HEALTHY INFECTED** 4 **PREDICTED HEALTHY** 93





Imagine we always report back "healthy"

AC7	ГП	Δ	ı
AC	ı	'∕	L

INFECTED HEALTHY

INFECTED 0 0

PREDICTED

HEALTHY 5 95





Imagine we always report back "healthy"

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95
	,		

(0+95)/100 = 95% Accuracy

- Accuracy:
 - How often is the model correct?

95% accuracy for a model that always returns "healthy"!





 You may be thinking, "The numbers here are arbitrary, we just happen to get good accuracy in this made up case. Real world data would reflect poor accuracy if a model always returned the same result".



- This is the accuracy paradox!
 - Any classifier dealing with imbalanced classes has to confront the issue of the accuracy paradox.
 - Imbalanced classes will always result in a distorted accuracy reflecting better performance than what is truly warranted.





- Imbalanced classes are often found in real world data sets.
 - Medical conditions can affect small portions of the population.
 - Fraud is not common (e.g. Real vs. Fraud credit card usage).



- If a class is only a small percentage (n%), then a classifier that always predicts the majority class will always have an accuracy of (1-n).
- In our previous example we saw infected were only 5% of the data.
- Allowing the accuracy to be 95%.





- This means we shouldn't solely rely on accuracy as a metric!
- This is where precision, recall, and f1-score will come in.
- Let's explore these other metrics in the next lecture.



Classification Performance Metrics

Part Two: Precision and Recall





- We already know how to calculate accuracy and its associated paradox.
- Let's explore three more metrics that can help give a clearer picture of performance:
 - Recall (a.k.a. sensitivity)
 - Precision
 - F1-Score





	ACTOAL	
	INFECTED	HEALTHY
INFECTED	4	2
HEALTHY	1	93
		INFECTED 4

ΔΟΤΙΙΔΙ

Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

(TP)/Total Actual Positives





	ACTUAL	
	INFECTED	HEALTHY
ECTED	4	2
ALTHY	1	93
	ECTED ALTHY	ECTED 4

Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

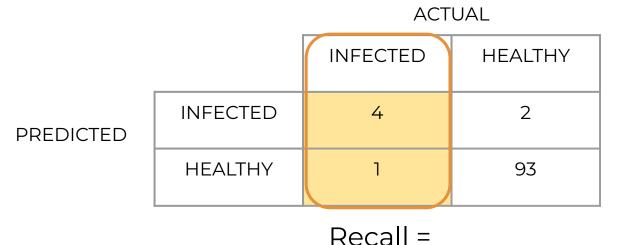
Recall = (TP)/Total Actual Positives

 $\Lambda \subset T \cup \Lambda \cup I$

(TP)/Total Actual Positives







Recall:

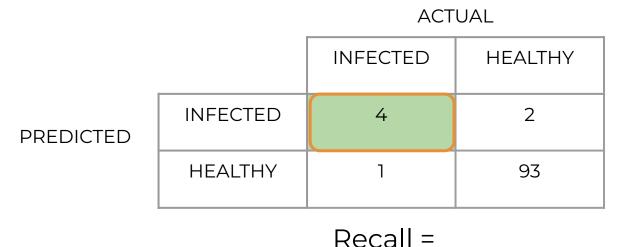
When it
 actually is a
 positive case,
 how often is it
 correct?

(TP)/Total Actual Positives

(٦







(4)/5

Recall:

When it
 actually is a
 positive case,
 how often is it
 correct?

(TP)/Total Actual Positives





Let's begin with recall.

		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	
PREDICTED		1	93	

Recall = 0.8

 $\Lambda \subset T \cup \Lambda \cup I$

- Recall:
 - How many relevant cases are found?

(TP)/Total Actual Positives





 What's the recall if we always classify as "healthy"?

ACTUAL

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall:

 How many relevant cases are found?

(TP)/Total Actual Positives

Recall = (TP)/Total Actual Positives





 What's the recall if we always classify as "healthy"?

ACTUAL

11	h	е	a	lt	h	y'	"?

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall = (0)/5!

- Recall:
 - How many relevant cases are found?

(TP)/Total Actual Positives





 A recall of 0 alerts you the model isn't catching cases! **ACTUAL**

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall:

How many relevant cases are found?

(TP)/Total Actual **Positives**

Recall = (0)/5!





	ACTUAL		
	INFECTED	HEALTHY	
INFECTED	4	2	
HEALTHY	1	93	
		INFECTED 4	

Precision = (TP)/Total Predicted Positives

 $\Lambda \subset T \cup \Lambda$

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?





		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	

Precision = (TP)/Total Predicted Positives

- Precision:
 - When prediction is positive, how often is it correct?





		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	

Precision =

- Precision:
 - When prediction is positive, how often is it correct?





		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	

Precision = (TP)/6

- Precision:
 - When
 prediction is
 positive, how
 often is it
 correct?





		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	

Precision = (4)/6

- Precision:
 - When prediction is positive, how often is it correct?





		ACTUAL		
		INFECTED	HEALTHY	
PREDICTED	INFECTED	4	2	
	HEALTHY	1	93	

Precision = 0.666

- Precision:
 - When prediction is positive, how often is it correct?





 What's the **precision** if we always classify as "healthy"?

ACTUAL

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Precision:

 When prediction is positive, how often is it correct?

Precision = (TP)/Total Predicted Positives





 What's the **precision** if we always classify as "healthy"?

ACTUAL

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Precision = 0/0

- Precision:
 - When prediction is positive, how often is it correct?





- Recall and Precision can help illuminate our performance specifically in regards to the relevant or positive case.
- Depending on the model, there is typically a trade-off between precision and recall, which we will explore later on with the ROC curve.





• Since precision and recall are related to each other through the numerator (TP), we often also report the F1-Score, which is the harmonic mean of precision and recall.

$$F = \frac{2 \times precision \times recall}{precision + recall}$$



• The harmonic mean (instead of the normal mean) allows the entire harmonic mean to go to zero if **either** precision or recall ends up being zero.

$$F = \frac{2 \times precision \times recall}{precision + recall}$$



 As a final note on the confusion matrix, there are many more metrics available:

		True cond	ition		
Predicted condition	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma}{\Gamma}$ True positive + $\frac{\Sigma}{\Gamma}$ True negative $\frac{\Sigma}{\Gamma}$ Total population
	Predicted condition positive	True positive	False positive, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) = Σ False positive Σ Predicted condition positive
	Predicted condition negative	False negative, Type II error	True negative	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$
		True positive rate (TPR), Recall, Sensitivity, probability of detection, Power = $\frac{\Sigma}{\Sigma}$ True positive Condition positive	$\label{eq:false-positive} \begin{aligned} & \text{False positive rate (FPR), Fall-out,} \\ & \text{probability of false alarm} = \frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}} \end{aligned}$	Positive likelihood ratio (LR+) = $\frac{TPR}{FPR}$	Diagnostic odds F ₁ score =
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	Specificity (SPC), Selectivity, True negative rate $(TNR) = \frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR-) = $\frac{FNR}{TNR}$	ratio (DOR) = $\frac{LR+}{LR-}$ 2 · $\frac{Precision \cdot Recall}{Precision + Recall}$





 Finally, let's explore a way to visualize the relationships between metrics such as precision and recall with curves.



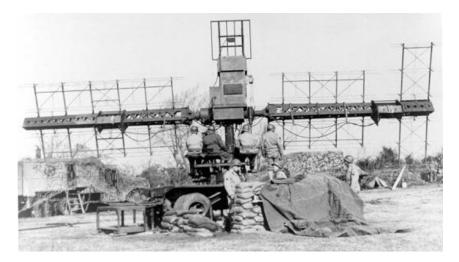
Classification Performance Metrics

Part Three: ROC Curves





 During World War 2, Radar technology was developed to help detect incoming enemy aircraft.







 The technology was so new, the US Army wanted to develop a methodology to evaluate radar operator performance.





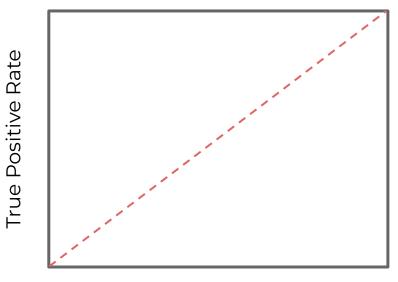


 They developed the Receiver Operator Characteristic curve.

True Positive Rate



 They developed the Receiver Operator Characteristic curve.

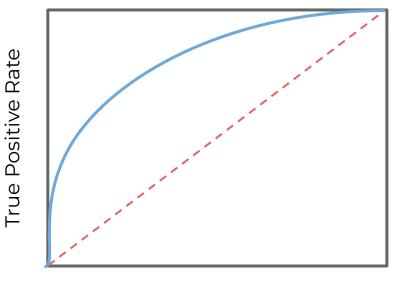




False Positive Rate



 They developed the Receiver Operator Characteristic curve.

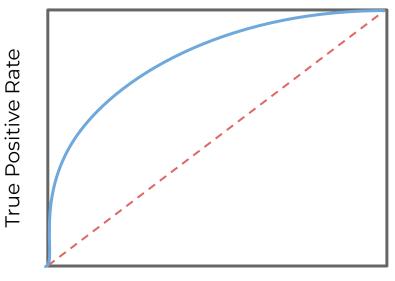




False Positive Rate



 There can be a trade-off between True Positives and False Positives.

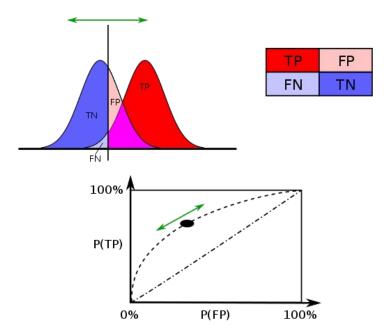




False Positive Rate



 There can be a trade-off between True Positives and False Positives.

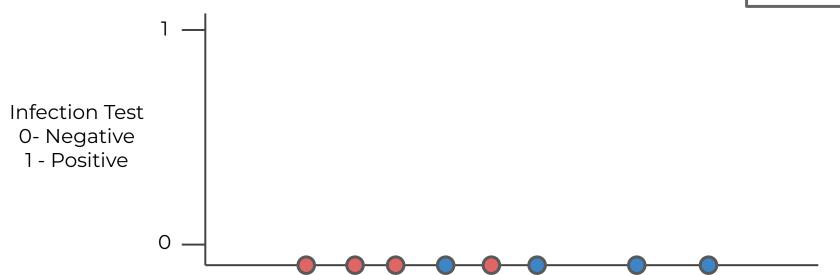






• Our previous infection test.

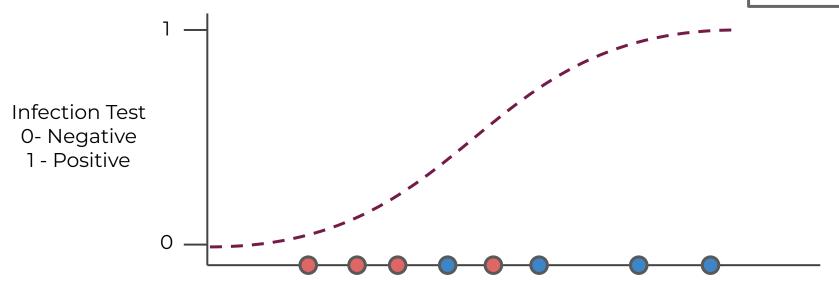






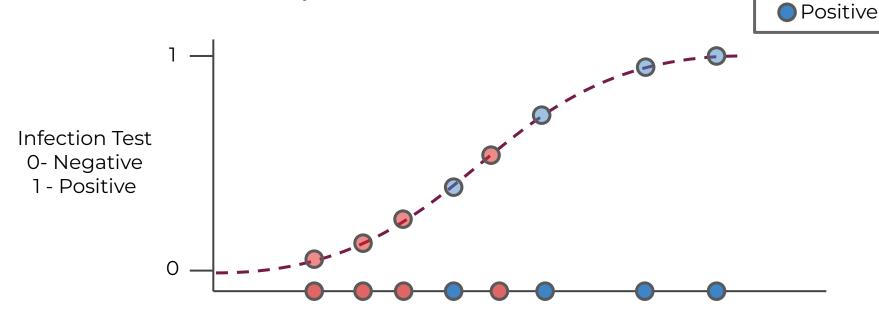
• Fit logistic regression model.







• Given X we predict 0 or 1.



Actual Status

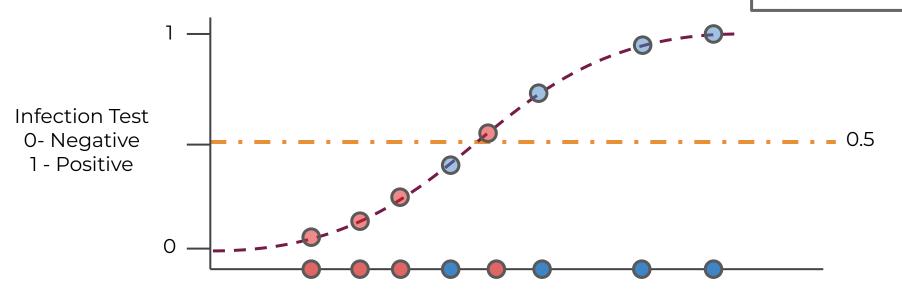
Negative



Default is to choose 0.5 as cut-off.

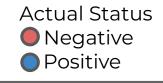
Actual Status

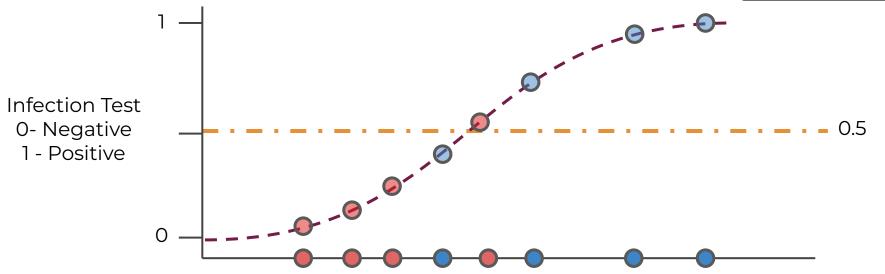
Negative
Positive



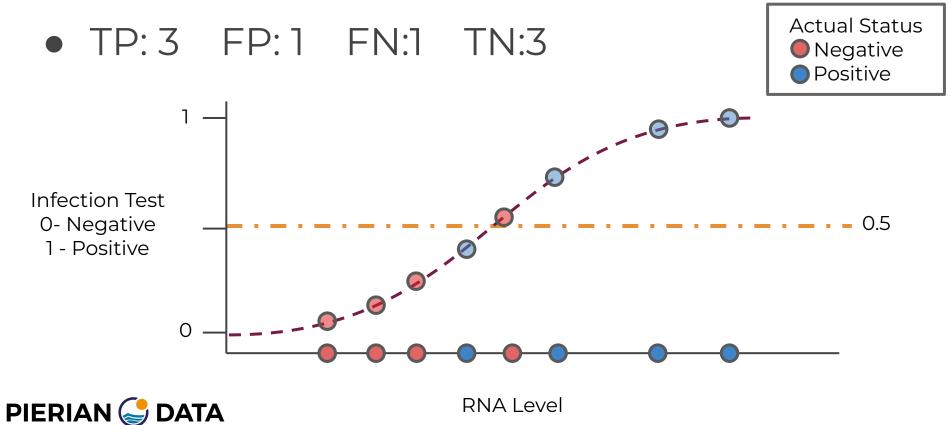


How many TP vs FP?



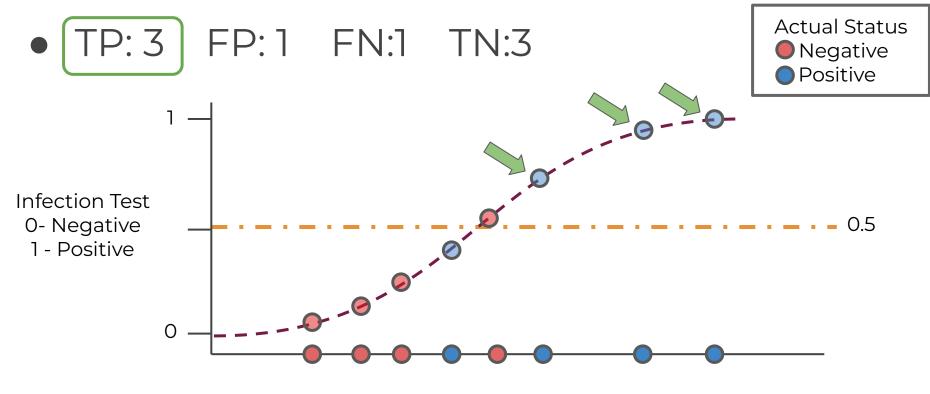




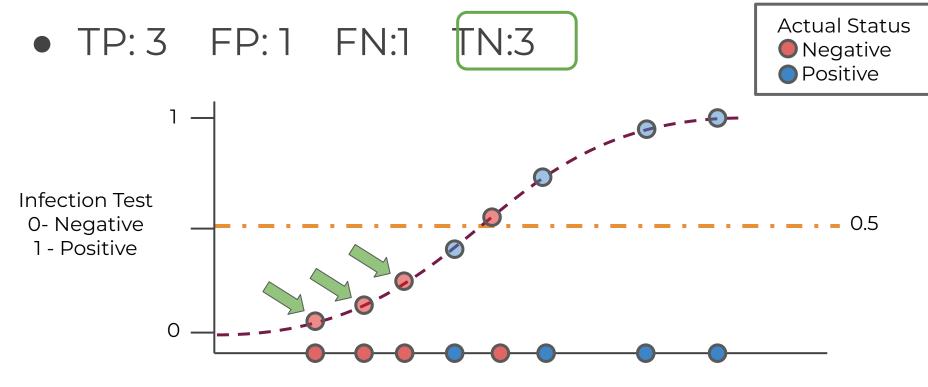




Classification Metrics

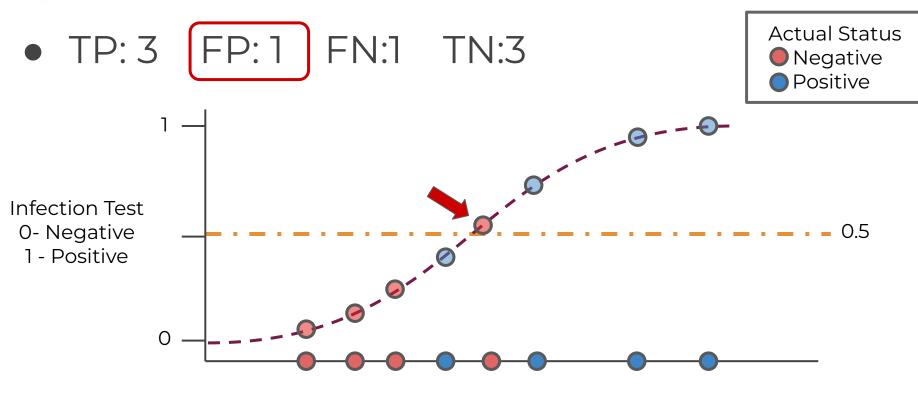






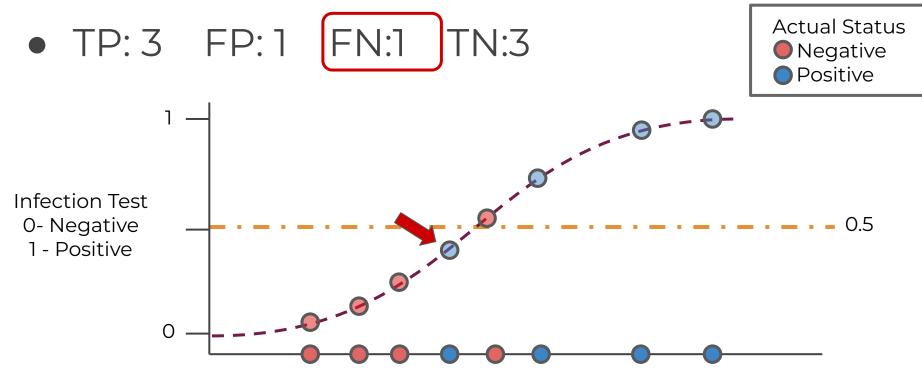


PIERIAN 🈂 DATA



RNA Level

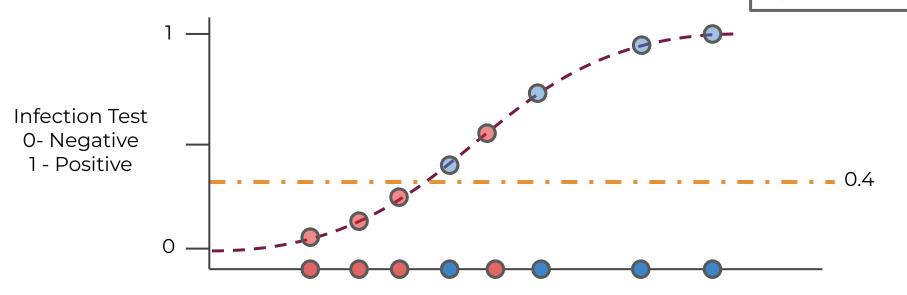




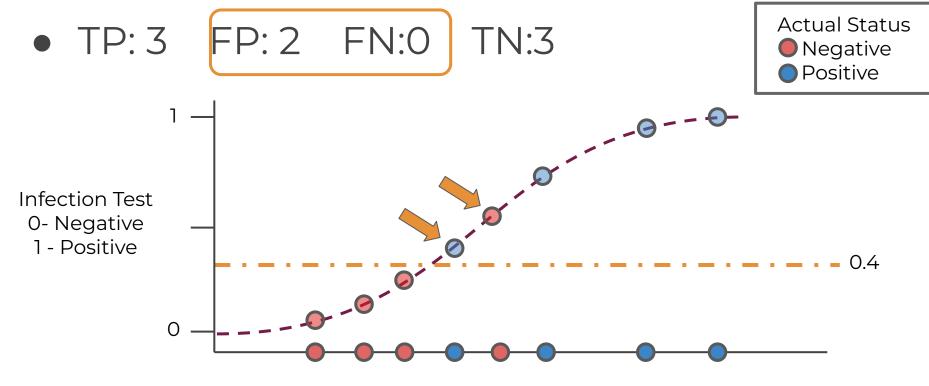


What if we lowered the cut-off?

Actual Status
NegativePositive









- In certain situations, we gladly accept more false positives to reduce false negatives.
- Imagine a dangerous virus test, we would much rather produce false positives and later do more stringent examination than accidentally release a false negative!





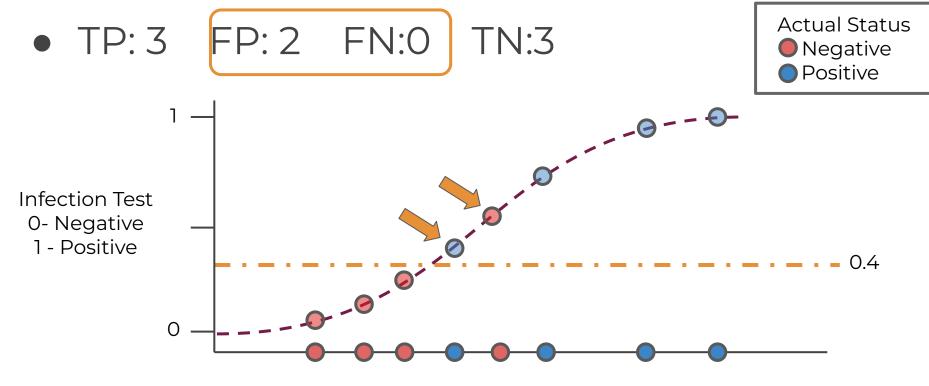
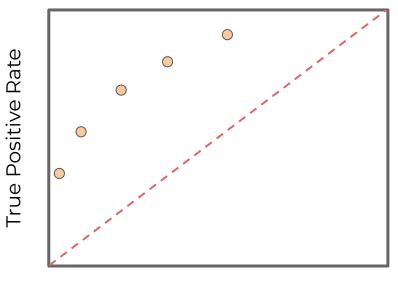




 Chart the True vs. False positives for various cut-offs for the ROC curve.

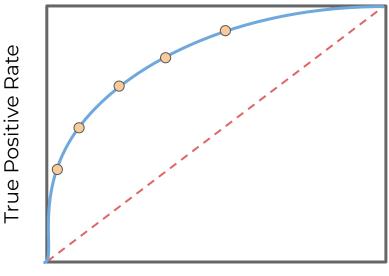




False Positive Rate



 By changing the cut-off limit, we can adjust our True vs. False Positives!

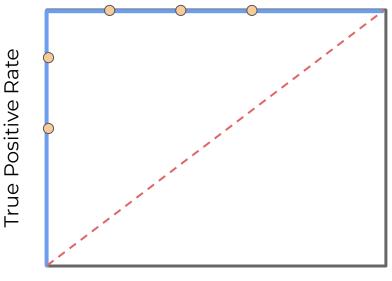




False Positive Rate



- A perfect model would have a zero FPR.
- Random guessing is the red line.

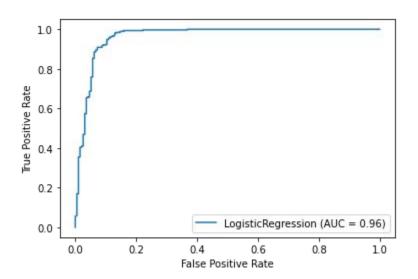




False Positive Rate



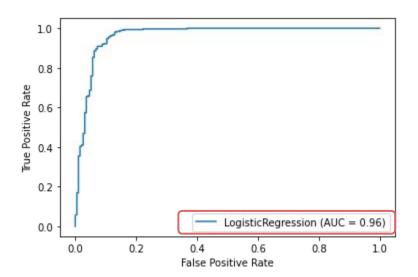
 Realistically with smaller data sets the ROC curves are not as smooth.







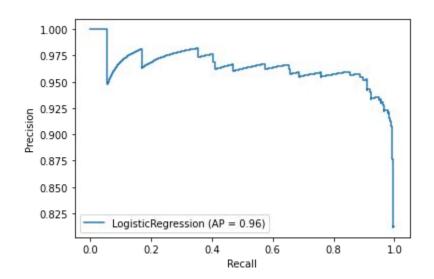
 AUC - Area Under the Curve, allows us to compare ROCs for different models.







Can also create precision vs. recall curves:







Logistic Regression with Scikit-Learn

Part Three: Performance Metrics





Logistic Regression Multi-Class Problems

Part One: Data and Model





Logistic Regression Multi-Class Problems

Part Two: Training and Performance Evaluation





Logistic Regression Exercise Overview





Logistic Regression Exercise Solutions

