Logistic Regression

Logistic Regression

- 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

- 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

- 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

- 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

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

Logistic Regression

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

Logistic Regression

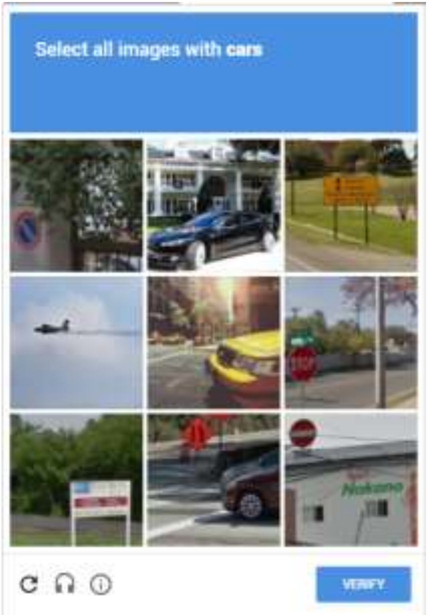
- Logistic Regression will allow us to predict a categorical label based on historical feature data.
- The categorical target column is two or more discrete class labels.

Logistic Regression

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

Logistic Regression

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



Logistic Regression

- 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

Logistic Regression

- 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

Logistic Regression

- 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.

Logistic Regression

- 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!

PIERIAN DATA

Logistic Regression Theory and Intuition

Part One: The Logistic Function

PIERIAN DATA

Logistic Regression

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

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

Logistic Regression

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

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

Logistic Regression

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

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

Logistic Regression

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

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

Logistic Regression

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

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

Logistic Regression

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

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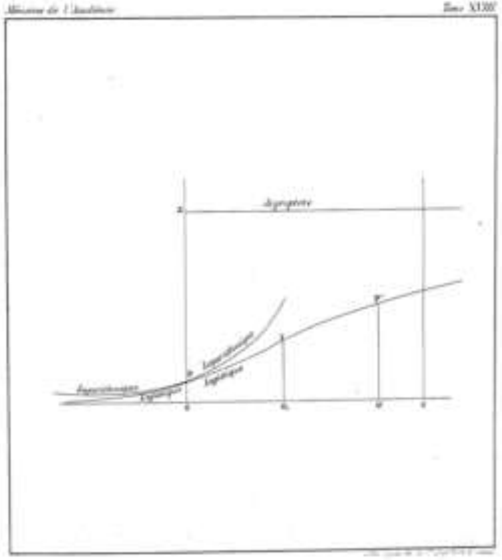
Logistic Regression

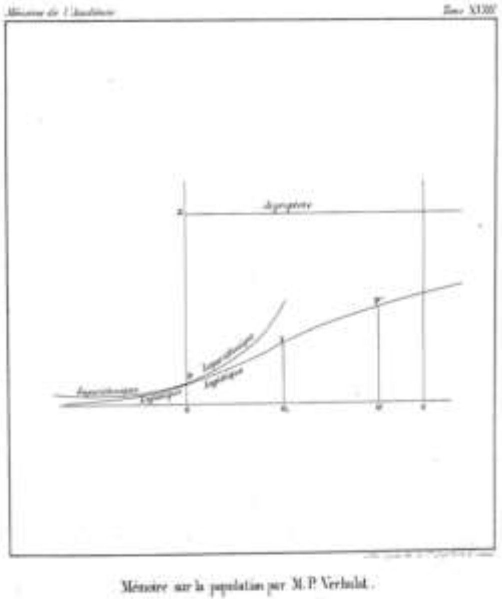
- 1830-1850: Developed for the purposes of modeling population growth.



Mémoire sur la population par M.P. Verhulst.

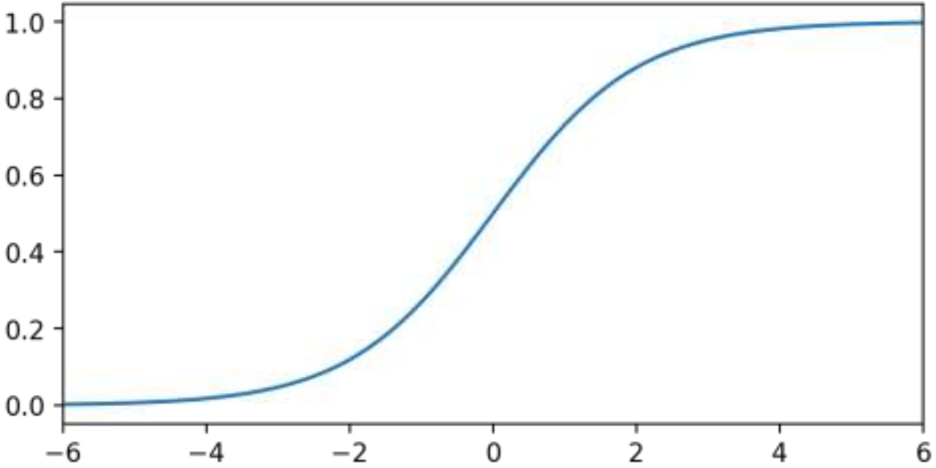
Logistic Regression

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



Logistic Regression

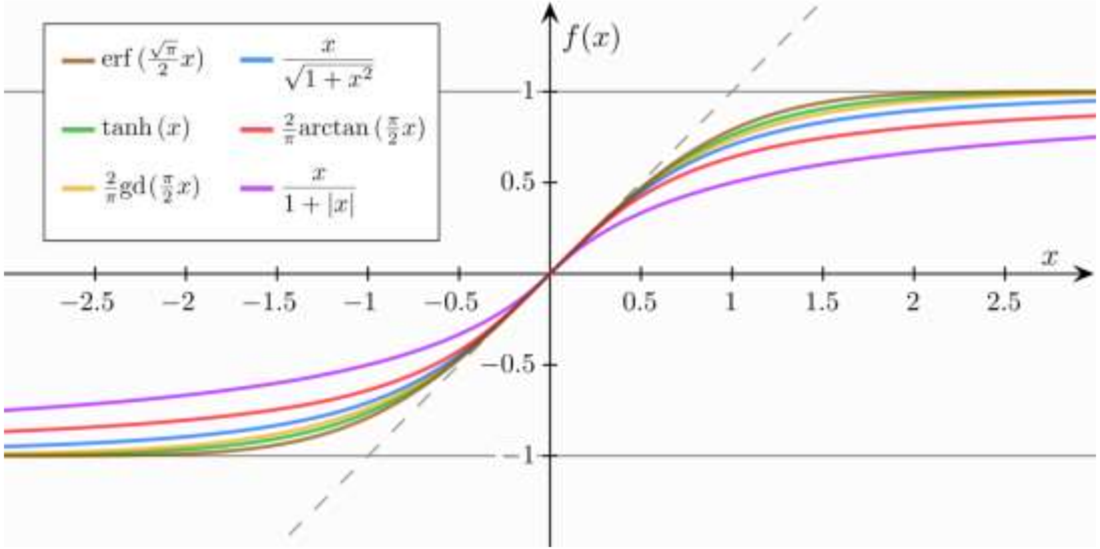
- Why the need for a logistic function versus a logarithmic function?



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

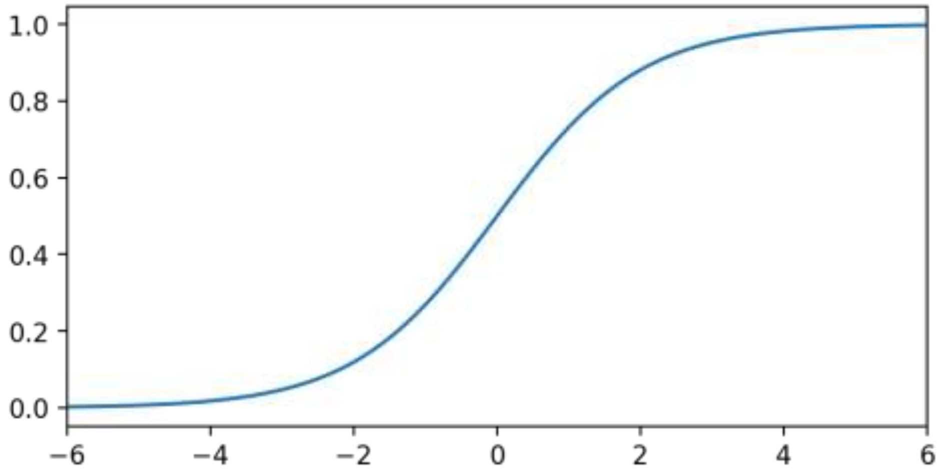
Logistic Regression

- Note: There is a “family” of logistic functions.



Logistic Regression

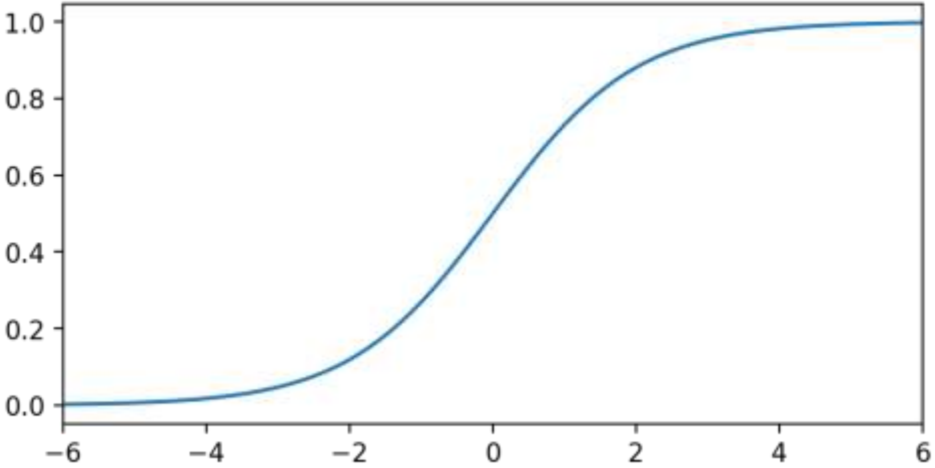
- Notice the “leveling off” behavior of the curve.



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

Logistic Regression

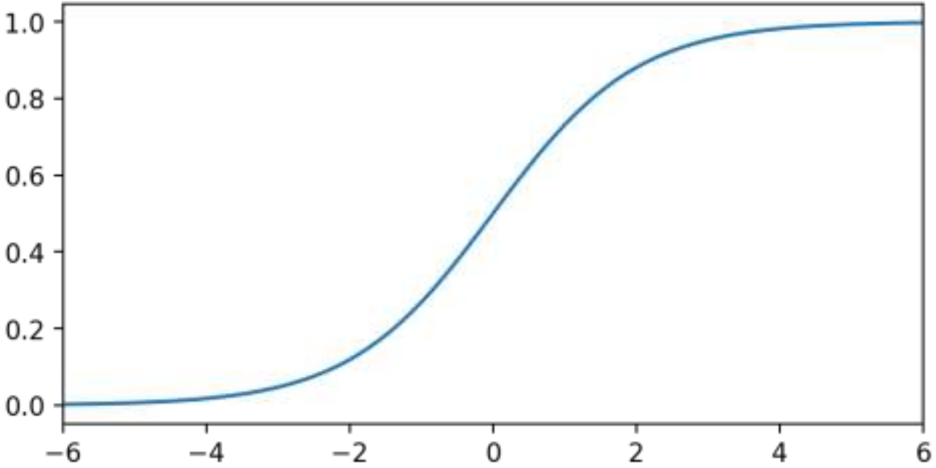
- Also notice **any** value of **x** will have an output range between 0 and 1.



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

Logistic Regression

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



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Logistic Regression

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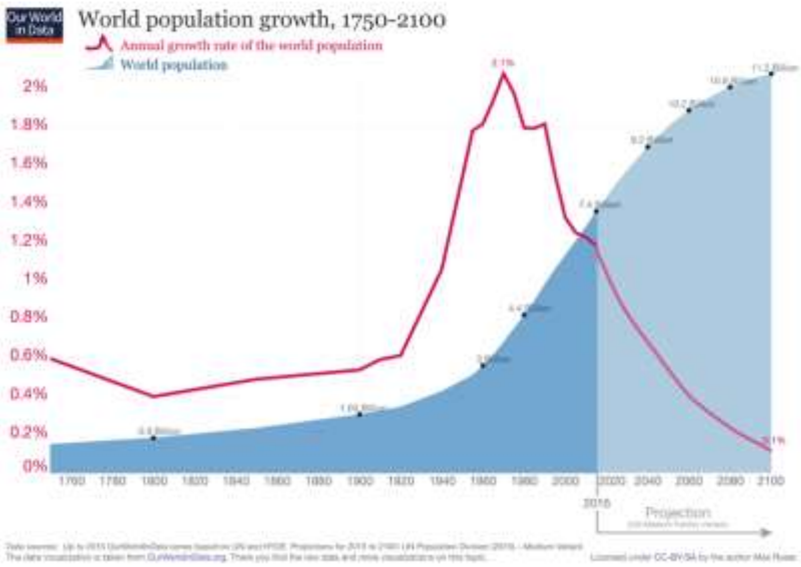

Logistic Regression

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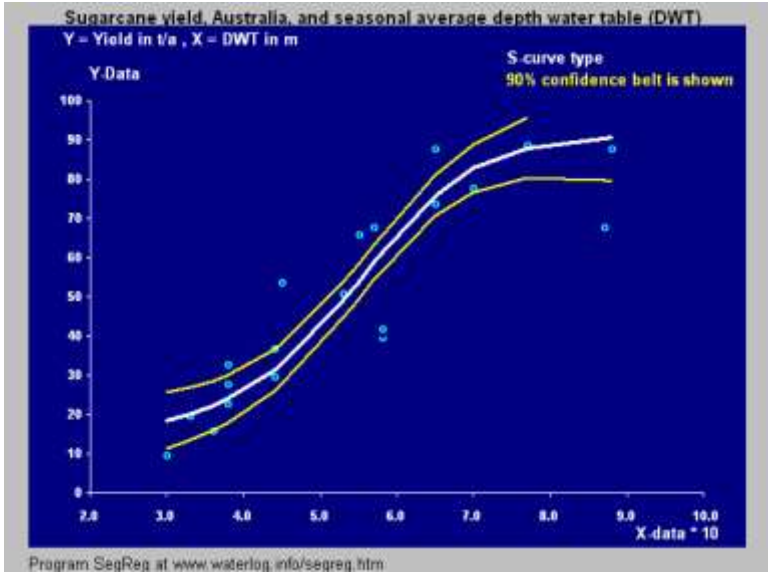
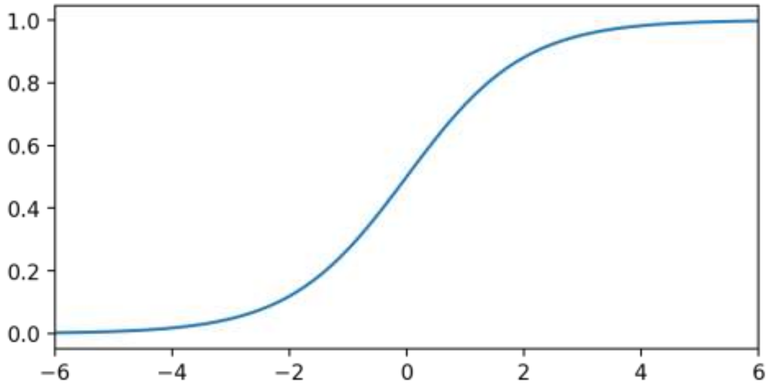


Logistic Regression

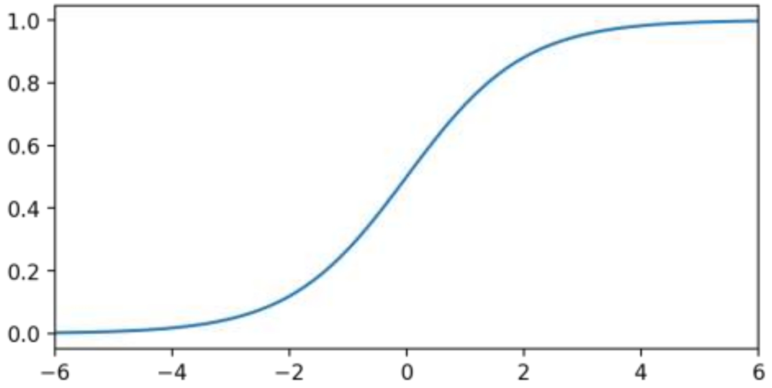
- 1940s: Using the logistic function for statistical modeling was developed by Joseph Berkson.



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

Logistic Regression

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



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

Logistic Regression

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

Logistic Regression

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


leaves another 'very doubtful'

Logistic Regression

- 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

Logistic Regression

- 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)

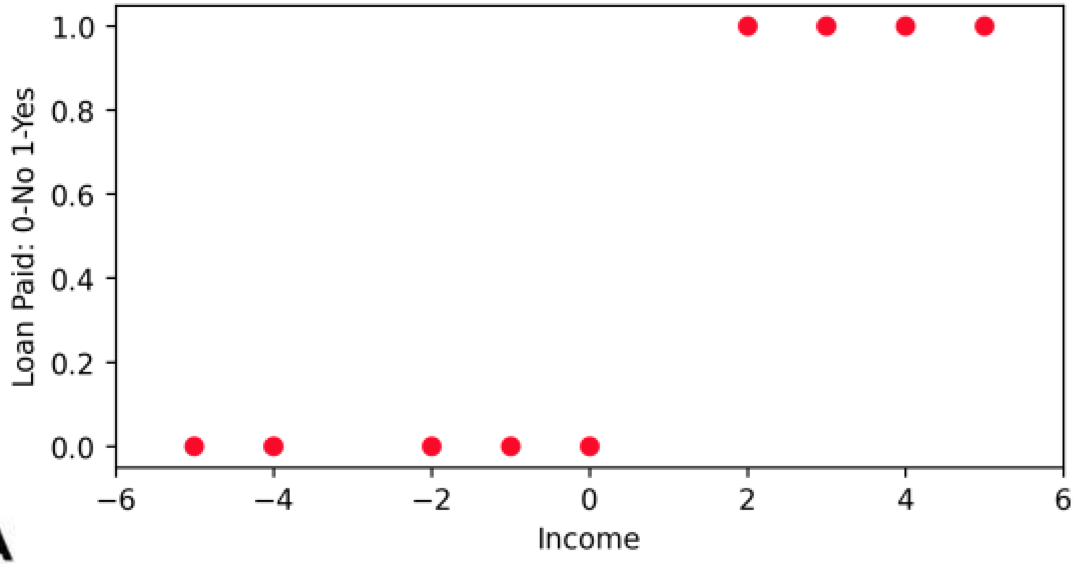
Logistic Regression

- Our data set:

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

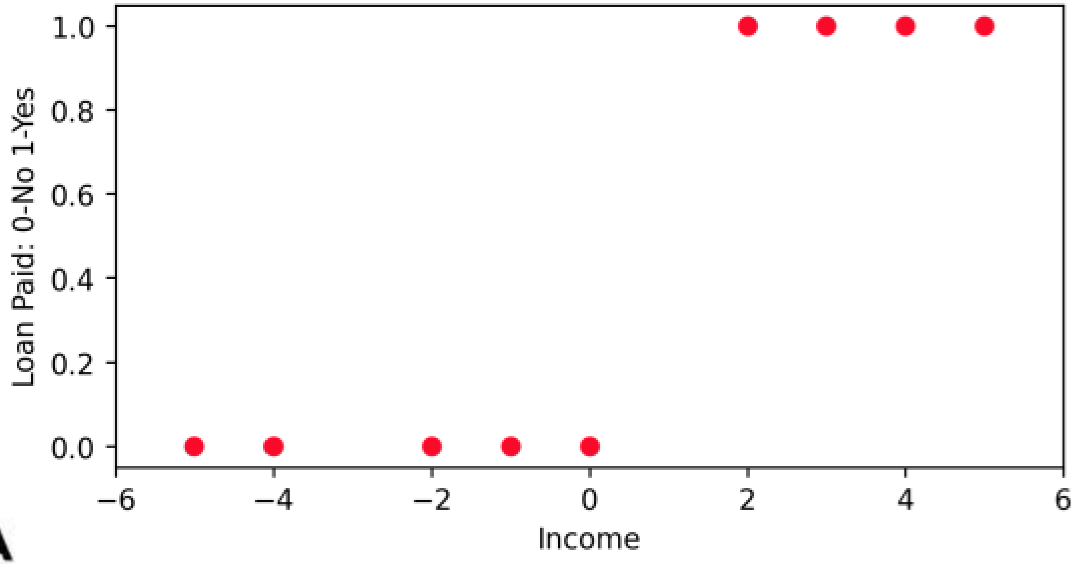
Logistic Regression

- Let’s begin by plotting income versus default:



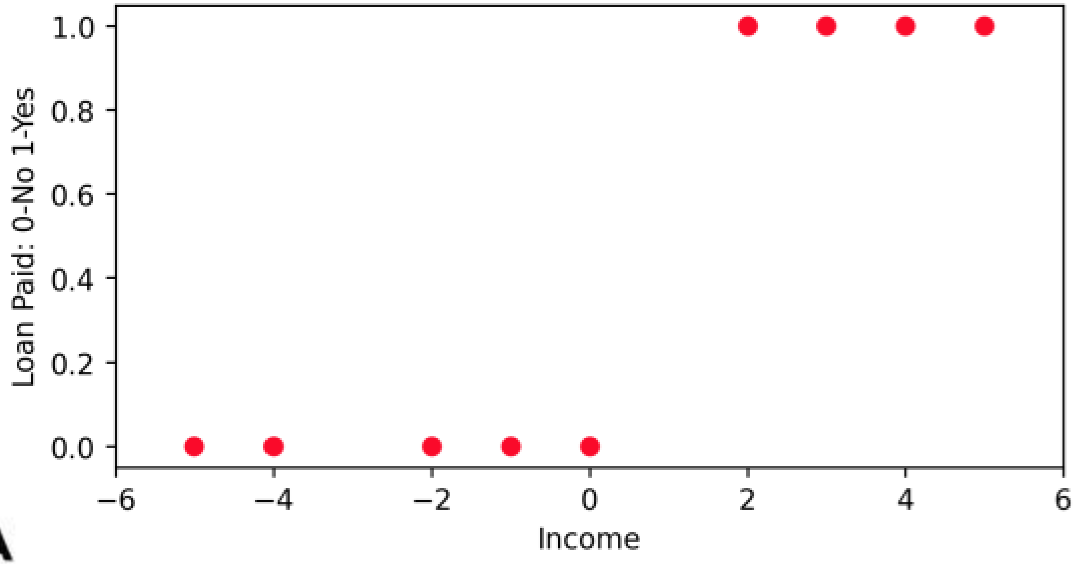
Logistic Regression

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



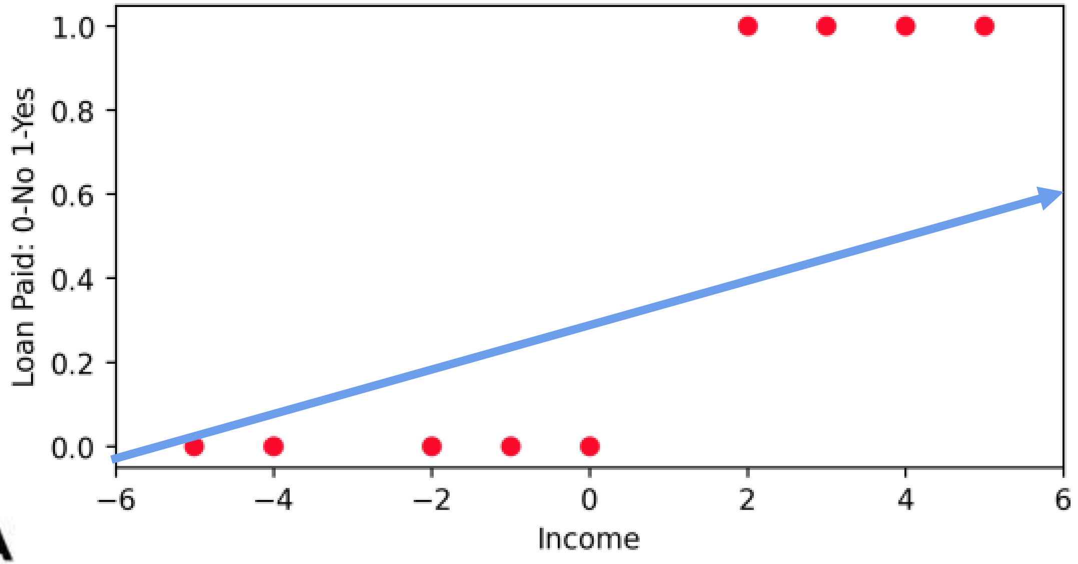
Logistic Regression

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



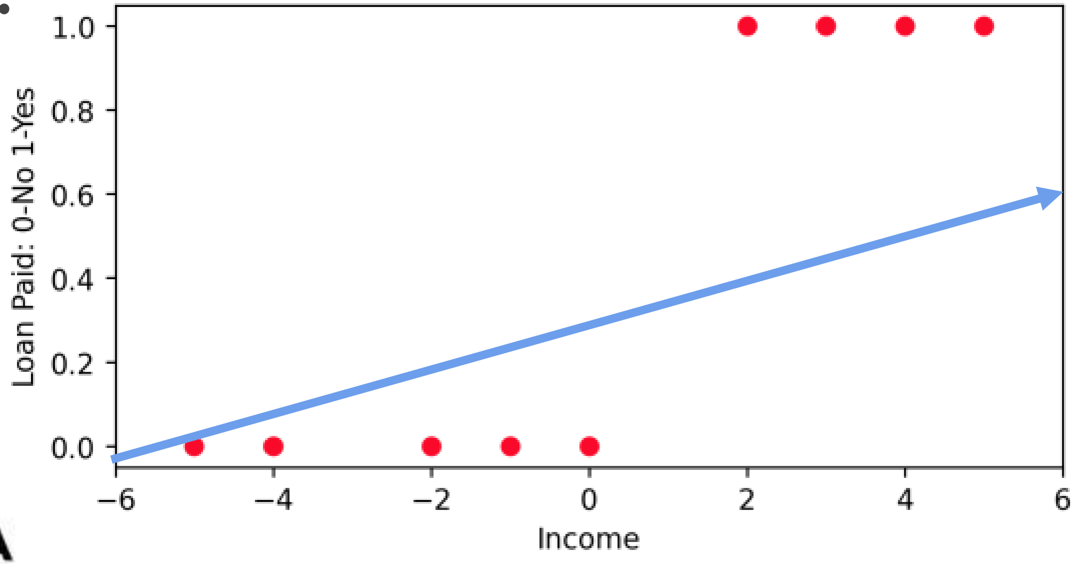
Logistic Regression

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



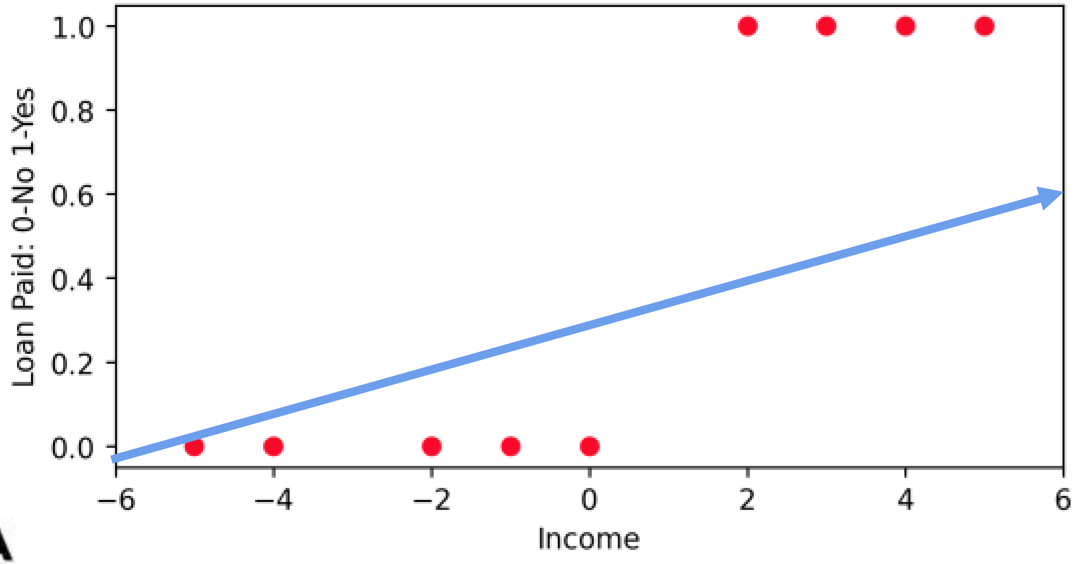
Logistic Regression

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



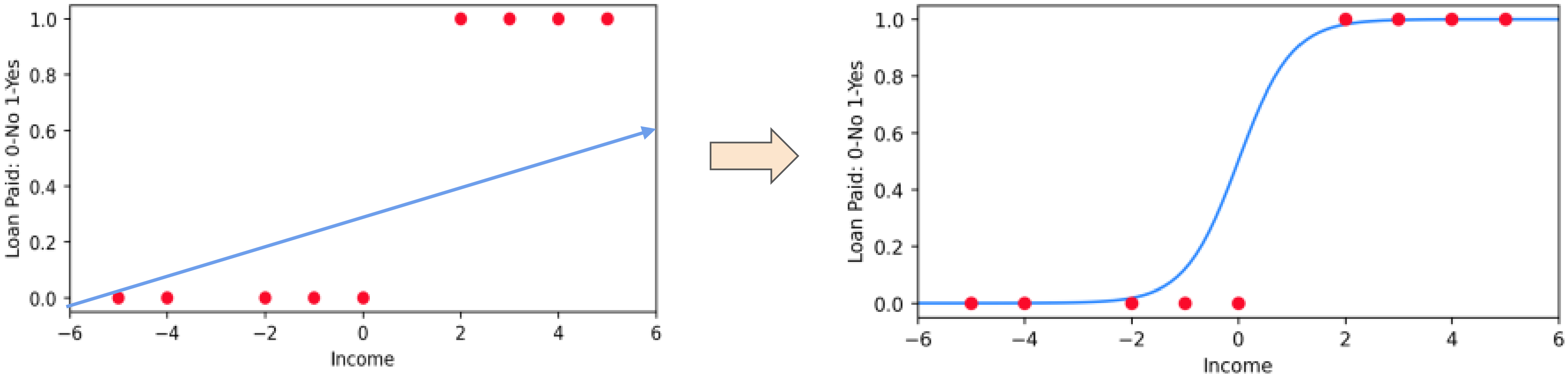
Logistic Regression

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



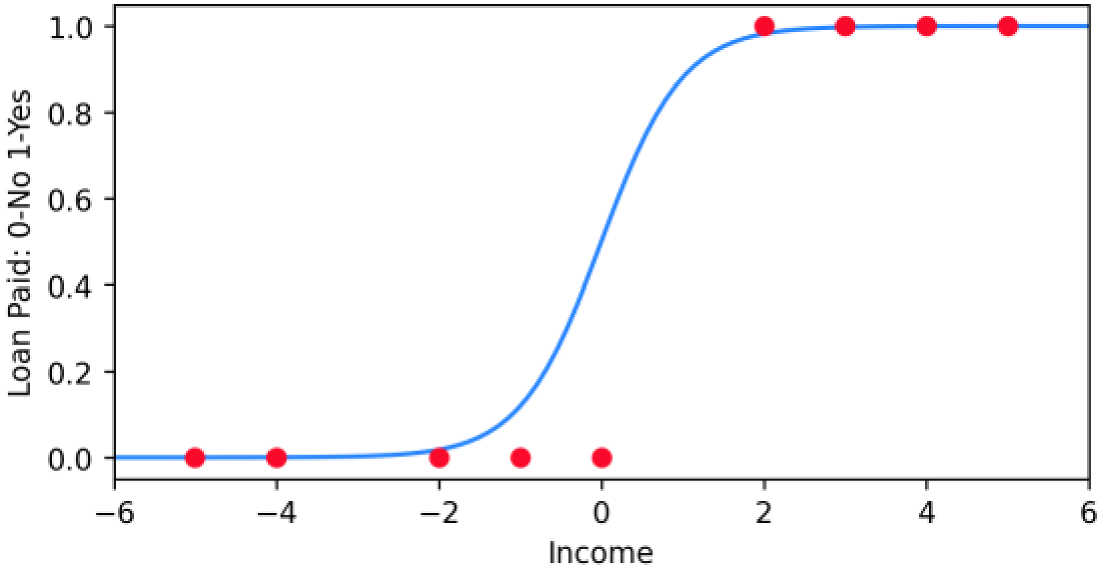
Logistic Regression

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



Logistic Regression

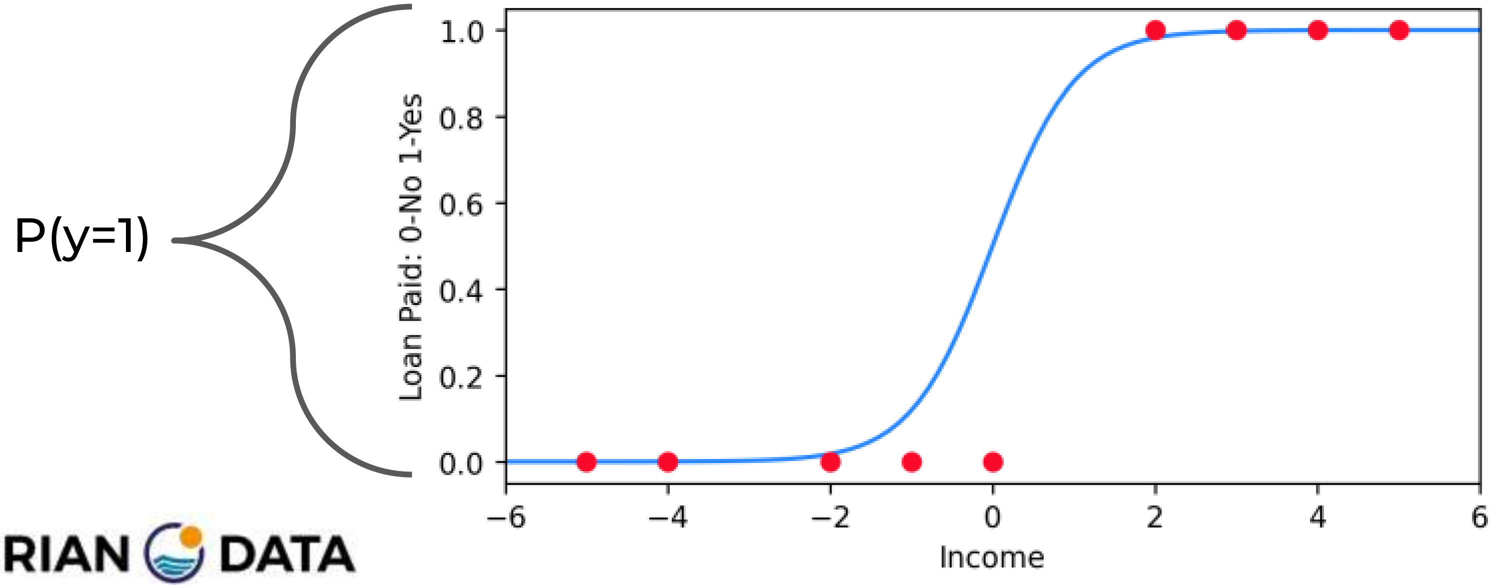
- Let's first focus on what this Logistic Regression would look like.



PIERIAN DATA

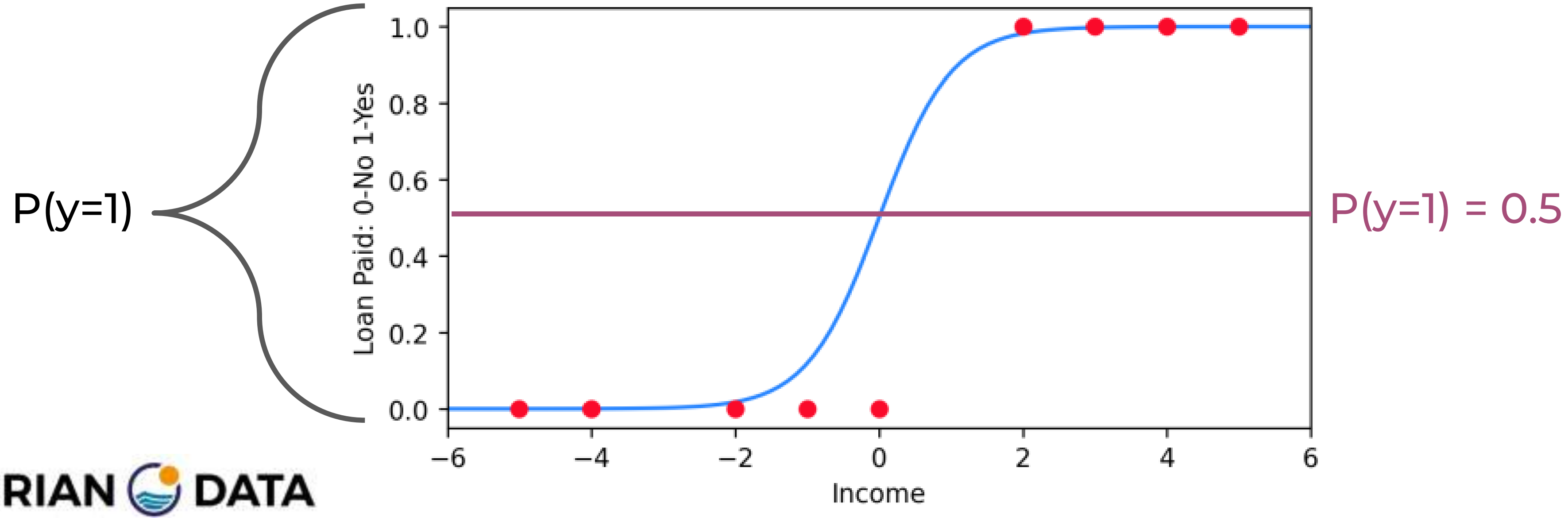
Logistic Regression

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



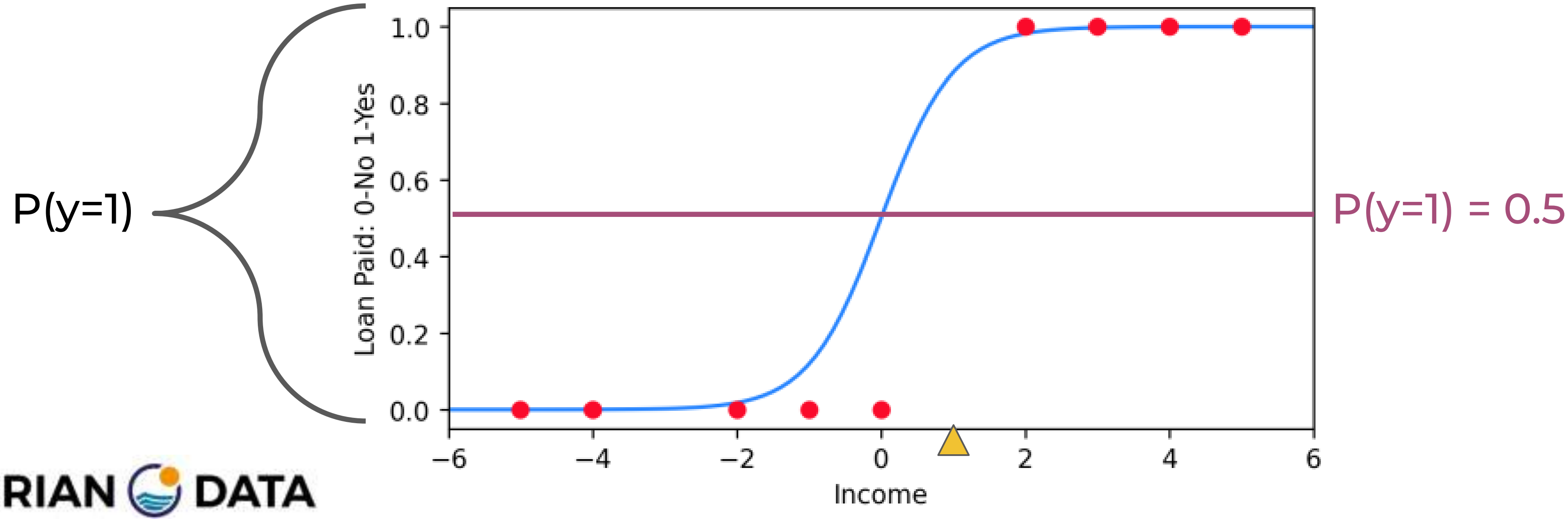
Logistic Regression

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



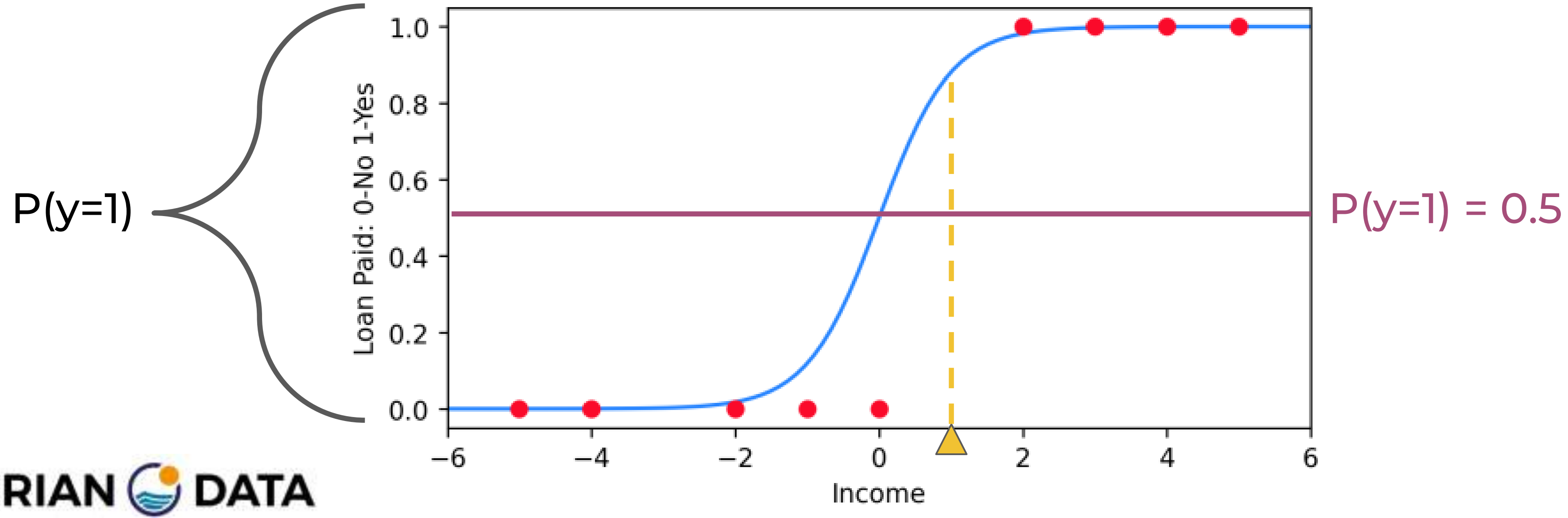
Logistic Regression

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



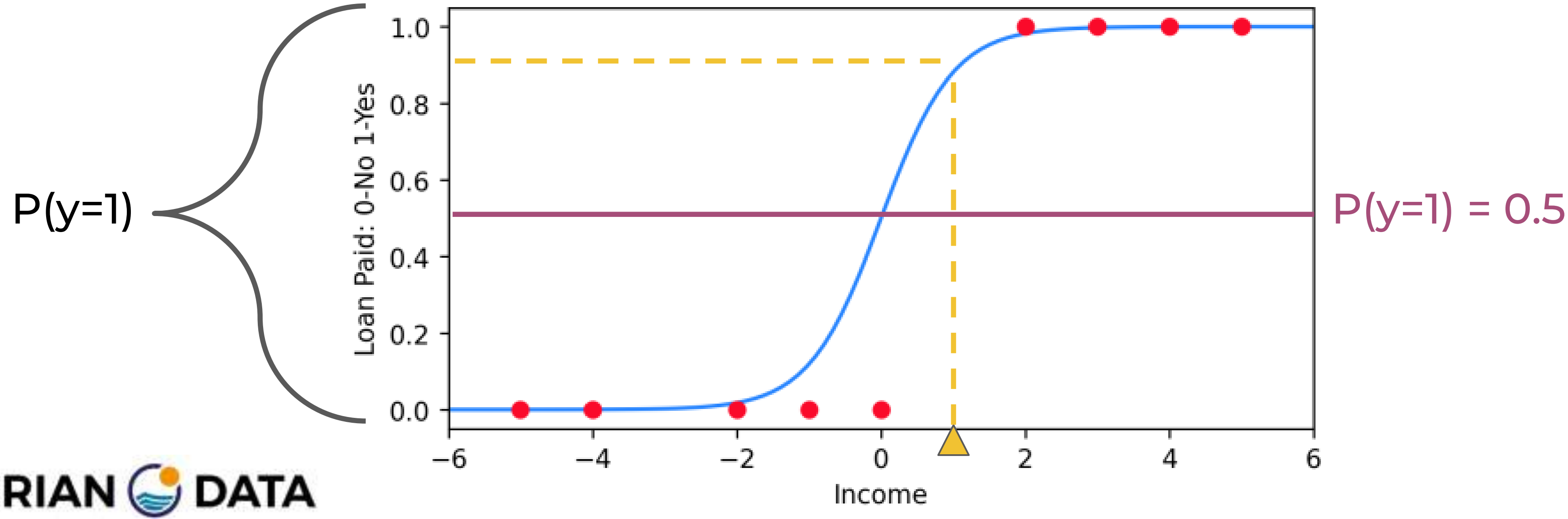
Logistic Regression

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



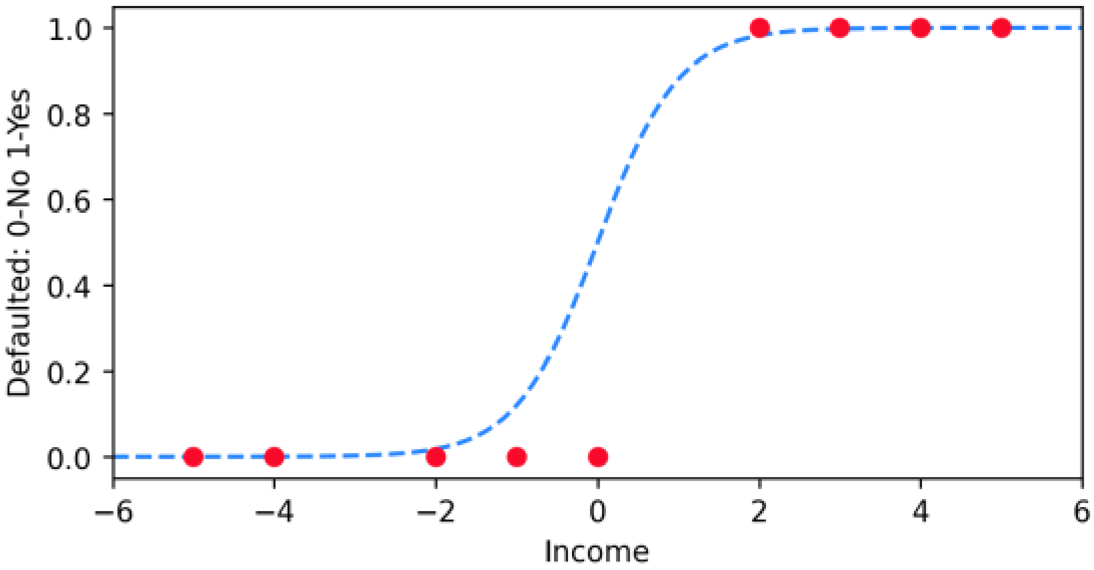
Logistic Regression

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



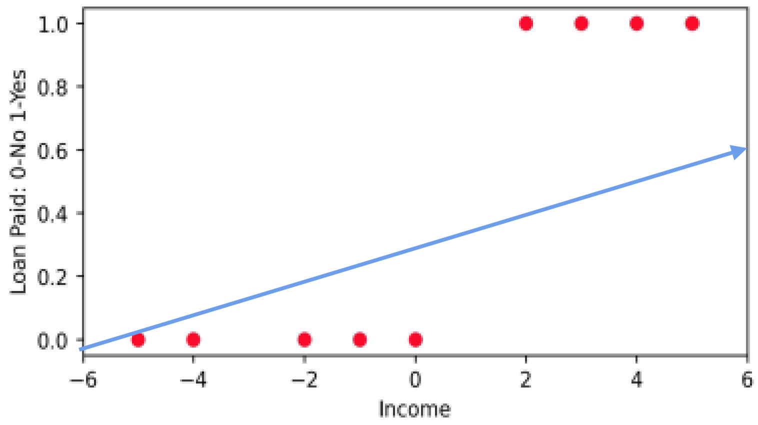
Logistic Regression

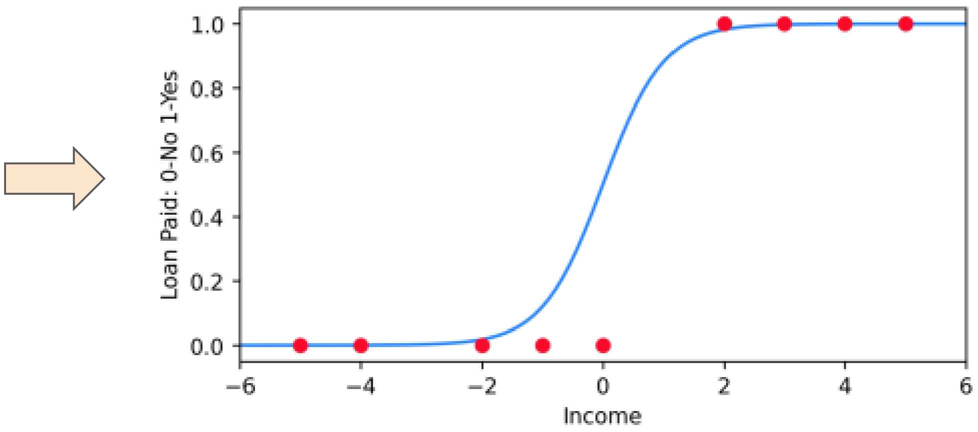
- But how do we actually create this line?



Logistic Regression

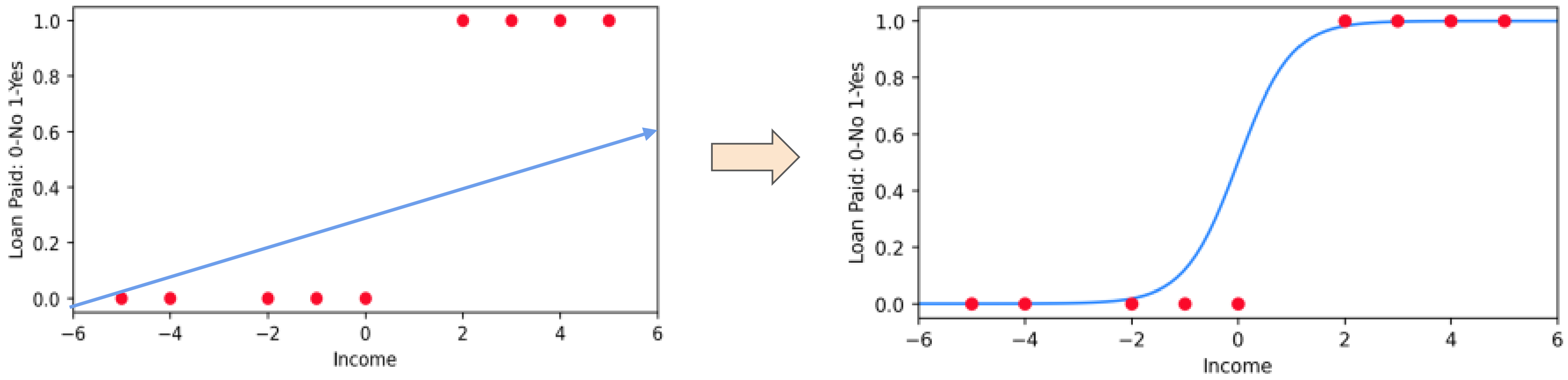
- Fortunately, the mathematics of the conversion are quite simple!





Logistic Regression

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

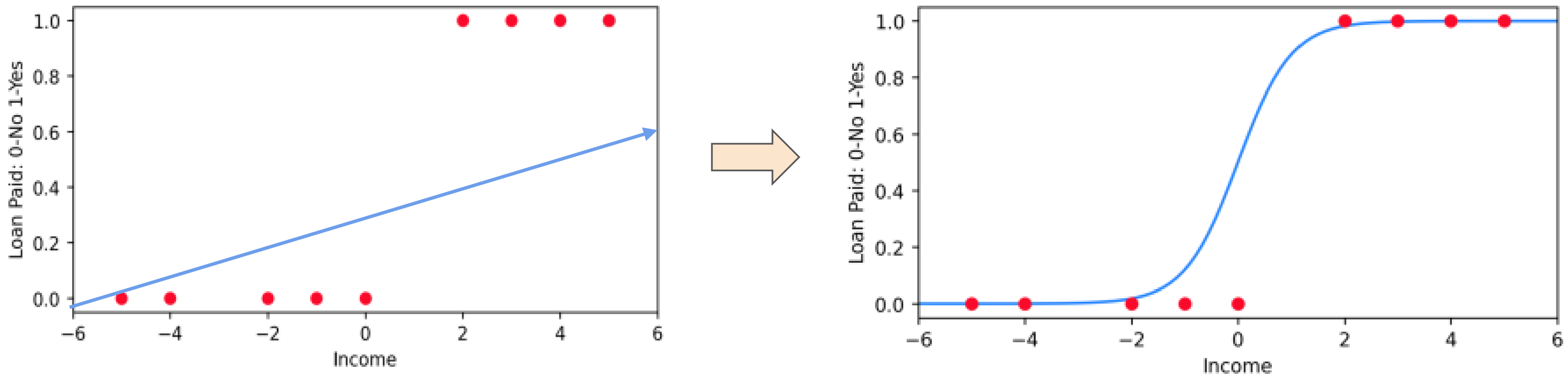


Logistic Regression Theory and Intuition

Part Two: Linear to Logistic Math

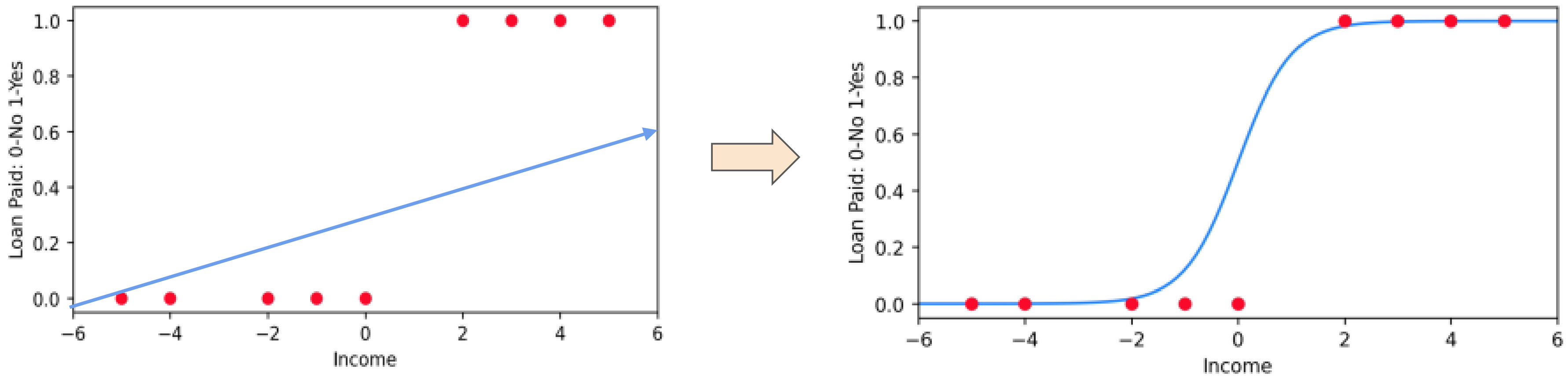
Logistic Regression

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



Logistic Regression

- Relevant ISLR Reading:
    - Section 4.3 Logistic Regression



Logistic Regression

- We already know the Linear Regression equation:

$$\hat{y} = \beta_0 x_0 + \cdots + \beta_n x_n$$

$$\hat{y} = \sum_{i=0}^{n} \beta_i x_i$$

Logistic Regression

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

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

Logistic Regression

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

$$\hat{y} = \beta_0 x_0 + \cdots + \beta_n x_n$$

$$\hat{y} = \boxed{\sum_{i=0}^{n} \beta_i x_i}$$

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

Logistic Regression

- Simply put in terms of the logistic function:

$$\hat{y} = \sigma(\beta_0 x_0 + \cdots + \beta_n x_n)$$

$$\hat{y} = \sigma\left(\sum_{i=0}^{n} \beta_i x_i\right)$$

Logistic Regression

- Writing it out fully:

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

Logistic Regression

- How do we interpret the coefficients and their relation to **ŷ** ?

$$\hat{y} = \frac{1}{1 + e^{-\sum_{i=0}^{n} \boxed{\beta_i} x_i}}$$

Logistic Regression

- First we need to understand the term **odds.**
- A term you may be familiar with from gambling **odds**.

Logistic Regression

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

Logistic Regression

- 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:

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

Logistic Regression

- Imagine an event with **50%** probability of occuring. 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.**

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

Logistic Regression

- 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.

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

Logistic Regression

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

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

Logistic Regression

- Solving for **log odds:**

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

Logistic Regression

- Solving for **log odds:**

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

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

Logistic Regression

- Solving for **log odds:**

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

Logistic Regression

- Solving for **log odds:**

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

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

Logistic Regression

- Solving for **log odds:**

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

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

$$\frac{\hat{y}}{1 - \hat{y}} = e^{\sum_{i=0}^{n} \beta_i x_i}$$

Logistic Regression

- Solving for **log odds:**

$$\frac{\hat{y}}{1-\hat{y}} = e^{\sum_{i=0}^{n} \beta_i x_i}$$

Logistic Regression

- Solving for **log odds:**

$$\frac{\hat{y}}{1-\hat{y}} = e^{\sum_{i=0}^{n} \beta_i x_i}$$

$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \beta_i x_i$$

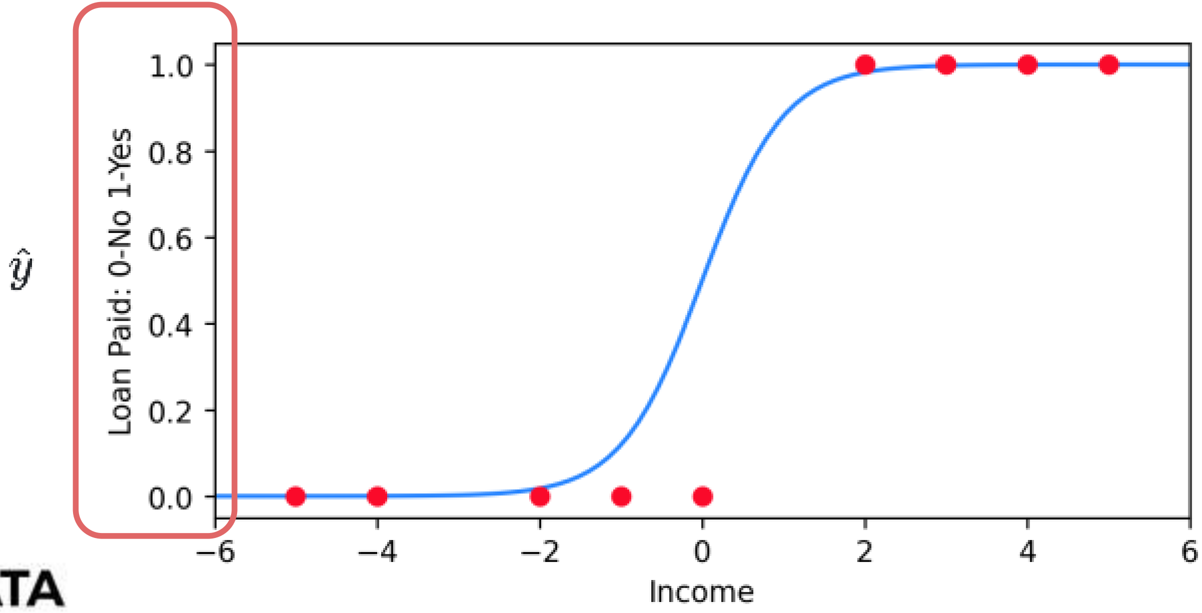
Logistic Regression

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

$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \beta_i x_i$$

Logistic Regression

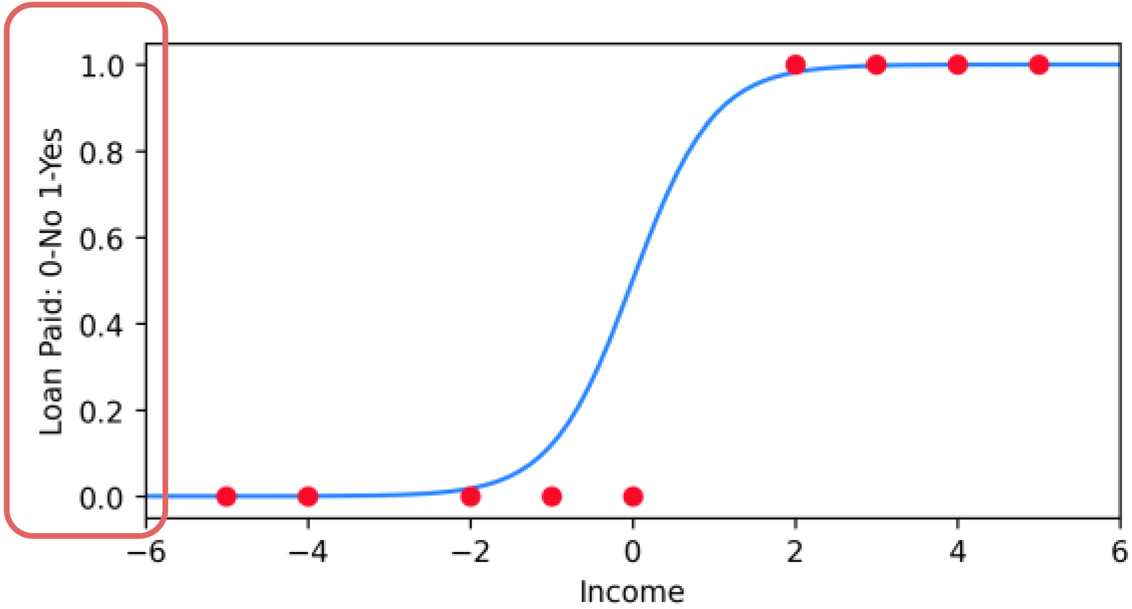
- What would the function curve look like in terms of log odds?



Logistic Regression

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

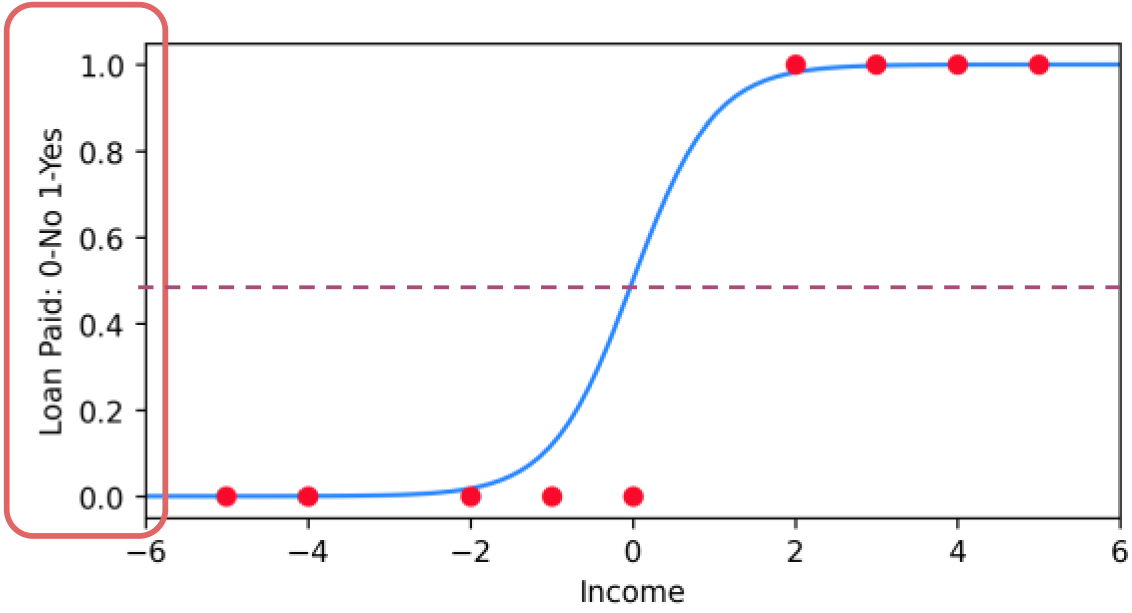
$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) \Leftarrow \hat{y}$$



Logistic Regression

- Consider p=0.5

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



Logistic Regression

- Consider p=0.5, halfway point now at 0.

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

Logistic Regression

- As p goes to 1 then log odds becomes ∞

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

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

Logistic Regression

- As p goes to 0 then log odds becomes -∞

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

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

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

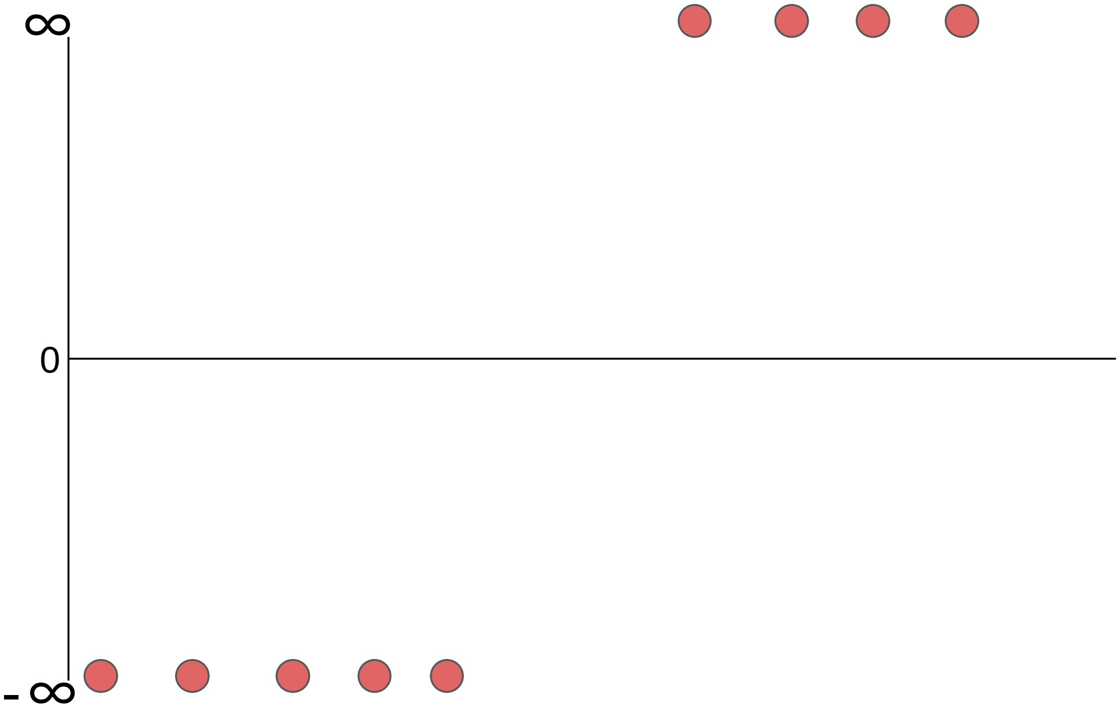
Logistic Regression

- Class points now at infinity

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

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

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



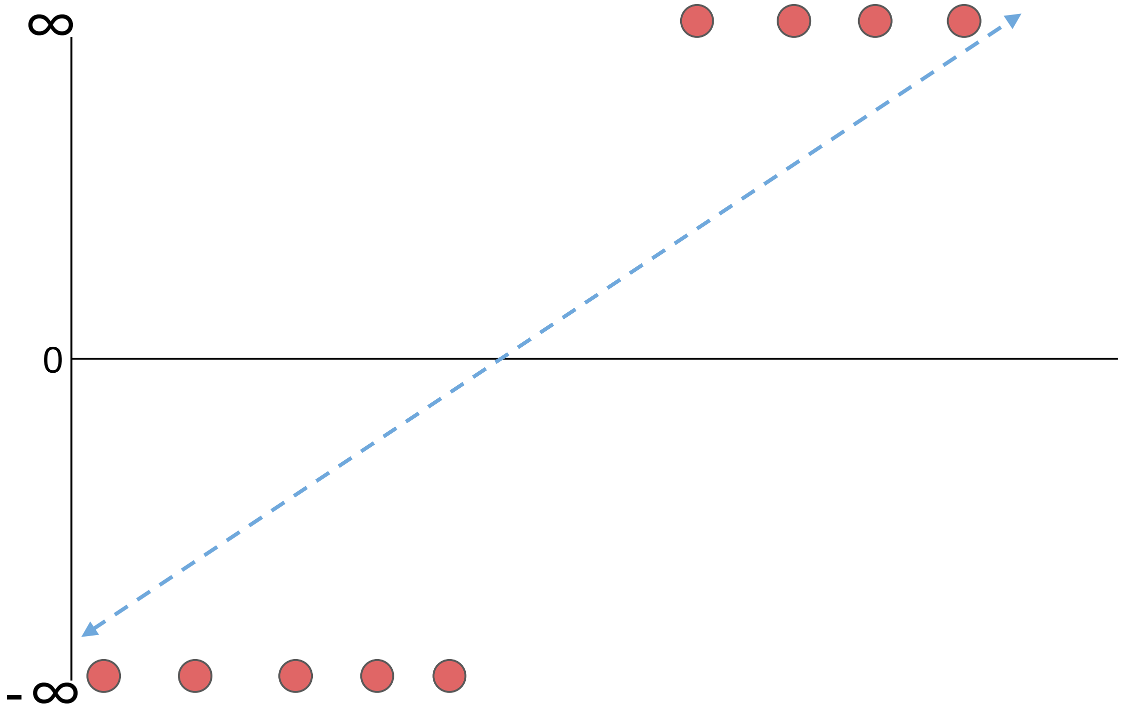
Logistic Regression

- On log scale logistic function is straight line

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

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

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



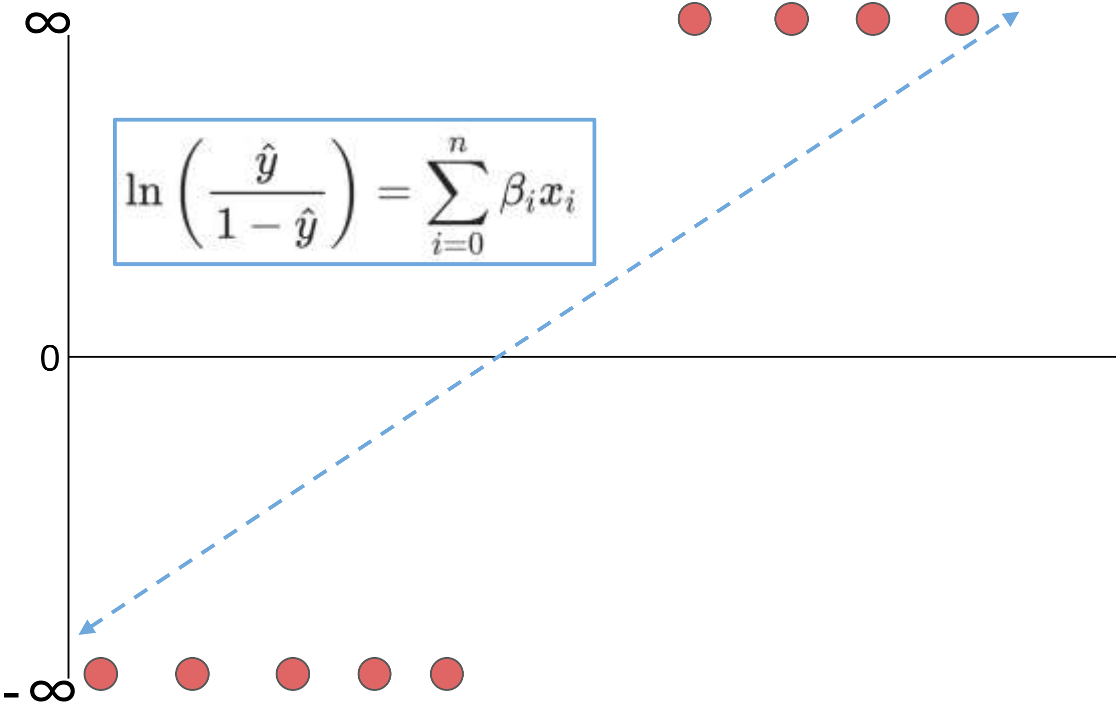
Logistic Regression

- Coefficients in terms of change in log odds.

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

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

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



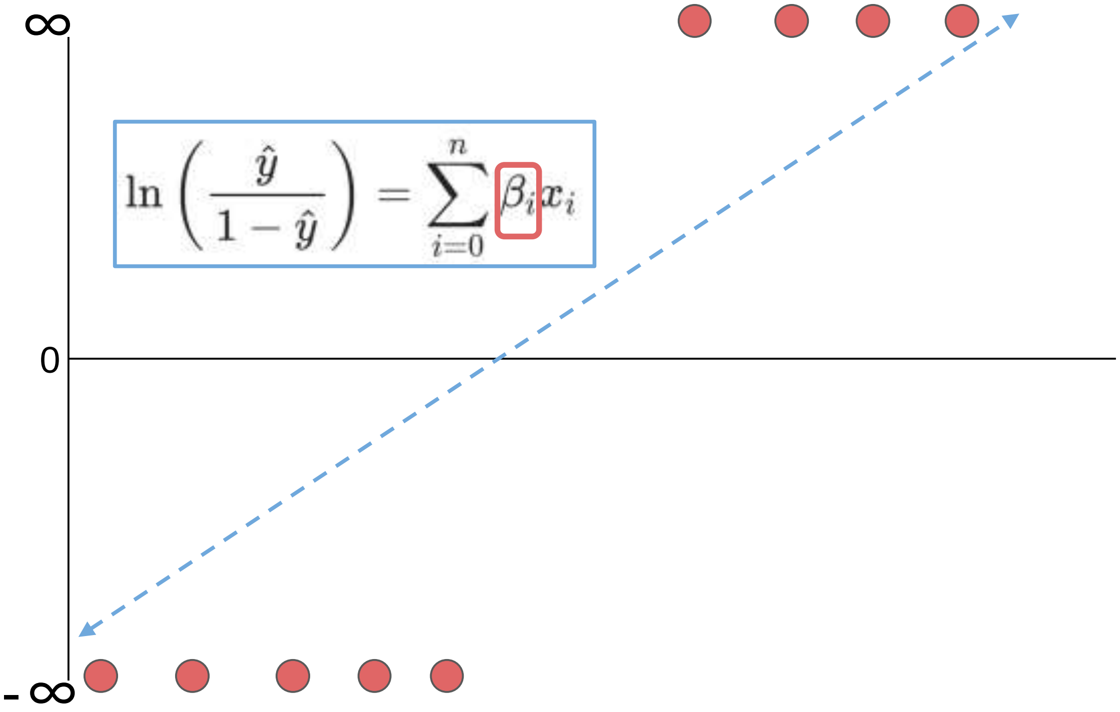
Logistic Regression

- Is β simple to interpret? Not really...

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

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

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



$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \boxed{\beta_i} x_i$$

Logistic Regression

- 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.

$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \beta_i x_i$$

Logistic Regression

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

$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \beta_i x_i$$

Logistic Regression

- Sign of Coefficient
  - Positive **β** indicates an increase in likelihood of belonging to 1 class with increase in associated **x** feature.
  - Negative **β** indicates an decrease in likelihood of belonging to 1 class with increase in associated **x** feature.

Logistic Regression

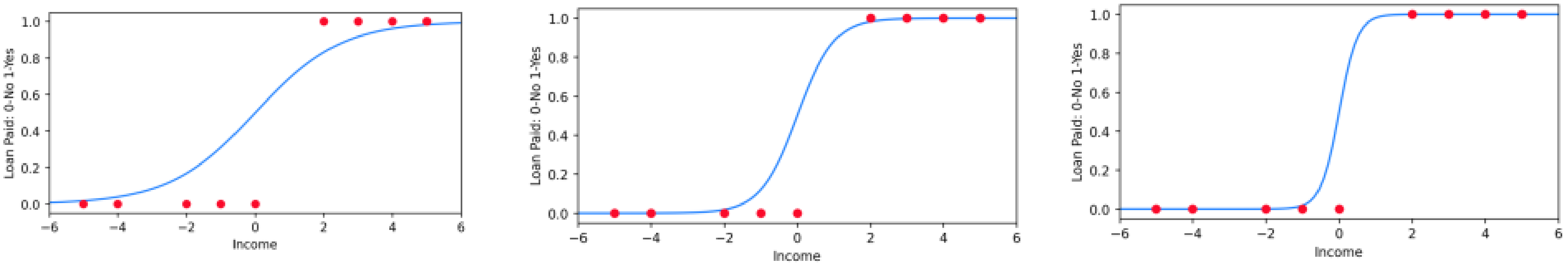
- Magnitude of Coefficient
  - Harder to directly interpret magnitude of β directly, especially when we could have discrete and continuous x feature values.
  - We can however begin to use **odds ratio**, essentially comparing magnitudes against each other.

Logistic Regression

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

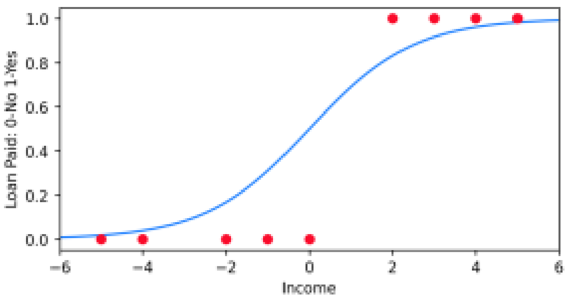
Logistic Regression

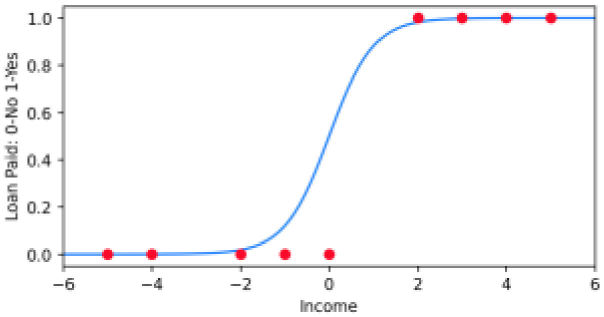
- The last mathematical topic we need to discuss concerning Logistic Regression is how we actually fit this curve!

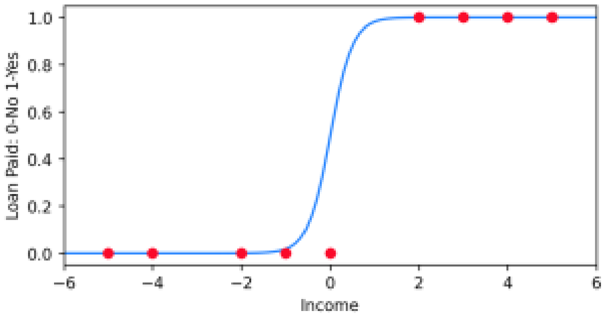


Logistic Regression

- 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

- 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.

Logistic Regression

- 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

Logistic Regression

- Quick Note: ISLR Section 4.3.2

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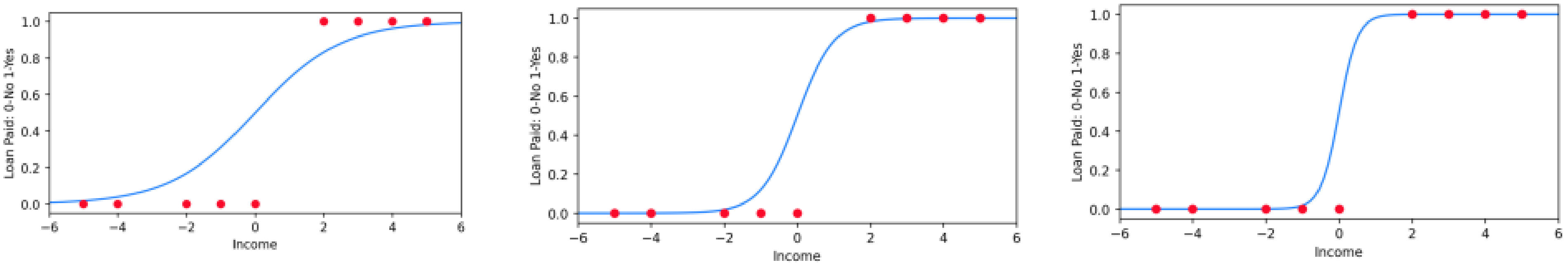
Logistic Regression

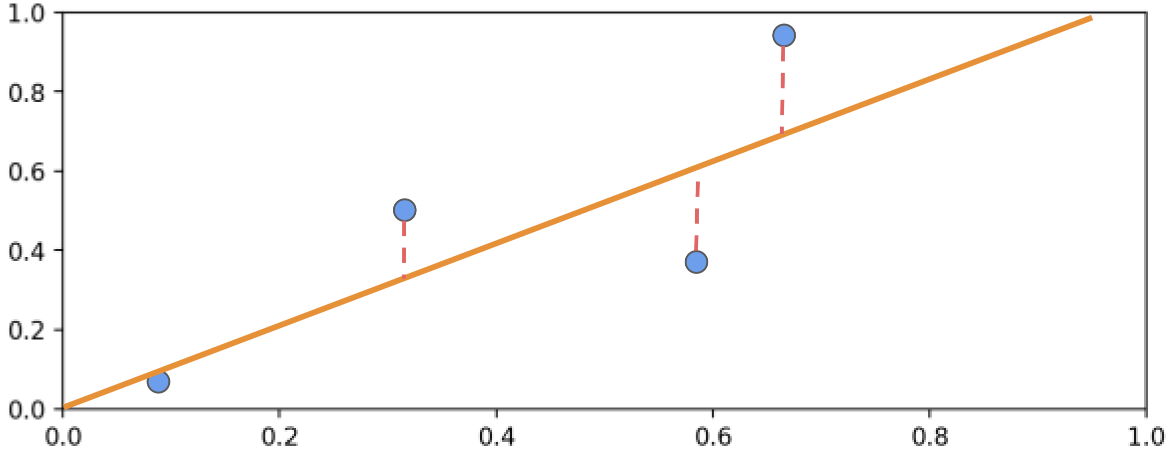
- Here we see three different Logistic Regression curves with different β values.
- How do we measure which is the best fit?



PIERIAN DATA

Logistic Regression

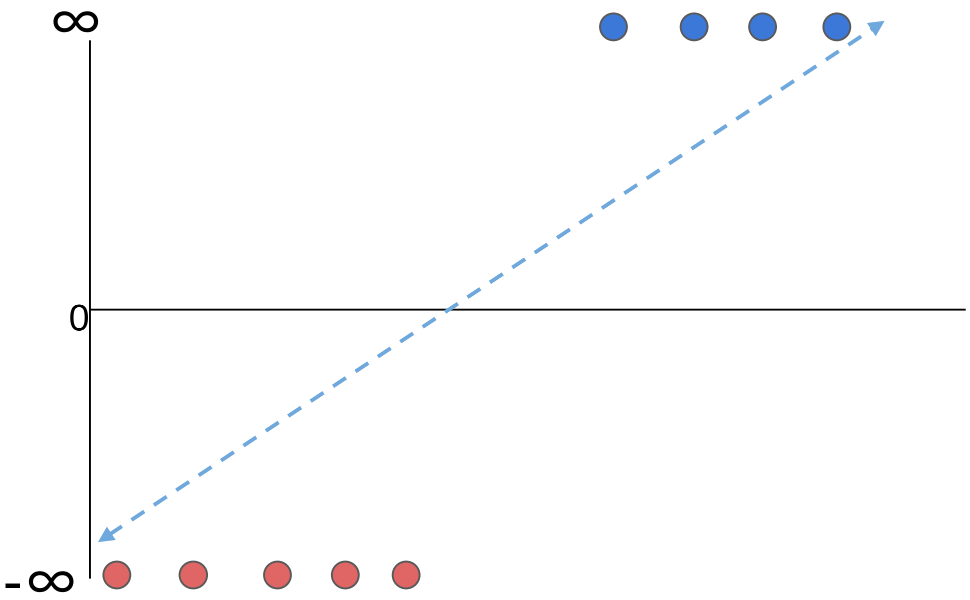
- Recall in Linear Regression we seek to minimize the Residual Sum of Squares (RSS).



Logistic Regression

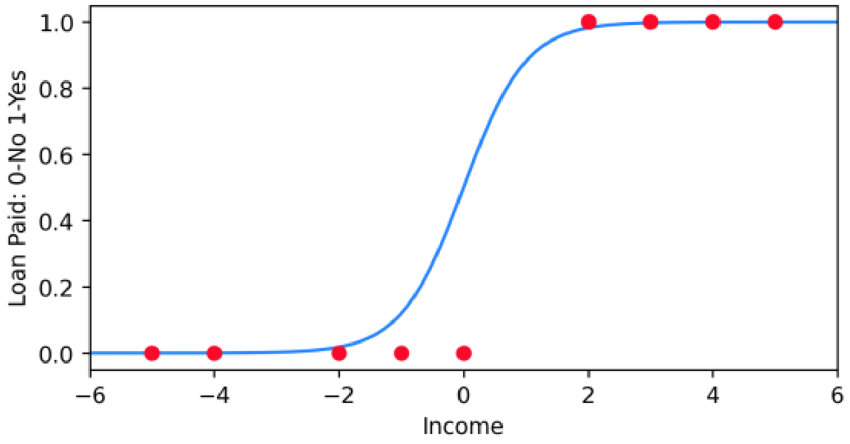
- Unfortunately, even in log odds targets are at infinity, making RSS unfeasible.

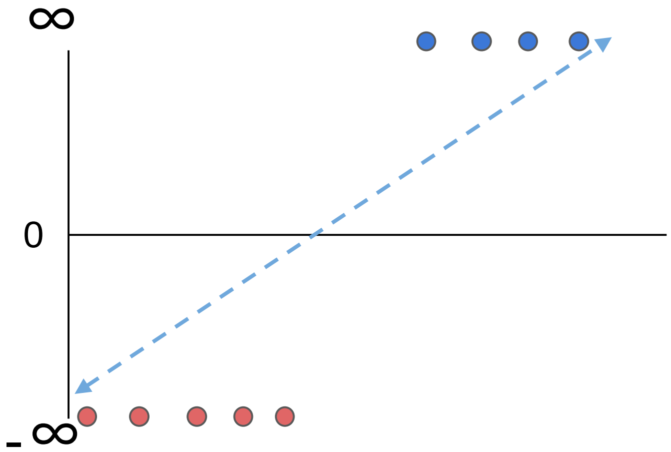
$$\ln\left(\frac{\hat{y}}{1-\hat{y}}\right) = \sum_{i=0}^{n} \beta_i x_i$$



Logistic Regression

- The first step for maximum likelihood is to go from log odds back to probability.





Logistic Regression

- The first step for maximum likelihood is to go from log odds back to probability.

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

Logistic Regression

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

Logistic Regression

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

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

Logistic Regression

- The first step for maximum likelihood is to go from log odds back to probability.

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Logistic Regression

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Logistic Regression

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

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

Logistic Regression

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

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

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

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

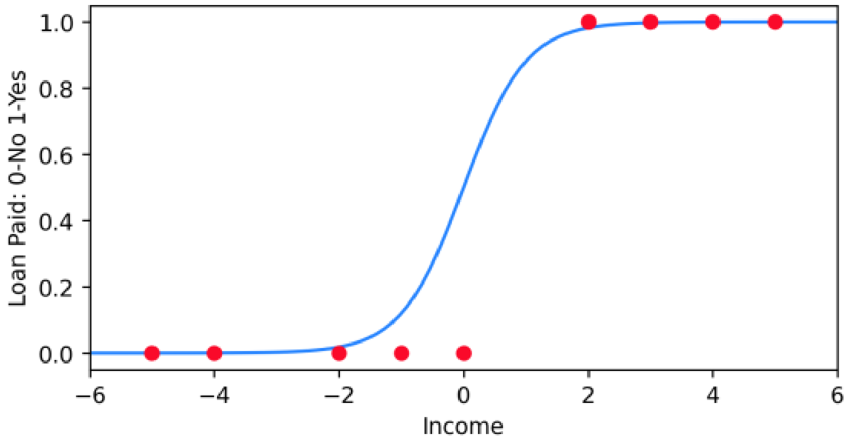
Logistic Regression

- The first step for maximum likelihood is to go from log odds back to probability.

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

Logistic Regression

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



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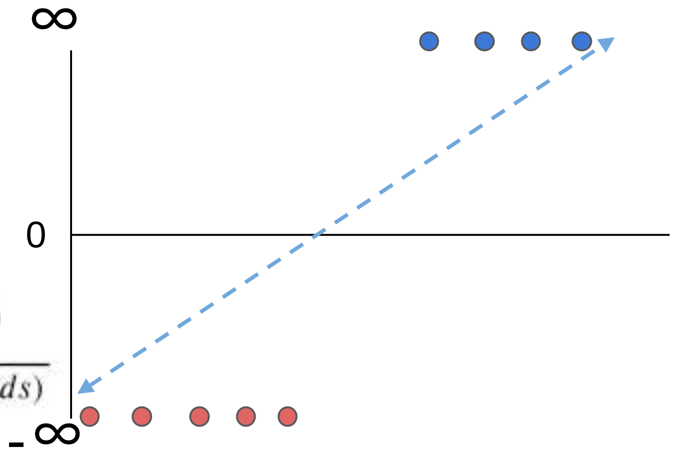
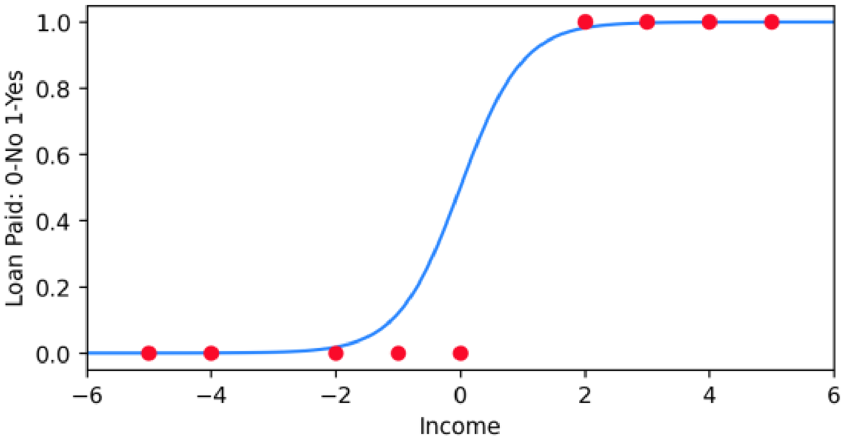


Logistic Regression

- Let's now explore the intuition behind **maximum likelihood.**



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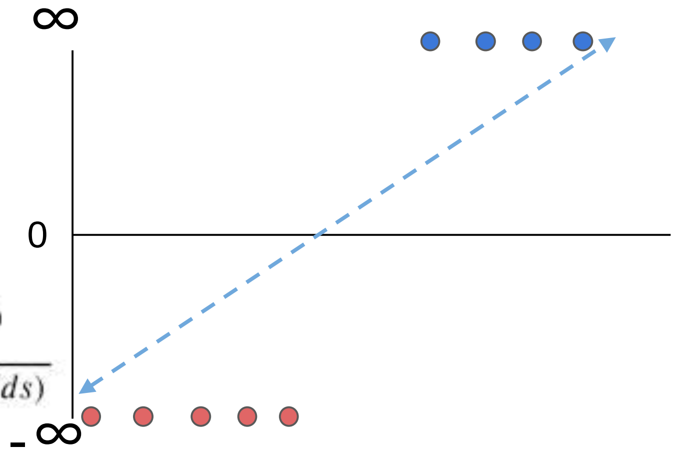
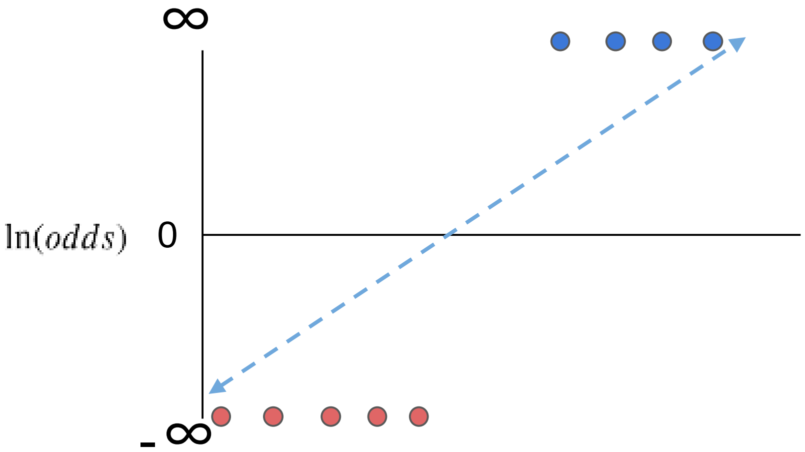


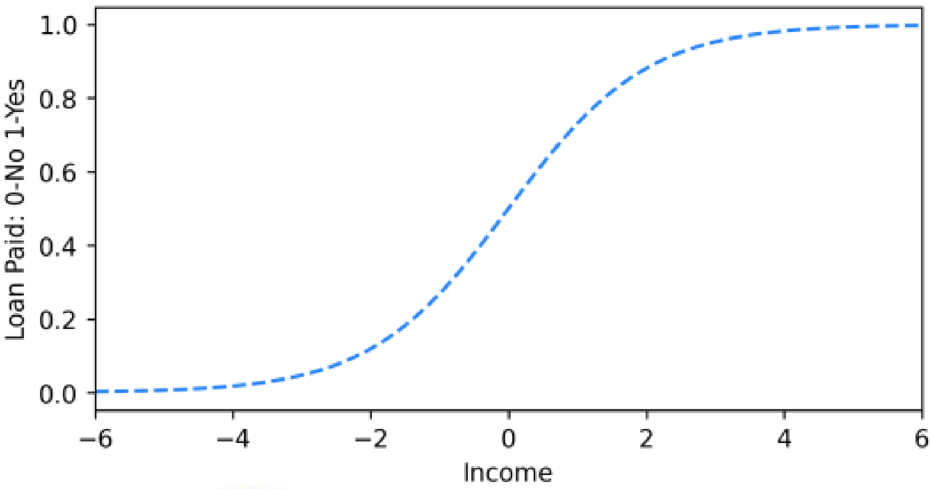
Logistic Regression

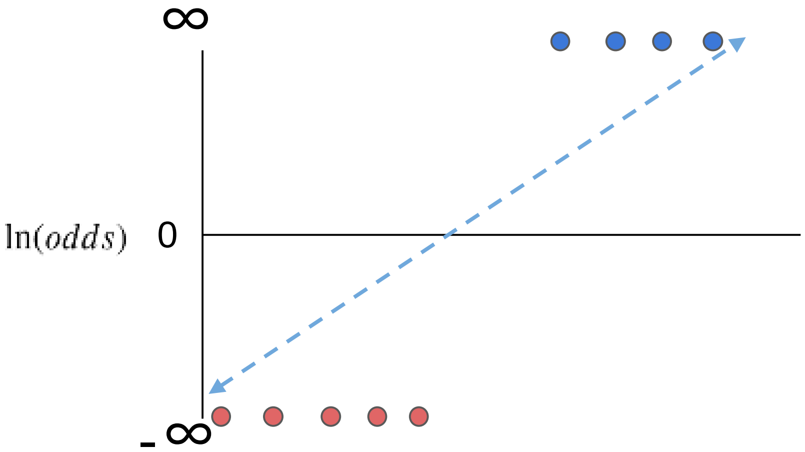
- We choose a line in the log(odds) axis and project the points on to the line:



Logistic Regression

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





PIERIAN DATA

Logistic Regression

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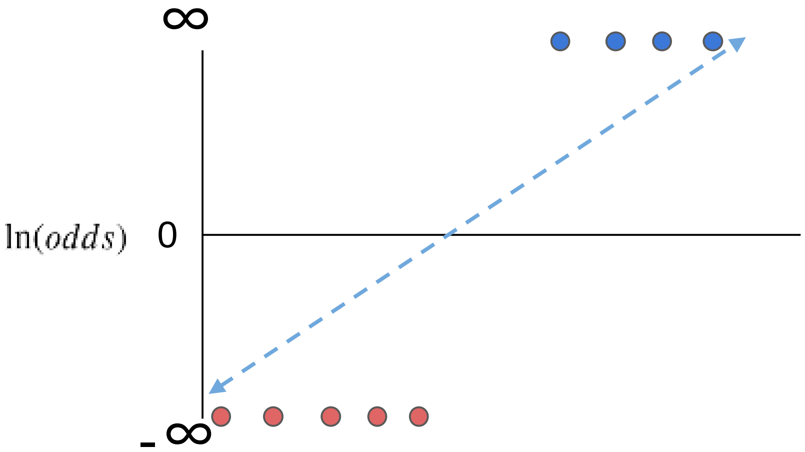

Logistic Regression

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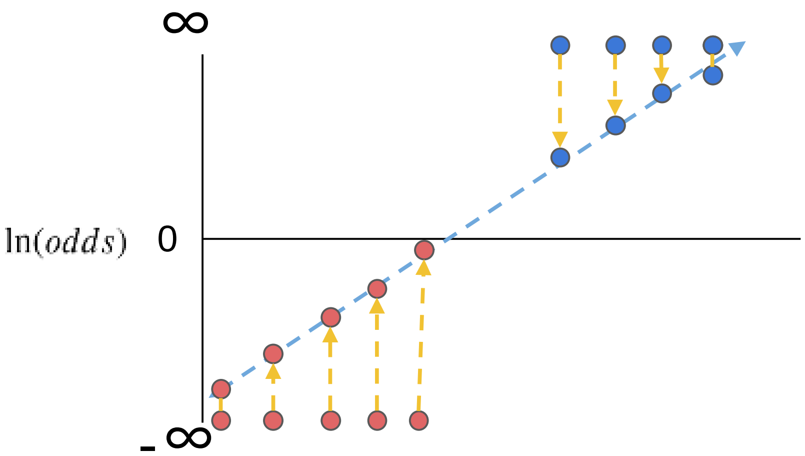
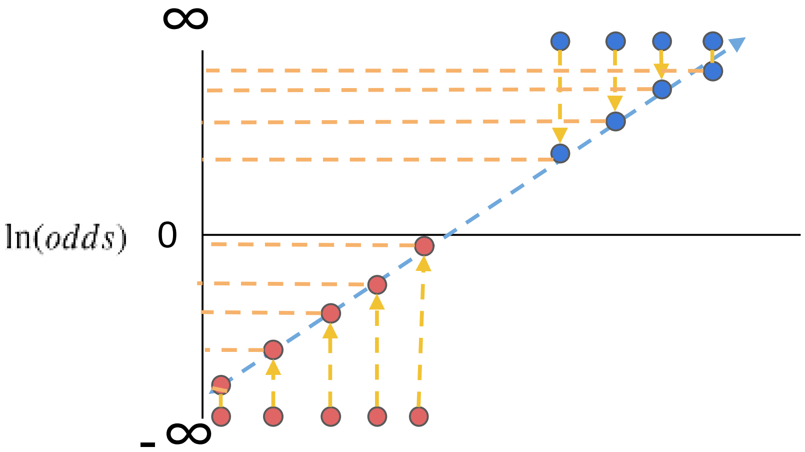


PIERIAN DATA

Logistic Regression

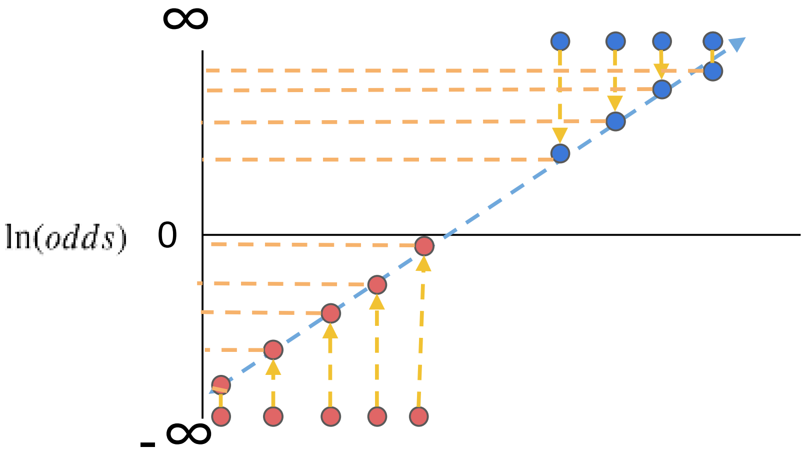
- Calculate the log odds for the projected points on this line.



Logistic Regression

- Plot these values as probabilities on the logistic regression model.

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



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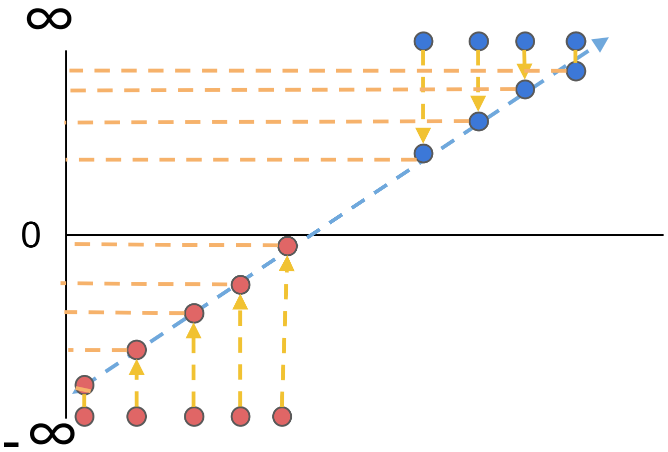
$\ln(odds)$



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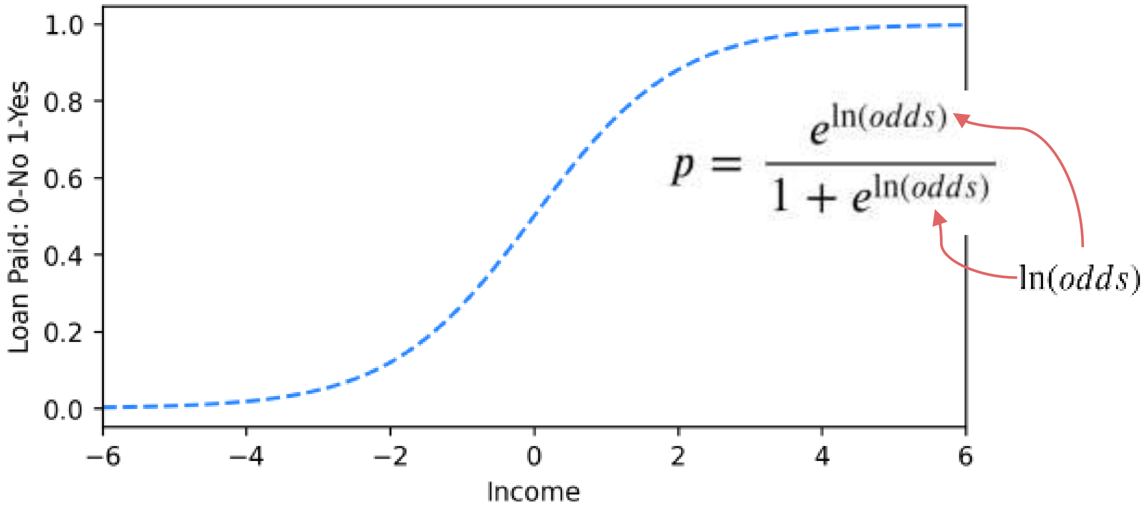
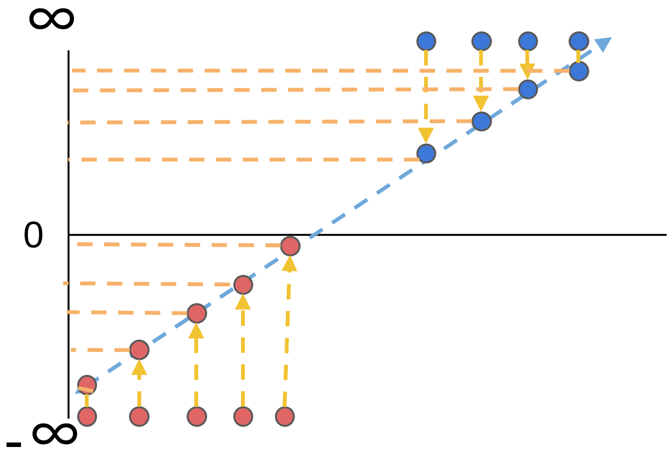
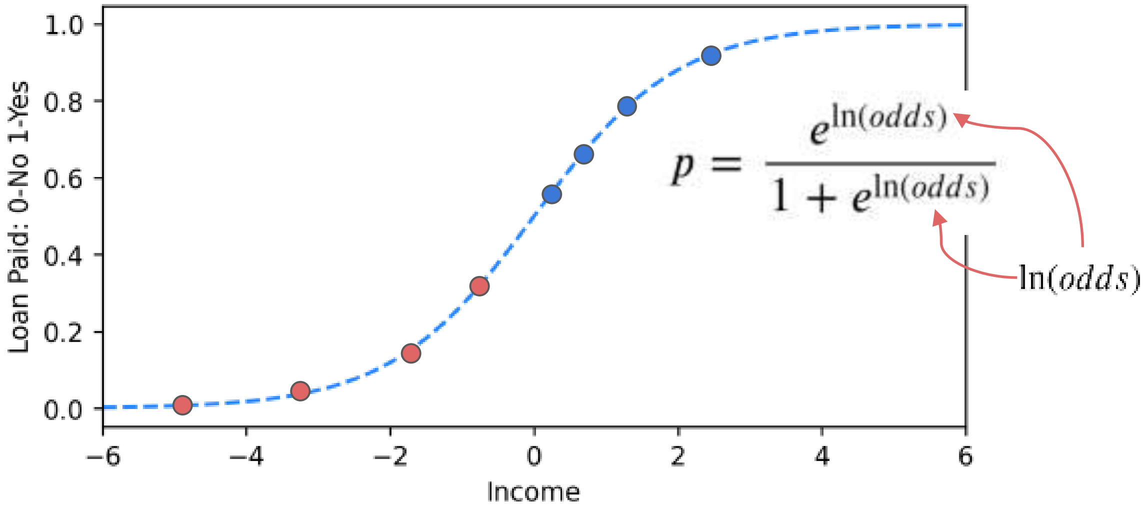
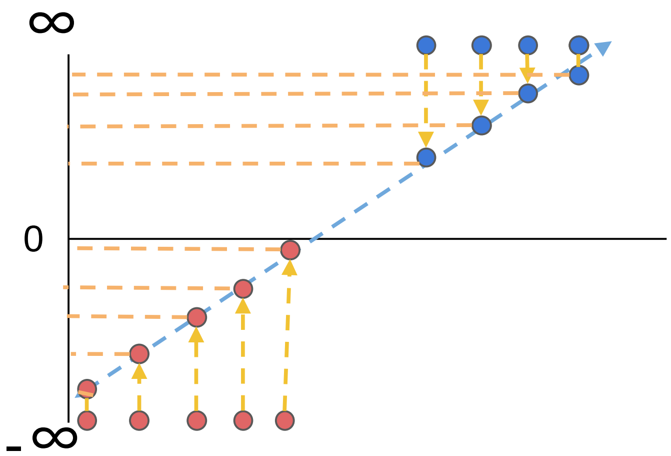




Logistic Regression

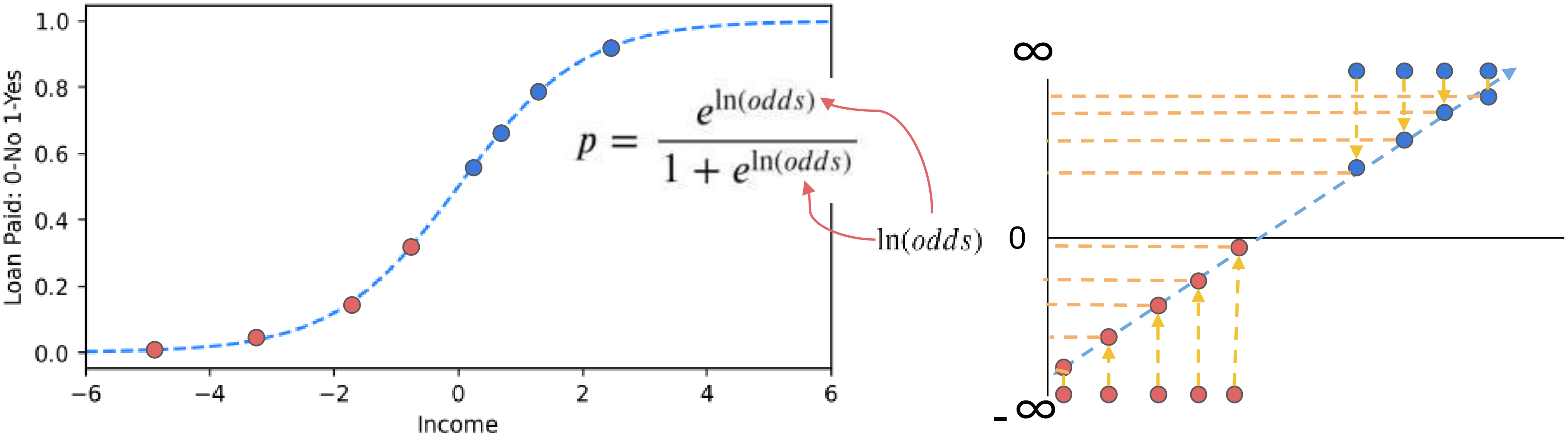
- Plot these values as probabilities on the logistic regression model.





Logistic Regression

- We now measure the likelihood of these probabilities.



Logistic Regression

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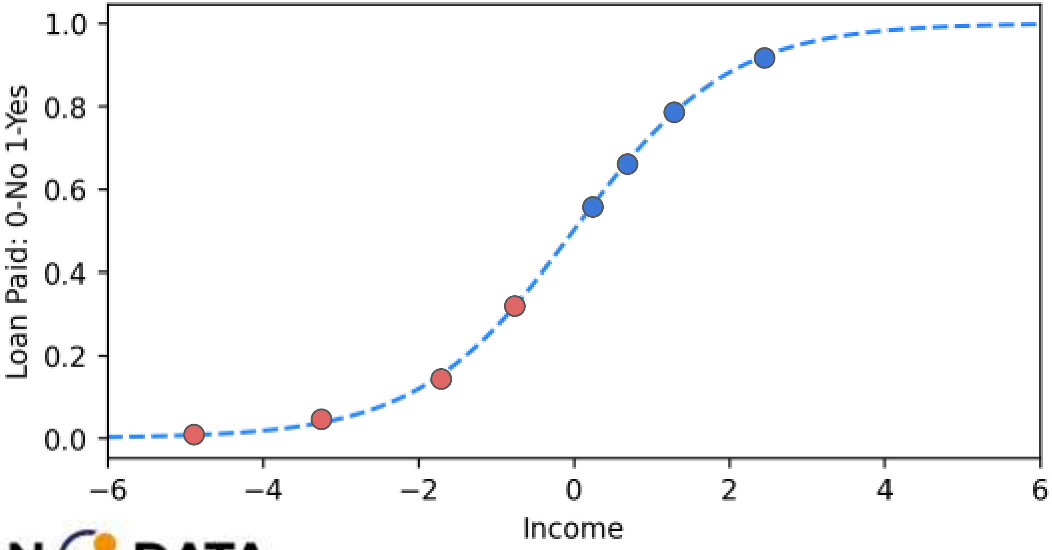
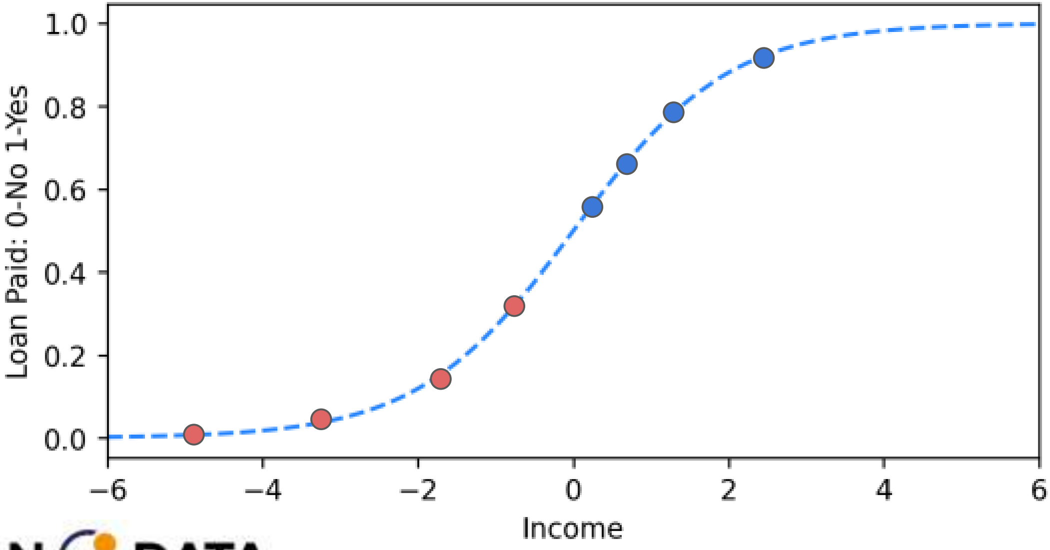


Logistic Regression

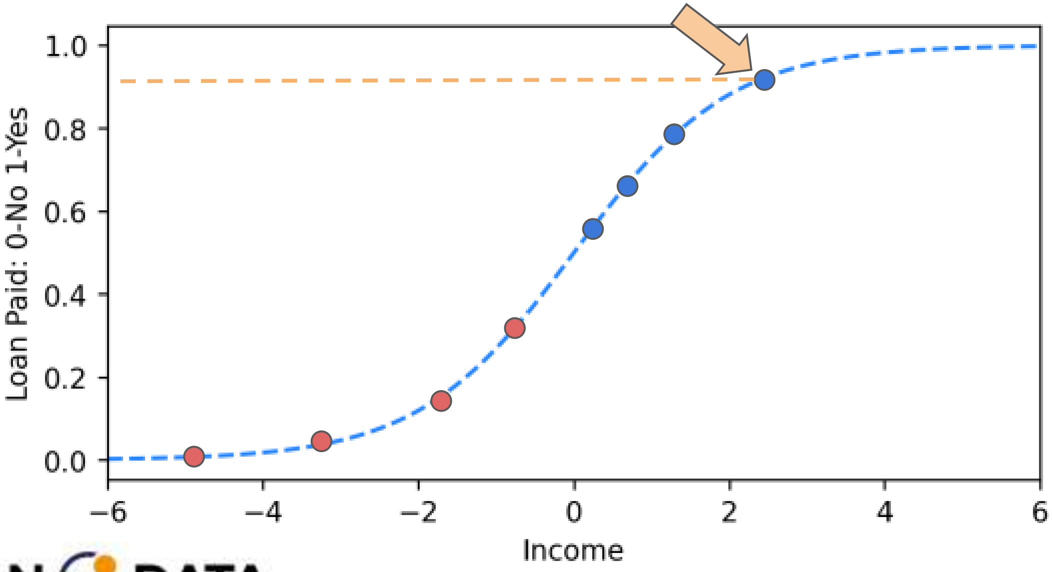
- Likelihood = Product of probabilities of belonging to class 1.



PIERIAN DATA

Logistic Regression

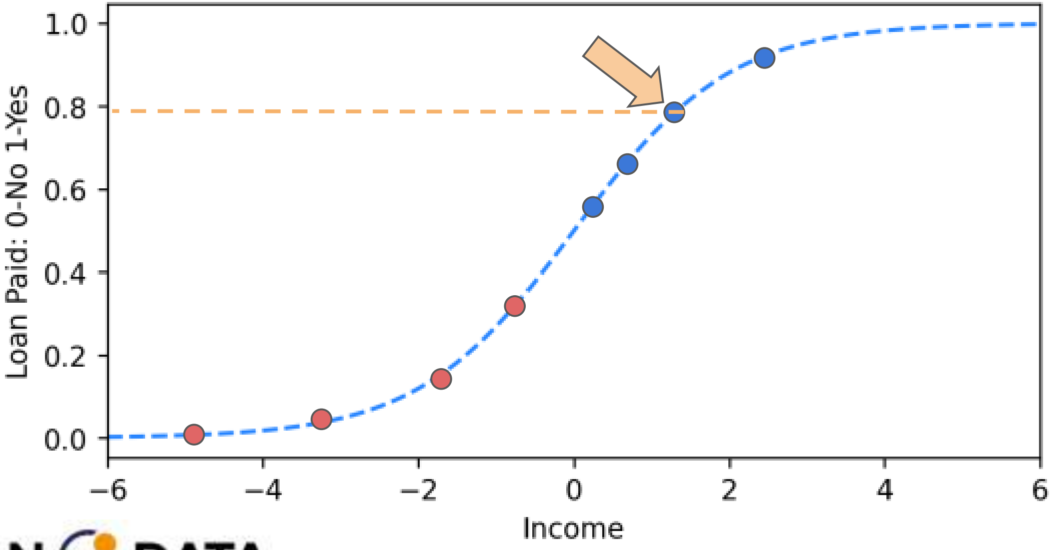
- Likelihood = 0.9 ...



PIERIAN DATA

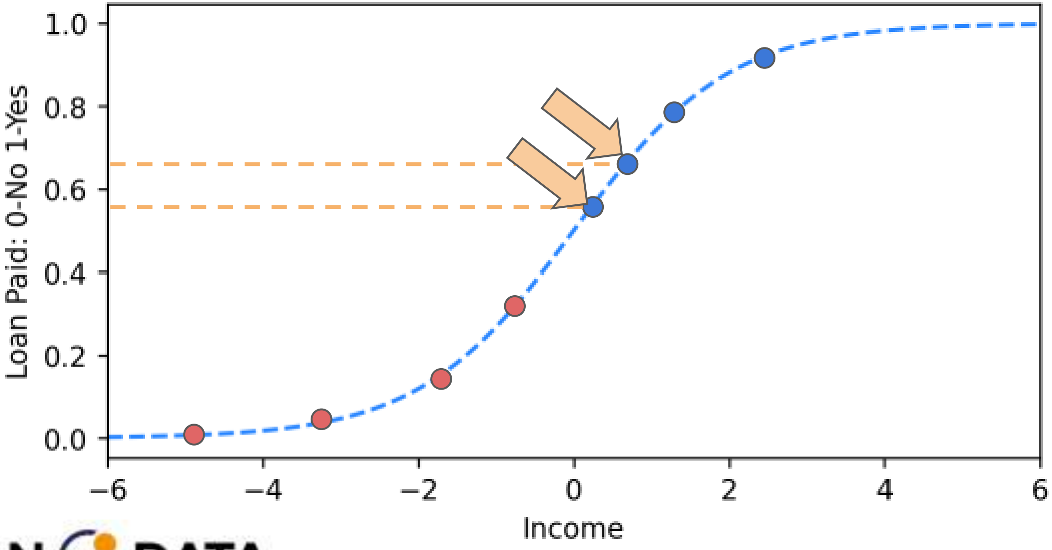
Logistic Regression

- Likelihood = 0.9 × 0.8 × …



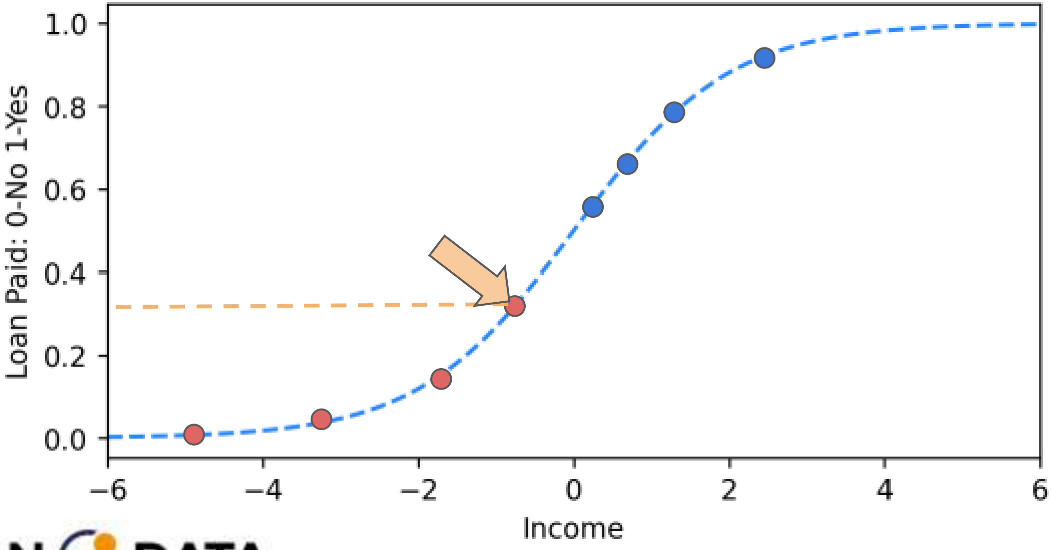
Logistic Regression

- Likelihood = 0.9 × 0.8 × 0.65 × 0.55 × …



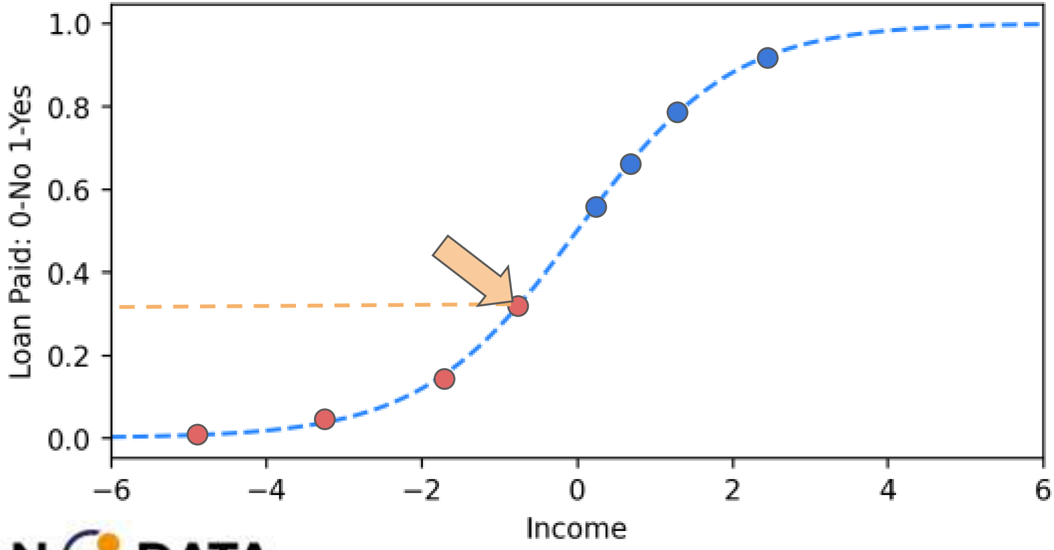
Logistic Regression

- Likelihood = 0.9 × 0.8 × 0.65 × 0.55 × (1-p) ×…



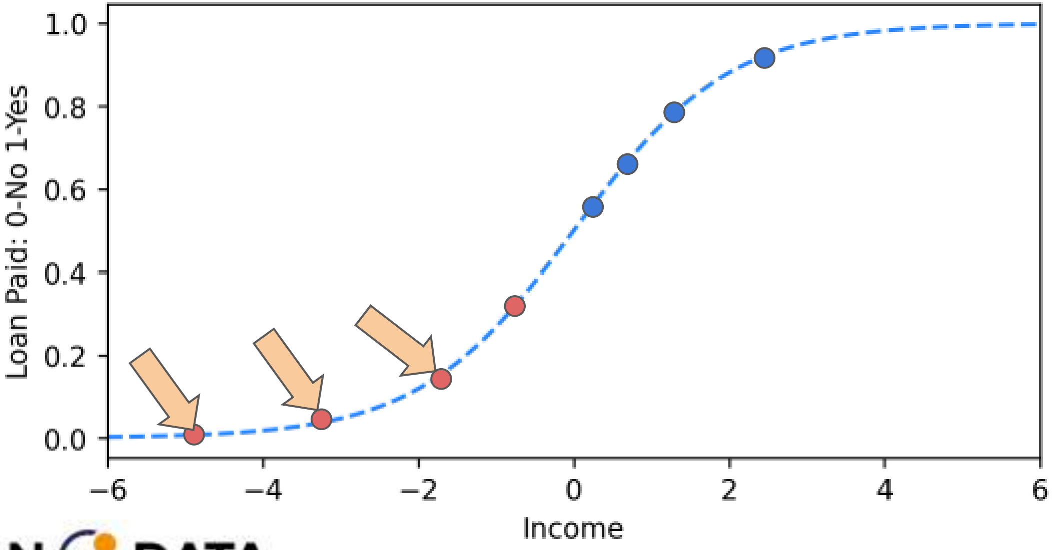
Logistic Regression

- Likelihood = 0.9 × 0.8 × 0.65 × 0.55 × (1-0.3) ×...



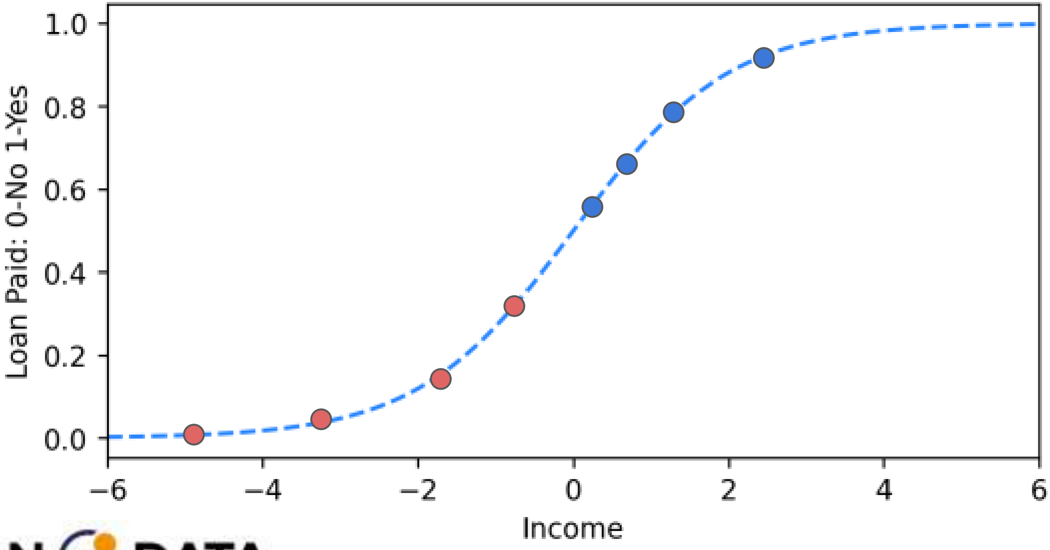
Logistic Regression

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



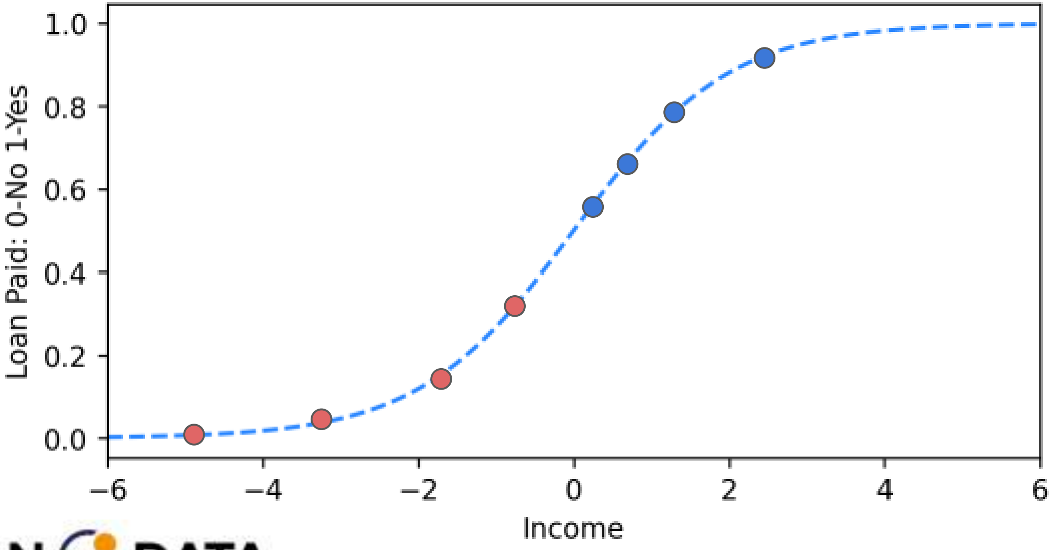
Logistic Regression

- Likelihood = 0.129



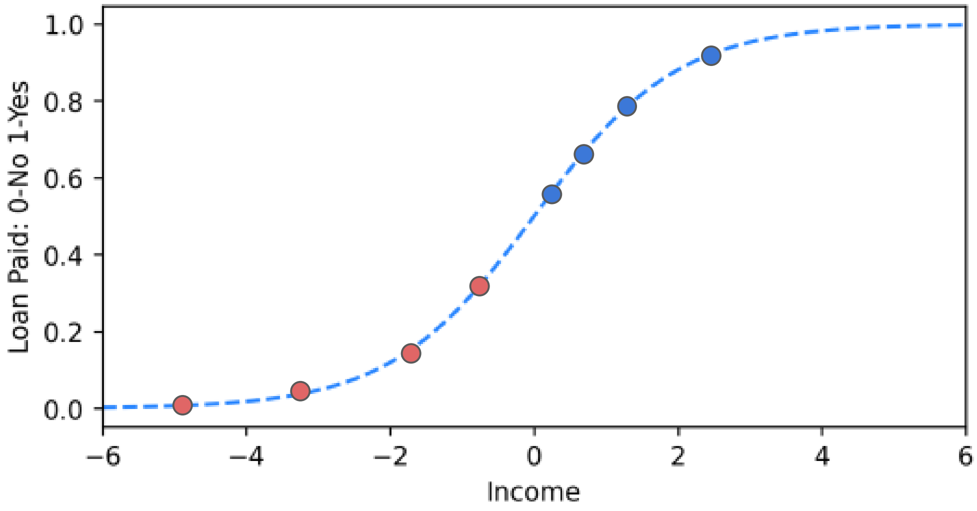
Logistic Regression

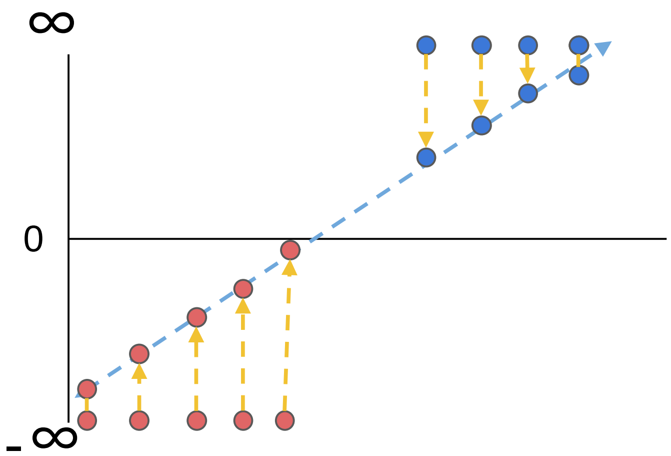
- Note in practice we actually maximize the **log** of the likelihoods. (e.g. ln(0.9)×ln(0.8)×...)



Logistic Regression

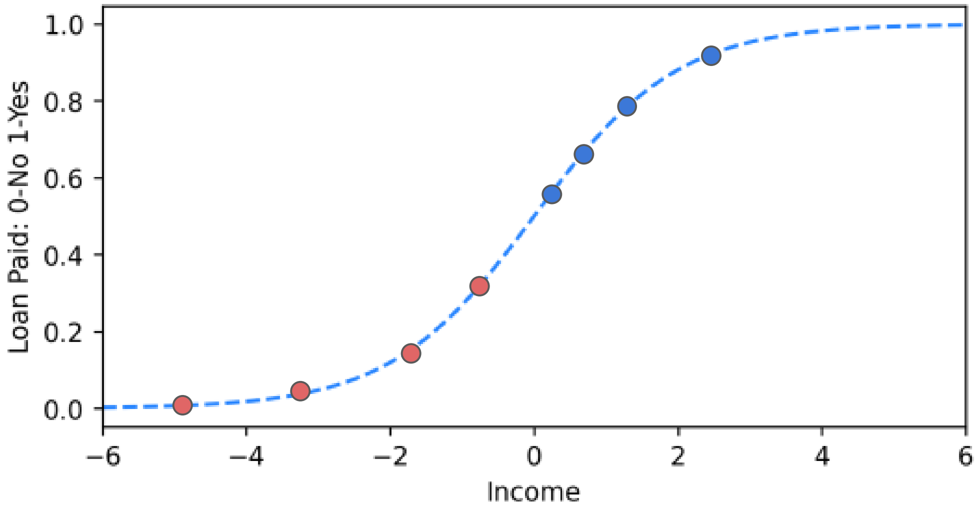
- There is some set of coefficients that will maximize these log likelihoods.

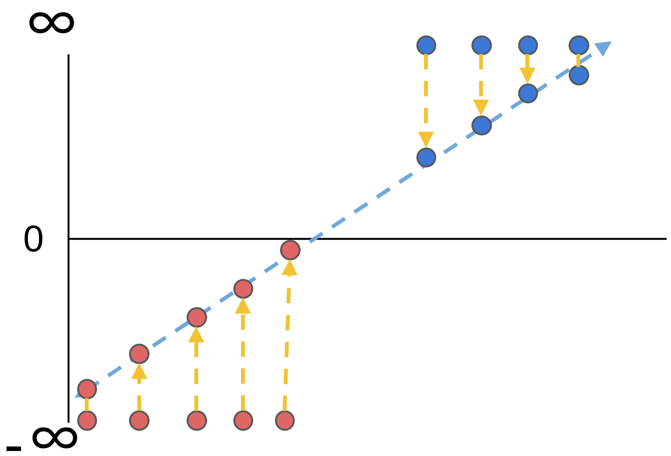




Logistic Regression

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





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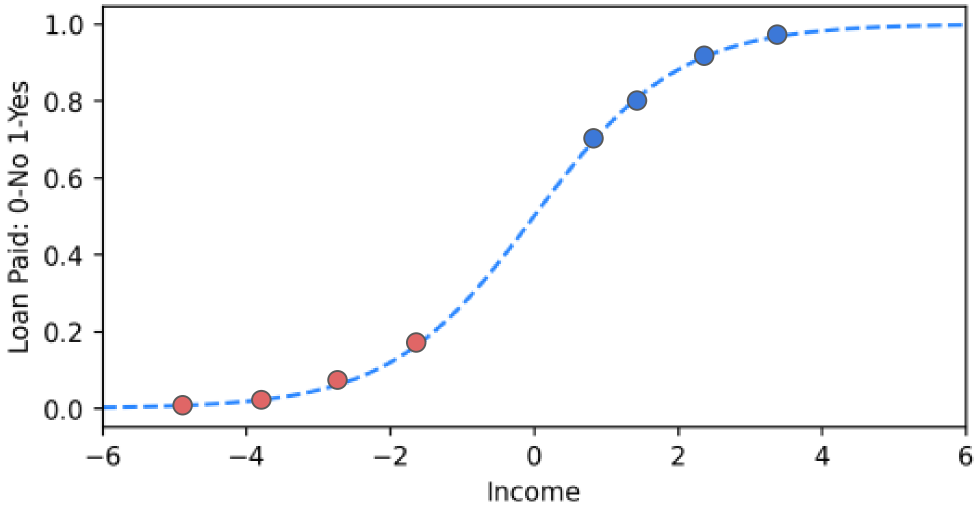
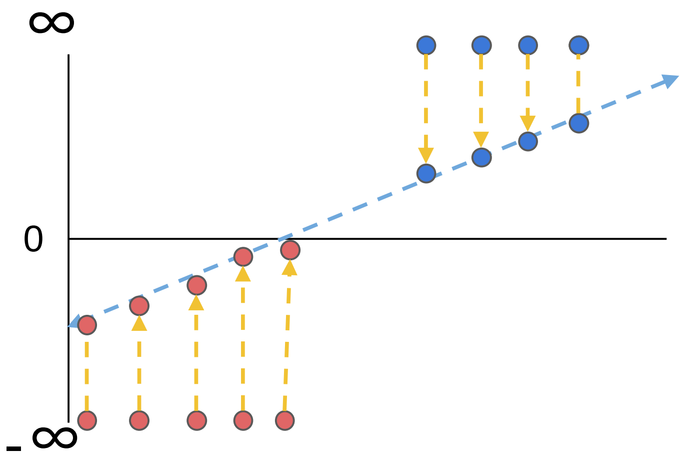




Logistic Regression

- 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.

Logistic Regression

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

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

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

Logistic Regression

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

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

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

Logistic Regression

- 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.

Logistic Regression

- 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

Classification Metrics

- 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?

Classification Metrics

- 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:
    - 0 - Not Infected (Tests Negative)
    - 1 - Infected (Tests Positive)

Classification Metrics

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

Classification Metrics

- 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...*

Classification Metrics

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

Classification Metrics

- 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.

Classification Metrics

- Confusion Matrix

ACTUAL

	INFECTED	HEALTHY

Classification Metrics

- Confusion Matrix

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED		
	HEALTHY		

Classification Metrics

- Confusion Matrix

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	TRUE POSITIVE	
	HEALTHY		

Classification Metrics

- Confusion Matrix

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	TRUE POSITIVE	
	HEALTHY		TRUE NEGATIVE

Classification Metrics

- Confusion Matrix

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

Classification Metrics

- Confusion Matrix

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

Classification Metrics

- Imagine a test group of 100 people:

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED		
	HEALTHY		

Classification Metrics

- 5 are infected. 95 are healthy.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED		
	HEALTHY		

Classification Metrics

- We tested all of them with these results:

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Classification Metrics

- What is accuracy?

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Classification Metrics

- What is accuracy?

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

- Accuracy:
  - How often is the model correct?

Acc = (TP+TN)/Total

Classification Metrics

- Calculating accuracy:

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

(4+93)/100 = 97% Accuracy

- Accuracy:
  - How often is the model correct?

Acc = (TP+TN)/Total

Classification Metrics

- Is this a good value for accuracy?

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

(4+93)/100 = 97% Accuracy

- Accuracy:
  - How often is the model correct?

Acc = (TP+TN)/Total

Classification Metrics

- 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?

Acc = (TP+TN)/Total

Classification Metrics

- Imagine we **always** report back “healthy”

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Classification Metrics

- Imagine we **always** report back “healthy”

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Classification Metrics

- 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”!

Classification Metrics

- **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*”.

Classification Metrics

- 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.

Classification Metrics

- **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).

Classification Metrics

- 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%.

Classification Metrics

- 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

Classification Metrics

- 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

Classification Metrics

- Let's begin with recall.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

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

(TP)/Total Actual Positives

Classification Metrics

- Let's begin with recall.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Recall =
(TP)/Total Actual Positives

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

(TP)/Total Actual Positives

Classification Metrics

- Let's begin with recall.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Recall =
(TP)/5

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

(TP)/Total Actual Positives

Classification Metrics

- Let's begin with recall.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Recall =
(4)/5

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

(TP)/Total Actual Positives

Classification Metrics

- Let's begin with recall.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Recall = 0.8

- Recall:
  - How many relevant cases are found?

(TP)/Total Actual Positives

Classification Metrics

- What’s the recall if we always classify as “healthy”?

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall =
(TP)/Total Actual Positives

- Recall:
  - How many relevant cases are found?

(TP)/Total Actual Positives

Classification Metrics

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

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall =
(0)/5 !

- Recall:
  - How many relevant cases are found?

(TP)/Total Actual Positives

Classification Metrics

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

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Recall =
(0)/5 !

- Recall:
  - How many relevant cases are found?

(TP)/Total Actual Positives

Classification Metrics

- Now let's explore **precision**.

		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?

(TP)/Total Predicted Positives

Classification Metrics

- Now let's explore **precision.**

		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?

(TP)/Total Predicted Positives

Classification Metrics

- Now let's explore **precision**.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Precision =
(TP)/6

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

(TP)/Total Predicted Positives

Classification Metrics

- Now let's explore **precision.**

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Precision =
(TP)/6

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

(TP)/Total Predicted Positives

Classification Metrics

- Now let's explore **precision**.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Precision =
(4)/6

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

(TP)/Total Predicted Positives

Classification Metrics

- Now let's explore **precision**.

		ACTUAL	
		INFECTED	HEALTHY
PREDICTED	INFECTED	4	2
	HEALTHY	1	93

Precision = 0.666

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

(TP)/Total Predicted Positives

Classification Metrics

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

ACTUAL

		INFECTED	HEALTHY
PREDICTED	INFECTED	0	0
	HEALTHY	5	95

Precision =
(TP)/Total Predicted Positives

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

(TP)/Total Predicted Positives

Classification Metrics

- 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?

(TP)/Total Predicted Positives

Classification Metrics

- 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.

Classification Metrics

- 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.

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

Classification Metrics

- 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.

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

Classification Metrics

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

		True condition				
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition	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) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
	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 = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$	F_1 score = $2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$
		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−) = $\frac{\text{FNR}}{\text{TNR}}$		

Classification Metrics

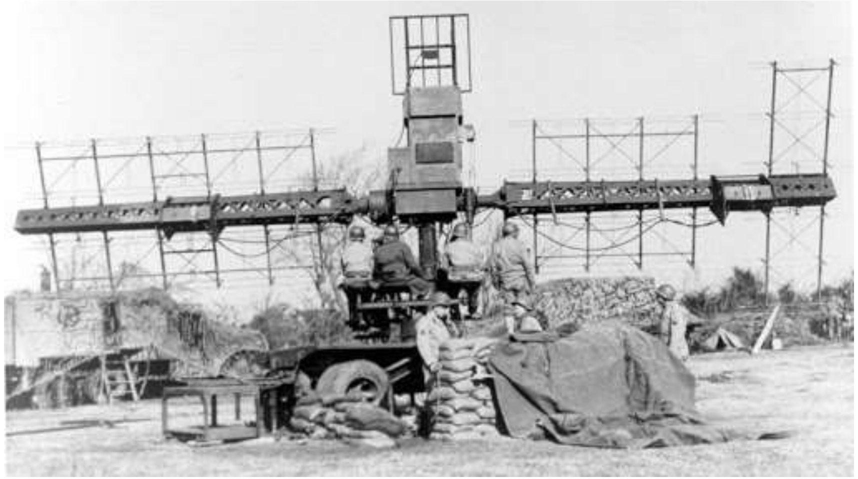
- Finally, let’s explore a way to visualize the relationships between metrics such as precision and recall with curves.

Classification Performance Metrics

Part Three: ROC Curves

Classification Metrics

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

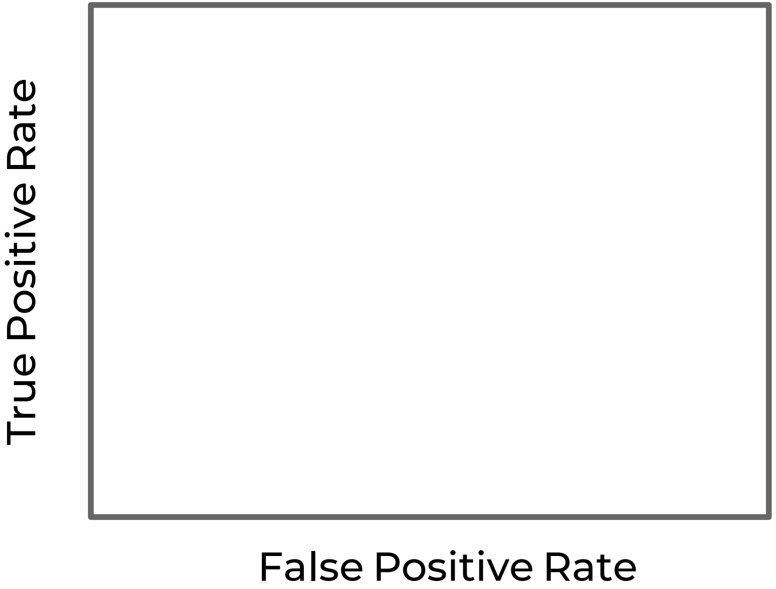


Classification Metrics

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

Classification Metrics

- They developed the Receiver Operator Characteristic curve.



Classification Metrics

- They developed the Receiver Operator Characteristic curve.

Classification Metrics

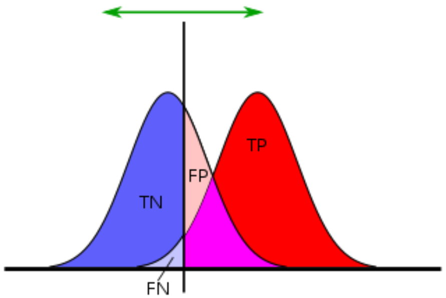
- They developed the Receiver Operator Characteristic curve.

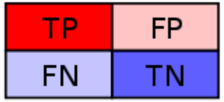
Classification Metrics

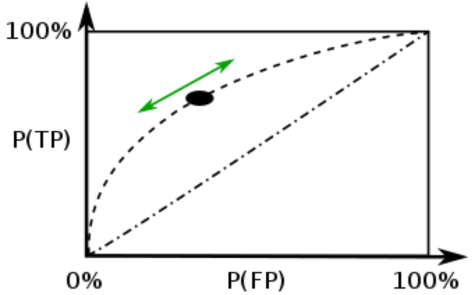
- There can be a trade-off between True Positives and False Positives.

Classification Metrics

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

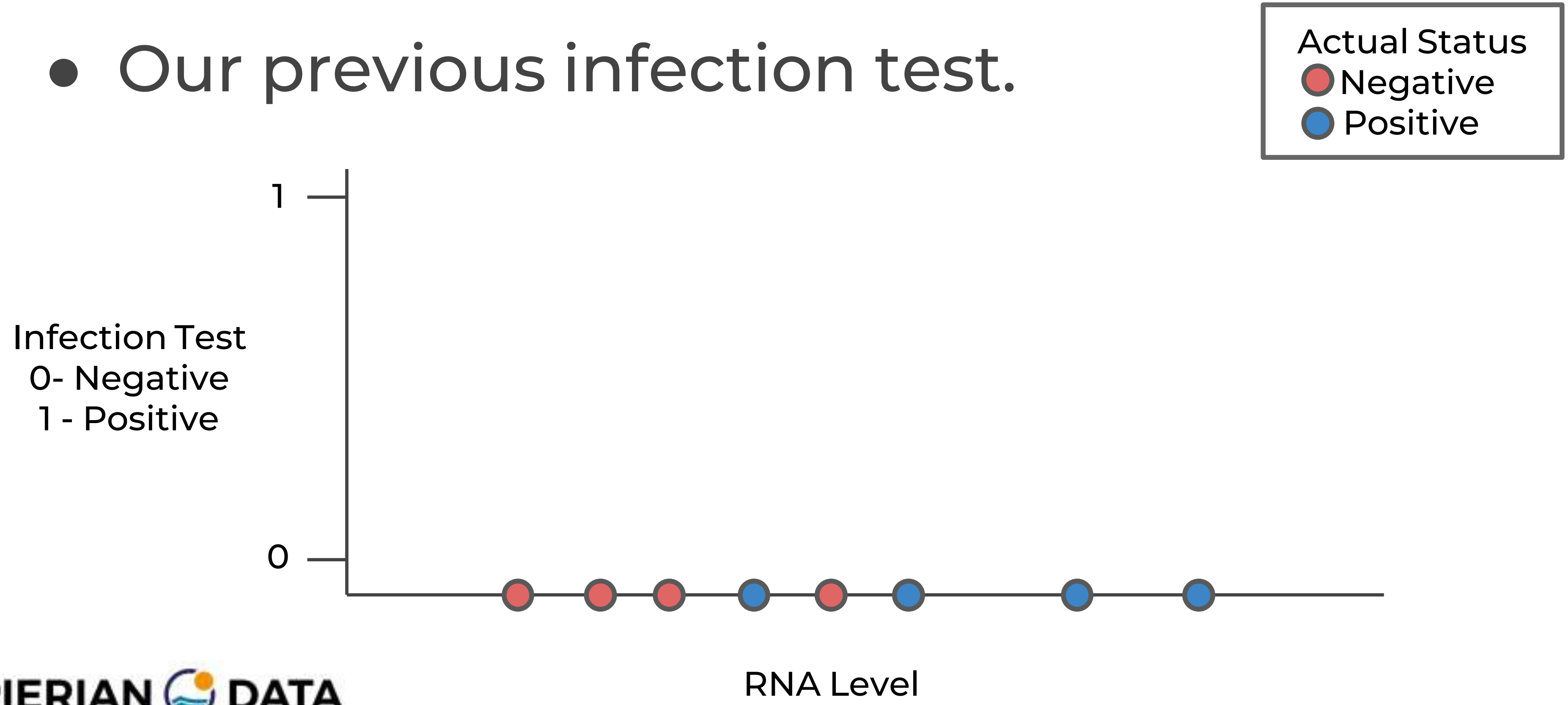






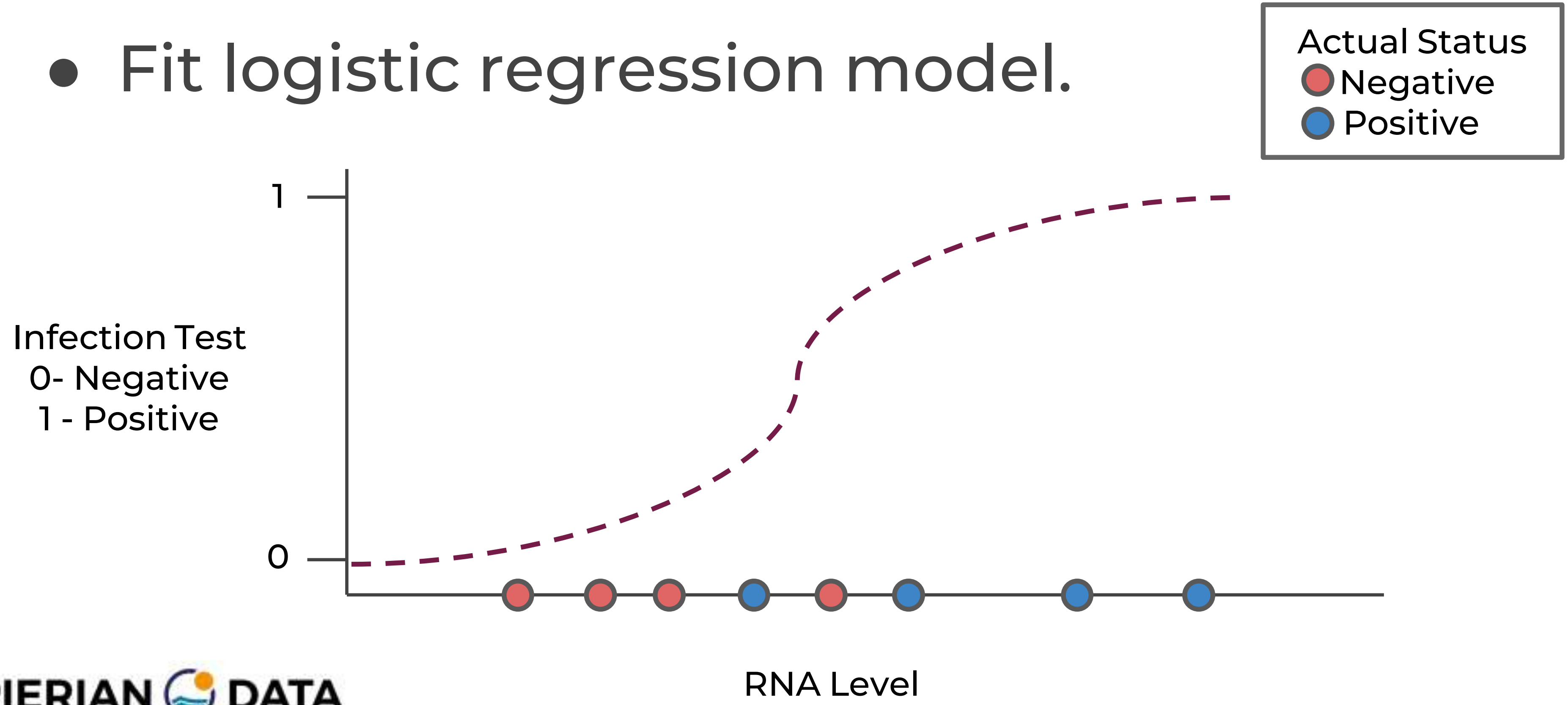
Classification Metrics

- Our previous infection test.



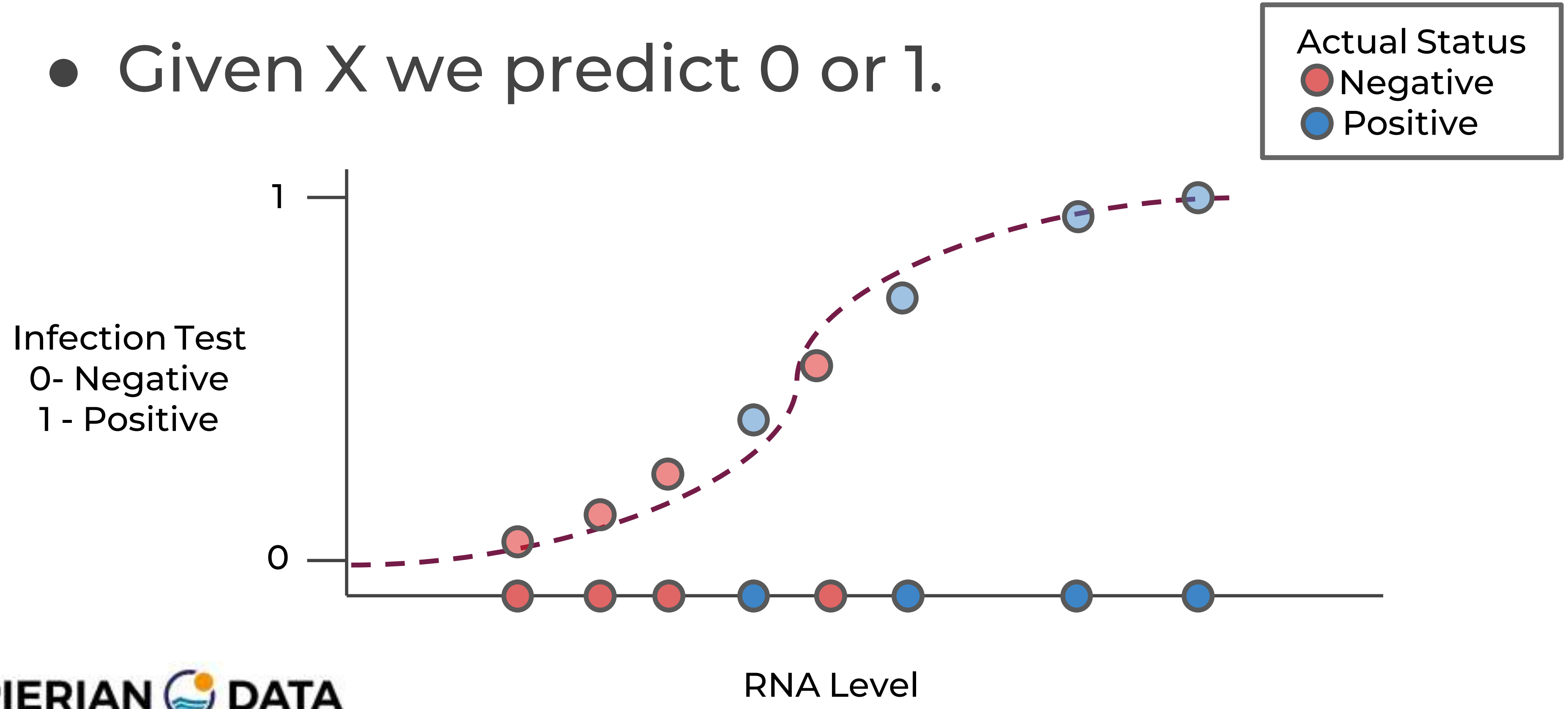
Classification Metrics

- Fit logistic regression model.



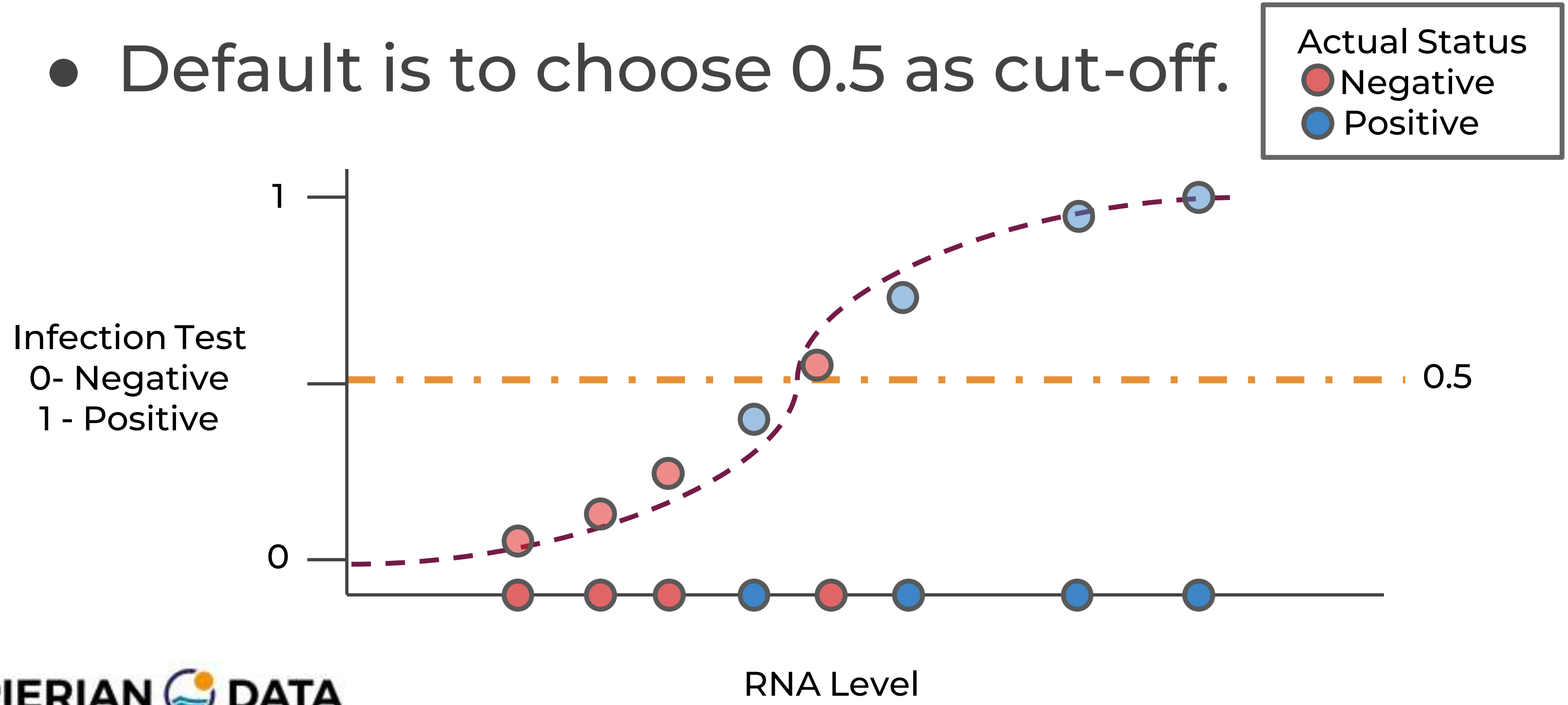
Classification Metrics

- Given X we predict 0 or 1.



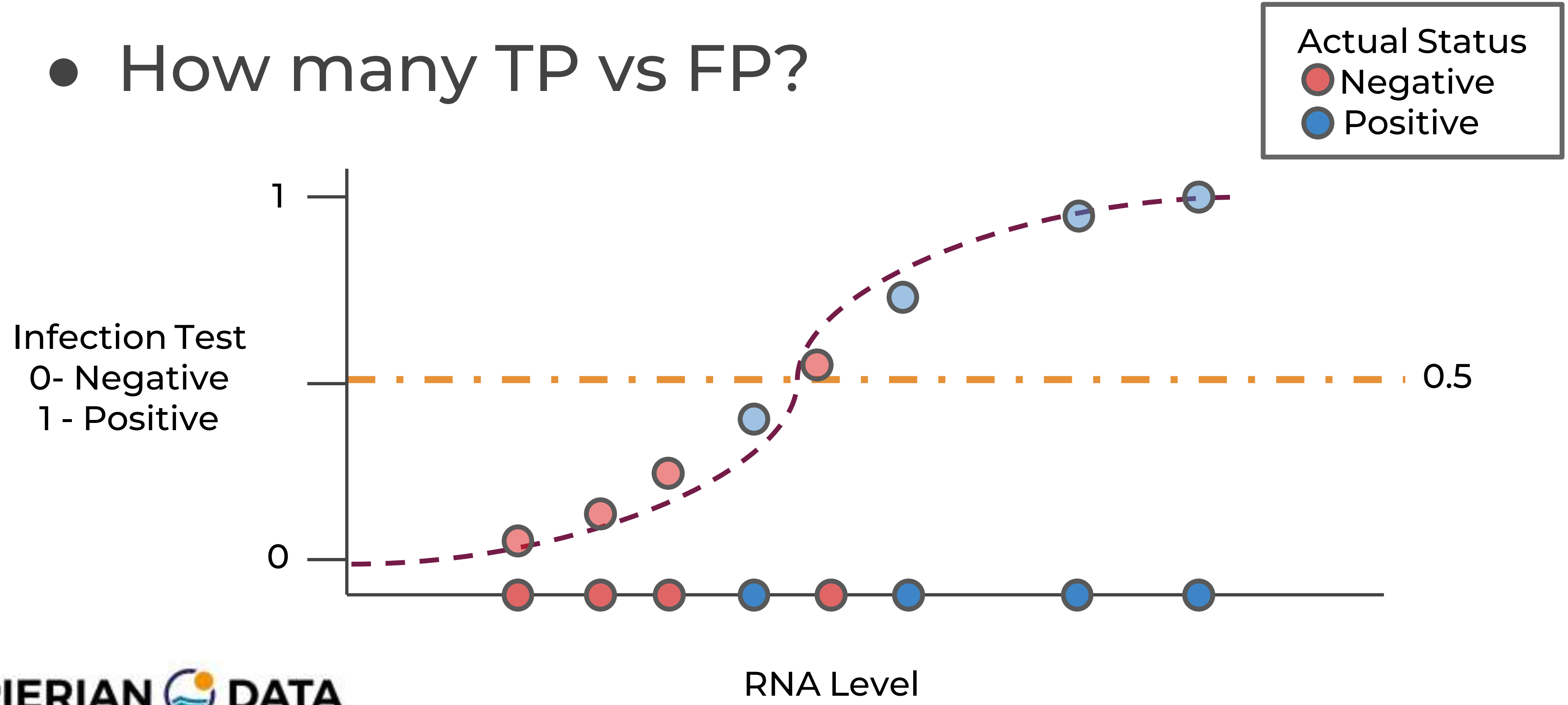
Classification Metrics

- Default is to choose 0.5 as cut-off.



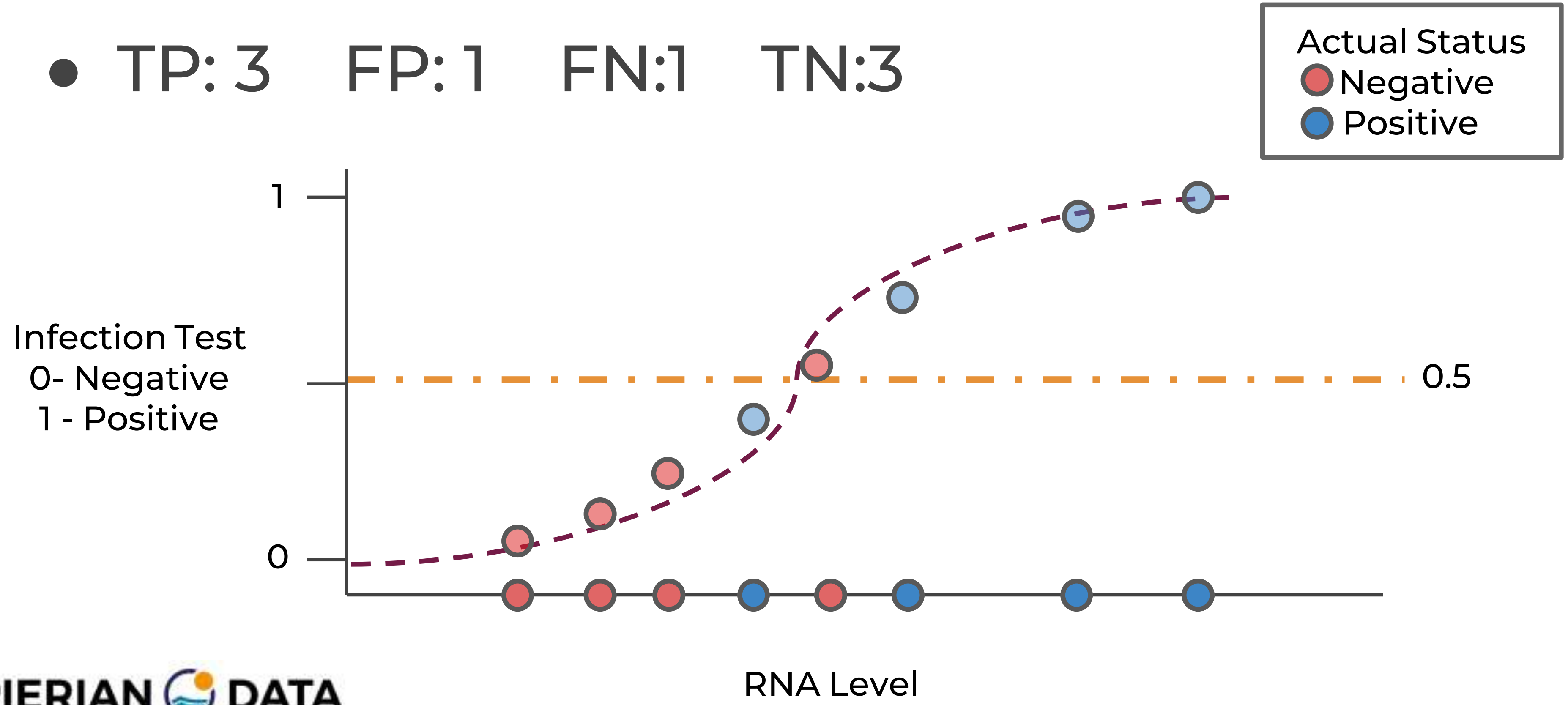
Classification Metrics

- How many TP vs FP?



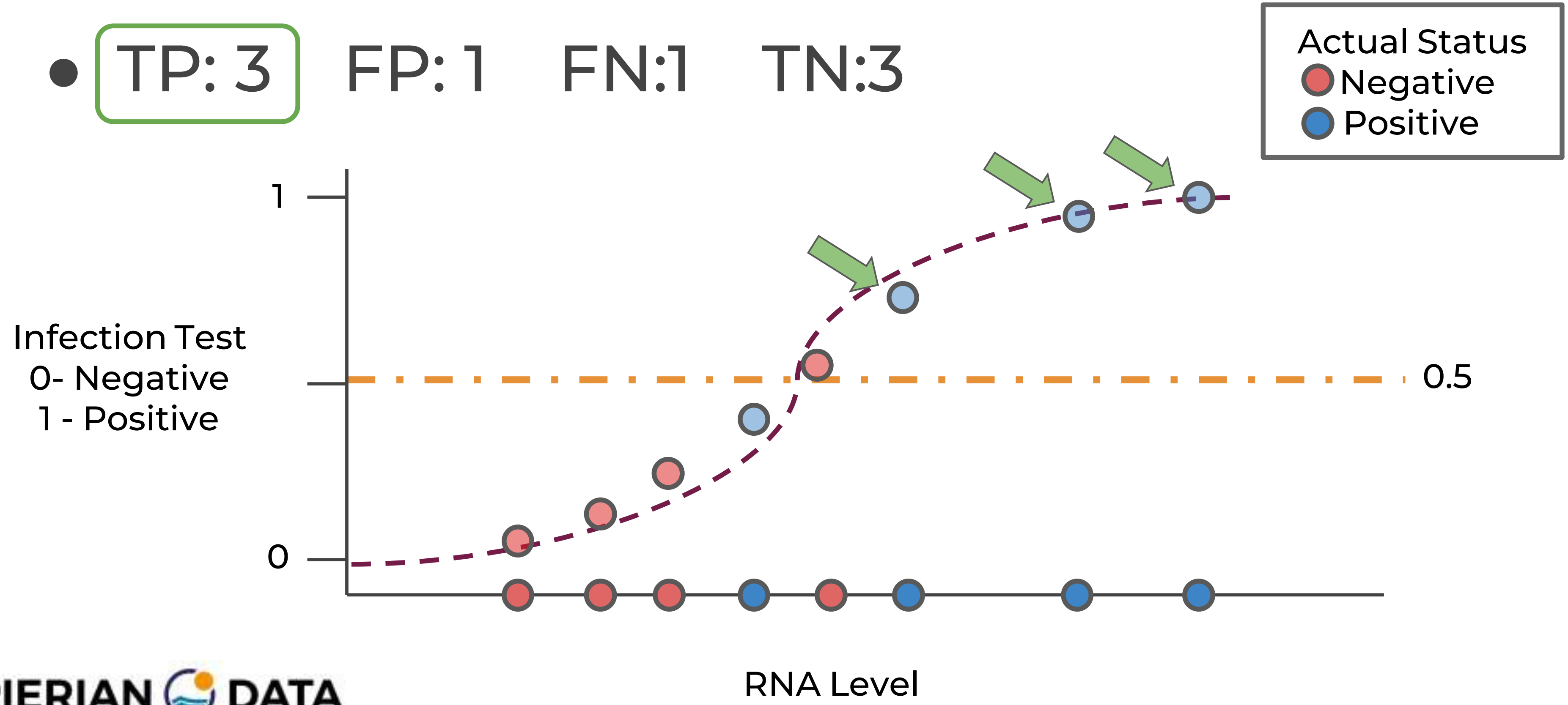
Classification Metrics

- TP: 3 FP: 1 FN:1 TN:3



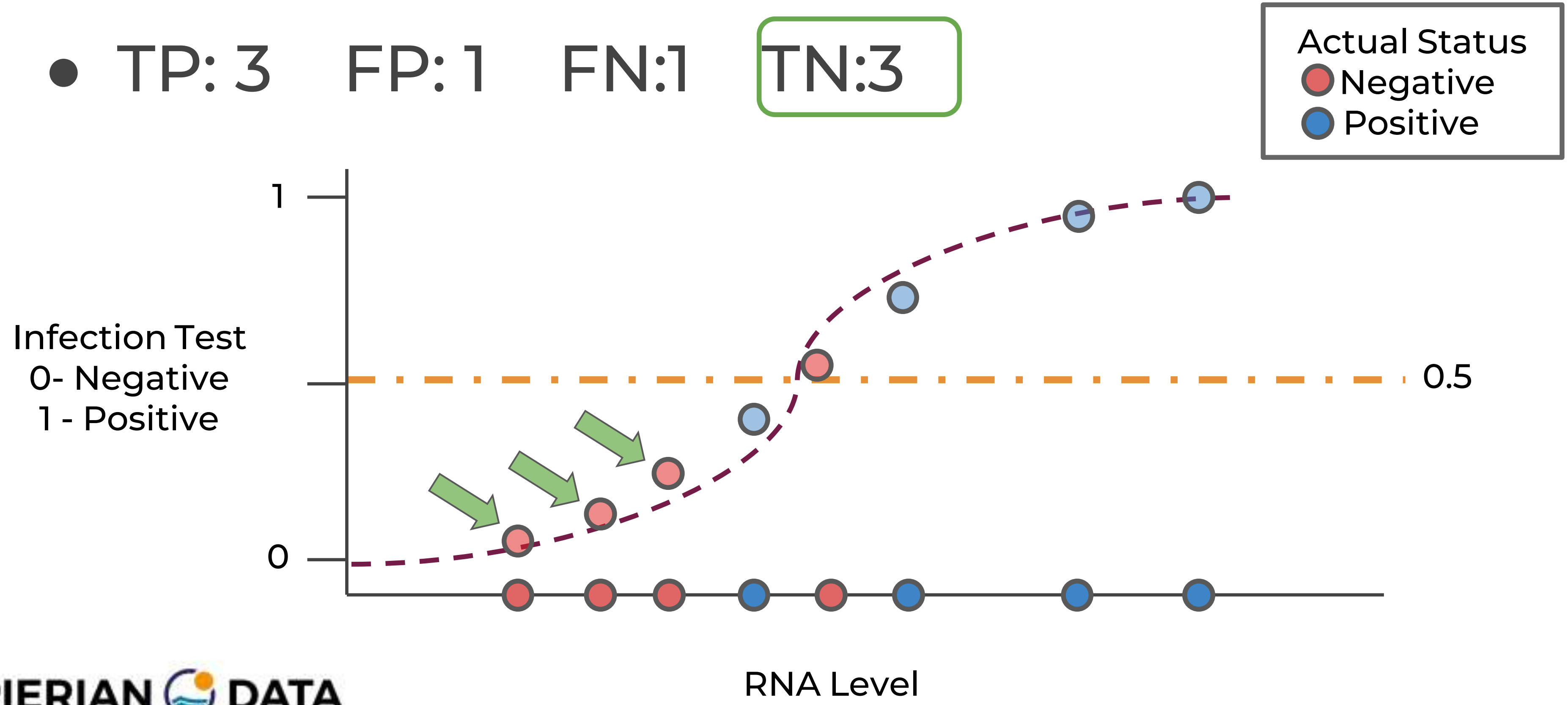
Classification Metrics

- TP: 3   FP: 1   FN:1   TN:3



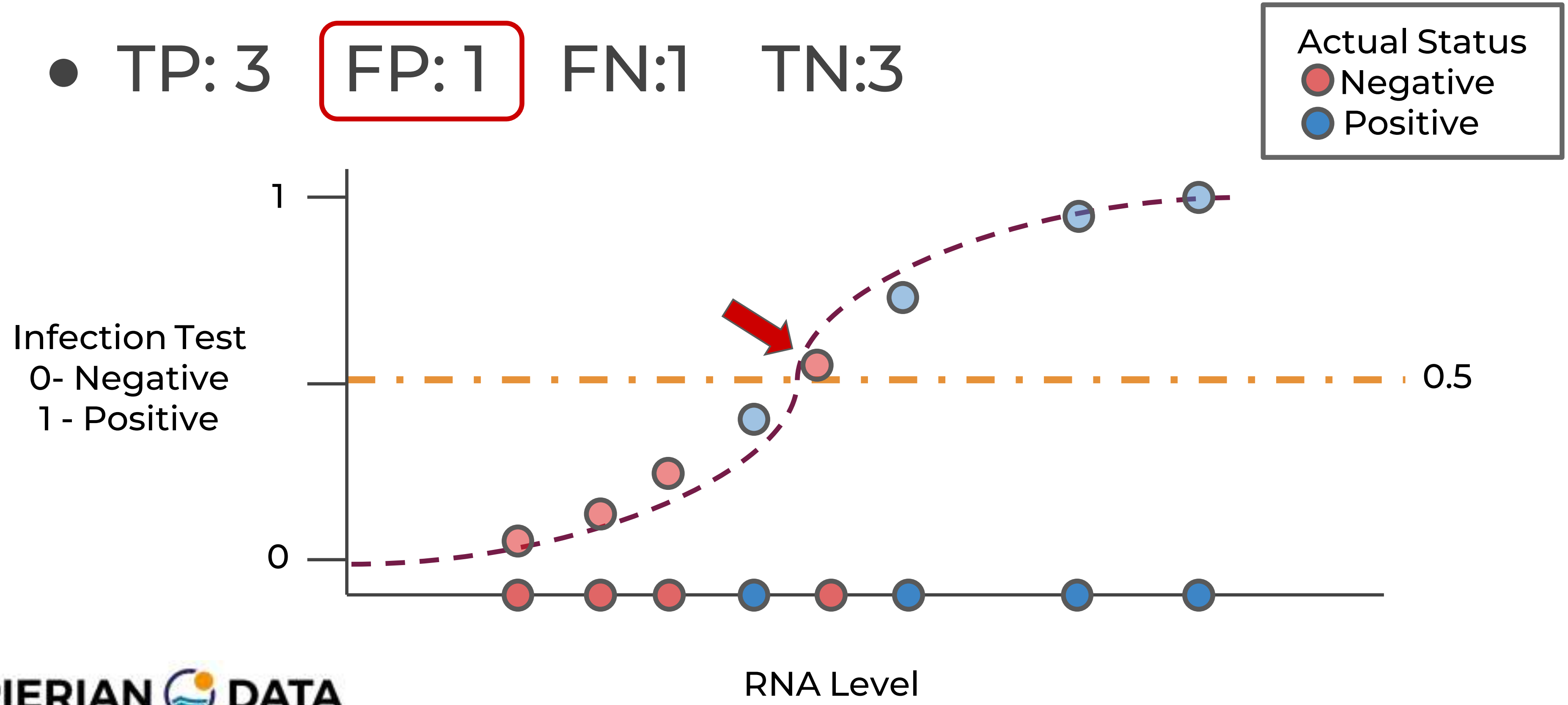
Classification Metrics

- TP: 3 FP: 1 FN:1 TN:3



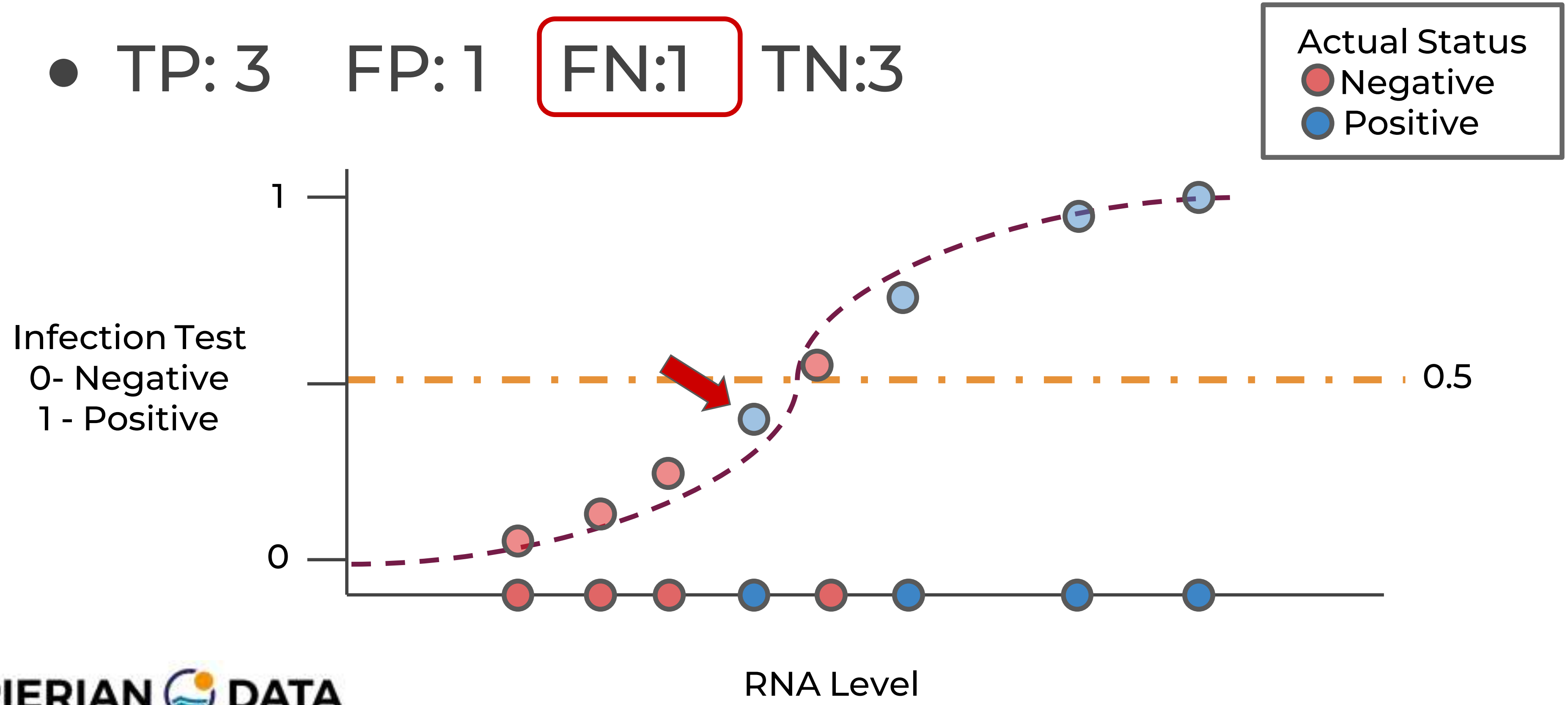
Classification Metrics

- TP: 3 $\boxed{\text{FP: 1}}$ FN:1 TN:3



Classification Metrics

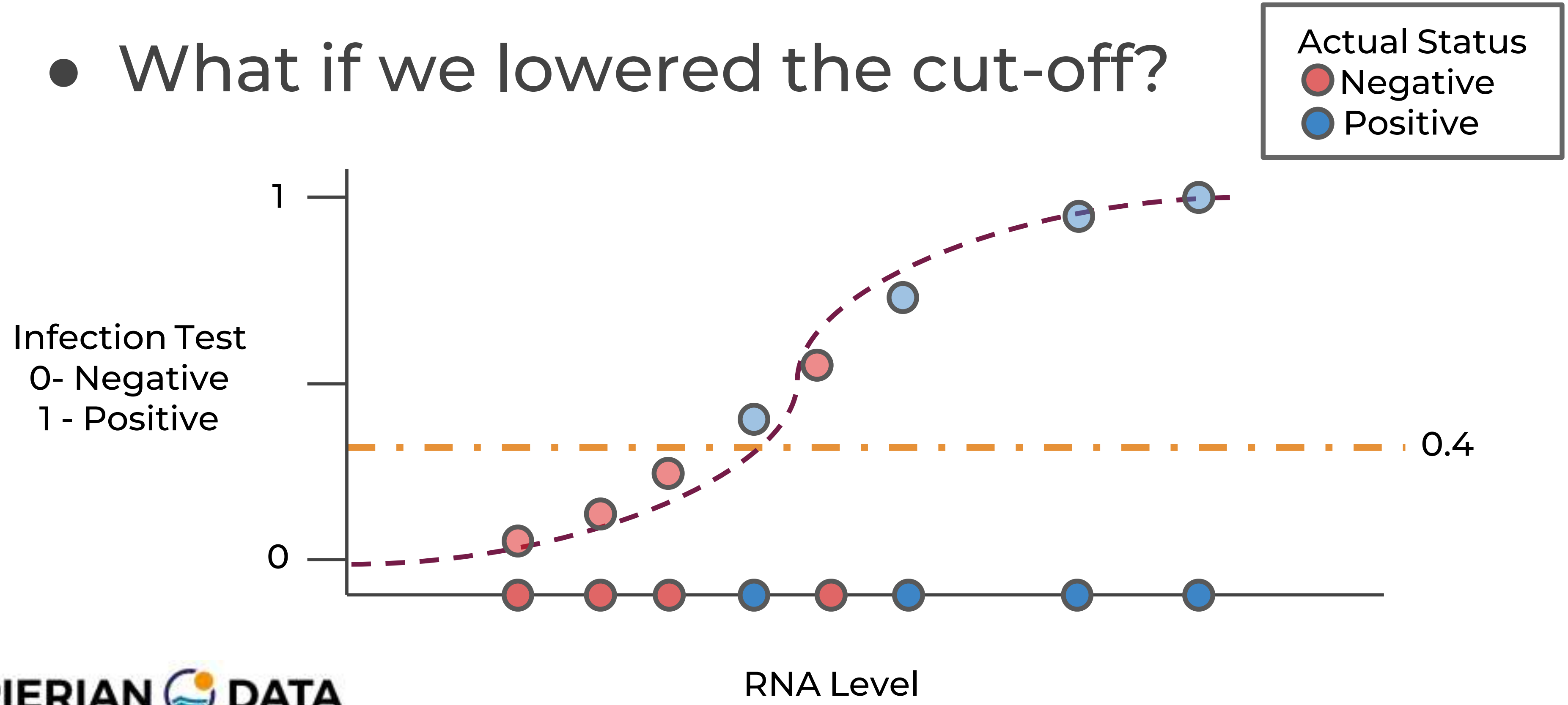
- TP: 3 FP: 1 FN:1 TN:3



PIERIAN DATA

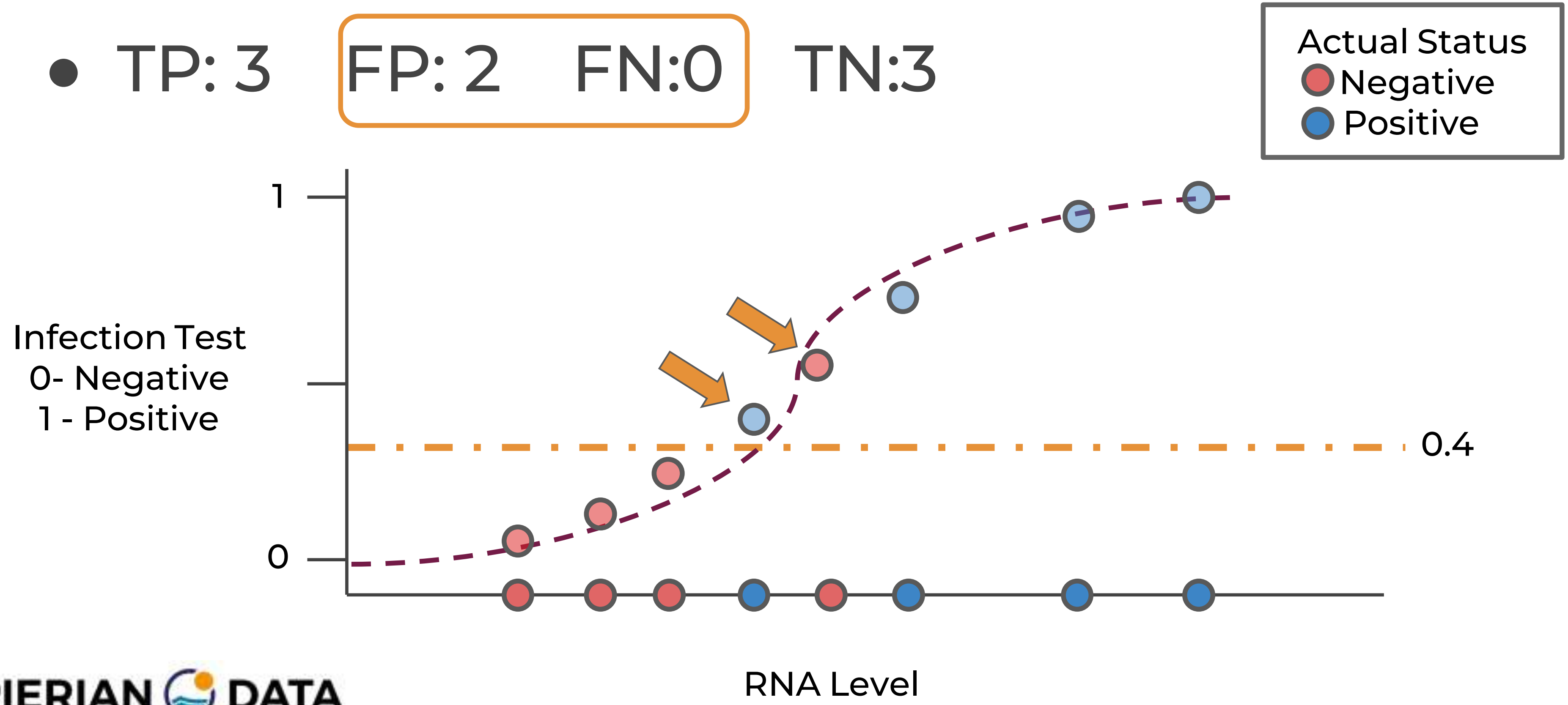
Classification Metrics

- What if we lowered the cut-off?



Classification Metrics

- TP: 3 FP: 2 FN:0 TN:3



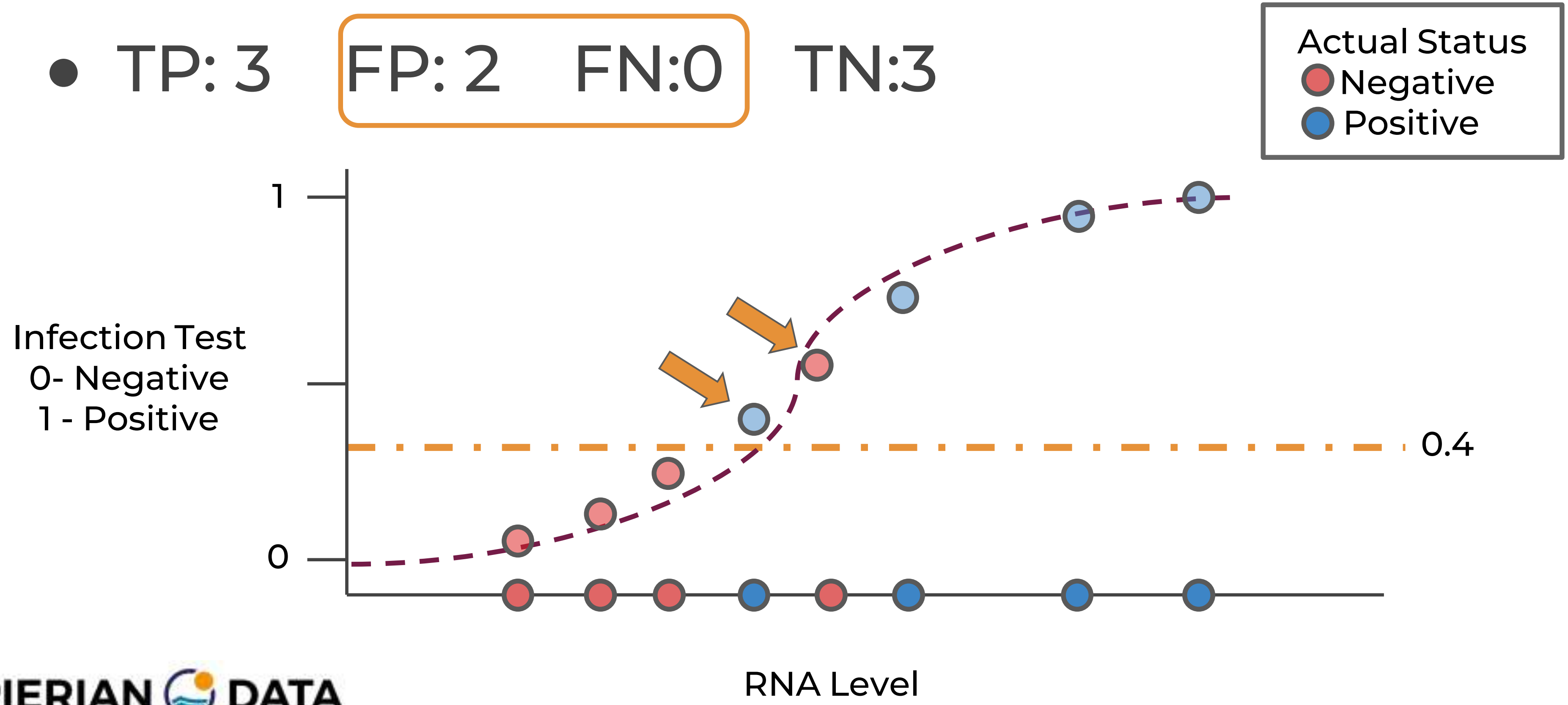
PIERIAN DATA

Classification Metrics

- 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!

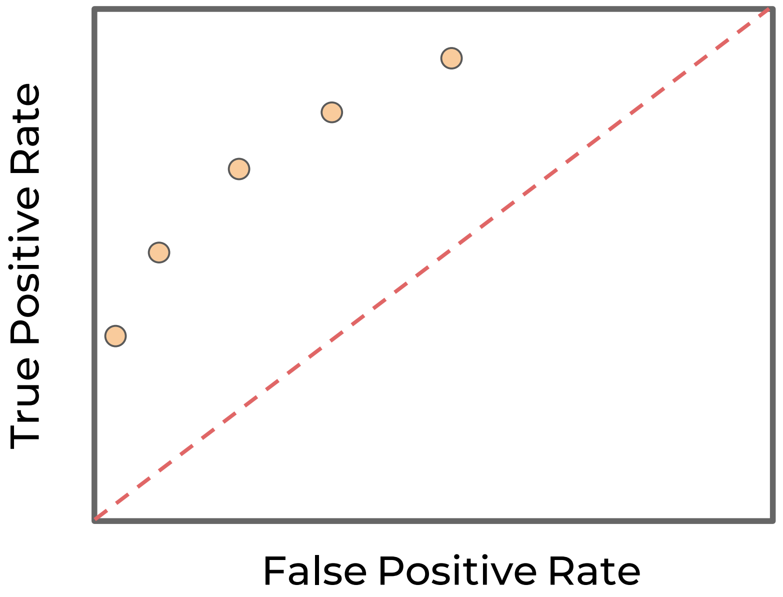
Classification Metrics

- TP: 3 FP: 2 FN:0 TN:3



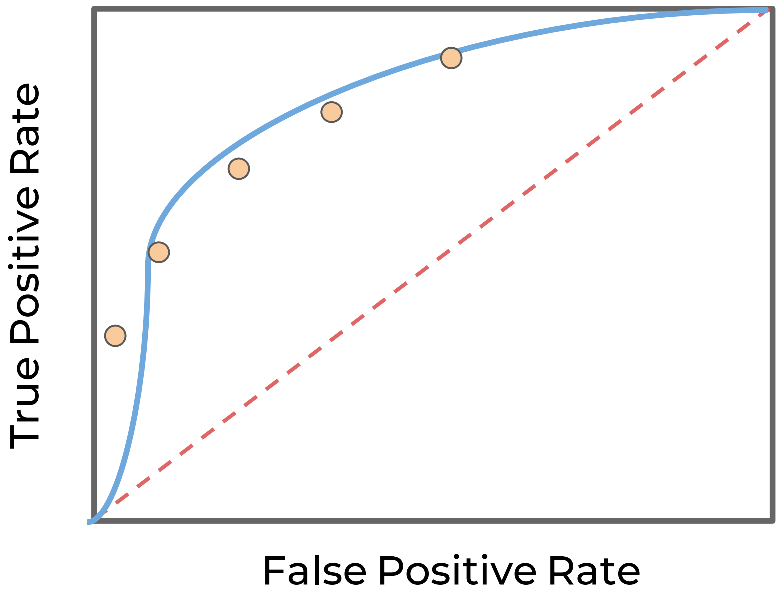
Classification Metrics

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



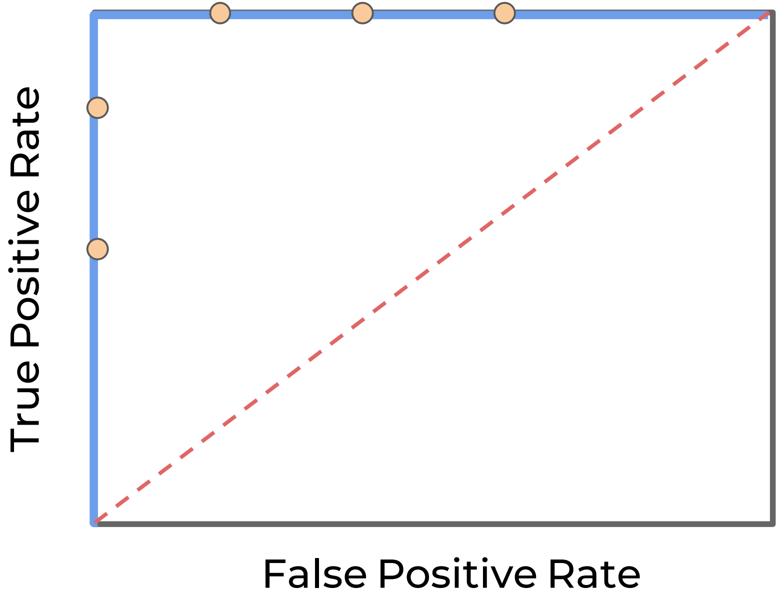
Classification Metrics

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



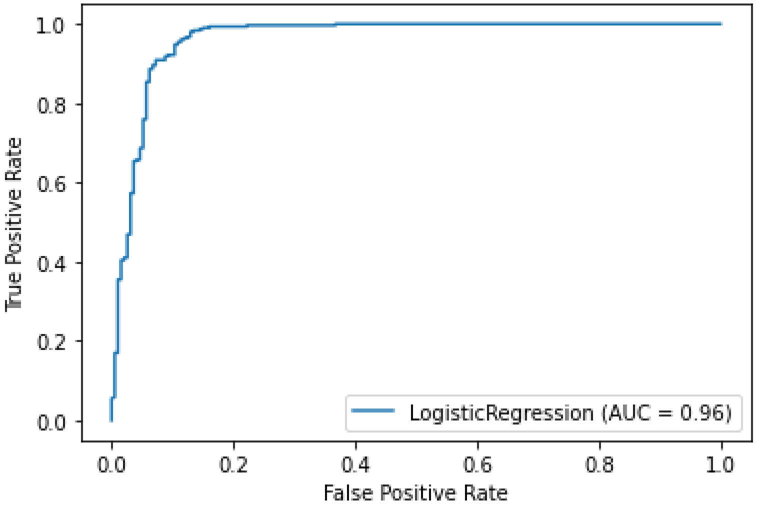
Classification Metrics

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



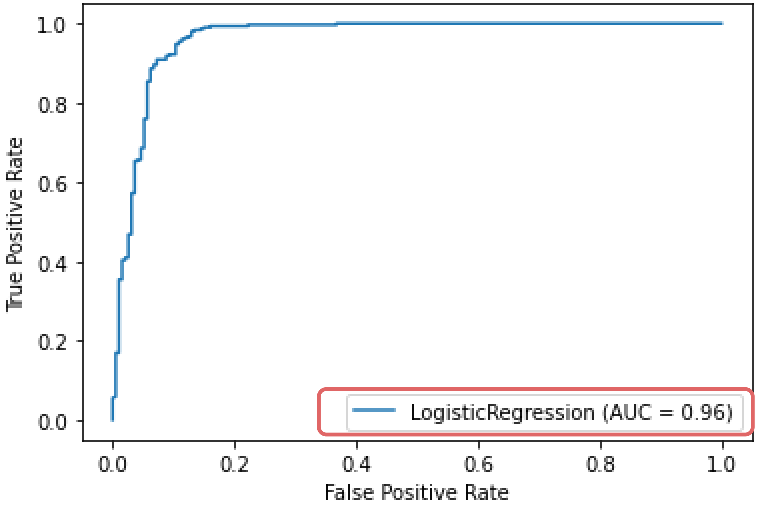
Classification Metrics

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



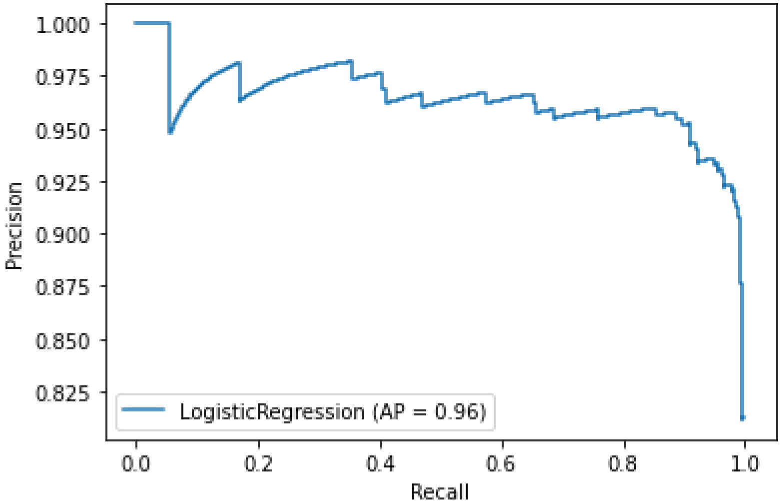
Classification Metrics

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



Classification Metrics

- Can also create precision vs. recall curves:



PIERIAN DATA

Logistic Regression with Scikit-Learn

Part Three: Performance Metrics

PIERIAN DATA

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

PIERIAN DATA