

Guillem & Roderic, Summer 2025



Mathematical Modeling

Dynamical Systems

Game Theory

Machine Learning

Supervised

Linear/Logistic Regression, SVMs, Neural Networks

Unsupervised

PCA, t-SNE, k-means, Neural Networks

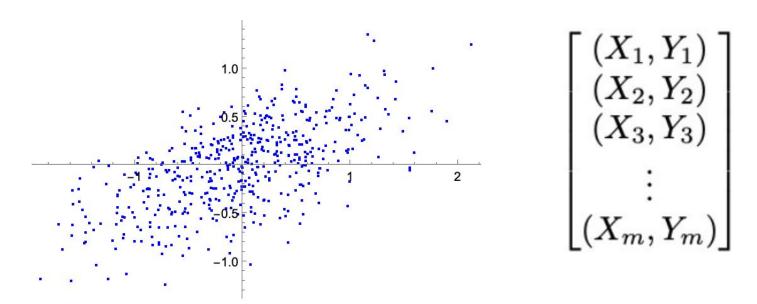
Learning Types

- Supervised:
 - Classification (logistic regression, Random Forests, SVM, NNs)
 - Regression (linear regression, Random Forests, NNs)
- Unsupervised:
 - Dimensionality Reduction (PCA, t-SNE, UMAP)
 - Clustering (k-means)
- Other:
 - Reinforcement Learning (Q-learning, PPO)
 - 0 ..

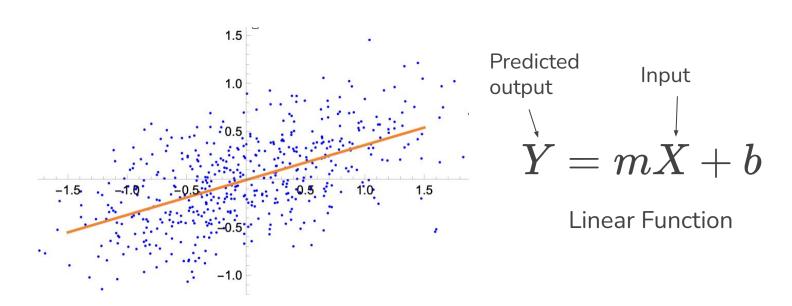
Data Types

- Numerical:
 - Price of a home
 - Quality of a Wine
- Categorical:
 - Edible and poisonous mushrooms
 - Survival in the Titanic
 - Iris Type
 - Handwritten digit

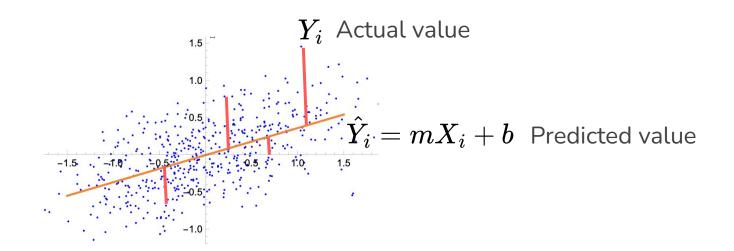
Suppose we have a dataset with two (numerical) variables:



How can we model the linear dependency of Y on X

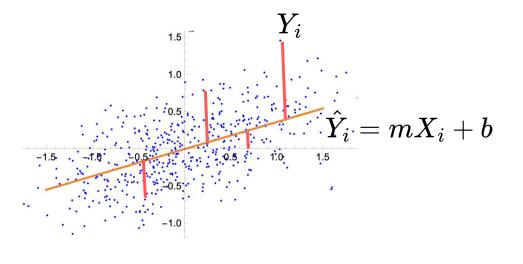


Minimize **residual sum of squares** (vertical distance): Y=mX+b



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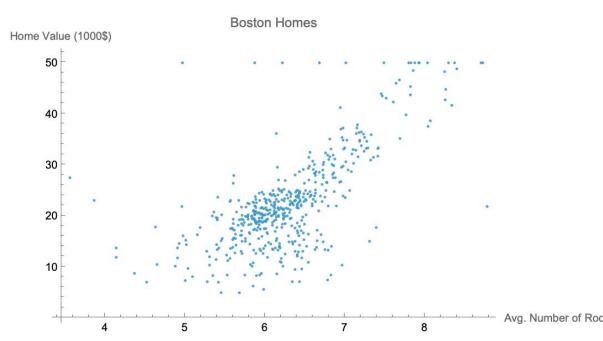
$$Y = mX + b$$



Goal: minimize the prediction error (residual sum of squares)

$$RSS = \sum_{i=1}^m \left(\hat{Y}_i - Y_i
ight)^2$$

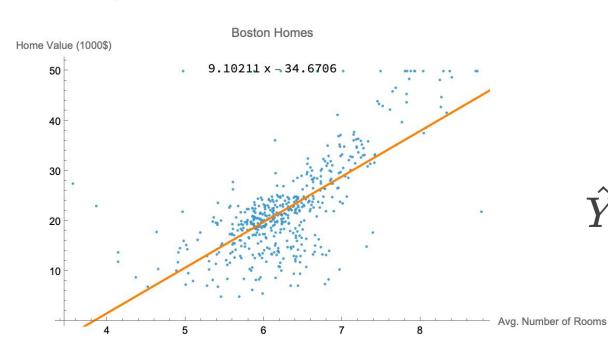




X = avg. number of rooms

Y = home value (1000\$)





X = avg. number of rooms

Y = home value (1000\$)

$$\hat{Y} = 9.1X - 34.67$$

What is the meaning of the slope 9.1 in the equation $\hat{Y}=9.1X-34.67$?



| Each additional room increases of price by 91 | .00\$ |
|---|-------|
|---|-------|

0%

On average, each additional room increase the price by 9100\$

0%

The price of a house with one room is 9100

0%



What is the meaning of the intercept -34.67 in the equation $\hat{Y}=9.1X-34.67$?



The expected price of a house with 0 rooms is -34670\$

0%

It has no real meaning

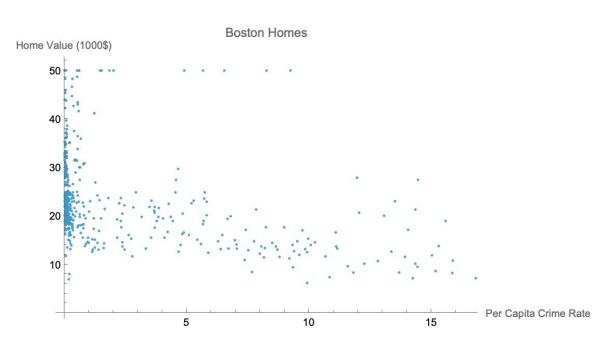
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If you reduce the number of rooms, the price decreases by -34670\$

0%





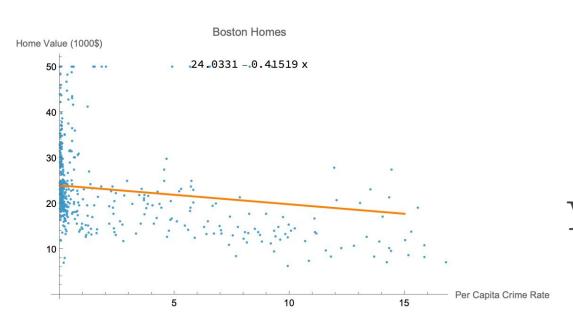


X = per capita crime rate

Y = home value (1000\$)



Example: Boston Homes



X = per capita crime rate

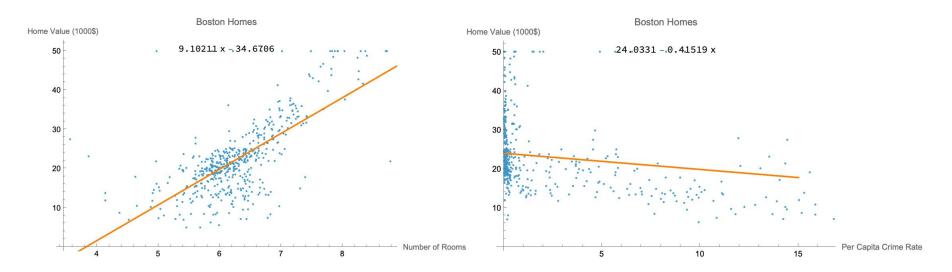
Y = home value (1000\$)

$$\hat{Y} = -0.42X + 24.03$$

Example: Boston Homes

RSS = 148.532

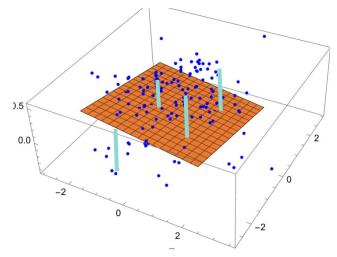
RSS = 190.461



Multidimensional Linear Regression

Suppose we have two (or more) predictor variables

Stil minimize residual sum of squares (vertical distances)



$$Y = m_1 X_1 + m_2 X_2 + b$$

If I use two predictors (crime rate and number of rooms) the RSS, when compared to the individual RSSs, will

Increase

Decrease

It depends on the data



If I use two predictors (crime rate and number of rooms) the RSS, when compared to the individual RSSs, will

Decrease

O%

It depends on the data

O%



If I use two predictors (crime rate and number of rooms) the RSS, when compared to the individual RSSs, will

Decrease

O%

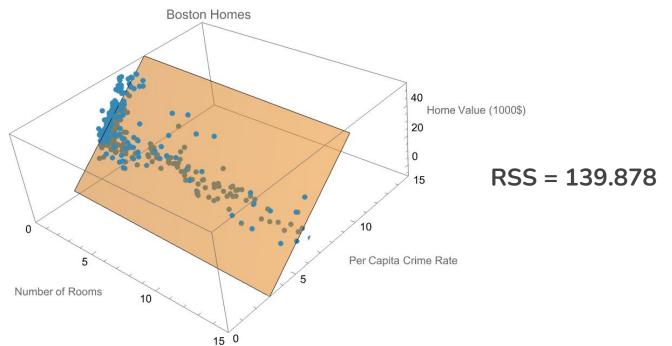
It depends on the data

O%



Example: Boston Homes

$$\hat{Y} = -29.24 - 0.26X_1 + 8.39X_2$$



Example: Boston Homes

$$\hat{Y} = 9.1X_1 - 34.67$$

$$RSS = 190.461$$

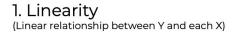
$$\hat{Y} = -0.42X_2 + 24.03$$

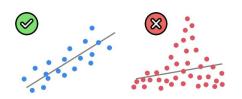
Rooms + Crime
$$RSS = 139.878$$

$$\hat{Y} = -29.24 - 0.26 X_2 + 8.39 X_1$$

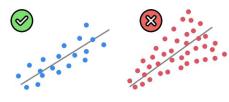
Linear Regression: When to Use?

When both the predictor and output are **numerical variables**, and:

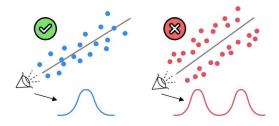




2. Homoscedasticity (Equal variance)



3. Multivariate Normality (Normality of error distribution)

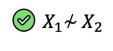


4. Independence (of observations. Includes "no autocorrelation")

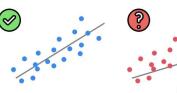


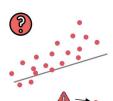
5. Lack of Multicollinearity (Predictors are not correlated with each other)

 $\boxtimes X_1 \sim X_2$



6. The Outlier Check (This is not an assumption, but an "extra")



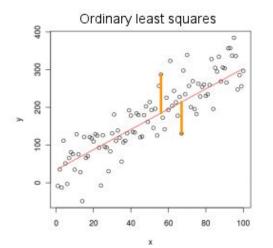


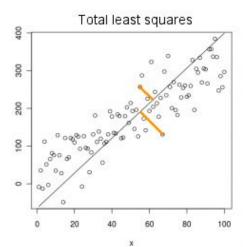
(From SuperDataScience)

Linear Regression vs PCA

Linear Regression: using X as a predictor, what is the equation that best describes Y

PCA: What linear combination of X and Y (direction/component) is the best predictor of our data?

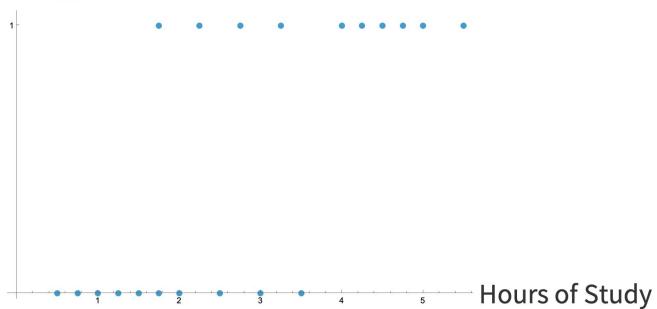




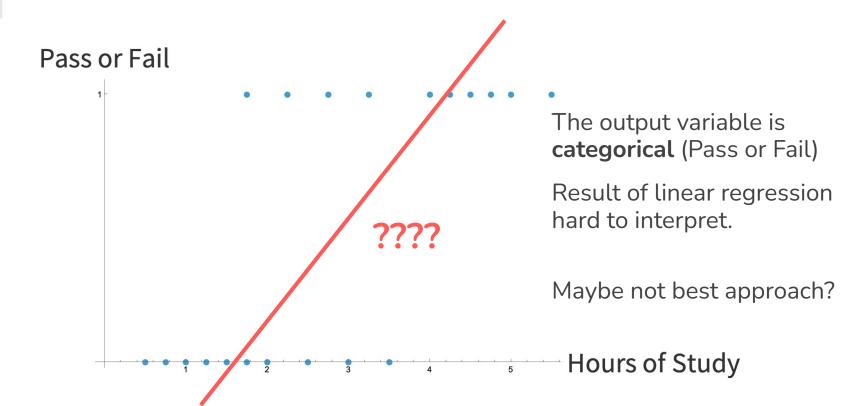
Logistic Regression

Example: Pass/Fail





Example: Pass/Fail



Logistic Regression: Main Idea

Instead of modeling the categorical variable (Pass=1, Fail=0), we model the **probability** of each class:

The probability of passing given you study X hours is $P\left(1\mid X\right)$

Logistic Regression: The Logit

Probability: P in (0,1)

Odds:
$$\frac{P}{1-P}$$
 in $(0,\infty)$

Logit (Log Odds):
$$logit(P) = log\left(\frac{P}{1-P}\right)$$
 in $(-\infty, \infty)$

Logit Regression: logit(P) = mX + b

Solving for P we get the **Sigmoid Function** $P = \frac{1}{1 + e^{-mX - b}}$

If P(1)=0.75, what are the $\mathrm{Odds}(1)$?

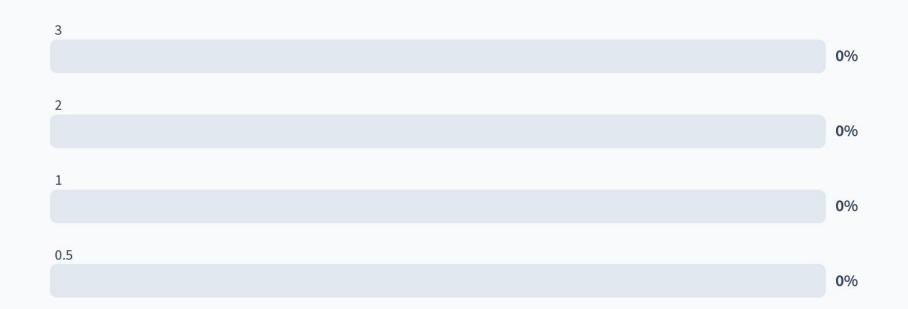
3

1

0.5

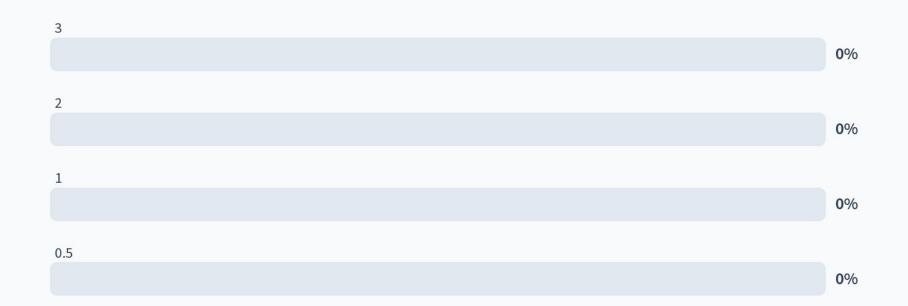


If P(1)=0.75, what are the $\mathrm{Odds}(1)$?





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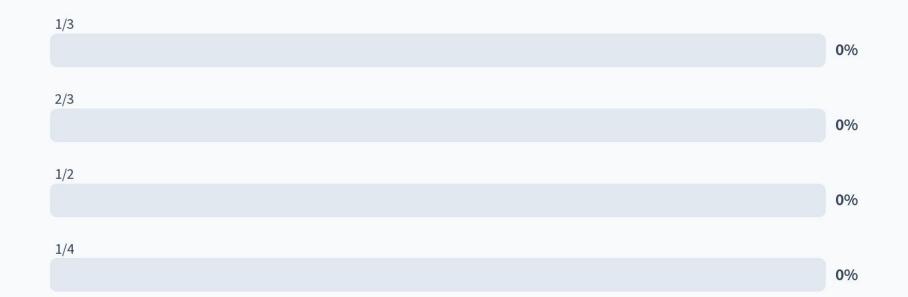


If $\mathrm{Odds}(1)=2$, what is P(1) ?



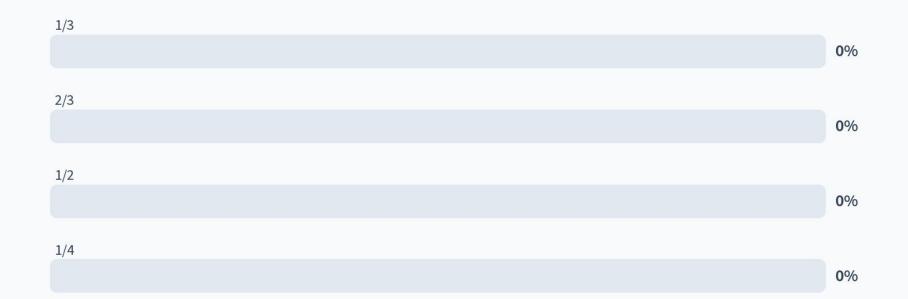


If $\mathrm{Odds}(1)=2$, what is P(1) ?





If $\mathrm{Odds}(1)=2$, what is P(1) ?





Logistic Regression

The predicted P(Y) value is interpreted as the probability that, given x, the categorical variable Y belongs to a class 1.

$$\hat{P}\left(Y=1\mid x
ight)=rac{1}{1+e^{-(mx+b)}}$$

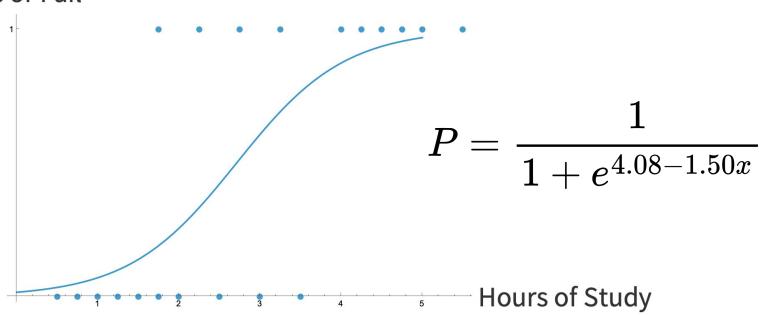
Goal: minimize the Log Loss
$$-\sum_{k=1}^n \left[Y_k \ln \left(\hat{P}_k \right) + (1-Y_k) \ln \left(1-\hat{P}_k \right) \right]$$

Logistic Regression: The Quantities

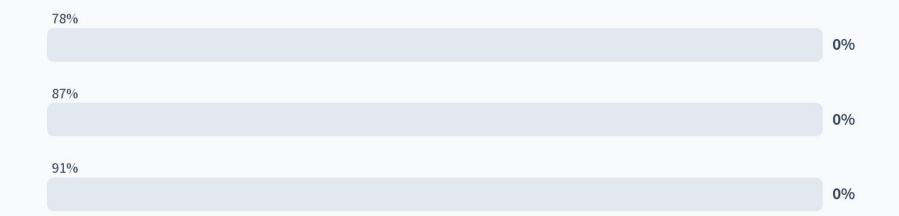
| Logit, Odds, And Probability Table | | | | |
|------------------------------------|-----------------|--------------------|--------------------------|--|
| | Probability (p) | Odds (p / (1 - p)) | Logit (log(p / (1 - p))) | |
| 1 | 0.01 | 0.0101 | -4.5951 | |
| 2 | 0.1 | 0.1111 | -2.1972 | |
| 3 | 0.25 | 0.3333 | -1.0986 | |
| 4 | 0.5 | 1.0 | 0.0 | |
| 5 | 0.75 | 3.0 | 1.0986 | |
| 6 | 0.9 | 9.0 | 2.1972 | |
| 7 | 0.99 | 99.0 | 4.5951 | |

Example: Pass/Fail



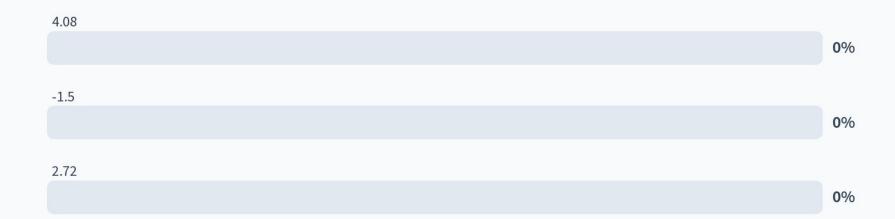


Consider the logistic model $\frac{1}{1+e^{4.08-1.5x}}$. If you study 4 hours, what is your probability of passing?



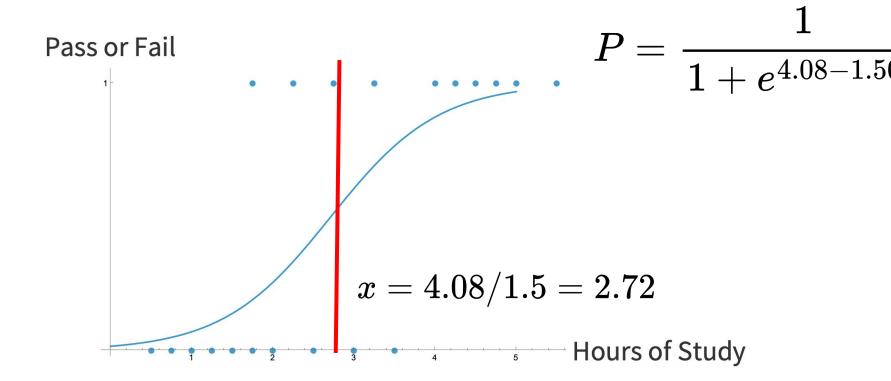


Consider the logistic model $\frac{1}{1+e^{4.08-1.5x}}$. The number of hours you should study so that the probability of passing is greater than the probability of failing is:

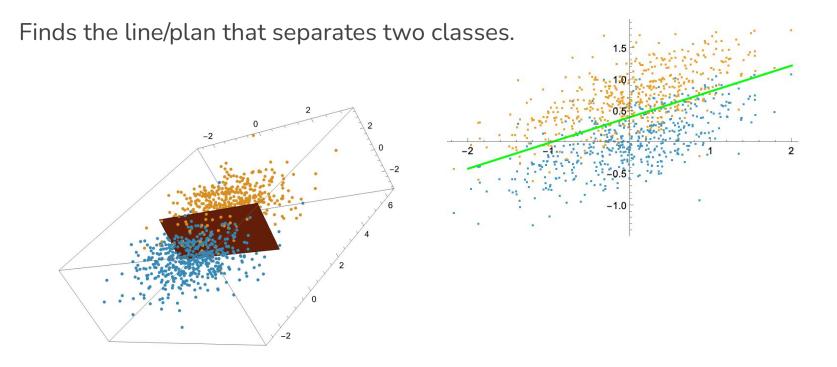




Example: Pass/Fail



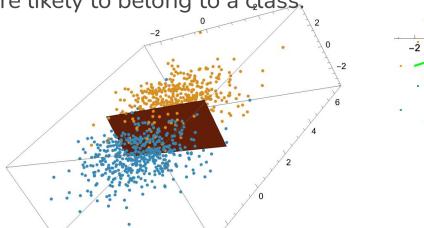
Logistic Regression: Visually

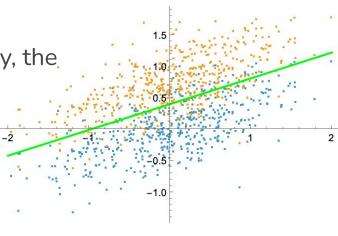


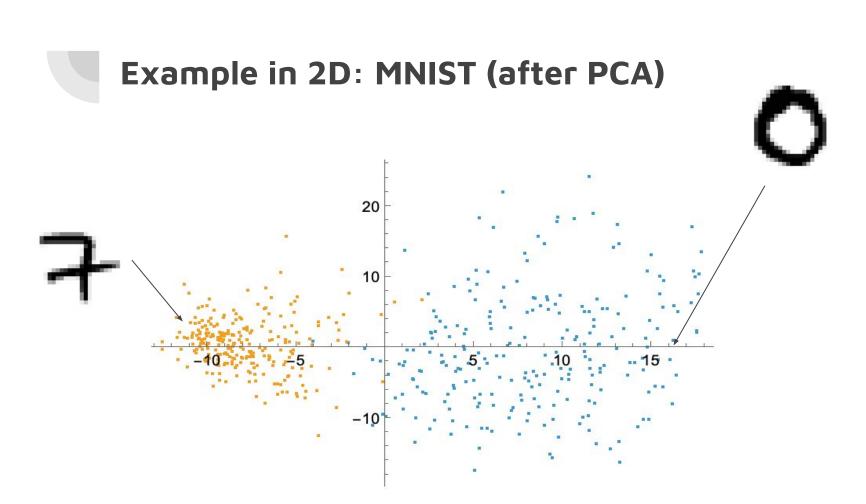
Logistic Regression: Visually

Tells us the likelihood of a point belonging to a class.

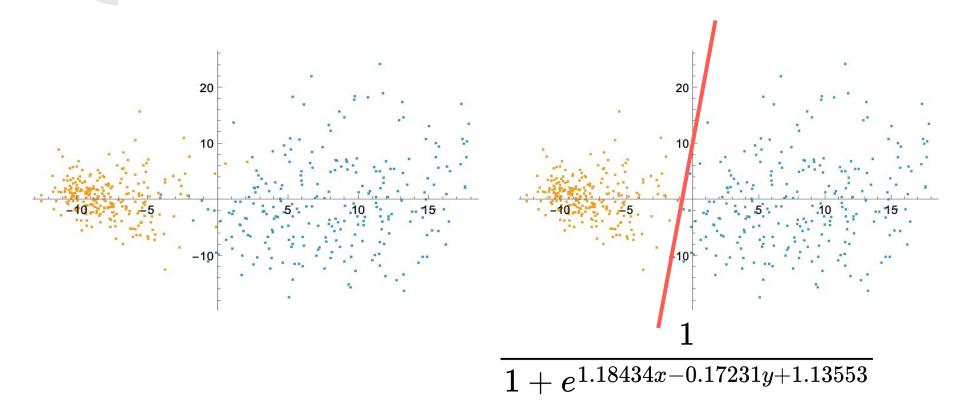
The farther the point is from the boundary, the more likely to belong to a class.







Example in 2D: MNIST (after PCA)



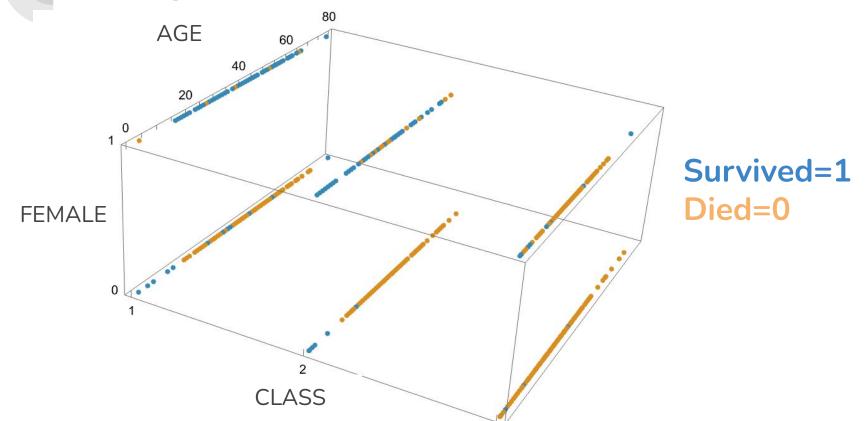
Example in 3D: The Titanic

"Classify whether a passenger on board the maiden voyage of the Titanic in 1912 survived given their age, sex and class."

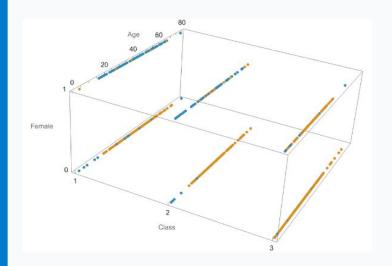


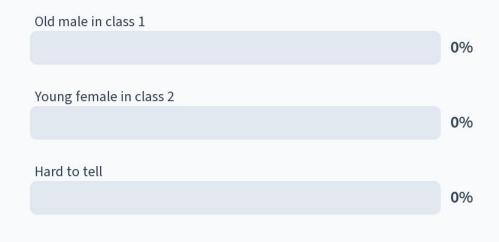
| Class | Age | Sex | SurvivalStatus |
|-------|---------|--------|----------------|
| 3rd | 12. yr | male | survived |
| 3rd | 29. yr | male | died |
| 2nd | 28. yr | female | survived |
| 1st | 16. yr | female | survived |
| 3rd | _ | male | died |
| 3rd | 20. yr | male | died |
| 3rd | 43. yr | male | died |
| 3rd | 18. yr | male | died |
| 3rd | 28.5 yr | male | died |
| 1st | _ | male | died |





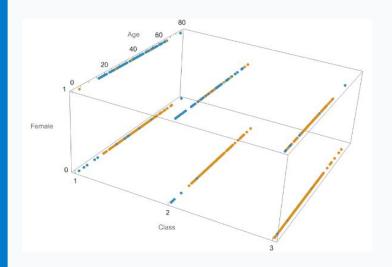
What has higher probability of surviving?

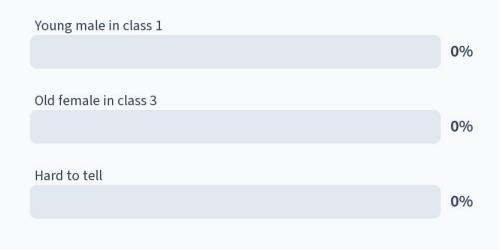






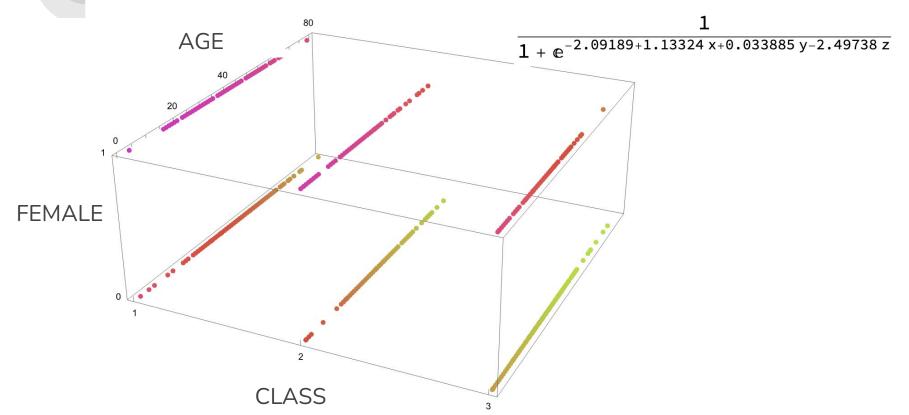
What has higher probability of surviving?



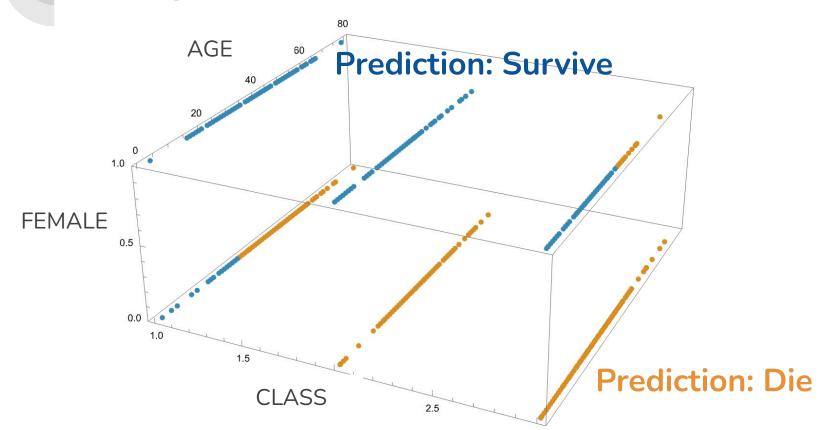








Example in 3D: The Titanic



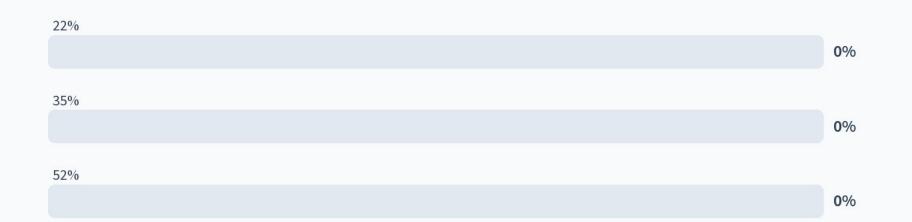
Given this logistic model $\frac{1}{1+e^{-2+x+0.05y-2.5z}}$, where x is class, y is age and z is gender, what is the probability that a 33 year old man in class 2 survived?





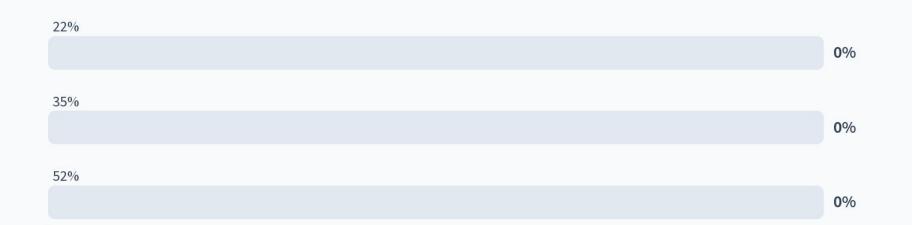
52%

Given this logistic model $\frac{1}{1+e^{-2+x+0.05y-2.5z}}$, where x is class, y is age and z is gender, what is the probability that a 33 year old man in class 2 survived?





Given this logistic model $\frac{1}{1+e^{-2+x+0.05y-2.5z}}$, where x is class, y is age and z is gender, what is the probability that a 33 year old man in class 2 survived?





Linear vs Logistic Regression Summary

Linear Regression:

- Purpose:
 - Establish potential relationships between input/output variables
 - Make predictions for newly observed data
 - Best for
 - i. Numerical predictor
 - ii. Numerical output

Logistic Regression:

- Purpose:
 - Estimate the probability that an input belongs to a particular class
 - Classify new data points based on a threshold
 - Best for
 - i. Numerical Predictor
 - i. Categorical Output