Machine Learning from Scratch

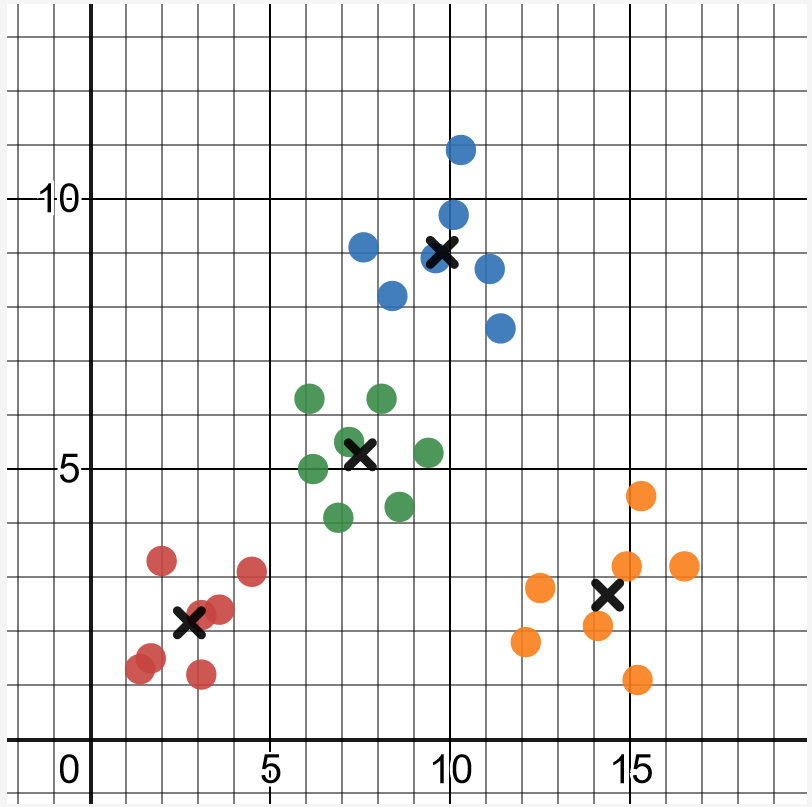
Hacking ML without Libraries

Section I
Overview

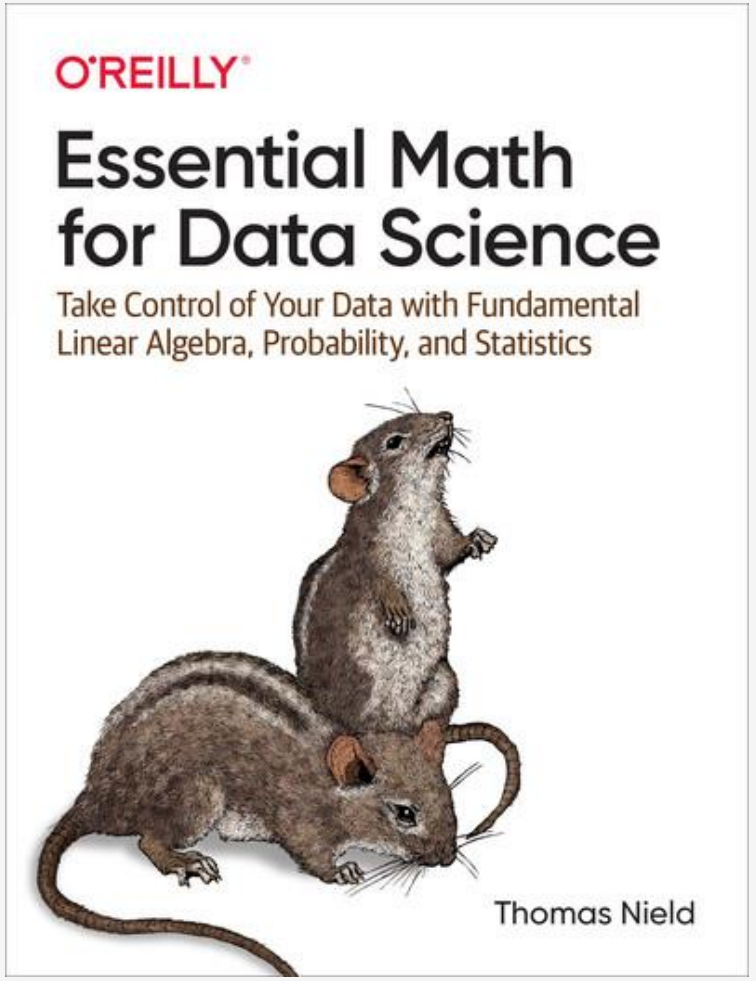
Agenda

Here is what we will do for the next 4 hours:

1. **Introduction** and what to expect
2. **Linear Regression** and **K-Means Clustering**
3. Text classification with **Naive Bayes**
4. Binary classification with **Logistic Regression**
5. **Decision trees** and **Random Forests**
6. Brief Introduction to **Neural Networks**



Supplemental Material



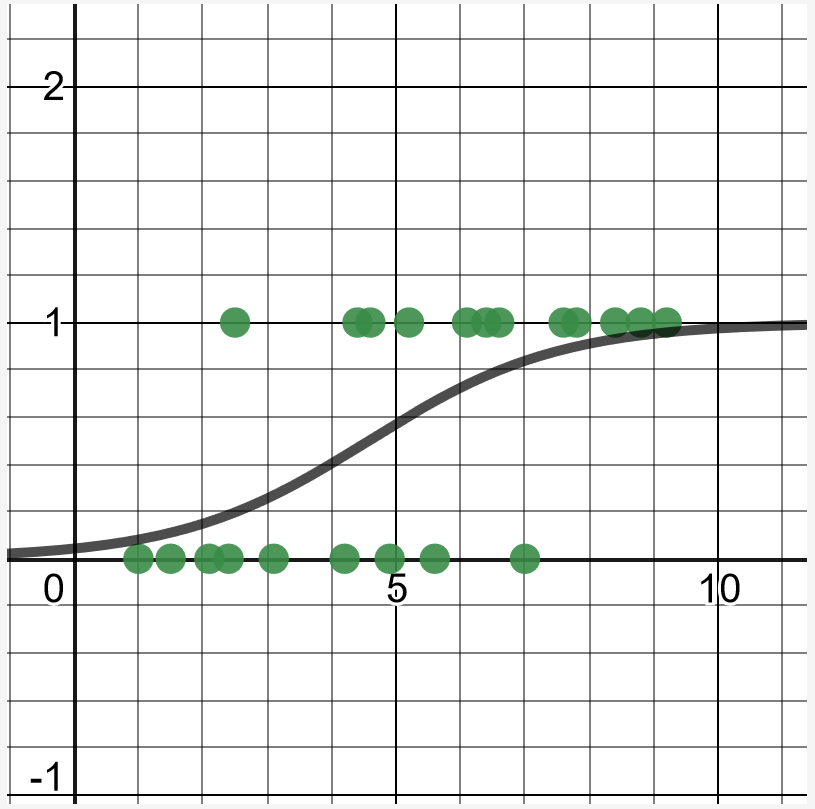
What to Expect

How to build machine learning algorithms from scratch to develop intuition and understanding.

Remove some unnecessary barriers to get started with machine learning:

- No calculus or partial derivatives
- Little to no linear algebra
- All Python code

While we may take some unconventional approaches, we will be doing actual machine learning.

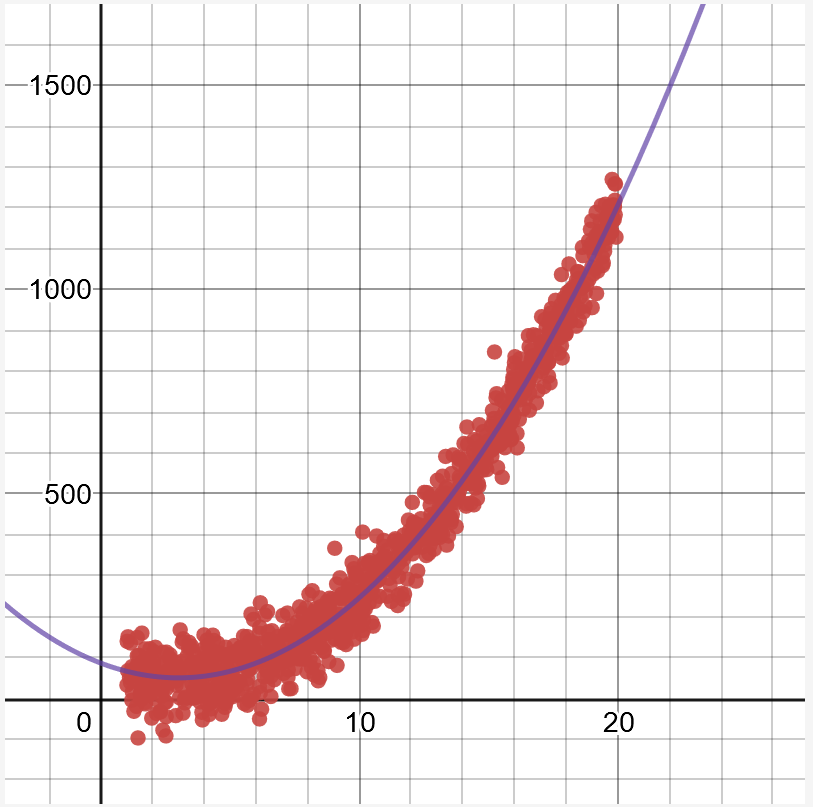


What Not to Expect

We will not be building state-of-the-art machine learning algorithms especially in regards to performance.

- We will primarily be using vanilla Python to build these algorithms, which has a high performance cost.
- Linear algebra libraries like NumPy can be used to gain efficiencies, and I will strive to include these alternate implementations in the code files.

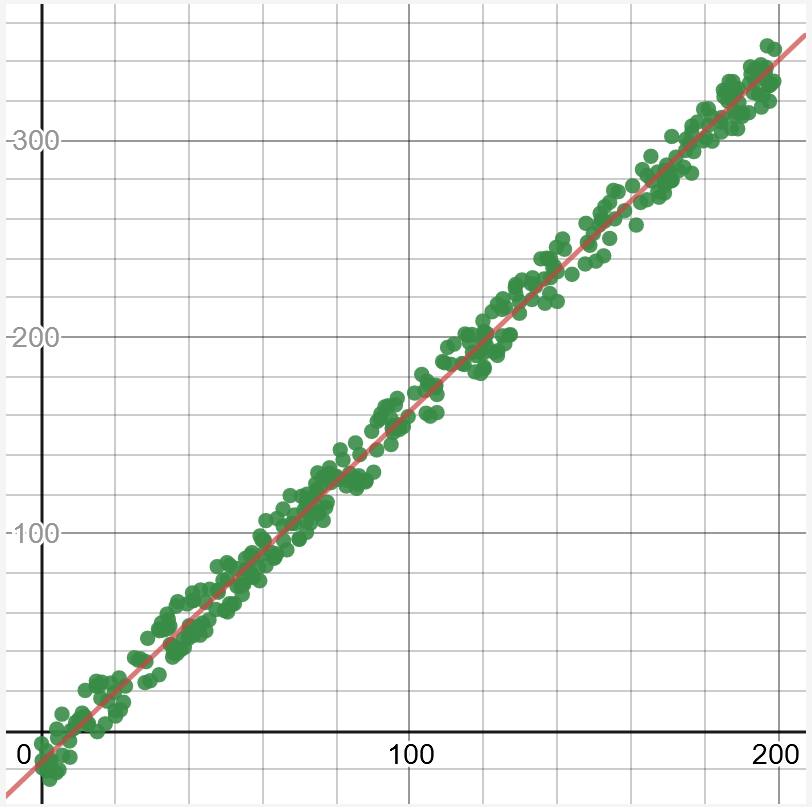
We will not be validating and analyzing our machine learning models formally, and instead focus on building the ML algorithms.



What Not to Expect

For model fitting we will not be using conventional methods like gradient descent and calculus.

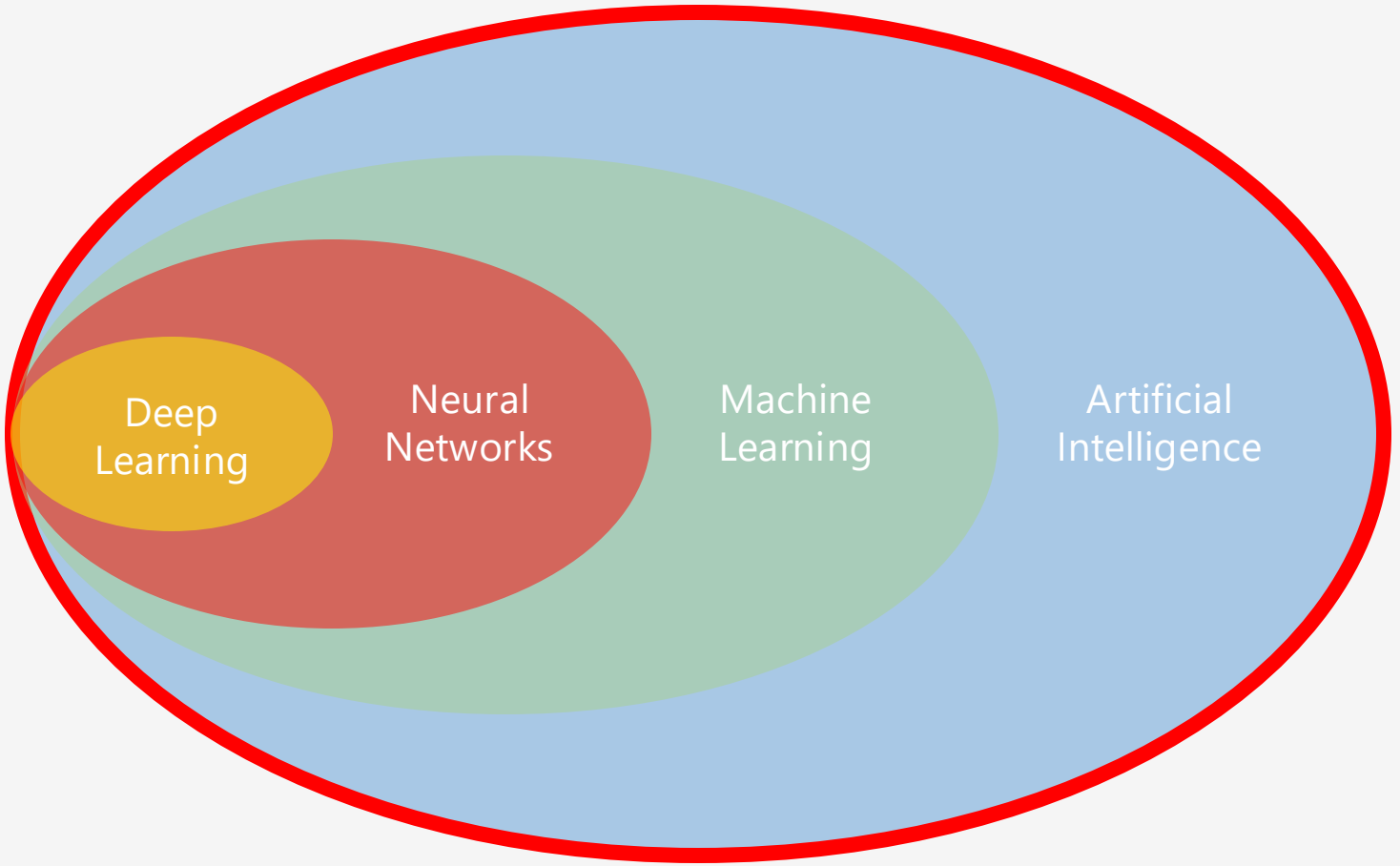
- Instead we will use simple hill-climbing algorithms.
- Optimization is optimization regardless if it is hill-climbing, simulated annealing, genetic algorithms, or gradient descent.
- Hill climbing is the simplest optimization algorithm to implement, and works remarkably well for basic machine learning.



Deep Learning vs *Neural Networks* vs *Machine Learning* vs *AI*

Artificial intelligence is a broad buzzword that can market any algorithm as "intelligent" including but not limited to…

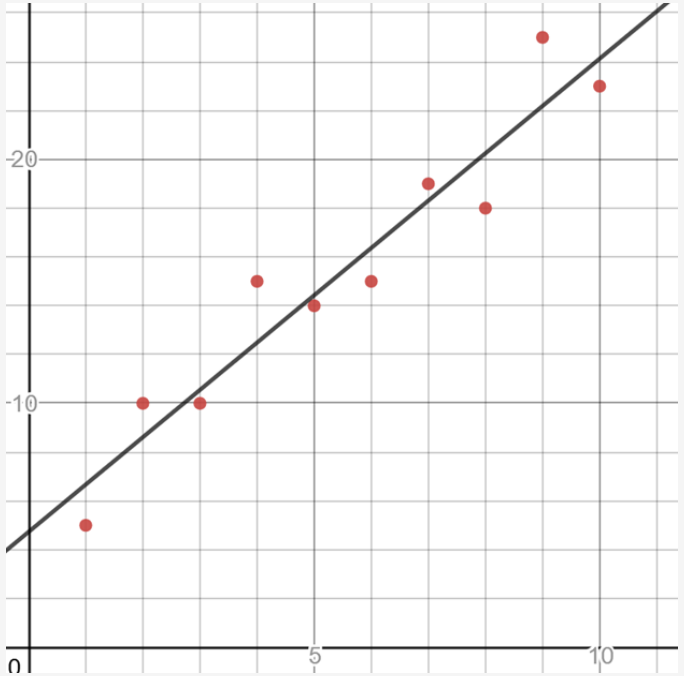
- Search algorithms
- Optimization algorithms
- Simple rule-based algorithms
- Monte Carlo simulations
- Machine learning



Artificial Intelligence Examples

Metaheuristics (e.g. Traveling Salesman Problem)

Linear programming (e.g. scheduling problems)

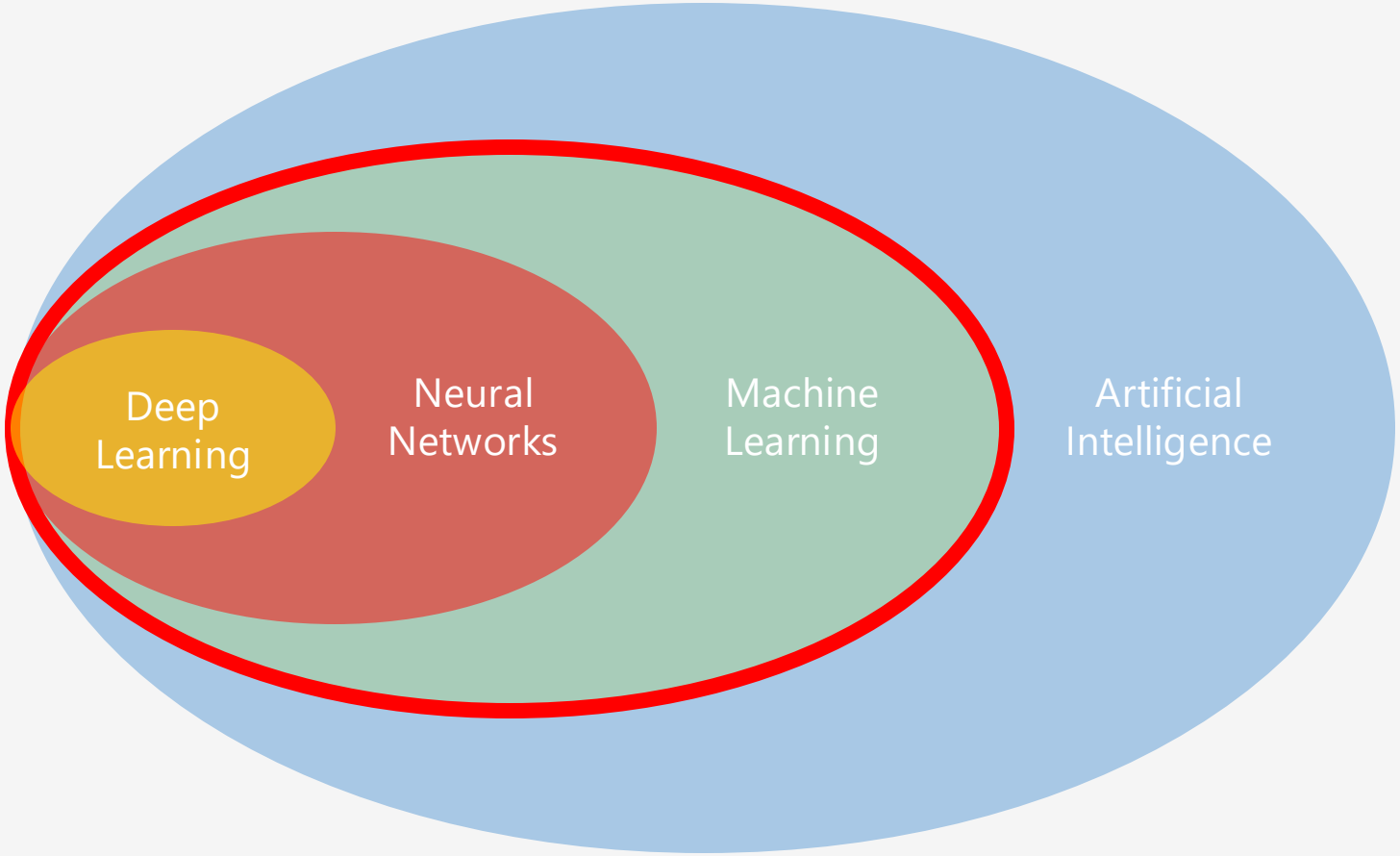


Machine learning (e.g. linear regression)

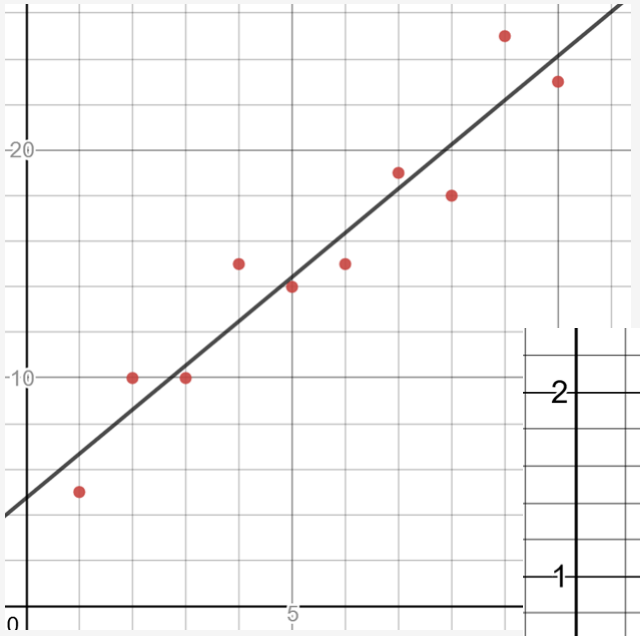
Deep Learning vs *Neural Networks* vs *Machine Learning* vs *AI*

Machine Learning is a family of data-driven algorithms that infer relationships between variables in data for the purposes of prediction.

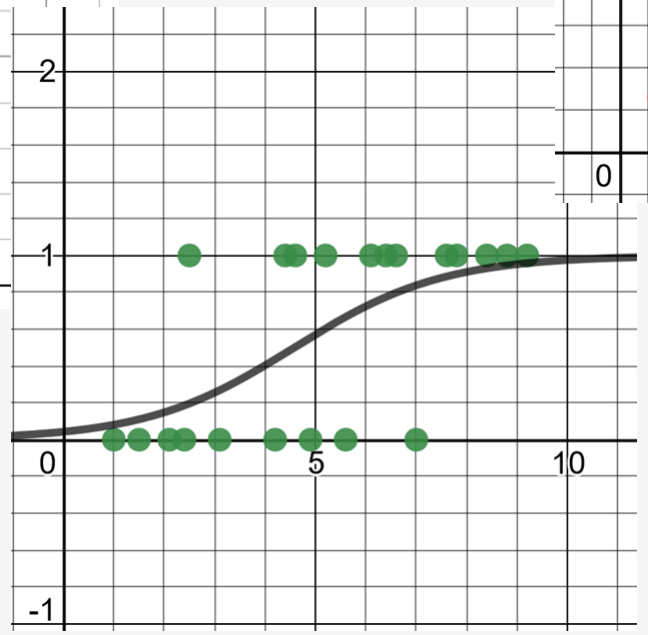
- Supervised learning – linear regression, logistic regression, Naïve Bayes, Decision trees/random forests, neural networks.
- Unsupervised learning – principal component analysis (PCA), k-means clustering
- Reinforcement Learning – Pairing supervised learning with simulations to generate data.



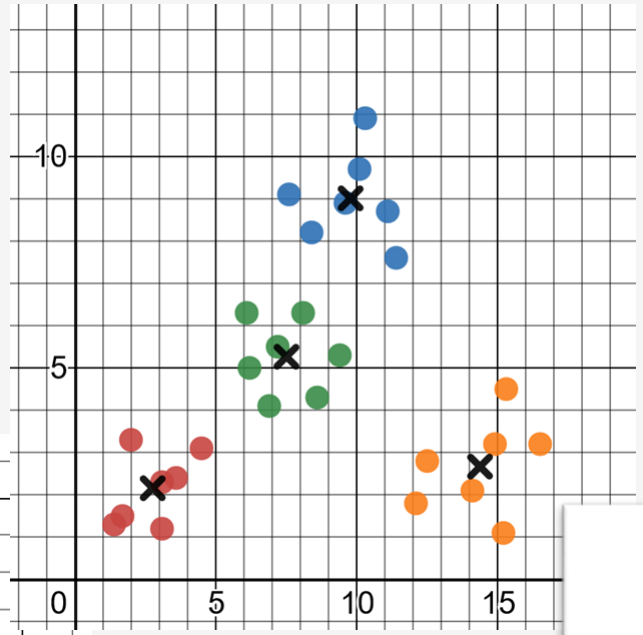
Machine Learning Examples



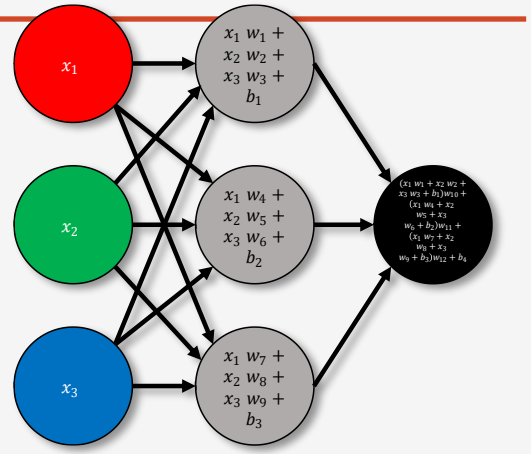
Linear Regression



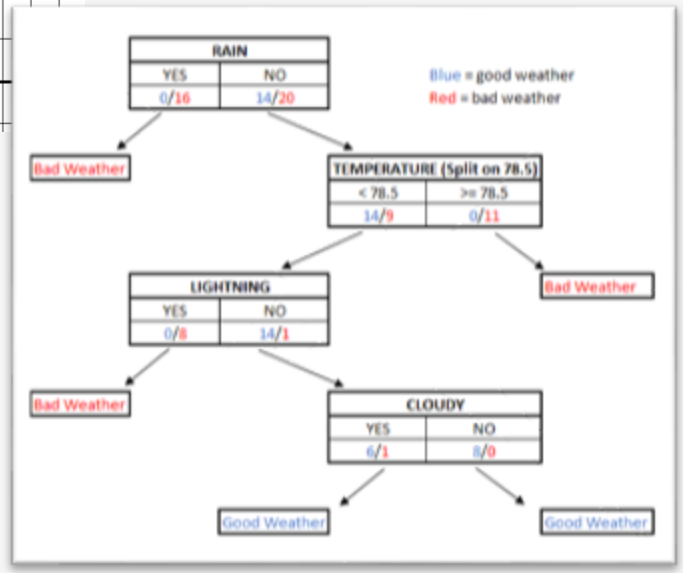
Logistic Regression



K-Means Clustering



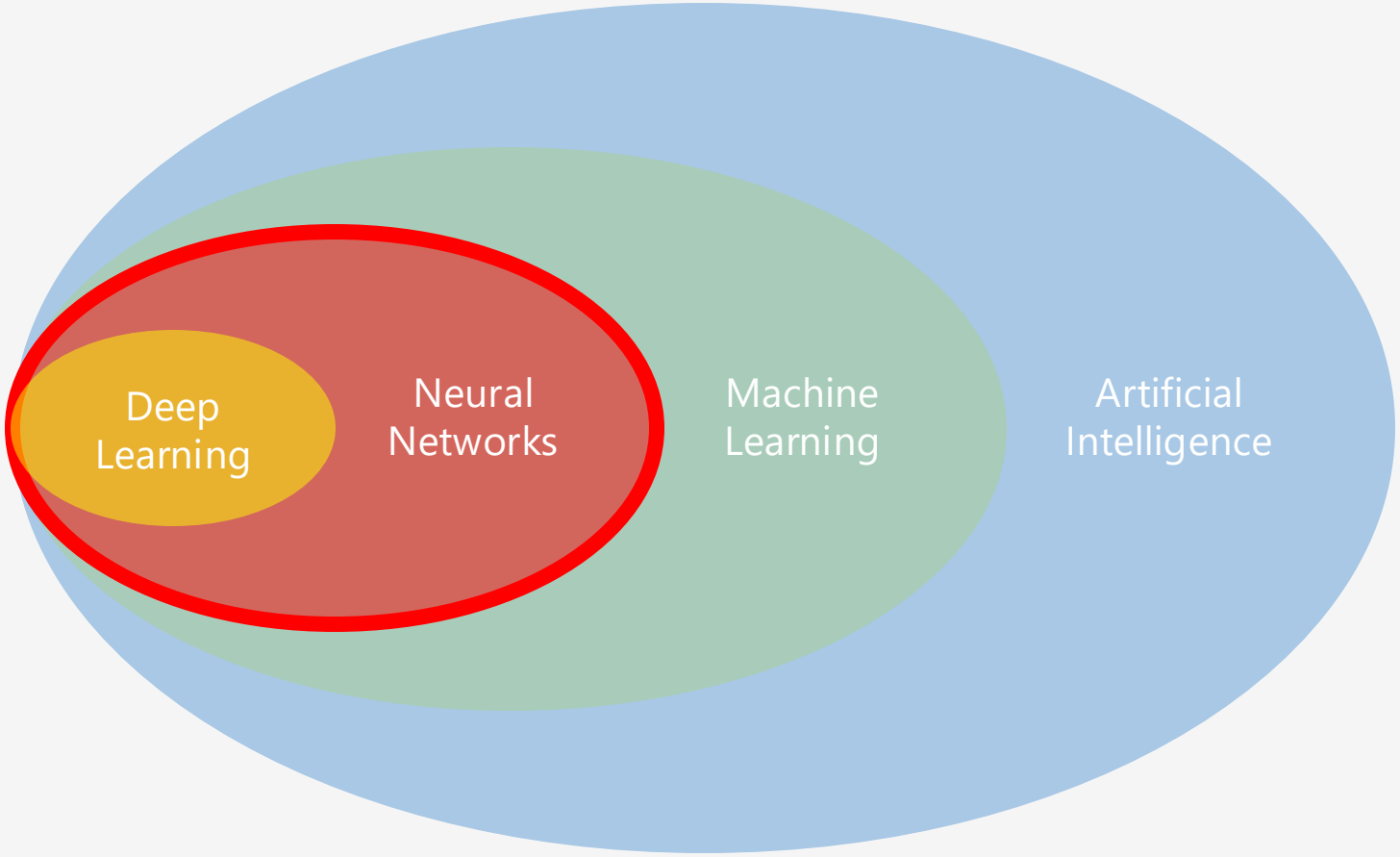
Neural Networks



Decision Trees

Deep Learning vs *Neural Networks* vs *Machine Learning* vs *AI*

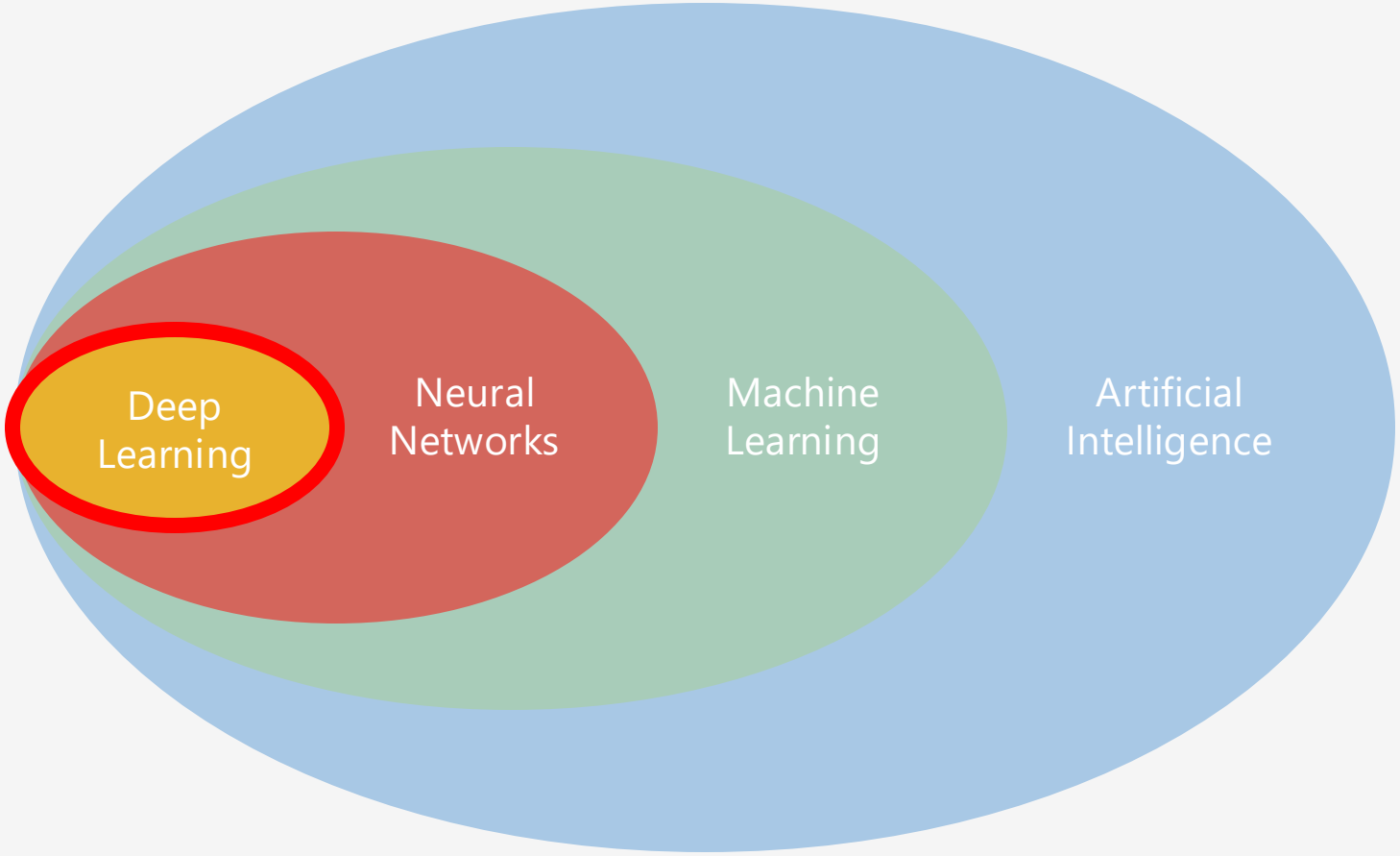
Neural networks are a type of supervised machine learning that utilizes nested layers of linear and nonlinear functions.



Deep Learning vs *Neural Networks* vs *Machine Learning* vs *AI*

Deep learning is a type of neural network that has more than one middle layer.

We will focus on deep learning too!



Programming Languages and Performance

We will build some exciting from-scratch models in Python.

Python is a great, easy-to-learn language, but it is ***really*** slow because it is dynamically typed and interpreted.

- Pure Python models will struggle to scale, even with modestly sized data sets of thousands of records.
- This is going to be the cost of learning machine learning without libraries like NumPy.
- NumPy is necessary to scale Python because it is efficiently written in C, but it is also esoteric and distracting for first-time learners.

Programming Languages and Performance

Java, Kotlin, Scala, Swift, C, C++, C#, Go, and other statically typed/compiled languages will perform much faster than Python.

- You will have more success scaling machine learning algorithms built from scratch with these platforms.
- If you truly enjoy building machine learning algorithms from scratch, please learn one of these platforms!

At this level with our toy examples, Python is going to work just fine.

Section II
Linear Regression and K-Means Clustering

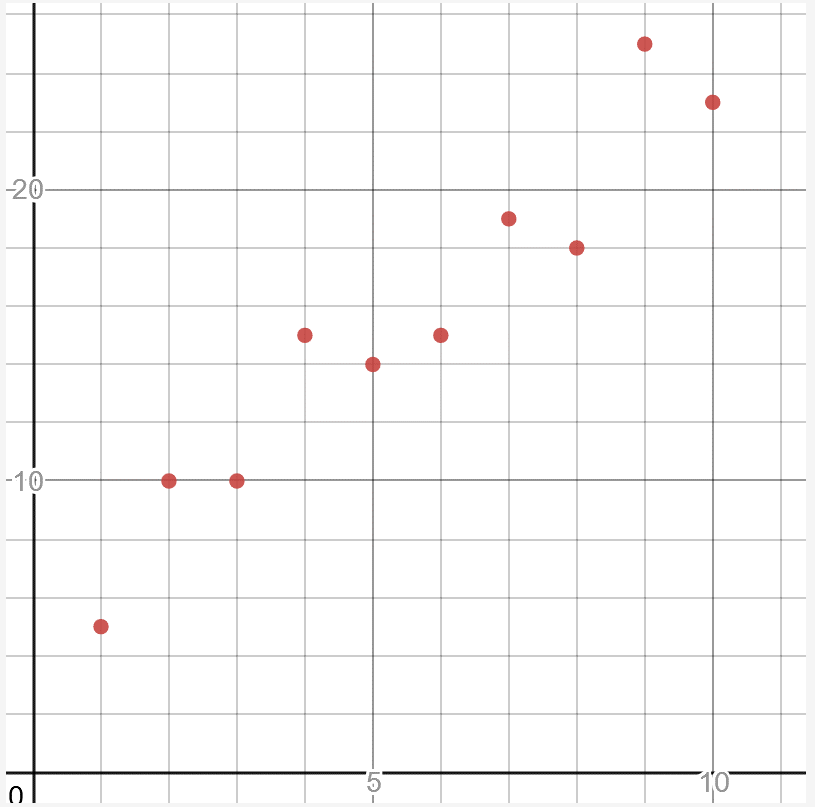
Simple Linear Regression

In practicality, machine learning is often about two tasks: regression and classification.

Let's start with regression, particularly the simplest one called **linear regression** which finds the best fit straight line through some points.

Here is a simple 2-dimensional plot of two variables, where x is independent and y is dependent.

- **Independent variables** are observed values that will serve as inputs into a function.
- **Dependent variables** are the outputted variables derived off the independent variables.



https://www.desmos.com/calculator/fmhotfn3qm

Simple Linear Regression

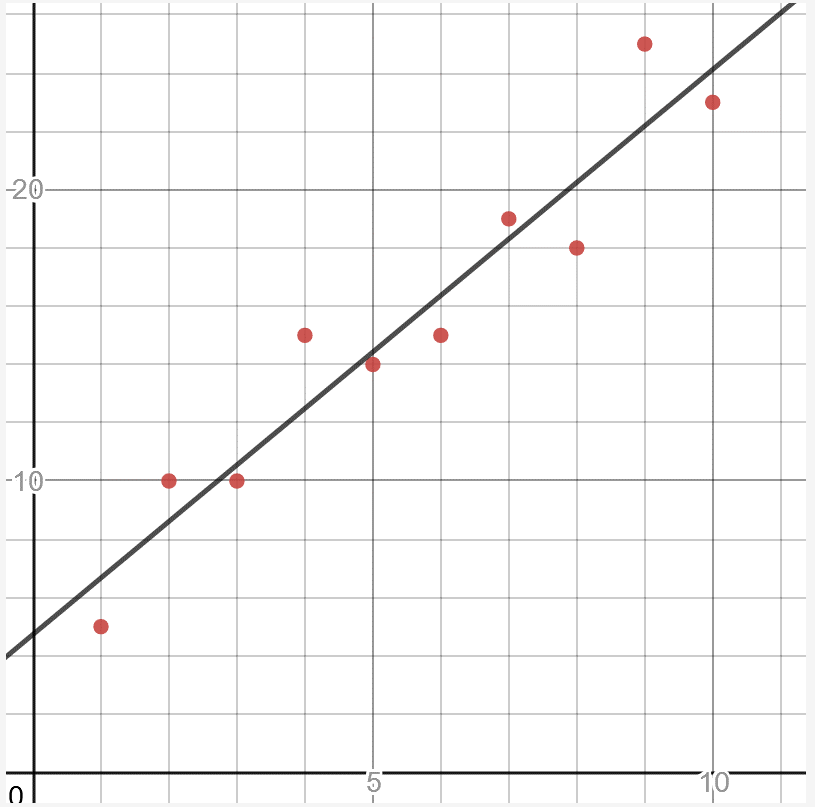
For a simple linear regression, we want to find a function $\boldsymbol{y = mx + b}$ that best fits to these points.

$$y = mx + b$$

We already know the $\boldsymbol{x}$ and $\boldsymbol{y}$ values from our existing data (the red points).

So the missing information is "what $\boldsymbol{m}$ and $\boldsymbol{b}$ values will create the best fit line"?

But before we solve for the $\boldsymbol{m}$ and $\boldsymbol{b}$ values, let's first ask "what defines a best fit anyway?"



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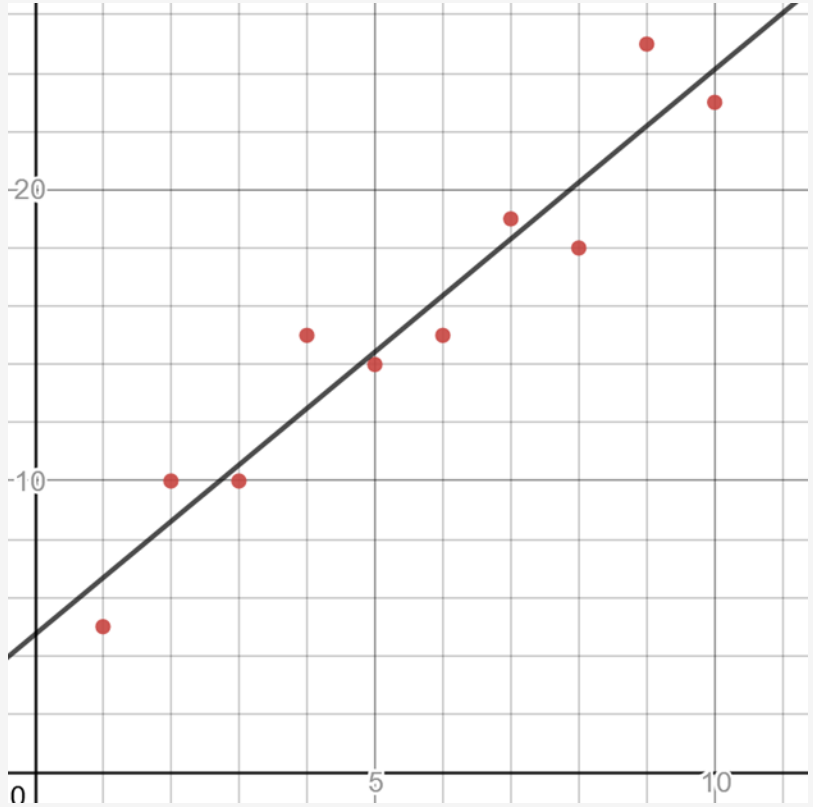
Simple Linear Regression

Pretend you drew any straight line through the points.

You will not be able to fit a perfect line, because the points do not exist on a straight line.

- Machine learning models are never perfect, as real-world data is never perfect.
- But you can fit a line to estimate a new y value for a given x value, even if there is an inevitable margin of error called loss.

Even if there is loss, it can be helpful in estimating predictions, such as how much y growth there will be at x time in the future.



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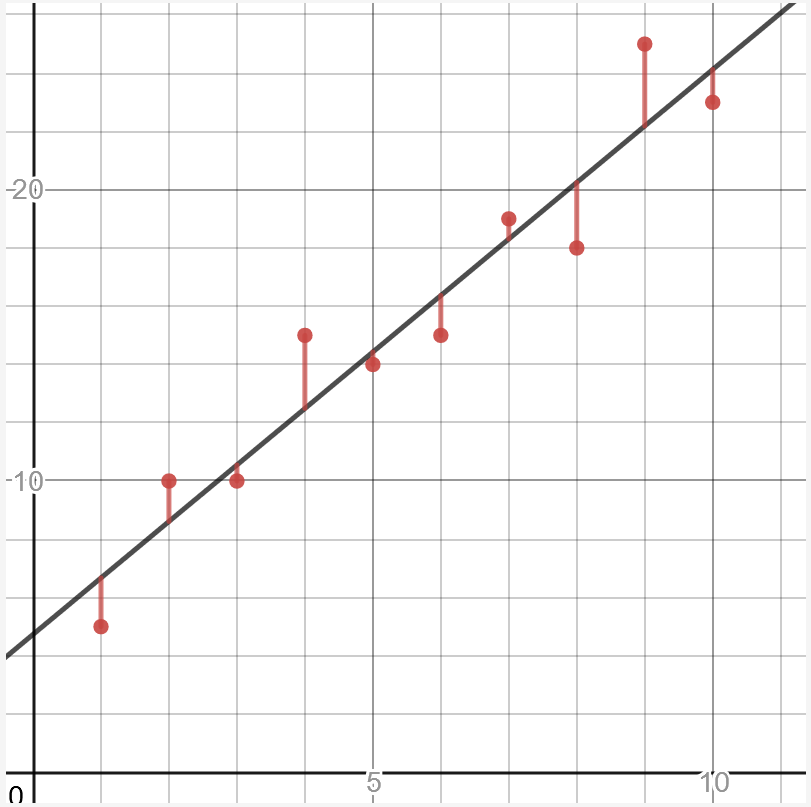
Simple Linear Regression

When you plot a given line, notice that there is a difference between the predicted y values and actual y values with our observed data.

These are called **residuals**, and in machine learning we want to minimize them.

So how do we minimize residuals in aggregate?



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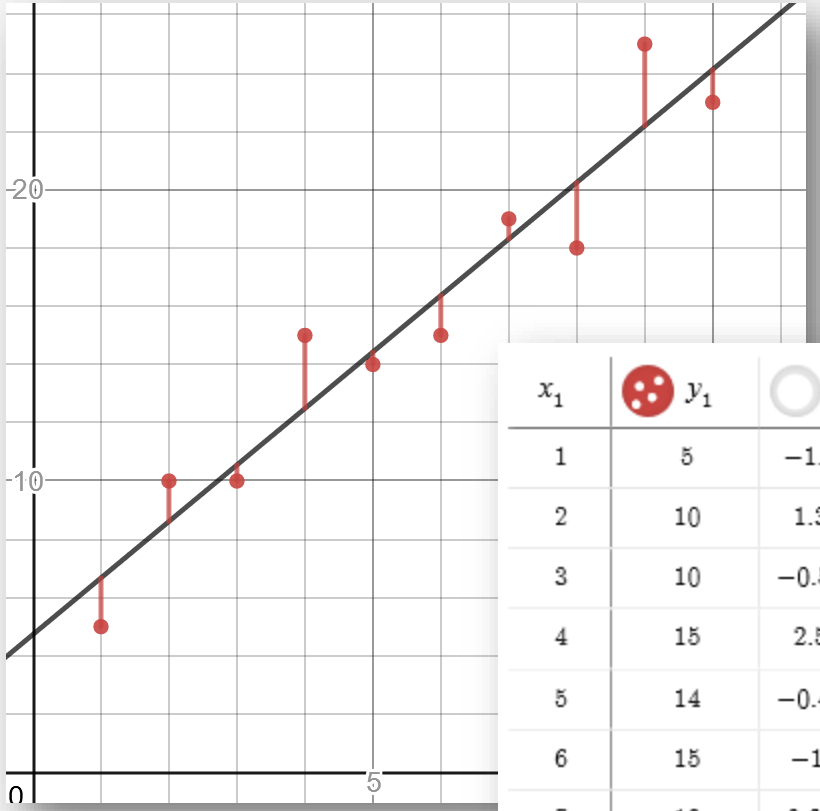
Loss Function

When we solve for $\boldsymbol{m}$ and $\boldsymbol{b}$ values, we need an objective to minimize total residuals using a **loss function**.

- We do not necessarily want to sum up the residuals, as the negatives will cancel out the positives.
- We can sum the absolute values, but that does not amplify larger residuals, and absolute values are mathematically difficult to work with.

So what is the best approach to total all the residuals to evaluate the quality of the fit?



x_1	y_1	e_1
1	5	−1.6727273
2	10	1.3878788
3	10	−0.55151515
4	15	2.5090909
5	14	−0.43030303
6	15	−1.369697
7	19	0.69090909
8	18	−2.2484848
9	25	2.8121212
10	23	−1.1272727

Sum of Least Squares

The best approach: we can square the residuals and sum them!

- Squaring will penalize large residuals by making them even larger!
- Squaring will also conveniently turn negatives into positives.
- Although we are not going to dive into calculus, squares are much easier to take the derivative of.

We can then find the $\boldsymbol{m}$ and $\boldsymbol{b}$ values that will find the sum of least squares.

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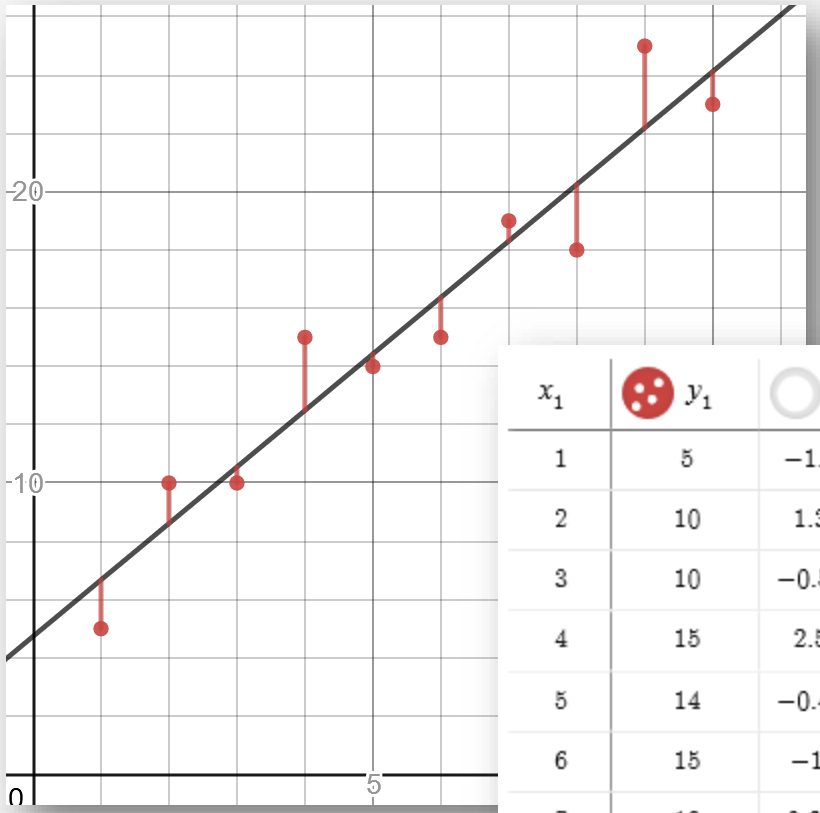

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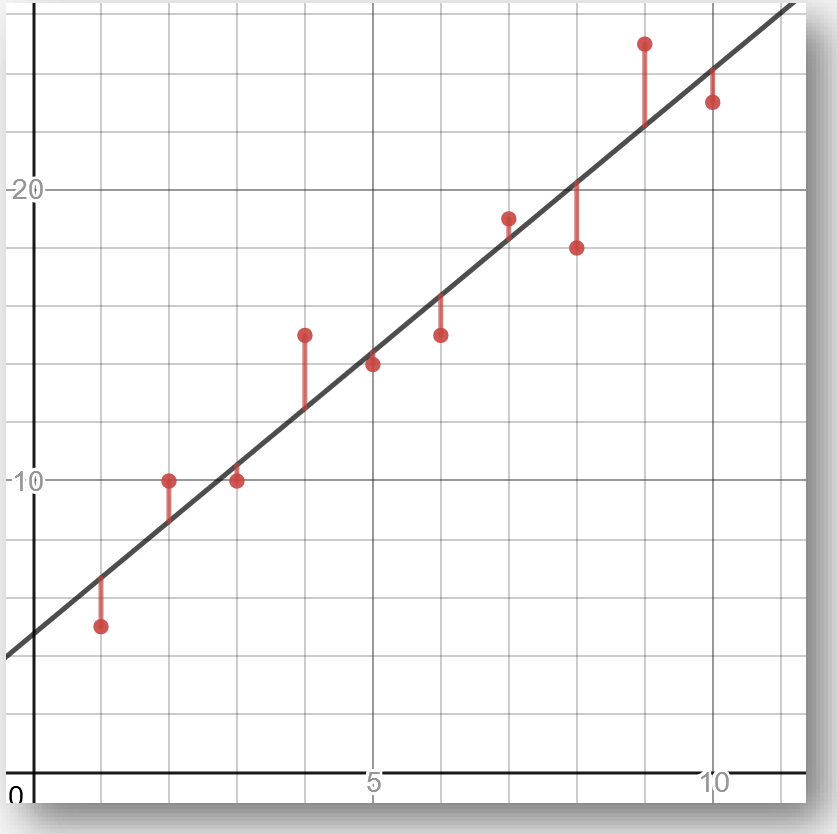
Calculating Sum of Squares

m	b			
1.93939	4.73333			
x	**y**	**y_predict (mx+b)**	**residual**	**residual squared**
1	5	6.67272	-1.67272	2.797992198
2	10	8.61211	1.38789	1.926238652
3	10	10.5515	-0.5515	0.30415225
4	15	12.49089	2.50911	6.295632992
5	14	14.43028	-0.43028	0.185140878
6	15	16.36967	-1.36967	1.875995909
7	19	18.30906	0.69094	0.477398084
8	18	20.24845	-2.24845	5.055527402
9	25	22.18784	2.81216	7.908243866
10	23	24.12723	-1.12723	1.270647473
			Sum of Squares	28.0969697



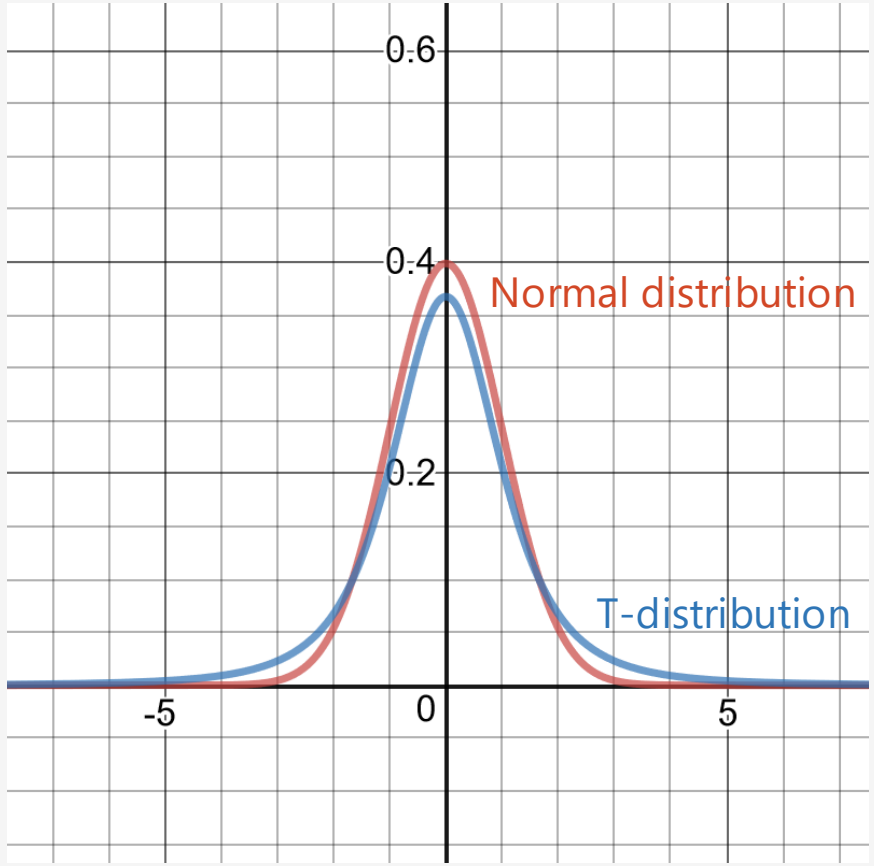
Solving for a Fit

Now that we have a loss function (the sum of squared residuals), how do we find the **m** and **b** values to minimize it?

- We randomly increase/decrease **m** and **b** with random values from a standard normal distribution, or even better a T-Distribution which has fatter tails.

- Fatter tails = more smaller/larger values = more diverse moves.

We can use these random adjustments to **m** and **b** as our moves in **hill climbing**.



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Hill Climbing – A Simple Optimization Algorithm

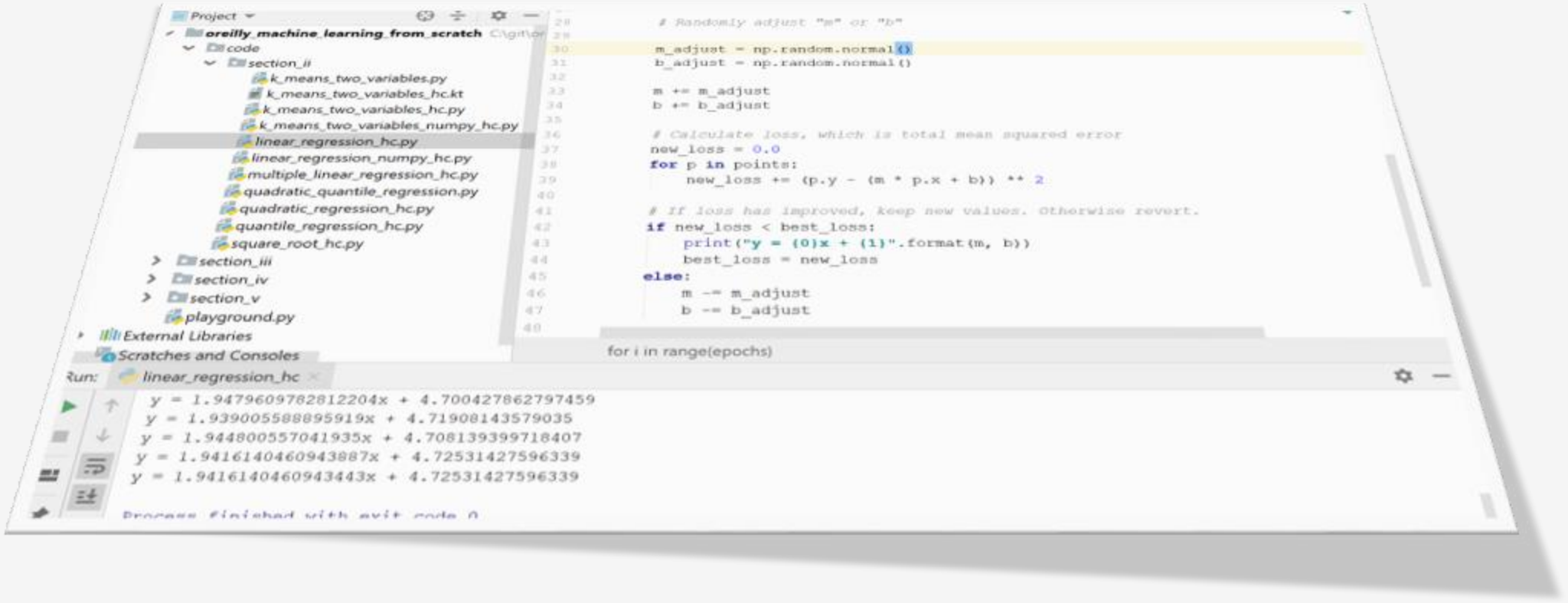
1. Start with a random or initial solution, even if it is poor quality.

2. Repeat the following steps for a number of iterations and/or until the solution cannot improve anymore.

    1. Select a random part of the solution and change it.

    2. If that results in an improvement, keep it.

Hands-On: Simple Linear Regression



Multiple Linear Regression

Solving for a function $\boldsymbol{y = mx + b}$ is elementary as it only has one independent variable $\boldsymbol{x}$.

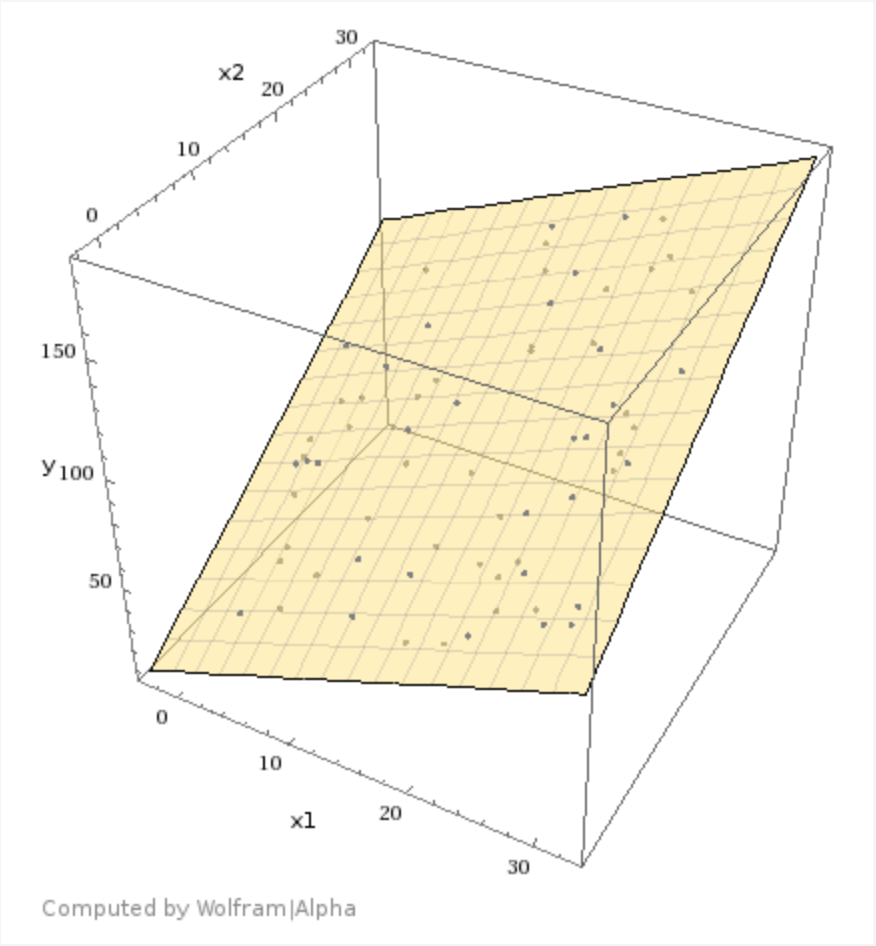
We can also solve for multiple independent variables, like x_1, x_2, x_3, and so on…

Let's say we have columns of independent variables x_1 and x_2, and a dependent variable y.

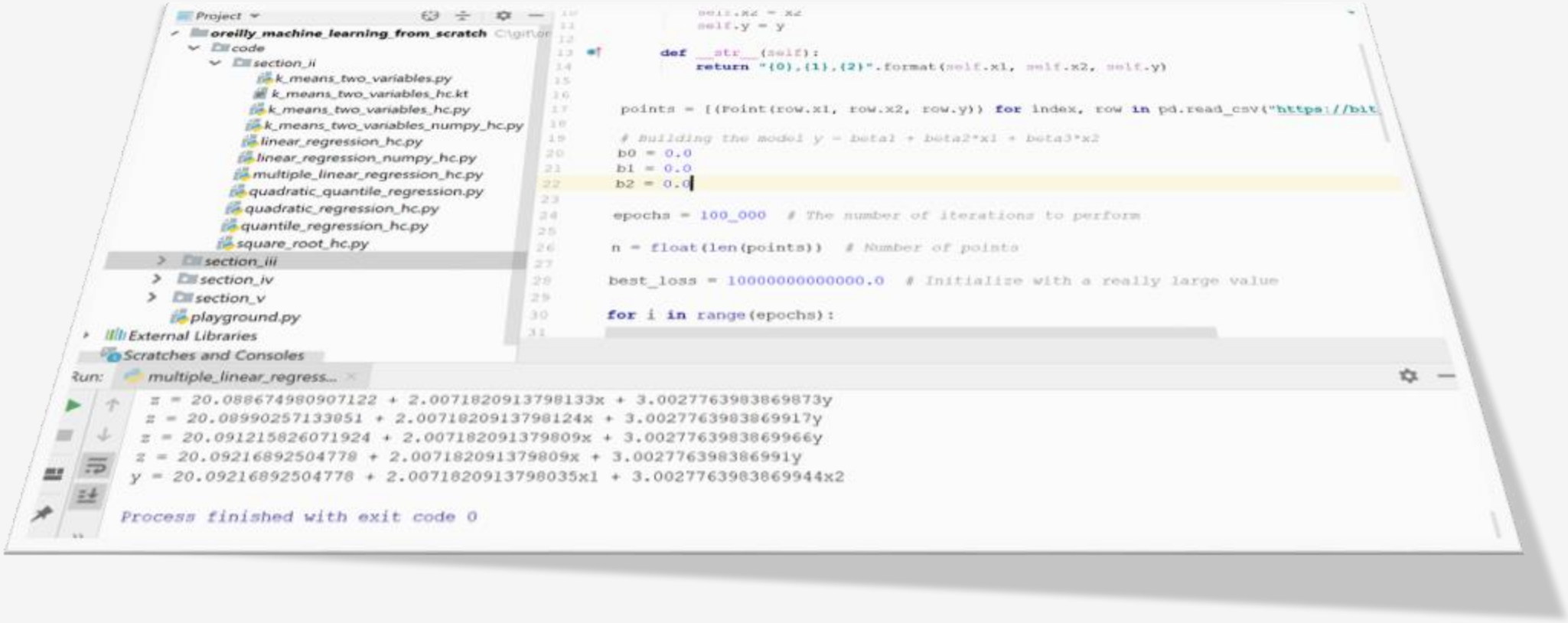
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

Instead of $\boldsymbol{m}$ and $\boldsymbol{b}$ constants, we now need to solve for each β parameter, where β_0 is the y-intercept and β_1 and β_2 are slopes for the respective x variables.

We can use the same hill-climbing technique as before!



Hands-On: Multiple Linear Regression

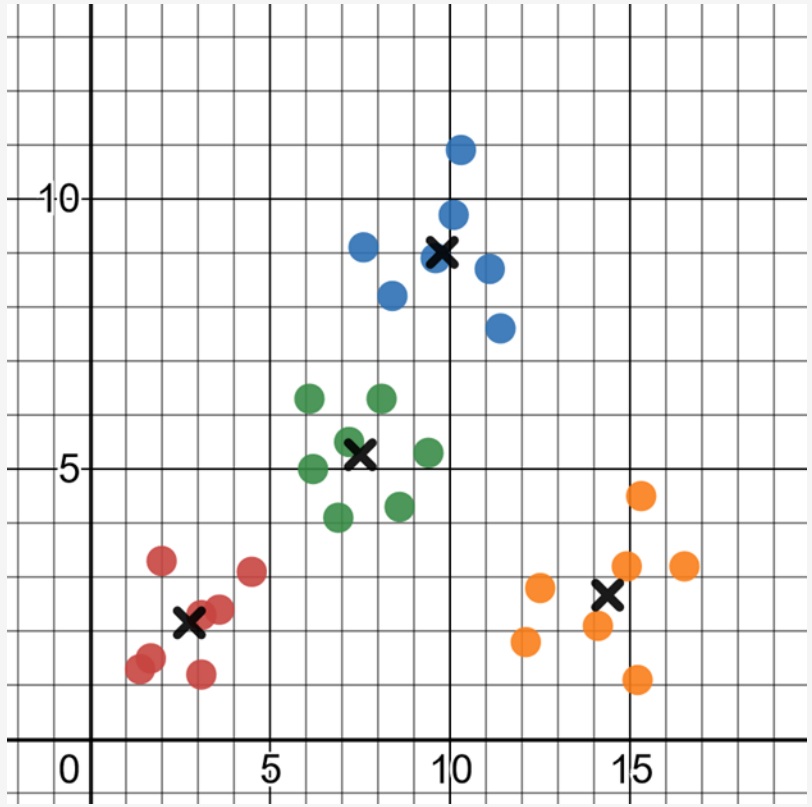


Clustering

Taking our exploration of machine learning with hill-climbing further, let's talk about k-means clustering!

Clustering groups up points based on a specified number of centroids.

- A **centroid** is a best-fit center for a cluster of points.
- To the right is some data, and we can easily eyeball there are approximately 4 groups of points.



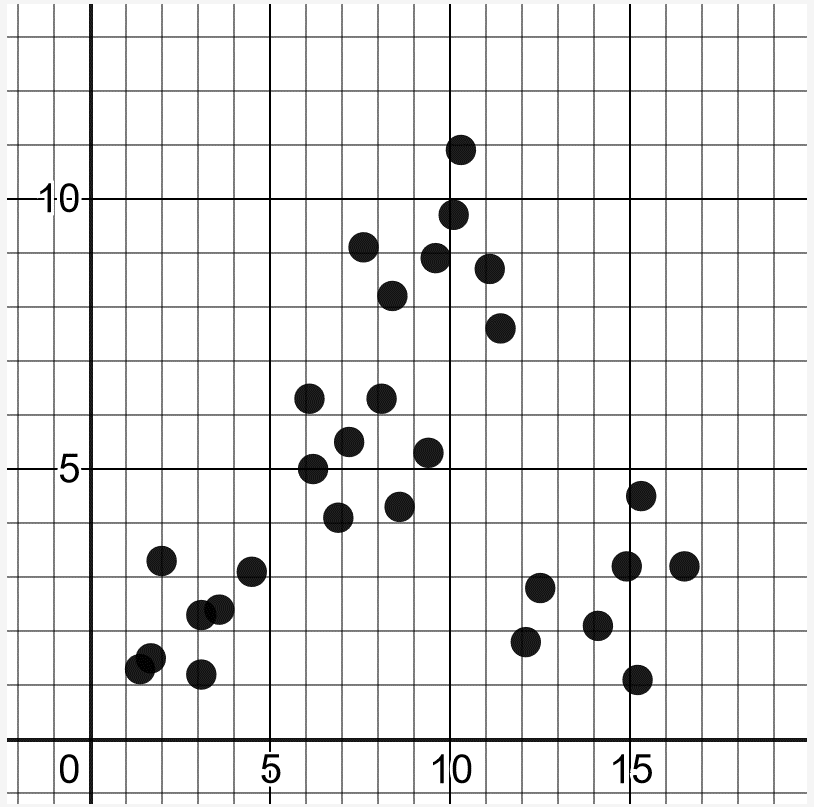
Clustering

Let's start with four centroids ($k = 4$) and use hill-climbing to center them on four clusters.

Each point will belong to the centroid it is closest to, and distance between a point and centroid is measured by:

$$d = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Our loss function will be the sum of squared distances between the centroids and their closest points.

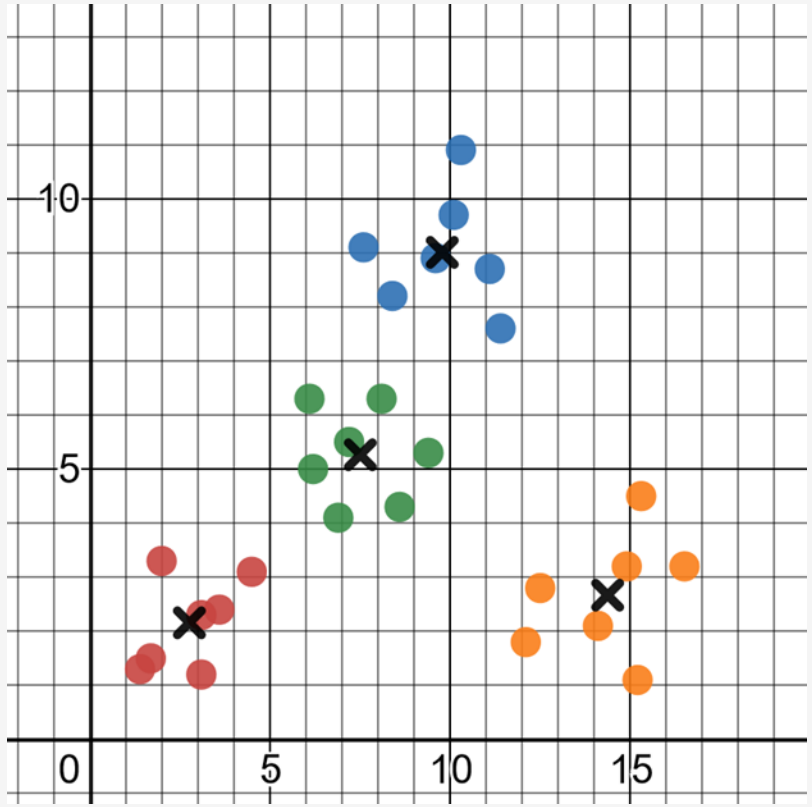


Clustering

We will start each centroid at (0,0).

For each iteration, we will:

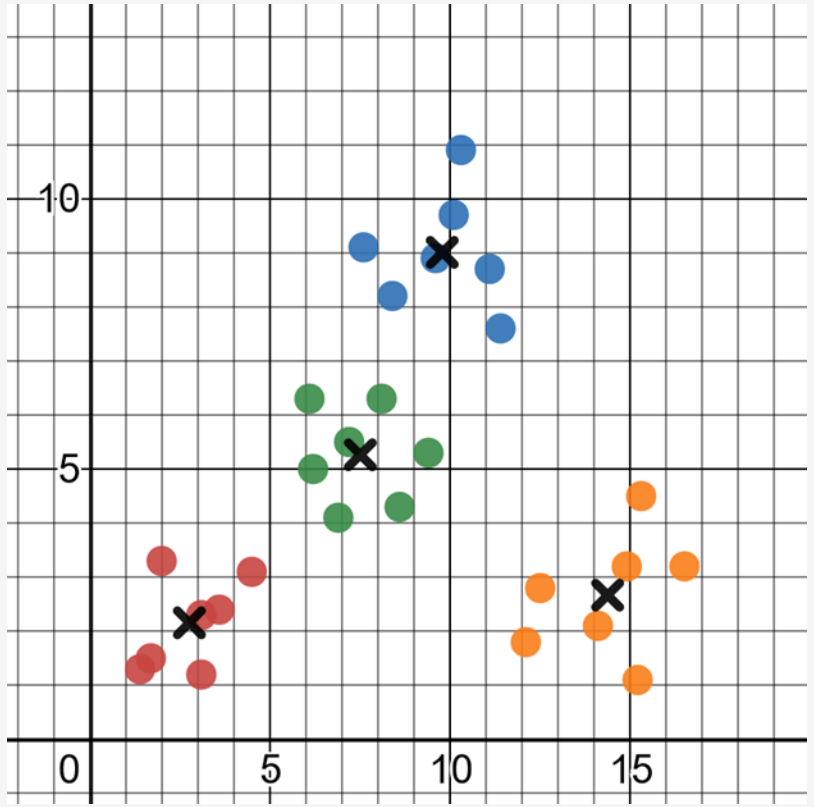
1. Select a centroid and randomly adjust its x and y value.
2. Calculate the distances between each point and their closest centroid, square them, and sum them.
3. If the sum of squared distances is reduced, keep the change.
4. Otherwise, revert the centroid back to its previous position.



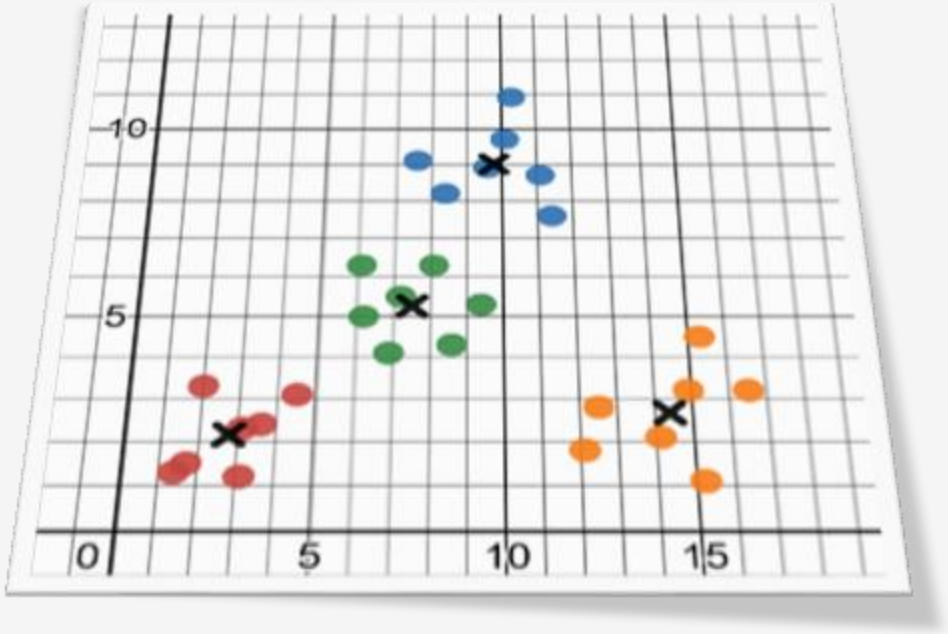
K-Means Clustering

Of course, there's a more efficient heuristic (search strategy) we can use for k-means clustering.

1. Take the average $\boldsymbol{x}$ and $\boldsymbol{y}$ values for the points nearest each centroid (hence, "k-means"!)
2. Set each centroid to that average $\boldsymbol{x}$ and $\boldsymbol{y}$.
3. Repeat until the centroids do not move anymore and are at the average of all their points.



Hands-On: K-Means Clustering



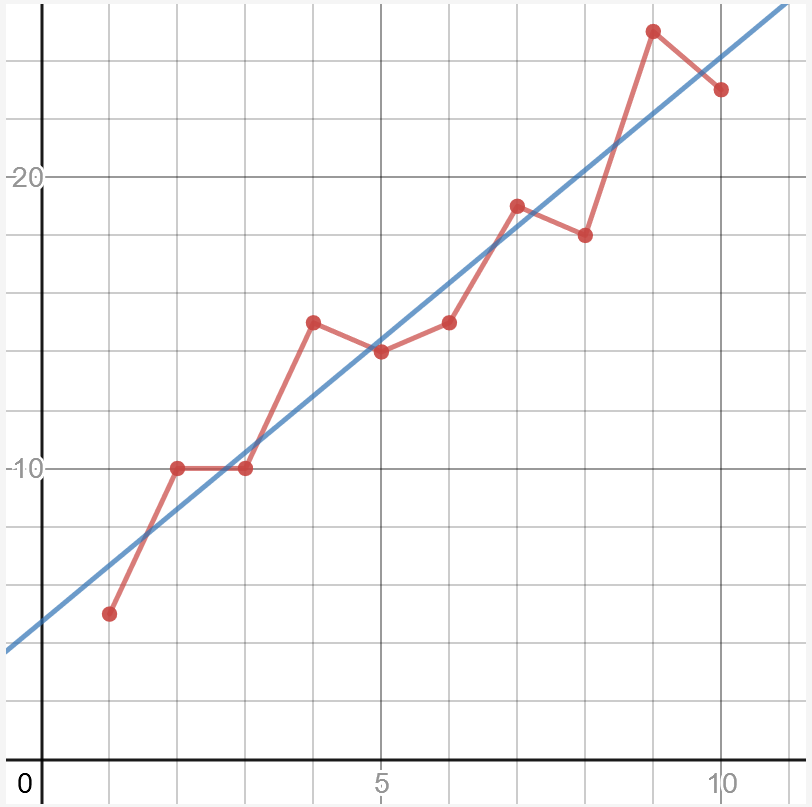
A Note About Overfitting

We are not going to focus too much on validating and analyzing machine learning models, but we should at least mention overfitting.

Overfitting means that our ML model works well with the data it was trained on but fails to predict correctly with new data.

- A common cause is the sampled data does not represent the larger population, but the model can simply be too flexible.
- The red line has high **variance**, meaning its predictions are sensitive to outliers and therefore can vary greatly.
- The blue "connect-the-dots" model has high **bias**, meaning the model is less sensitive to outliers because it prioritizes a method (maintaining a straight line) rather than bend and respond to variance.

The red "connect-the-dots" model is likely overfitted (high variance, low bias), but the blue linear regression line (low variance, high bias) is less likely to be overfit.



https://www.desmos.com/calculator/wmwfolbvdk

A Note About Overfitting

Linear regression is a highly biased method and is resilient to overfitting.

There are other remedies to mitigate overfitting, the most basic being separating **training data** and **test data**.

- The model is fit to the training data, and then is tested with the test data.
- If the test data performs poorly compared to the training data, there is a possibility of overfit (or just no correlation altogether).

You can also try to train with more data as well as utilize cross-validation, regularization, bagging, boosting, and other techniques.

Quiz Time!

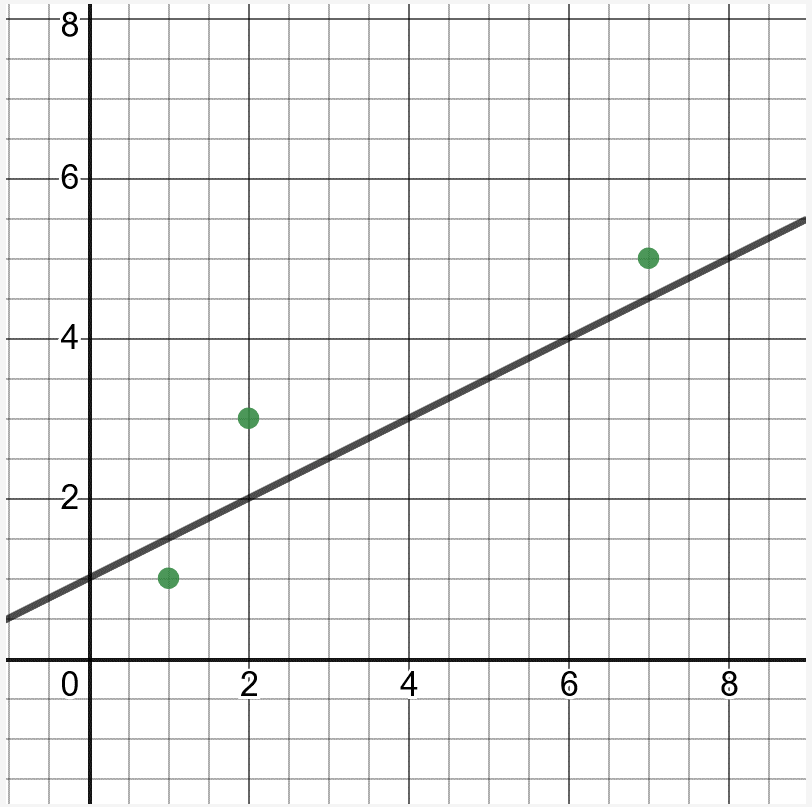
You have three points (1,1), (2,3), and (7,5). You are testing a fit for a line $y = \frac{1}{2}x + 1$. What is the loss calculated by sum of squares?

A) 1.5

B) 1.75

C) 1.0

D) -1.5



Quiz Time!

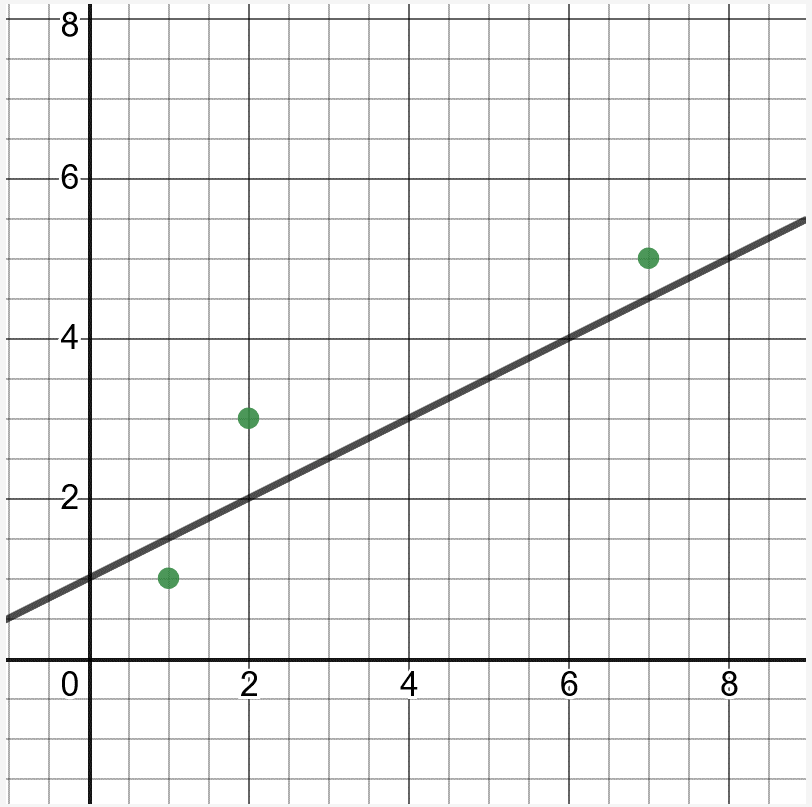
You have three points (1,1), (2,3), and (7,5). You are testing a fit for a line $y = \frac{1}{2}x + 1$. What is the loss calculated by sum of squares?

A) 1.5 $= (1 - (\frac{1}{2}1 + 1))^2 + (3 - (\frac{1}{2}2 + 1))^2 + 5 - (\frac{1}{2}7 + 1))^2$

B) 1.75

C) 1.0

D) -1.5

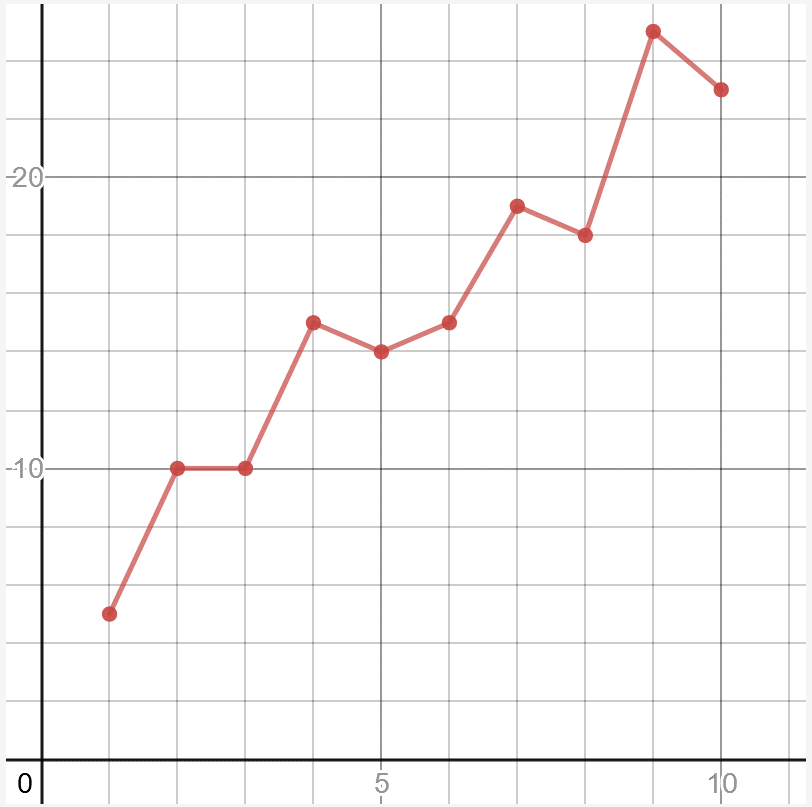


Quiz Time!

It is good to fit a regression as close to the points as possible, even if you just connect the points as shown to the right.

A) True

B) False



Quiz Time!

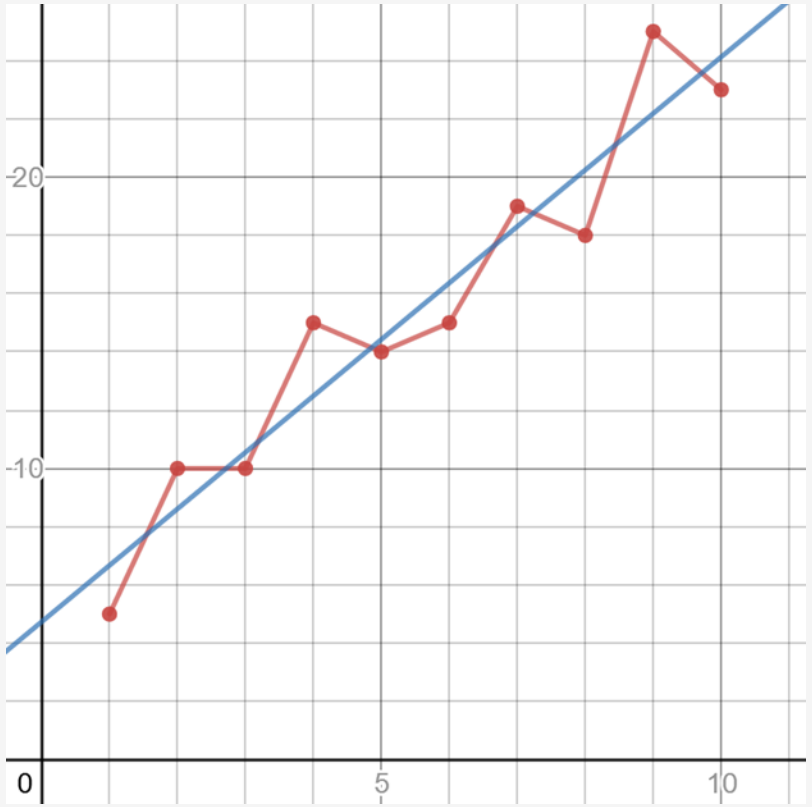
It is good to fit a regression as close to the points as possible, even if you just connect the points as shown to the right.

A) True

B) False

Doing a regression is a balancing act between fitting exactly to your data (variance) versus leaving some wiggle room (bias) to predict new data that will be different. Otherwise you will risk overfitting even if you have zero loss.

You might be better doing a linear regression (blue line) as shown to the right, which has a loss but is more likely to predict new data accurately.



Section III
Logistic Regression

Classifying Things

So far we just did regressions via linear regression.

However, linear regressions are awkward to use for classification.

- Lines extend in a straight direction for positive infinity and negative infinity, well outside a range of acceptable values.
- Lines do not do a good job representing a probability and staying within the limits of 0.0 and 1.0.
- When doing classification, probability is a critical tool.

Hot dog: 0.92

Classifying Things

Classification tasks are pretty common in machine learning:

- How do I classify images of *dogs* versus *cats*?
- Will a shipment be most likely be *late*, *early*, or *on-time*?
- Is this email *spam* or *not spam*?
- Will this movie get *1 star*, *2 stars*... or *5 stars*?

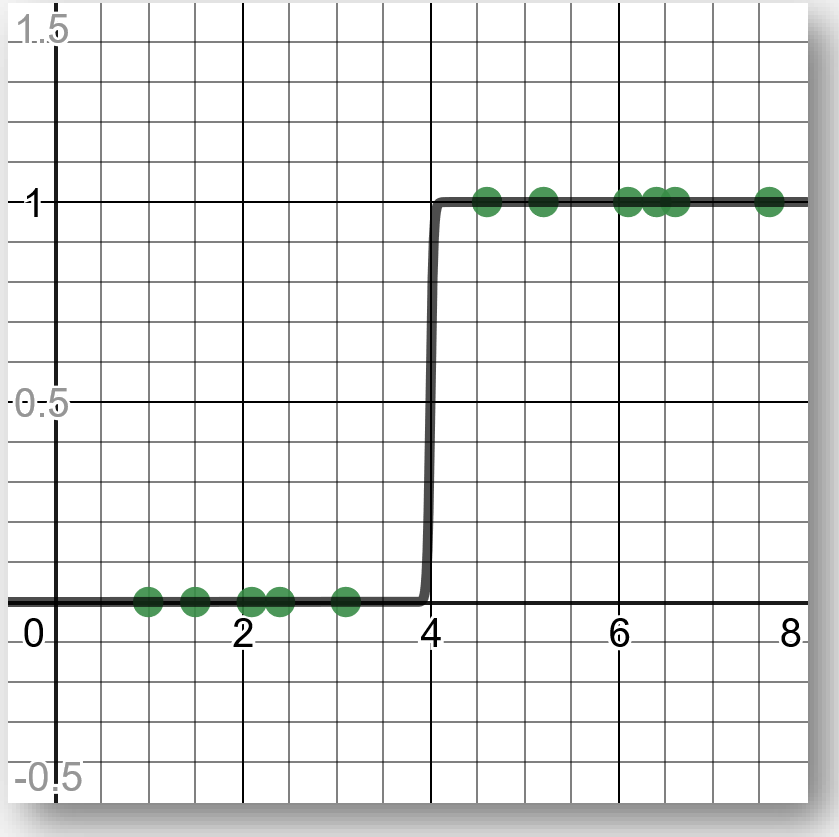
There are several machine learning algorithms that work well for classification, and we are going to learn first about Logistic Regression.

Hot dog: 0.92

Logistic Regression Intuition

Imagine you have 11 patients exposed to a chemical for x hours, and you plot whether they exhibited symptoms (1) or not (0).

Plotting our patient data (right), we can easily eyeball a clear cutoff at 4 hours where patients transition from ***not showing symptoms (0)*** to ***showing symptoms (1)***.



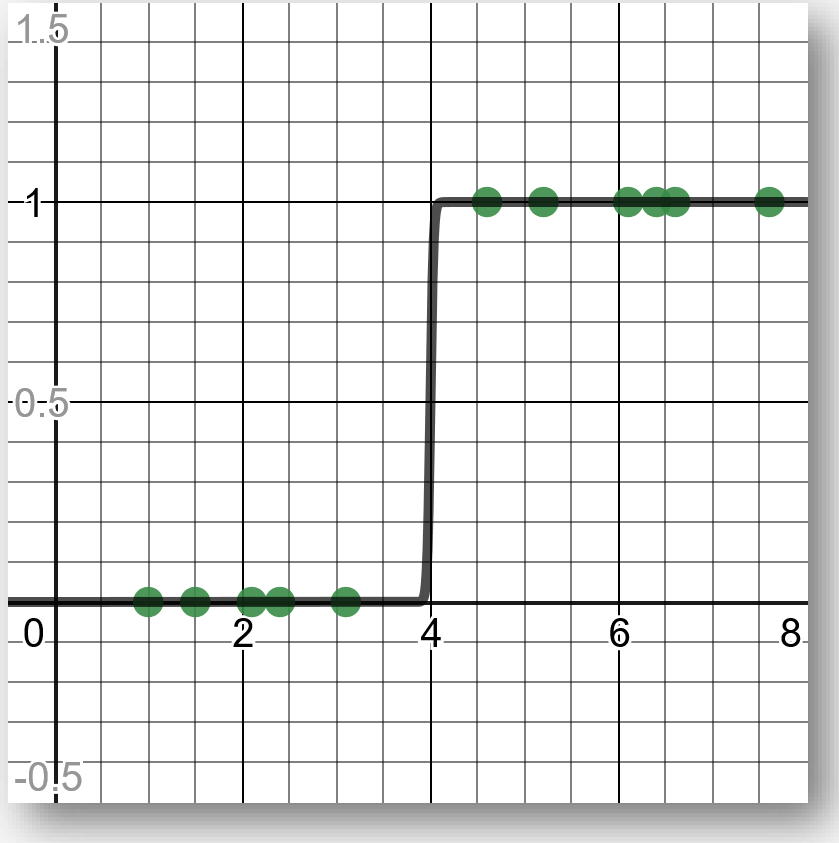
https://www.desmos.com/calculator/prs2p0sofc

Logistic Regression Intuition

This indicates any patient exposed for less than 4 hours will have a 0% chance of showing symptoms, but greater than 4 will have a 100% chance of showing symptoms.

Because there is a distinct separation at 4 hours, a logistic regression is going to “jump” from 0% to 100% at that boundary.

Of course, real life rarely works out this way…



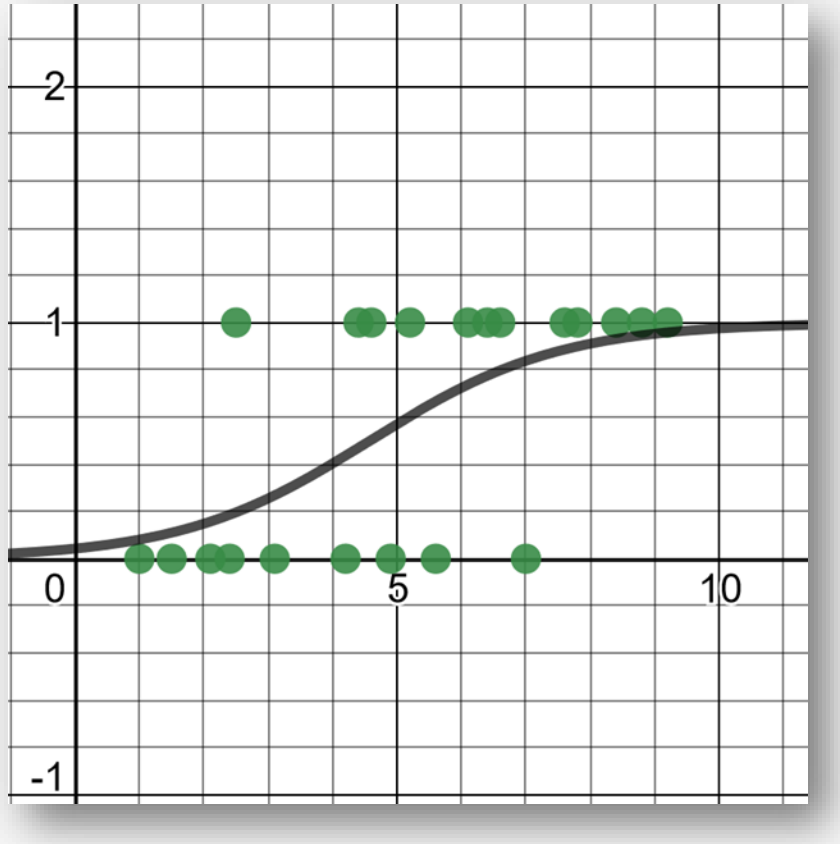
https://www.desmos.com/calculator/prs2p0sofc

Logistic Regression Intuition

Now let's say you gathered more data and got a realistic picture, where the middle of the range has a mix of patients showing symptoms and not showing symptoms.

The way to interpret this is the probability of patients showing symptoms gradually increases with each hour of exposure.

Because of this overlap of points in the middle, there is no distinct cutoff when patients show symptoms, but rather a gradual transition from 0% probability to 100% probability ("0" and "1").

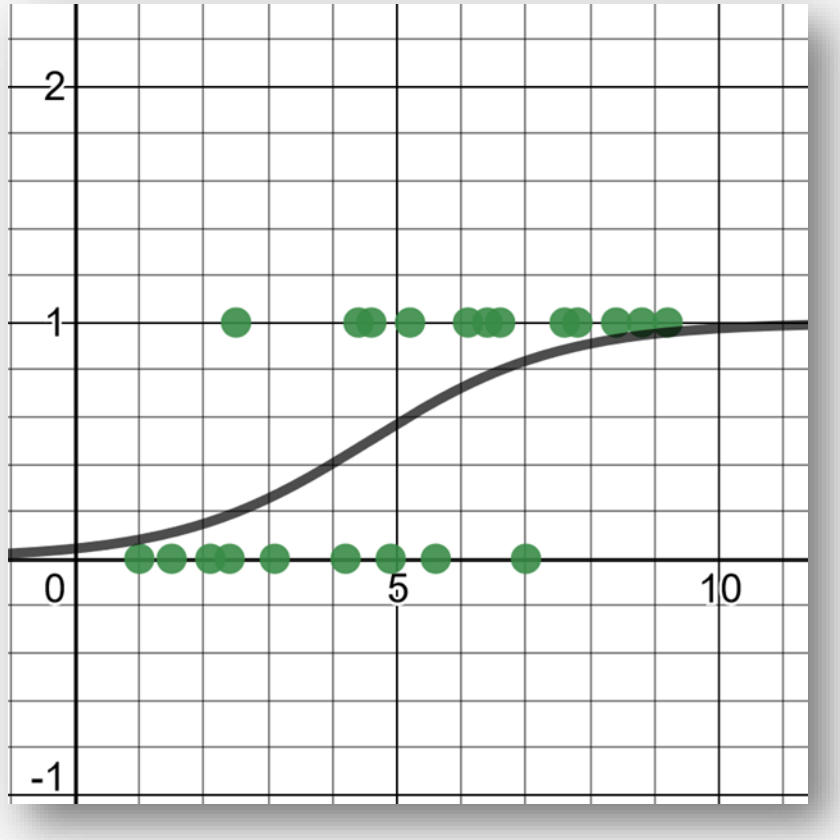


https://www.desmos.com/calculator/bsqtqfians

Logistic Regression Intuition

More technically, a logistic regression results in a curve indicating a probability of belonging to the **true** (1) category, which in this case means ***a patient showed symptoms***.

As the hours of chemical exposure increases, the number of patients showing symptoms increases, and thus the probability of showing symptoms increases.



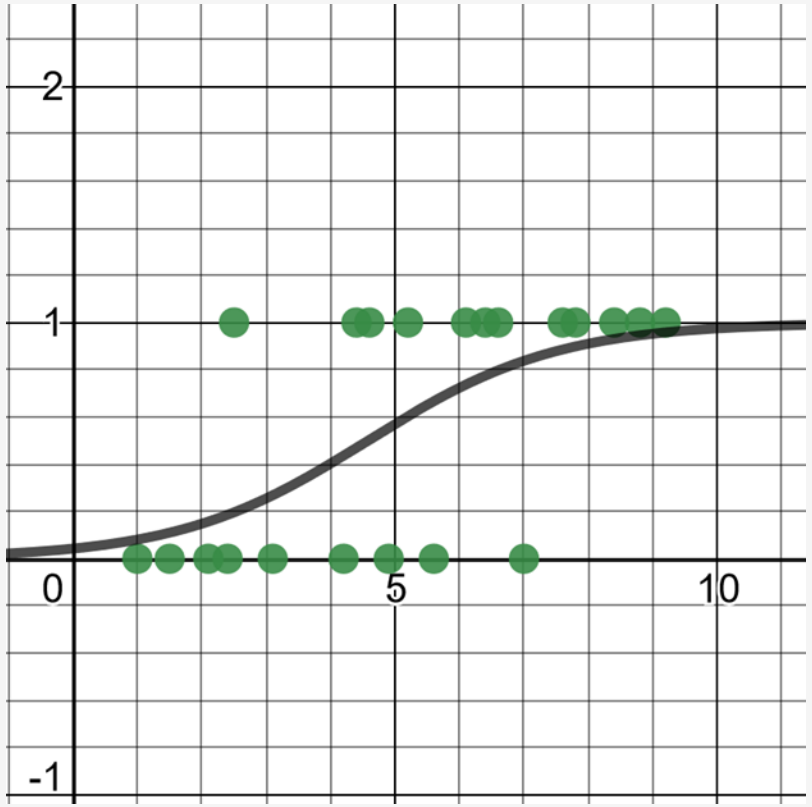
https://www.desmos.com/calculator/bsqtqfians

Logistic Regression

Logistic Regression is a classification tool that predicts a **true** or **false** value for one or more variables.

Training data must have outcomes of 0 (false) or 1 (true), but the regression will output a probability value between 0 and 1.

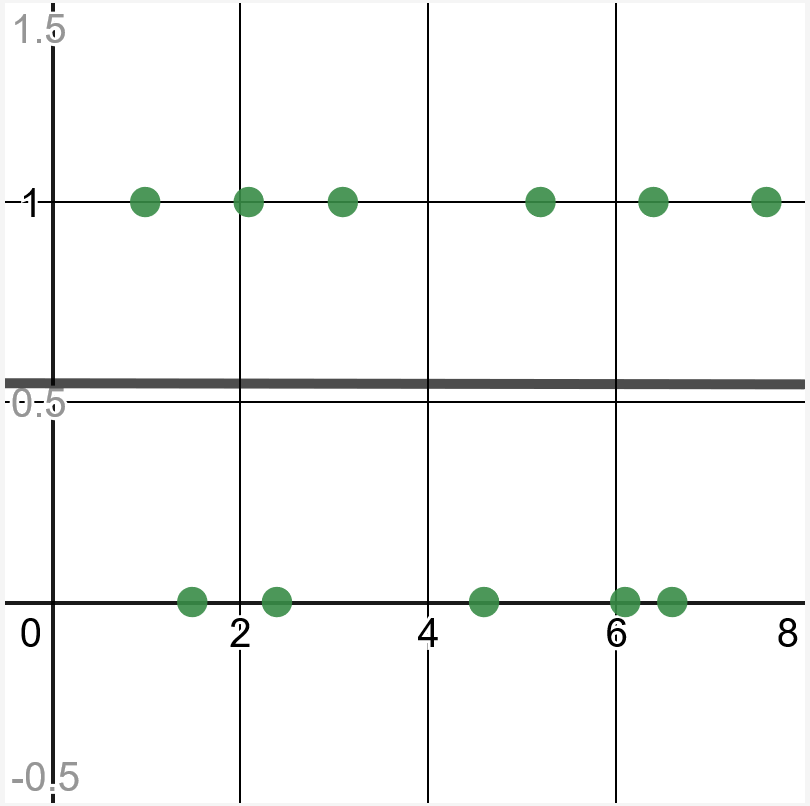
- An S-shaped curve (a **logistic function**) is fit to the points and then used to predict probability.
- If a predicted value (the y-axis) is less than .5 it is typically categorized as false (0), and if the predicted value is greater than/equal to .5 it is typically categorized as true (1).



https://www.desmos.com/calculator/bsqtqfians

When Not To Use Logistic Regression

Of course, if there is no transitional trend in your data then you should not use logistic regression.



https://www.desmos.com/calculator/cmeksxk5rk

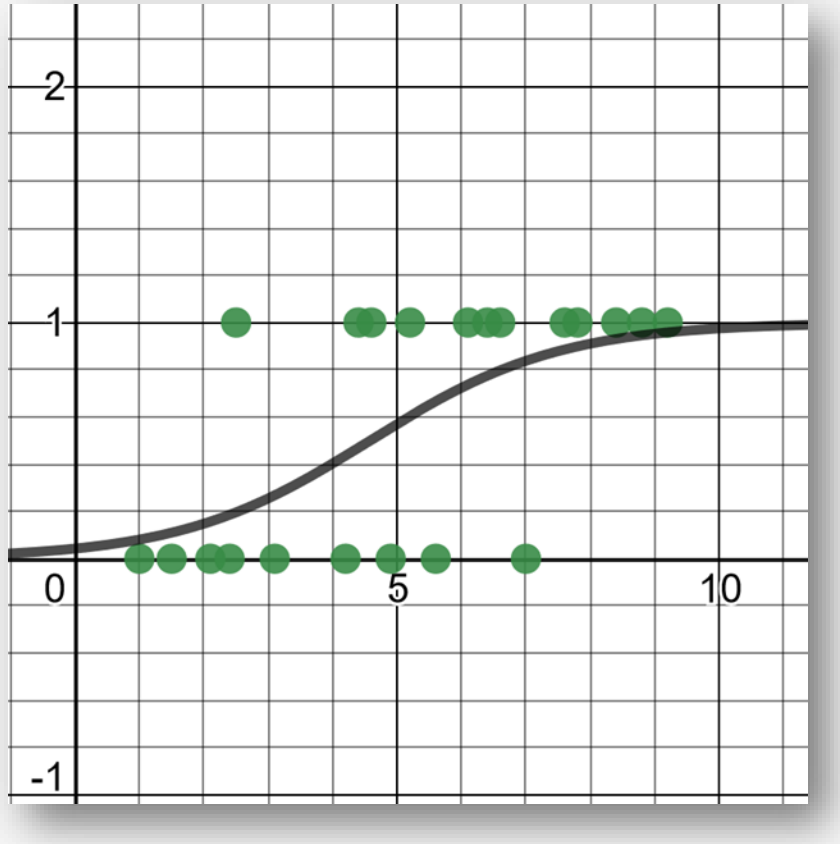
Just Show Me the Math!

For a single independent variable x to predict a dependent probability variable y, you need to fit the data to the logistic function:

$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

You can express this in Python as:

```
def predict_probability(x):
    p = 1.0 / (1.0 + math.exp(-(b0 + b1 * x)))
    return p
```



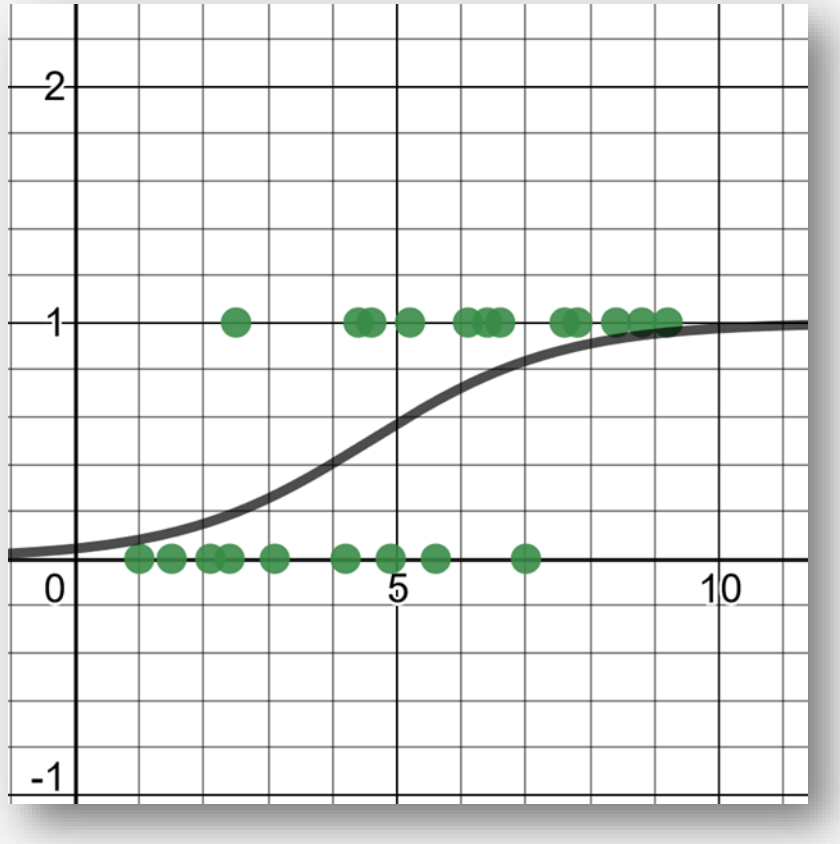
https://www.desmos.com/calculator/blfcwrlnuw

Just Show Me the Math!

You may see also see this logistic function expressed as:

$$y = \frac{e^{\beta_0+\beta_1 x}}{1.0 + e^{\beta_0+\beta_1 x}}$$

However it is the same and just algebraically expressed differently.



https://www.desmos.com/calculator/blfcwrlnuw

Just Show Me the Math!

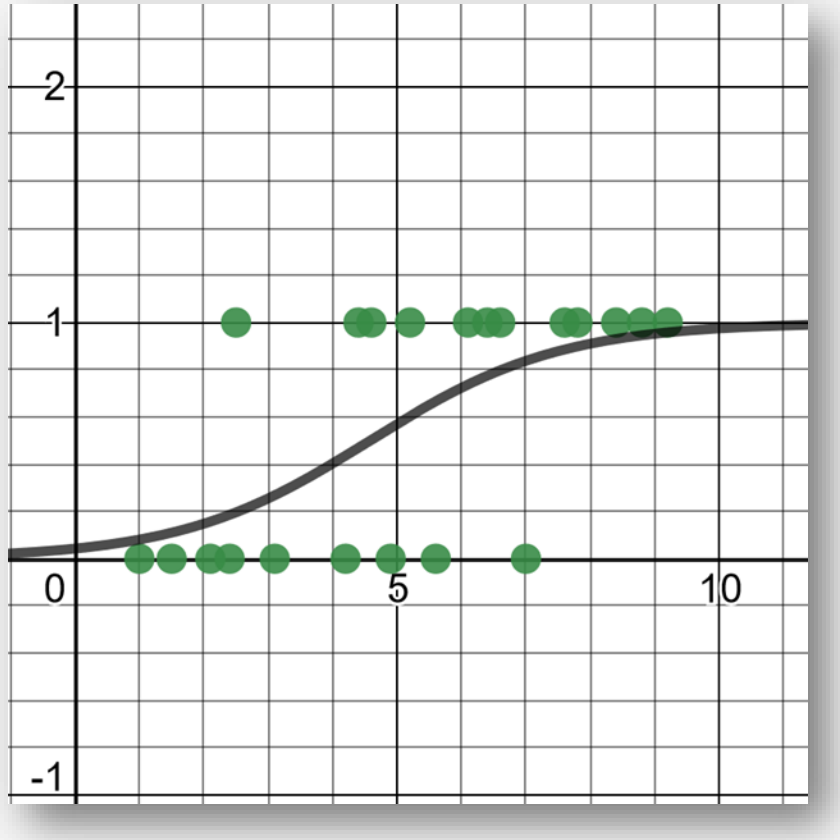
$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

```
def predict_probability(x):
    p = 1.0 / (1.0 + math.exp(-(b0 + b1 * x)))
    return p
```

Notice the expression $\beta_0 + \beta_1 x$ is linear, and this known as the **log odds function** which is translated logarithmically into a probability.

In the interest of time, we will avoid going into proofs and mathematical details about how this function works.

Just know it produces this S-shaped curve we need to output a probability between 0 and 1.



https://www.desmos.com/calculator/blfcwrlnuw

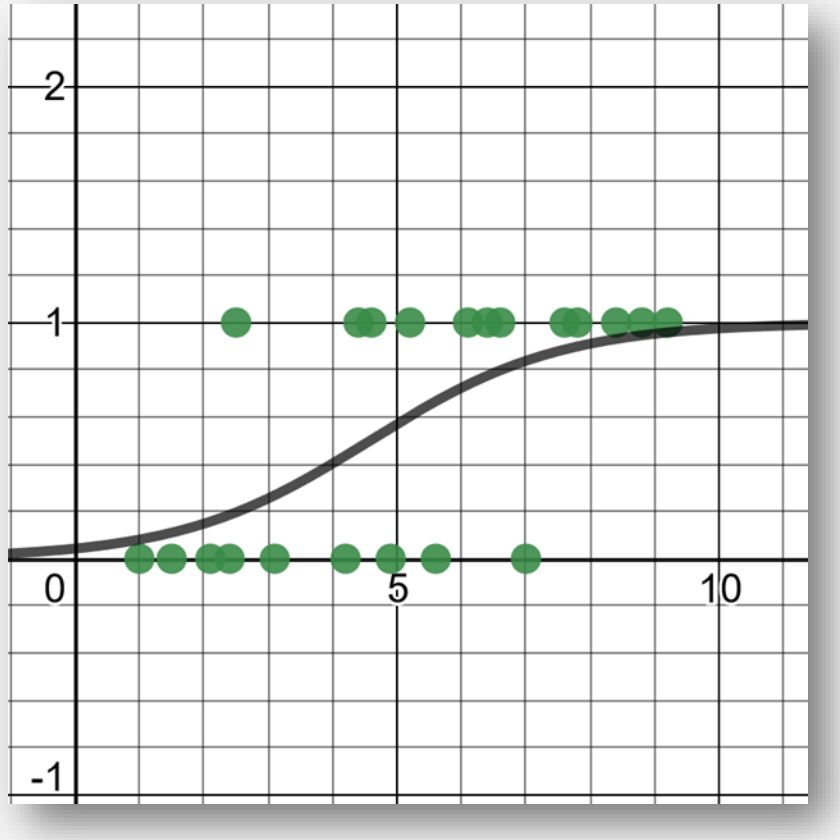
Just Show Me the Math!

$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

```
def predict_probability(x):
    p = 1.0 / (1.0 + math.exp(-(b0 + b1 * x)))
    return p
```

We need to solve for β_0 and β_1, but we cannot use least squares like in linear regression.

- We are trying to maximize probability of the curve predicting correctly, not finding the best fit.
- Using hill climbing, we need to find β_0 and β_1 that produces the maximum likelihood.



https://www.desmos.com/calculator/blfcwrlnuw

Maximum Likelihood

Maximum likelihood is a technique to estimate parameters that have the highest probability of outputting the observed data.

In our case, we need to find values for β_0 and β_1 that will yield the highest likelihood of outputting the correct true/false values.

Remember that our logistic function outputs a likelihood y for a given value x.

$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

Maximum Likelihood

Let's say during our hill-climbing, we test parameters $\beta_0 = -.3.17$ and $\beta_1 = 0.69$

$$y = \frac{1.0}{1.0 + e^{-(-3.17+0.69x)}}$$

To calculate the total likelihood for these parameters…

1. Get the true (1) data, calculate the likelihood $\boldsymbol{y}$ for each $\boldsymbol{x}$ value, and multiply them together.

2. Get the false (0) data, calculate the likelihood $(\boldsymbol{1.0 - y})$ for each $\boldsymbol{x}$ value, and multiply them together.

3. Multiply the two products above together, and that is your total likelihood.

Maximum Likelihood – Avoiding Floating Point Underflow

However, multiplying this many decimals together can cause floating point underflow.

With a clever mathematical hack, we can remedy this by using logarithmic addition instead of multiplication.

$$y = \log\left(\frac{1.0}{1.0 + e^{-(-3.17+0.69x)}}\right)$$

If you need to learn about logarithms, YouTube is the best place to get crash coursed.

PatrickJMT: https://youtu.be/AAW7WRFBKdw

Don't Memorize: https://youtu.be/4UNkQcBrLaQ

Maximum Likelihood – Avoiding Floating Point Underflow

$$y = \log\left(\frac{1.0}{1.0 + e^{-(-3.17+0.69x)}}\right)$$

To calculate the total likelihood for these parameters, but avoid floating point underflow…

1. Get the true (1) data, calculate the likelihood $\boldsymbol{y}$ for each $\boldsymbol{x}$ value, pass it to a $\boldsymbol{log}()$ function, then sum the values.

2. Get the false (0) data, calculate the likelihood $(\boldsymbol{1.0 - y})$ for each $\boldsymbol{x}$ value, pass it to a $\boldsymbol{log}()$ function, then sum the values.

3. Sum the two values above together, pass it to the $\exp()$ function to undo the logarithm, and that is your total likelihood.

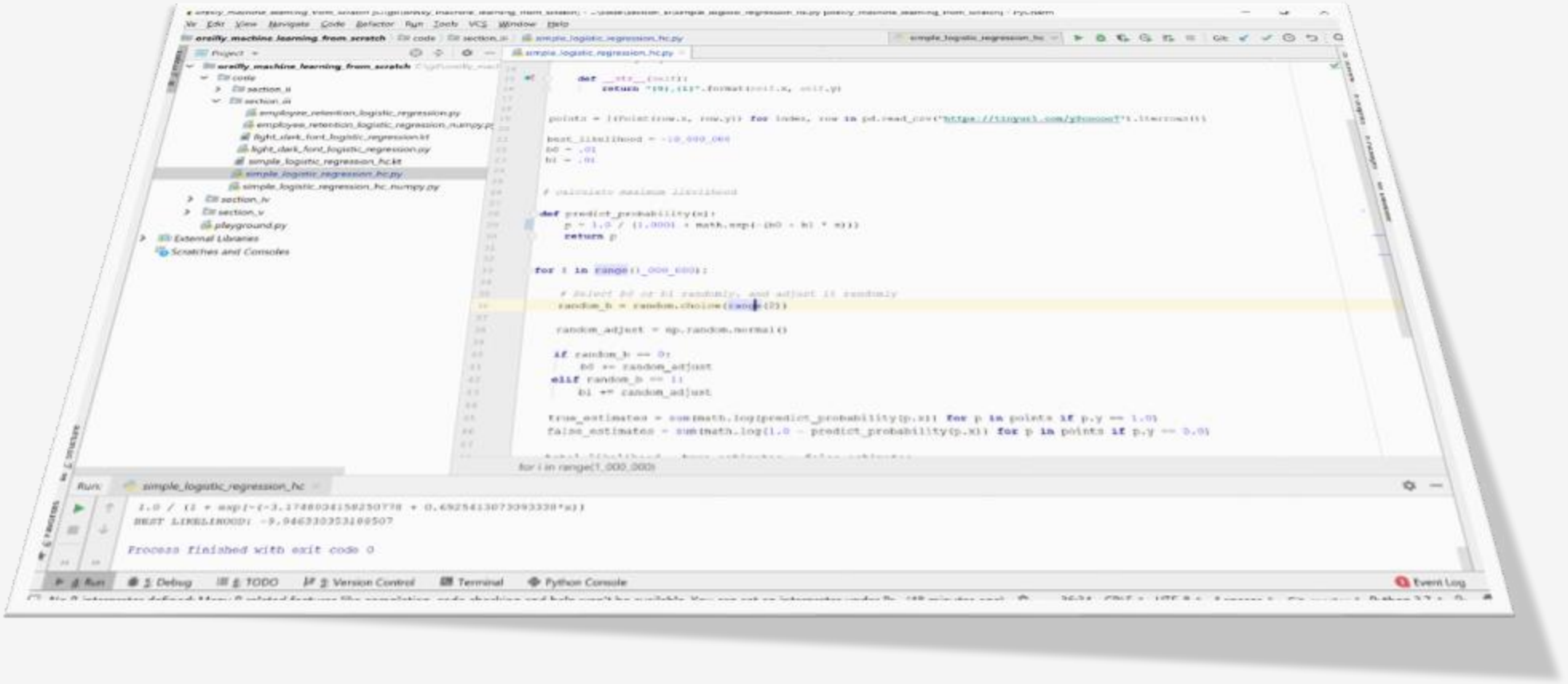
Maximum Likelihood

We now know how to calculate the likelihood for a given set of parameters.

To calculate the maximum likelihood…

1. Randomly adjust the β_0 and β_1 values (using hill-climbing, gradient descent, or other optimization)
2. Calculate the likelihood (as shown in the previous slide)
3. If the likelihood improves, keep the changes to β_0 and β_1 , otherwise revert.
4. Do this for as many iterations as necessary, until the likelihood stops improving.

Hands-On: Logistic Regression



Multivariable Logistic Regression

We can easily extend logistic regression to handle multiple independent variables, simply by adding more β_x variables for each additional variable.

We then solve for those β_x variables the same way as before.

$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \ldots + \beta_n x_n)}}$$

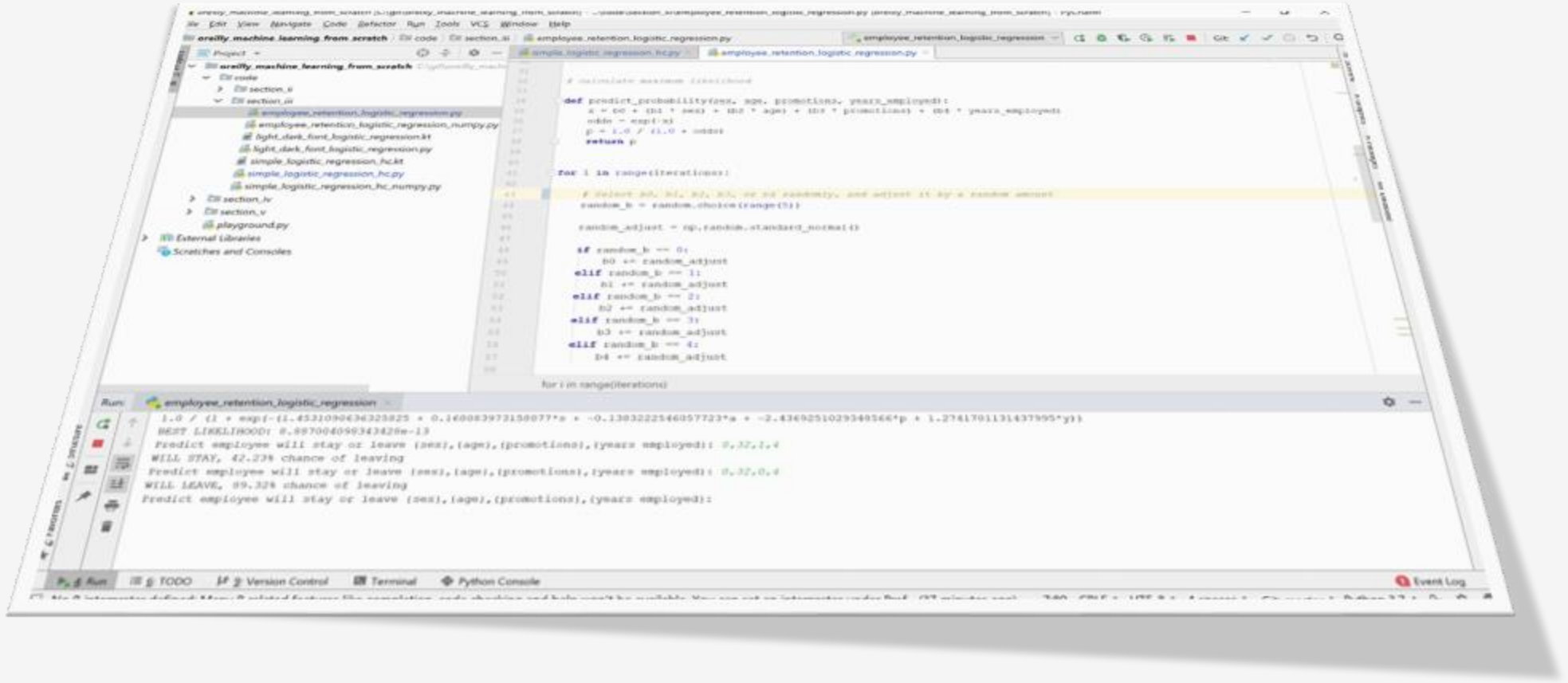
Multivariable Logistic Regression

We have some historical employee data (https://tinyurl.com/y6r7qjrp) and want to use it to predict whether an employee will quit or not.

SEX, AGE, $PROMOTIONS$, and $YEARS\_EMPLOYED$ are the predictor variables, and DID_QUIT is the outcome variable where 1 = true and 0 = false.

SEX	AGE	PROMOTIONS	YEARS_EMPLOYED	DID_QUIT
1	43	4	10	0
1	38	3	8	0
1	44	4	11	1
0	41	2	6	0
1	45	2	6	1
0	36	3	9	0
1	33	1	3	0
1	44	3	10	0
…				

Hands-On: Multivariable Logistic Regression



Using Logistic Regression for Classification

Logistic regression may seem limited in that it only supports two categories: true (1) or false (0).

But you can make it support any number of categories!

To use logistic regression for more than two categories:

1. Build a separate logistic regression for each category, where a given item belongs to that category (1) or doesn't belong to that category (0).

2. To predict which category an item belongs to, pass it through each category's logistic regression, and choose the one with the highest probability.

Exercise: "There's No Correlation"

It is one day from a manned space launch.

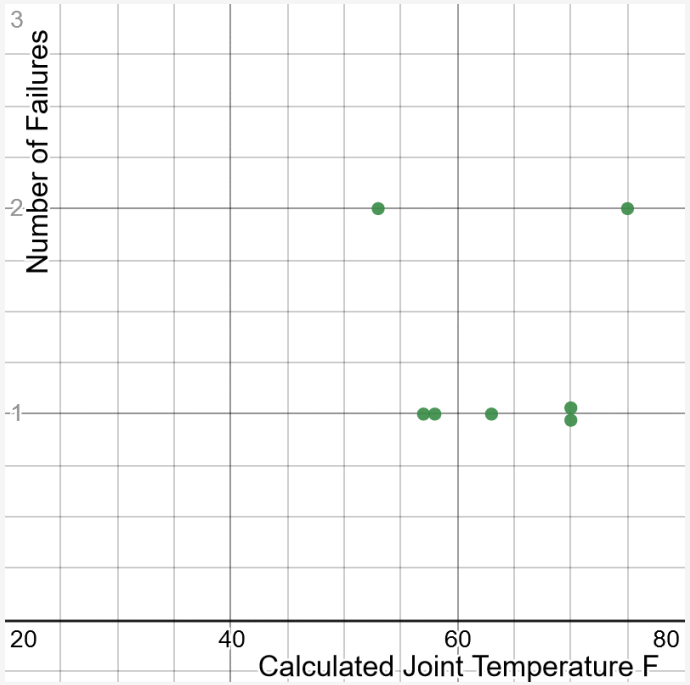
However, your engineering team has been expressing concern about the O-Rings that seal rocket gases from releasing, and whether they perform in colder temperatures.

You share this concern with other parties and are provided data of all 7 O-Ring failures from 24 launches and the temperature (shown to the right).

The consensus from other parties is there is no correlation between number of failures and temperature.

Is this assessment correct?

temperature	o_ring_failures
53	2
57	1
58	1
63	1
70	1
70	1
75	2



Data Source: http://www.math.usu.edu/~symanzik/teaching/2009_stat6560/RDataAndScripts/sharif_abbass_project1_challenger.csv

Exercise: "There's No Correlation"

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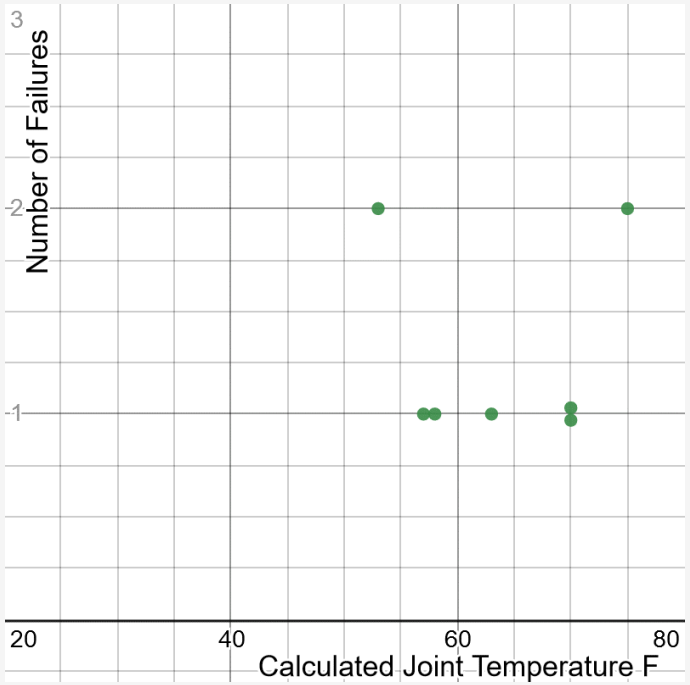
However, your engineering team has been expressing concern about the O-Rings that seal rocket gases from releasing, and whether they perform in colder temperatures.

You share this concern with other parties and are provided data of all **7 O-Ring failures** from **24 launches** and the temperature (shown to the right).

The consensus from other parties is there is no correlation between number of failures and temperature.

Is this assessment correct? **Is anything missing**?

temperature	o_ring_failures
53	2
57	1
58	1
63	1
70	1
70	1
75	2



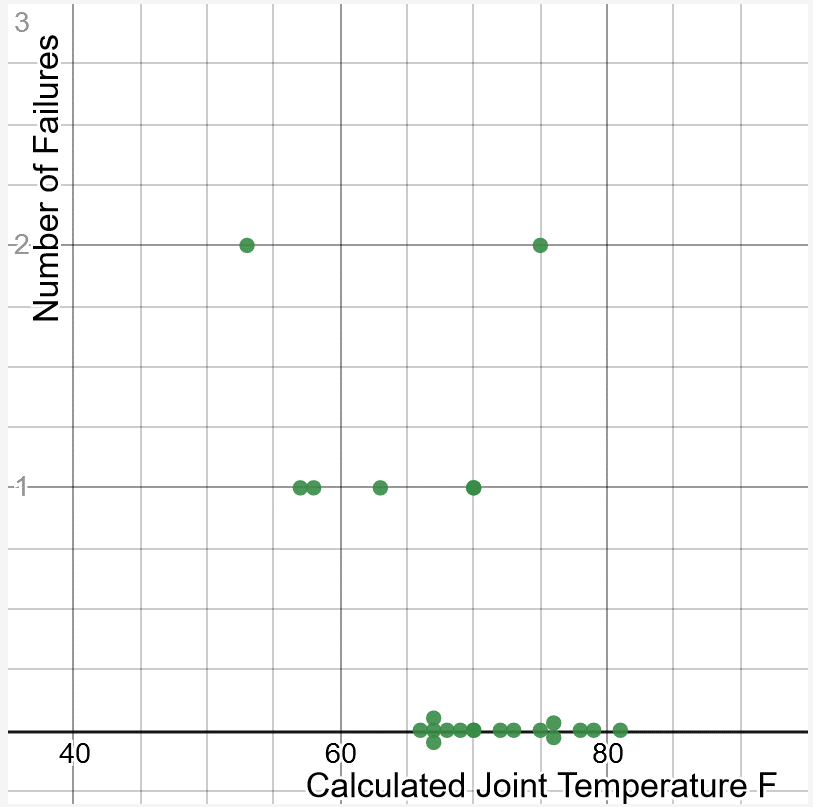
Data Source: http://www.math.usu.edu/~symanzik/teaching/2009_stat6560/RDataAndScripts/sharif_abbass_project1_challenger.csv

Exercise: "There's No Correlation"

Notice that data from successful launches were not included, which may tell an entirely different story.

What are your thoughts now? Is there a correlation? Is there a model that can be used to predict risk?

temperature	o_ring_failures
53	2
57	1
58	1
63	1
66	0
67	0
67	0
67	0
68	0
69	0
70	1
70	0
70	1
70	0
72	0
73	0
75	0
75	2
76	0
76	0
78	0
79	0
81	0



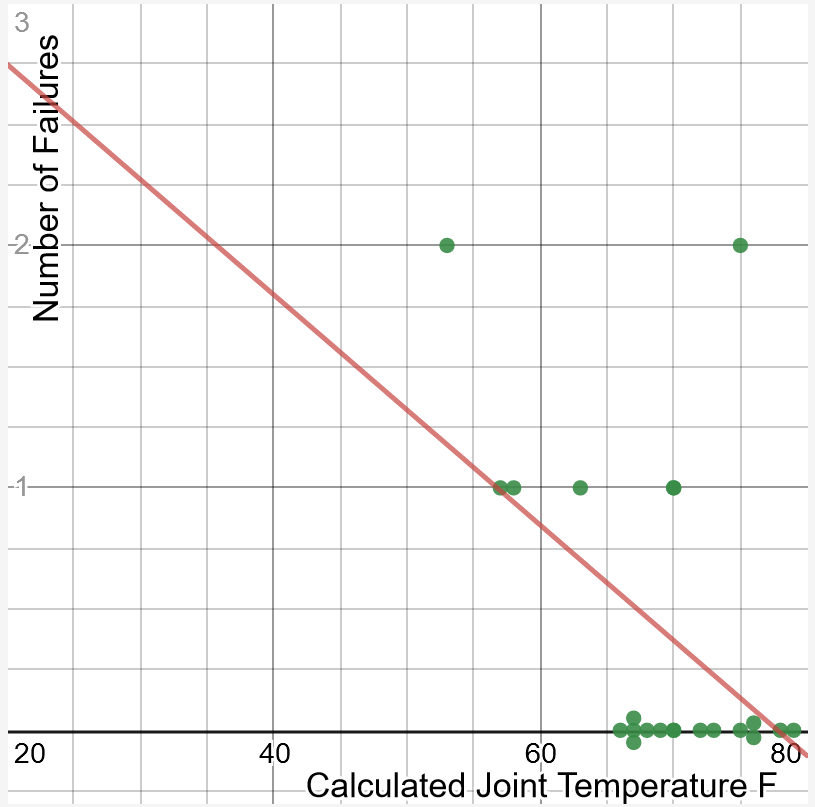
Exercise: "There's No Correlation"

You can try to apply a linear regression here, and while it does show a trend it is a little awkward especially since our data is sparse.

Should we transform our data somehow?

Are there any other models we can try?

temperature	o_ring_failures
53	2
57	1
58	1
63	1
66	0
67	0
67	0
67	0
68	0
69	0
70	1
70	0
70	1
70	0
72	0
73	0
75	0
75	2
76	0
76	0
78	0
79	0
81	0



Linear Regression Source Code

```
import pandas as pd
from sklearn.linear_model import LinearRegression

# Learn more: https://scikit-
learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html

# Import points

df = pd.read_csv('https://bit.ly/2DgjTk5', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Plain ordinary least squares
fit = LinearRegression().fit(X, Y)

# Print "m" and "b" coefficients
print("m = {0}".format(fit.coef_.flatten()))
print("b = {0}".format(fit.intercept_.flatten()))
```

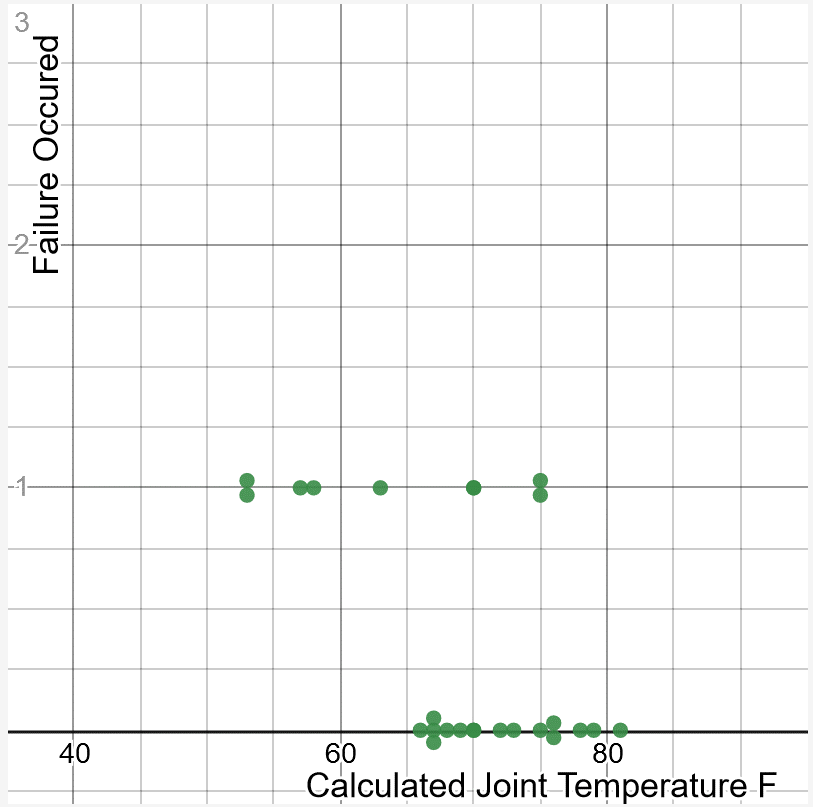
Exercise: “There’s No Correlation”

What if we converted the data to be binary, showing whether a failure occurred or not occurred, by separating each instance into its own record?

This reduces the domain of output variables to “0” and “1” creating a binary model.

Is a story now becoming clear? What model can we use to predict probability of failure at a given temperature?

temperature	o_ring_failures
53	1
53	1
57	1
58	1
63	1
66	0
67	0
67	0
67	0
68	0
69	0
70	1
70	0
70	1
70	0
72	0
73	0
75	0
75	1
75	1
76	0
76	0
78	0
79	0
81	0



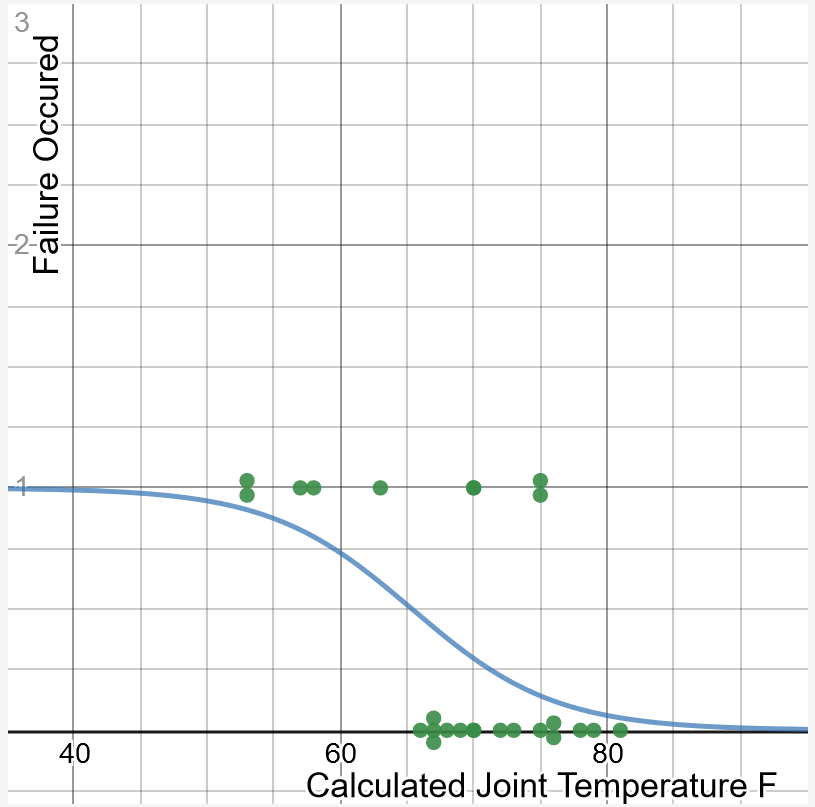
Exercise: "There's No Correlation"

Logistic regression might be the best way to model this risk.

Even though we lack freezing temperature data, the logistic regression points to a high probability of risk for O-ring failure.

If our launch is going to happen in freezing temperatures, this does not bode well.

temperature	o_ring_failures
53	1
53	1
57	1
58	1
63	1
66	0
67	0
67	0
67	0
68	0
69	0
70	1
70	0
70	1
70	0
72	0
73	0
75	0
75	1
75	1
76	0
76	0
78	0
79	0
81	0



Exercise: “There’s No Correlation”

This is exactly what happened to the space shuttle Challenger on January 28, 1986, and if you already have not figured out already, we are doing the analysis.

Through a series of unfortunate events, only partial data was accessible and omitted non-failure data, which showed a correlation with temperature and O-ring failure.

The analysis we just did should have happened before the accident, but unfortunately it occurred afterwards.

LESSON LEARNED: Don’t take your data at face value, ask where it came from and how it needs to be reshaped.

The space shuttle Challenger just moments before disaster on January 28, 1986 (above) and Richard Feynman famously demonstrating O-ring failure with a glass of ice water (left).

Space Shuttle Challenger: Logistic Regression Source Code

```
import numpy as np
import pandas as pd
import plotly.graph_objects as go
from sklearn.linear_model import LogisticRegression

# Load the data
df = pd.read_csv("https://bit.ly/2DgjTk5", delimiter=",")

# Duplicate and convert records to have binary outcomes
df = df.loc[df.index.repeat(df["o_ring_failures"])].append(df[df["o_ring_failures"] == 0])
df.loc[(df["o_ring_failures"] > 0), 'o_ring_failures'] = 1


# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]


model = LogisticRegression()
model.fit(X, Y)

# Print "m" and "b" coefficients
print("m = {0}".format(model.coef_.flatten()))
print("b = {0}".format(model.intercept_.flatten()))

# Plot results
fig = go.Figure()
fig.add_trace(go.Scatter(x=df["temperature"], y = df["o_ring_failures"], mode='markers', name="Observations"))
fig.add_trace(go.Scatter(x=np.arange(0.0,90.0,.1),
                         y= model.predict_proba(np.arange(0.0,90.0,.1).reshape(-1, 1))[:,-1],
                         mode='lines',
                         name='Logistic Regression'))
fig.show()
```

Quiz Time!

Logistic regression will only output a probability between 0 and 1 that an event will happen.

1) True

2) False

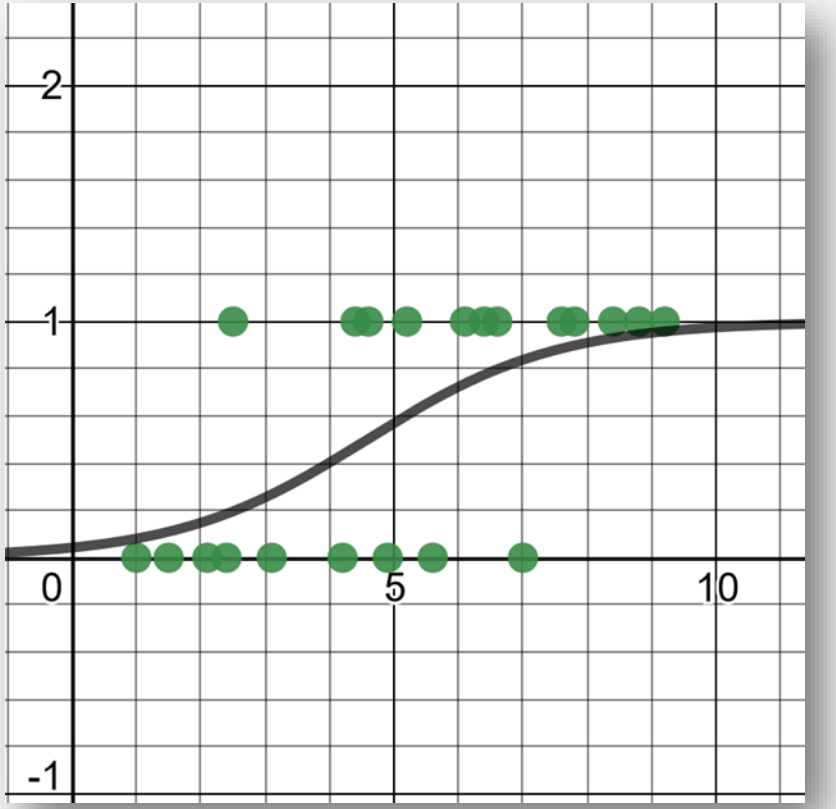
Quiz Time!

Logistic regression will only output a probability between 0 and 1 that an event will happen.

1) True

Like any probability model, logistic regression will output a percentage between 0 and 1

2) False



Quiz Time!

Logistic regression cannot be used for more than two categories.

A) True

B) False

Quiz Time!

Logistic regression cannot be used for more than two categories.

A) True

B) False

Logistic regression can support more than one category by doing a separate logistic regression for each category, and predicting the one that yields the highest probability.

Section IV
Naïve Bayes

What is Naïve Bayes?

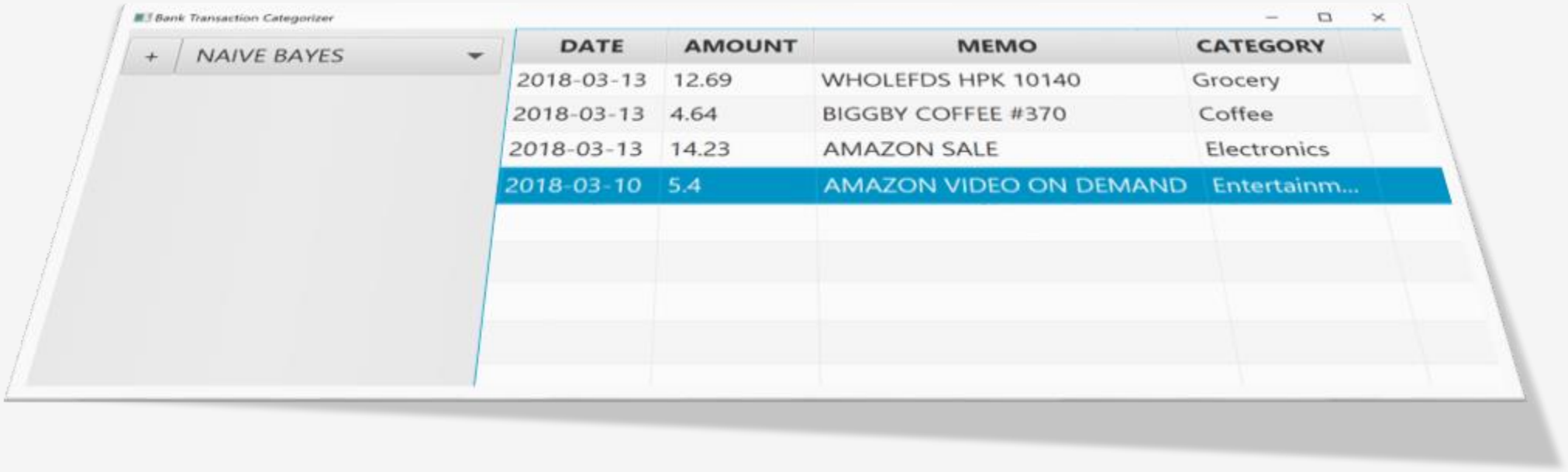
Naïve Bayes is a machine learning application of Bayes Theorem that merges probabilities of multiple features to predict a given category.

It is often used to classify text (e.g. email spam/not spam), which is the exercise the we will be doing today.

- Naïve Bayes is effective because it learns quickly, even with little data.
- Naive Bayes works by mapping probabilities of each individual feature occurring/not occurring for a given category (e.g. a word occurring in spam/not spam).
- While commonly used for discrete variables like words, it can also be used with continuous variables using statistical distributions (we will not cover this today).

Thomas Bayes, the inventor of Bayes Theorem

Demo: Categorizing Bank Transactions



How to Build a Naïve Bayes Text Classifier

To predict a category for a new set of features:

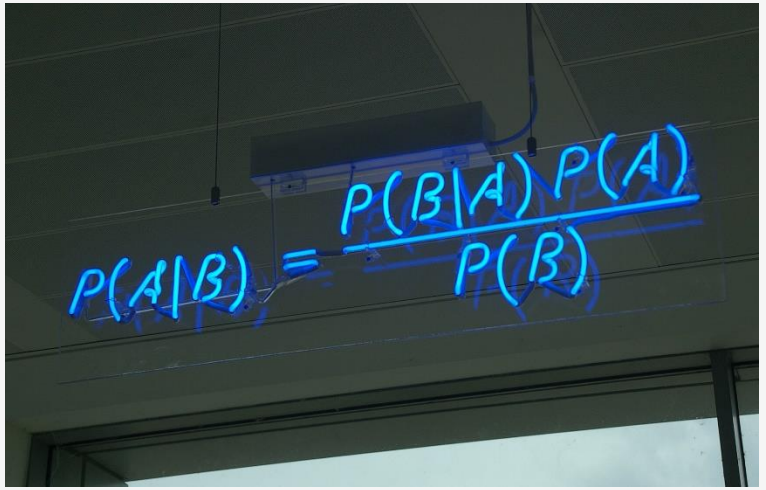
1) For a given category (like ***spam, grocery,*** etc), combine the probabilities of each feature ***occurring*** and ***not occurring*** by multiplying them.

$$Occur\ Product = P_{f1} * P_{f2} * P_{f3} * \ldots * P_{fn}$$

$$Not\ Occur\ Product = (1 - P_{f1}) * (1 - P_{f2}) * (1 - P_{f3}) * \ldots * (1 - P_{fn})$$

2) Combine the probabilities above with this division operation:

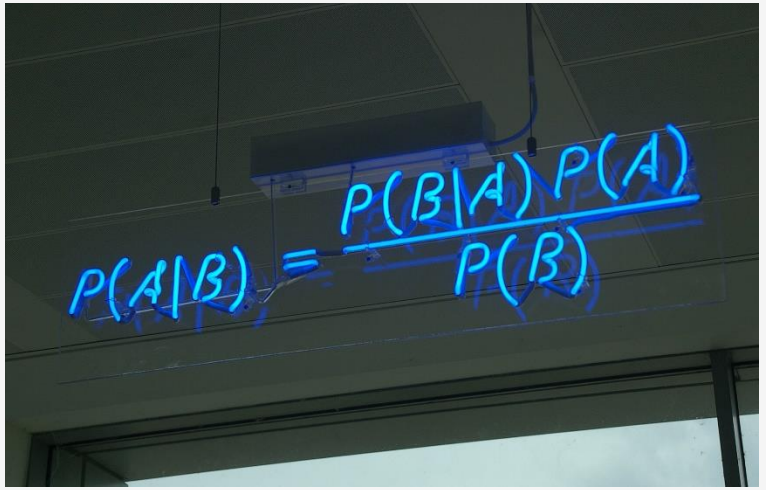
$$Combined\ Probability = \frac{(Occur\ Product)}{(Occur\ Product) + (Not\ Occur\ Product)}$$



How to Build a Naïve Bayes Text Classifier

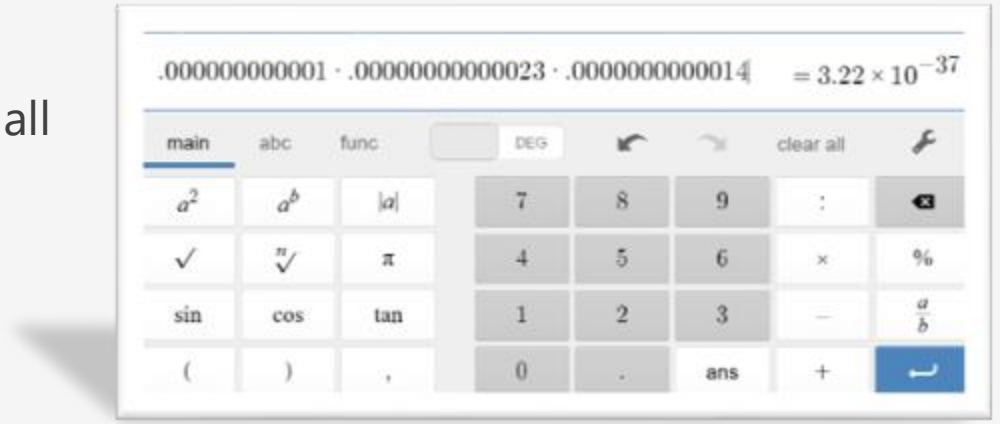
3) Calculate the combined probability for every category, and the one that is the highest is the category you predict.

Easy right? But there is one complication…



Dealing with Floating Point Underflow

Remember in logistic regression where we had floating point underflow issues, where multiplying small decimals gets so small the computer cannot handle them?



- We can remedy the issue here too by using logarithmic addition rather than multiplication.

- Transform each probability with a $\log()$ or $\ln()$ function and then sum them, then call $\exp()$ to convert the result back!

Dealing with Floating Point Underflow

$P_{fx} = Probability\ of\ feature$ x

$$Occur\ Product = exp(log(P_{f1}) + log(P_{f2}) + log(P_{f3}) + log(P_{fn}))$$

$$Not\ Occur\ Product = \exp(log(1 - P_{f1}) + log(1 - P_{f2}) + log(1 - P_{f3}) + \ldots + log(1 - P_{fn}))$$

$$Combined\ Probability = \frac{(Occur\ Product)}{(Occur\ Product) + (Not\ Occur\ Product)}$$

One More Thing…

Never let a feature have a zero probability, so add some small constants to the numerator and denominator like 0.1 and 0.2 to make a default probability.

"Fudging" the numbers in machine learning can be acceptable since machine learning deals with estimates anyway.

You can make these numbers smaller if you like.

$$Feature\ Probability\ = \frac{0.1 + (Occur\ Probability)}{0.2 + \ (Occur\ Probability) + (Not\ Occur\ Probability)}$$

Final Naïve Bayes Formulation

$P_{fx} = Probability\ of\ feature$ x, *with a fudged constant in numerator and denominator*

$$Occur\ Product = exp(log(P_{f1}) + log(P_{f2}) + log(P_{f3}) + log(P_{fn}))$$

$$Not\ Occur\ Product = \exp(log(1 - P_{f1}) + log(1 - P_{f2}) + log(1 - P_{f3}) + \ldots + log(1 - P_{fn}))$$

$$Combined\ Probability = \frac{(Occur\ Product)}{(Occur\ Product) + (Not\ Occur\ Product)}$$

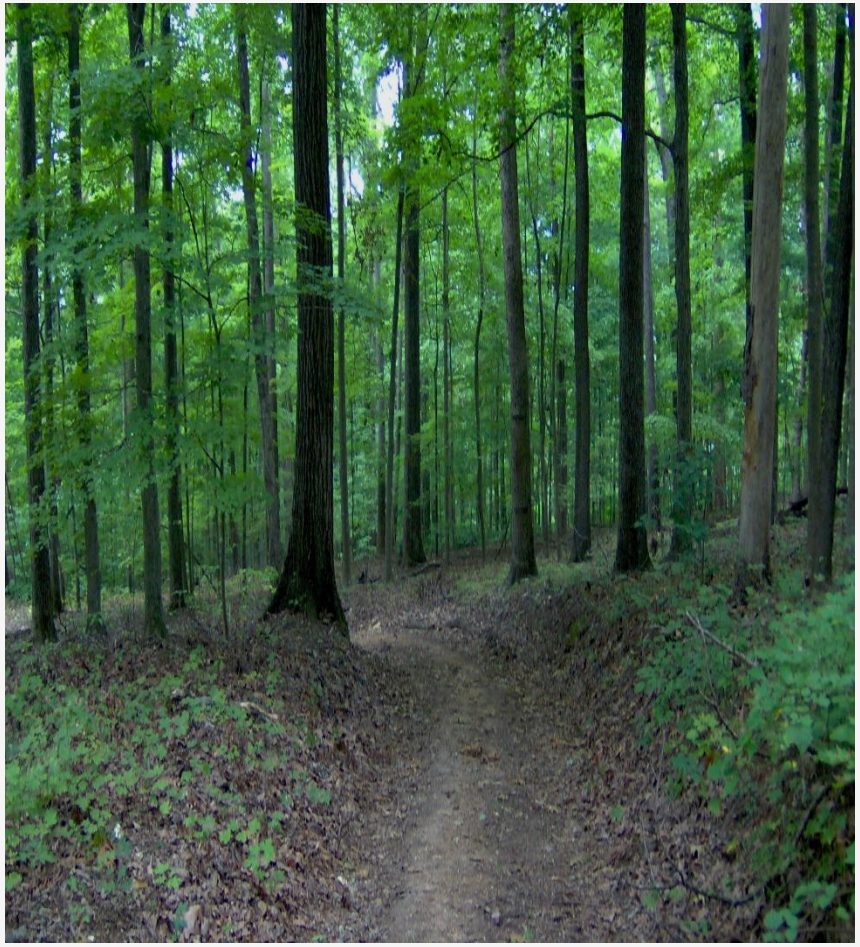
Section V
Decision Trees and Random Forests

What Are Decision Trees?

Decision trees are a powerful machine learning tool and work well for a lot of machine learning problems.

As a matter of fact, decisions trees work so well they are notorious for overfitting.

- This can be remedied with random forests which generates hundreds of decision trees with randomly sampled data.
- Decision trees can also be improved with gradient boosting and other techniques.
- Other flavors of decision trees exist, like regression trees.



Decision Tree Intuition

We have some weather data and labeled each record as being “1” (good weather) or “0” (bad weather).

We could solve this using a logistic regression but let us try using decision trees instead.

RAIN	LIGHTNING	CLOUDY	TEMPERATURE	GOOD_WEATHER_IND
0	1	1	74	0
0	0	0	69	1
1	0	1	58	0
0	0	0	71	1
0	0	0	73	1
0	1	1	80	0
0	1	1	74	0
0	0	0	73	1
…				

Decision Tree Intuition

Start with the variable that is most likely to separate good weather and bad weather as best as possible.

For reasons we will discuss later, you determine ***RAIN*** is good at separating good weather and bad weather, so you bucket records like this:

RAIN	
YES	NO
0/16	14/20

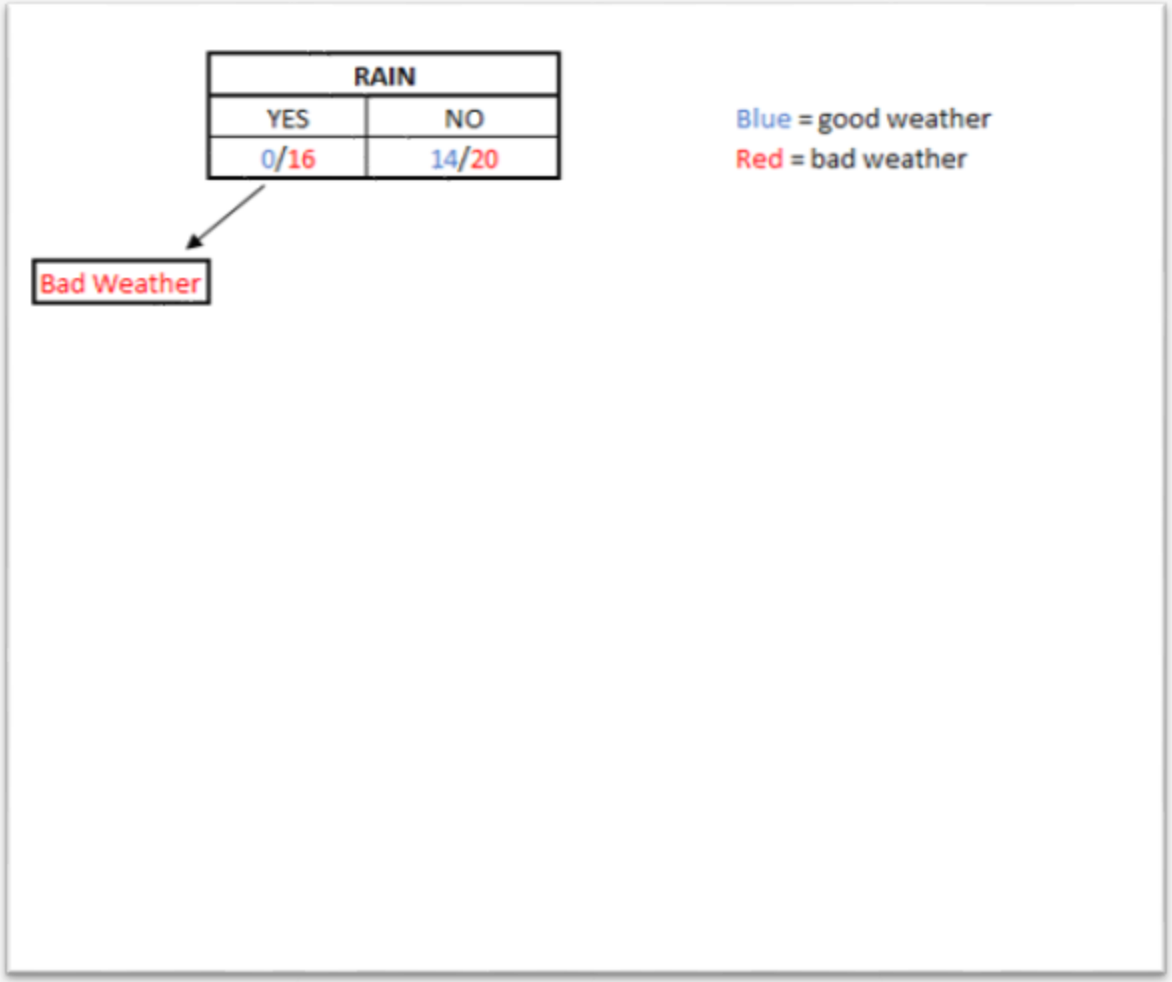
Blue = good weather

Red = bad weather

Decision Tree Intuition

Since all records where ***RAIN*** was present always yielded bad weather, we will simply predict any new record with ***RAIN*** as bad weather.

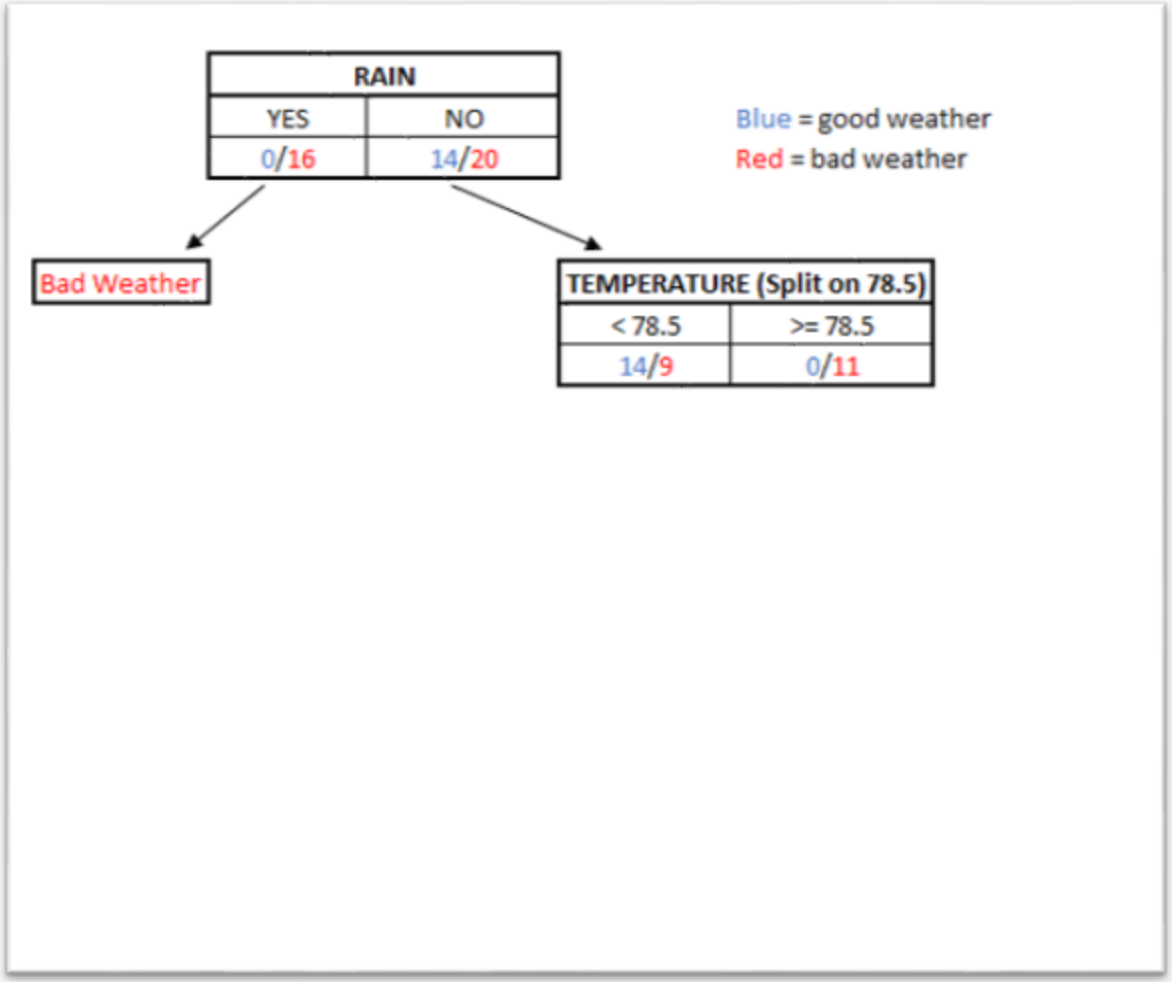
However, records that did not have ***RAIN*** are mixed, where some are good weather, and others are bad weather. These will need to be split again.



Decision Tree Intuition

We take records that did not have ***RAIN*** and now split them on ***TEMPERATURE***.

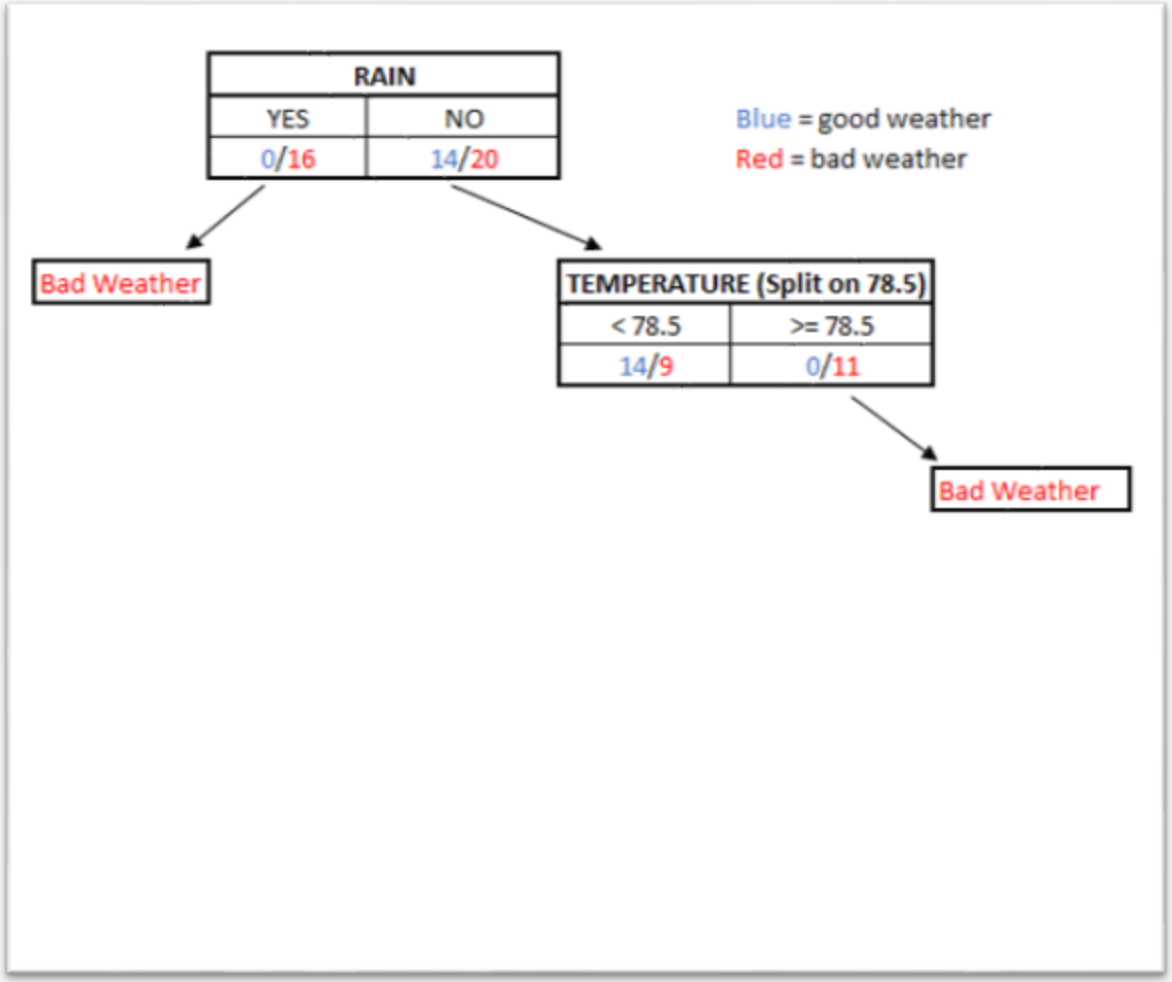
Since ***TEMPERATURE*** is continuous and not a simple *yes/no* binary, we split on a value 78.5 that optimizes the split (more on this later).



Decision Tree Intuition

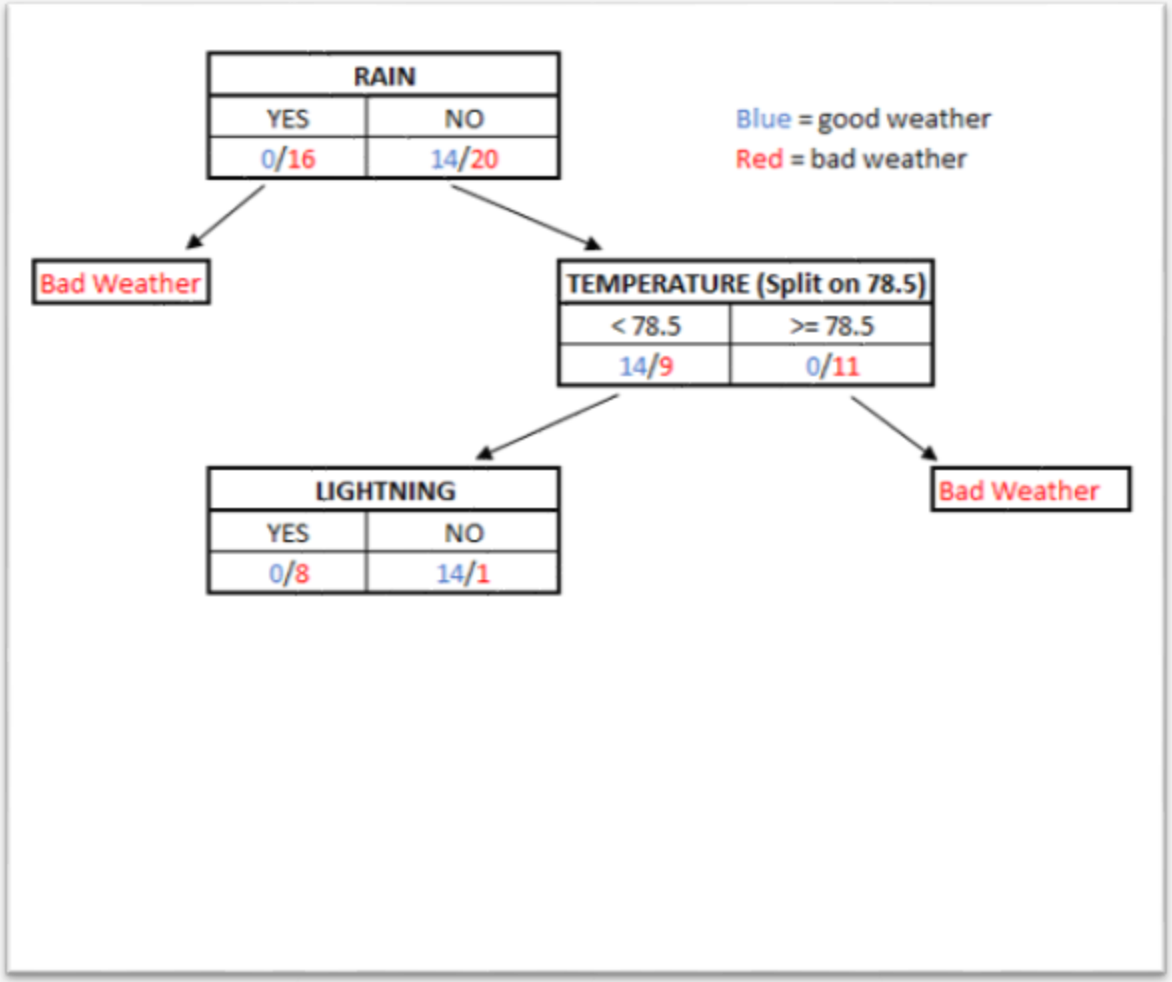
Notice how all records with ***TEMPERATURE*** greater than/equal to 78.5 are bad weather, so we will predict any records with a ***TEMPERATURE*** at least 78.5 as bad weather.

But records with a ***TEMPERATURE*** less than 78.5 have a mix of good weather and bad weather. So we need to split those again.



Decision Tree Intuition

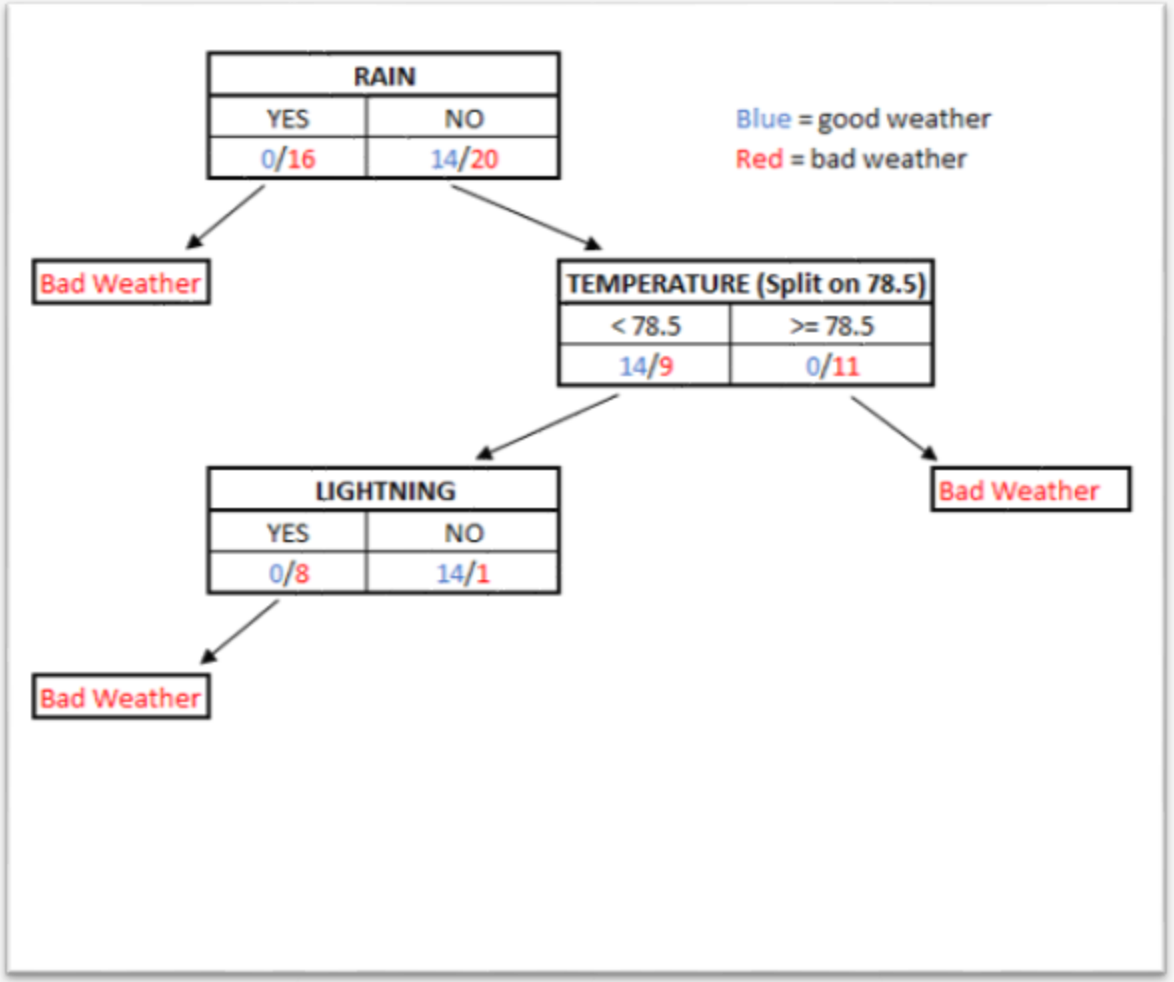
We take those records with ***TEMPERATURE*** less than 78.5 and now split them on whether ***LIGHTNING*** was present.



Decision Tree Intuition

We take those records with ***TEMPERATURE*** less than 78.5 and now split them on whether ***LIGHTNING*** was present.

Notice how all records with ***LIGHTNING*** are labelled as bad weather, so we can predict any new record with ***LIGHTNING*** as bad weather.

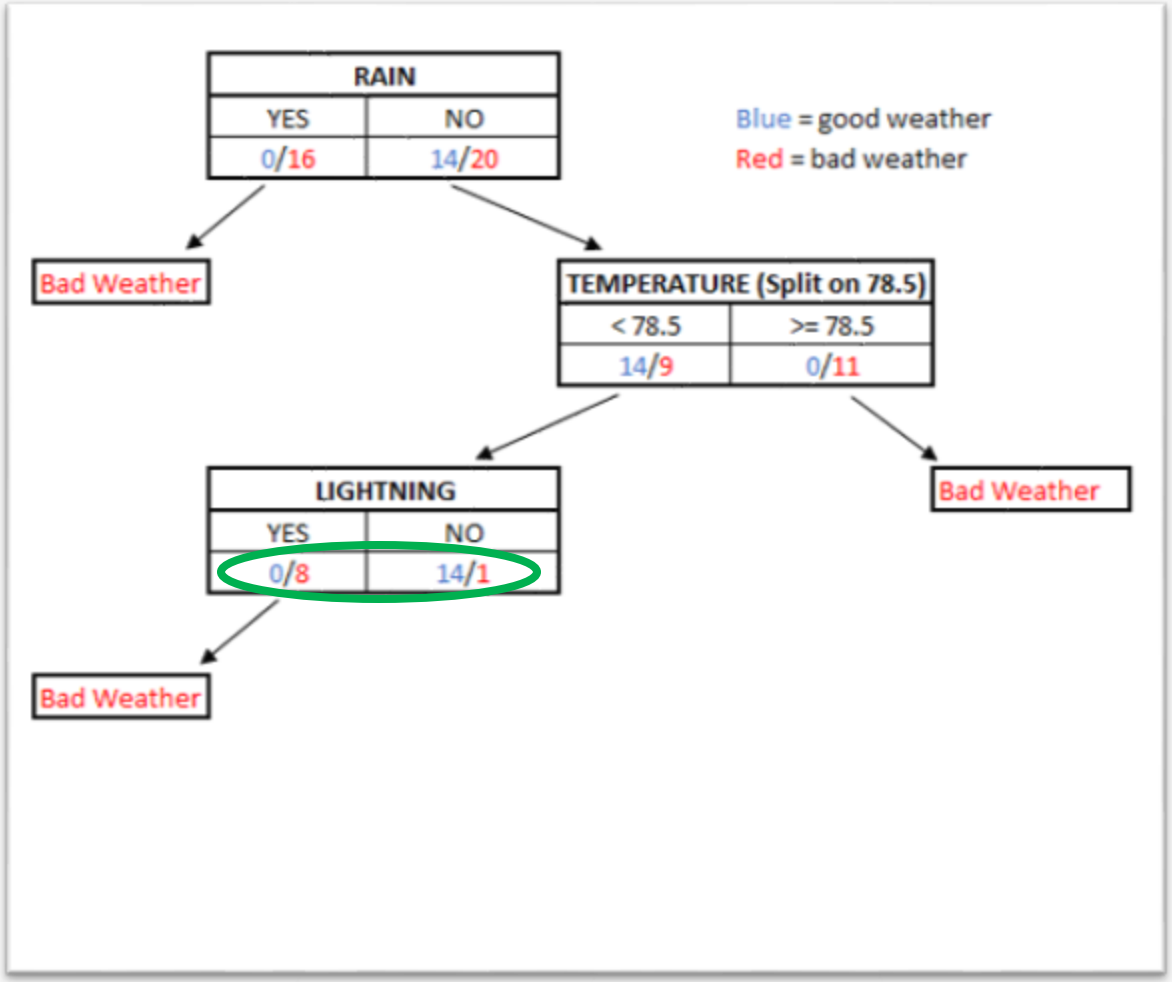


Decision Tree Intuition

We take those records with ***TEMPERATURE*** less than 78.5 and now split them on whether ***LIGHTNING*** was present.

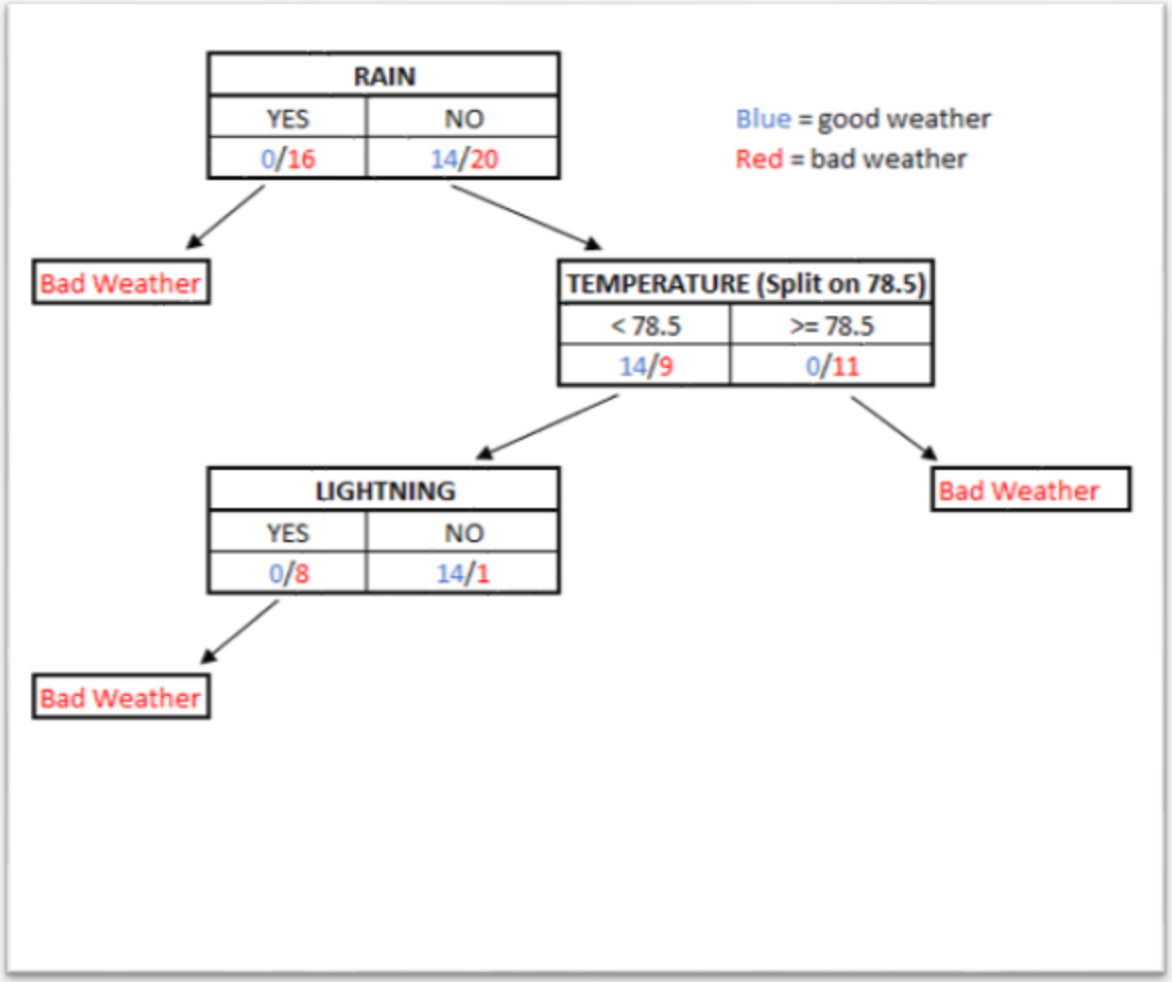
Notice how all records with ***LIGHTNING*** are labelled as bad weather, so we can predict any new record with ***LIGHTNING*** as bad weather.

Notice how close we are to a perfect clean split now!



Decision Tree Intuition

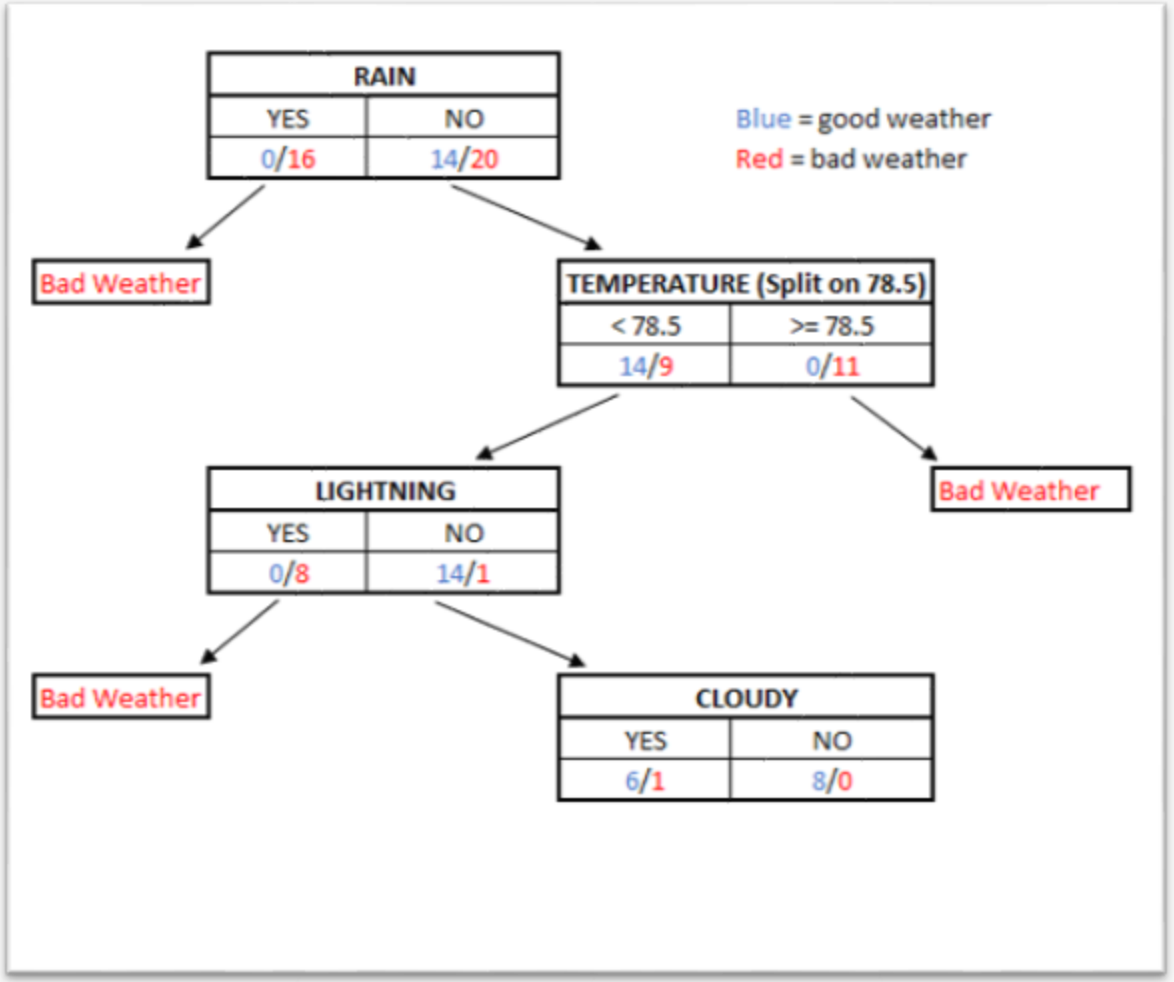
LIGHTNING almost gave us a perfect split, where lightning being present would predict bad weather and no lightning *almost* always meant good weather.



Decision Tree Intuition

LIGHTNING almost gave us a perfect split, where lightning being present would predict bad weather and no lightning *almost* always meant good weather.

We could probably stop here, but let's split these remaining records with no lightning. Finally we split on whether it was ***CLOUDY*** or not.

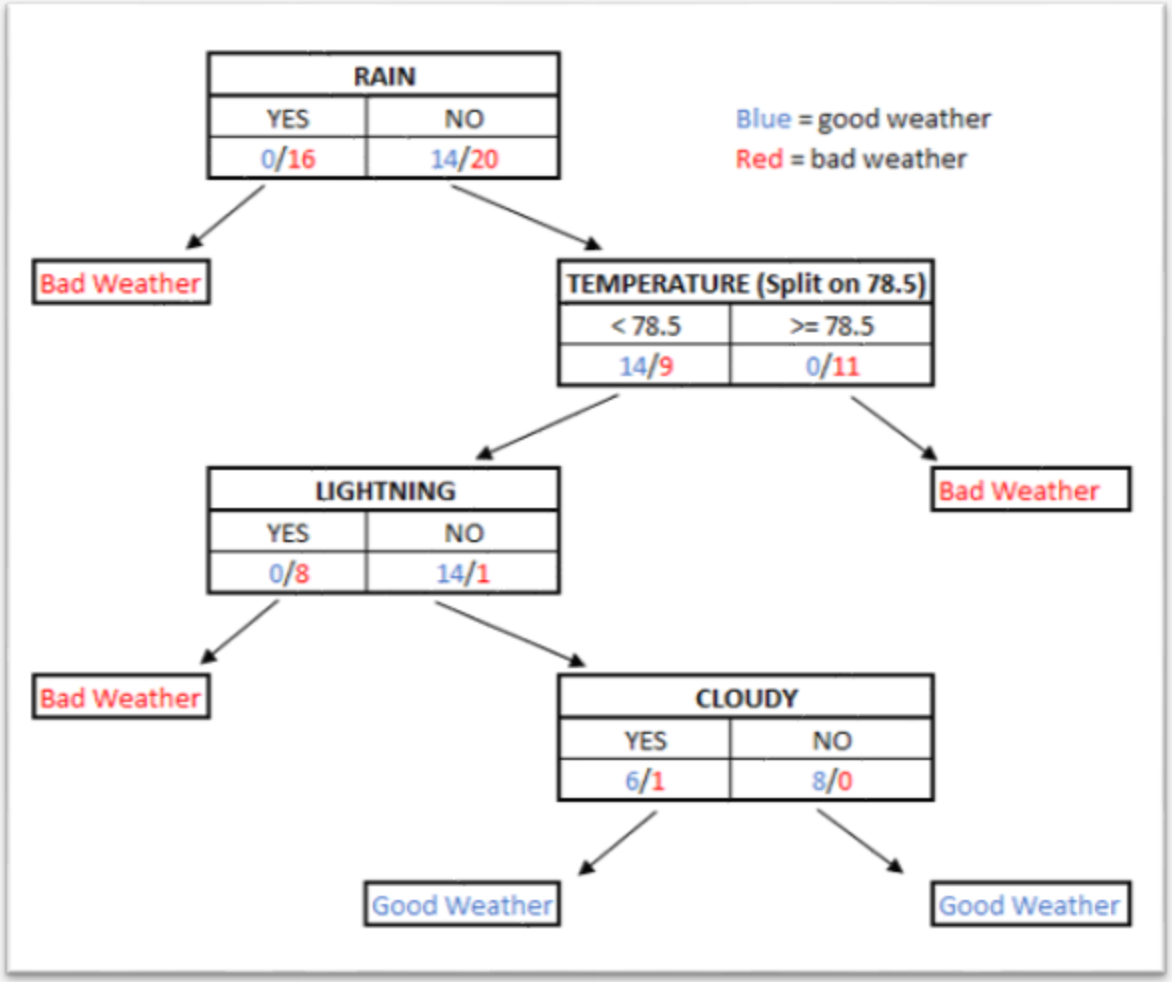


Decision Tree Intuition

At this point, we establish we cannot separate productively anymore and ***CLOUDY*** does not have any impact to our prediction.

It will always be good weather, given we already established there was no ***LIGHTNING***, the ***TEMPERATURE*** is less than 78.5, and there is no ***RAIN***.

Congratulations! We just built our first decision tree. But you might have a few questions…

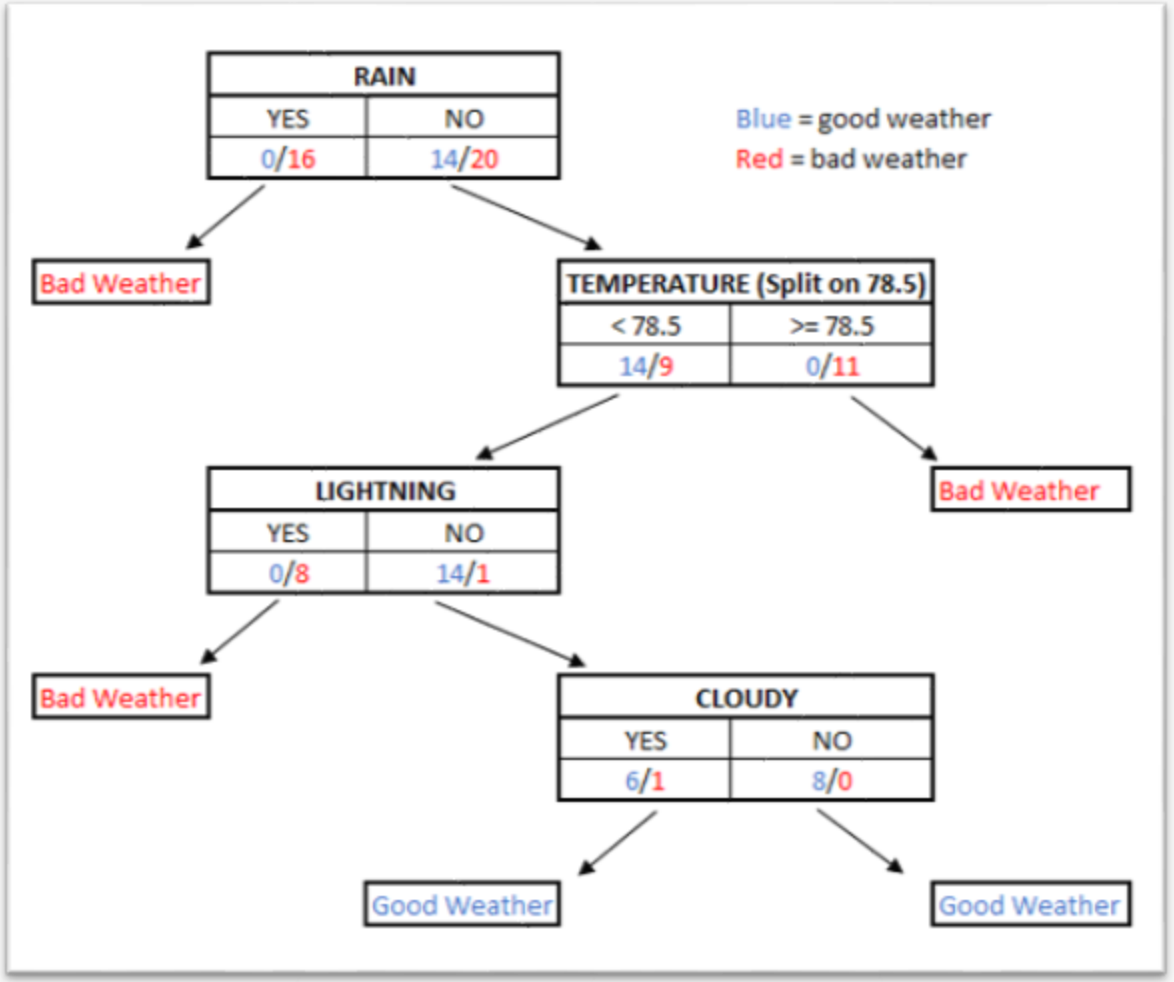


Decision Trees – Getting to the "Decision" Part

Hopefully by now, you have a strong intuition on what decision trees are trying to accomplish.

However, you may have some lingering questions on ***HOW*** to build a decision tree.

- At a given step, how do I determine which property is the best to split on?
- Where do I split continuous variables like ***TEMPERATURE***?
- When do I stop splitting and end my decision tree?



Gini Impurity

To build a decision tree, we must discuss the concept of **impurity** which describes how mixed something is.

EXAMPLE: If we have 6 dogs and 3 cats in a kennel, we do not purely have dogs or cats.

Gini Impurity is a common way to measure impurity using this function (for events *A* and *B*):

$$1 - (Probability\ of\ A)^2 - (Probability\ of\ B)^2$$

So the Gini impurity of dogs versus cats in the kennel:

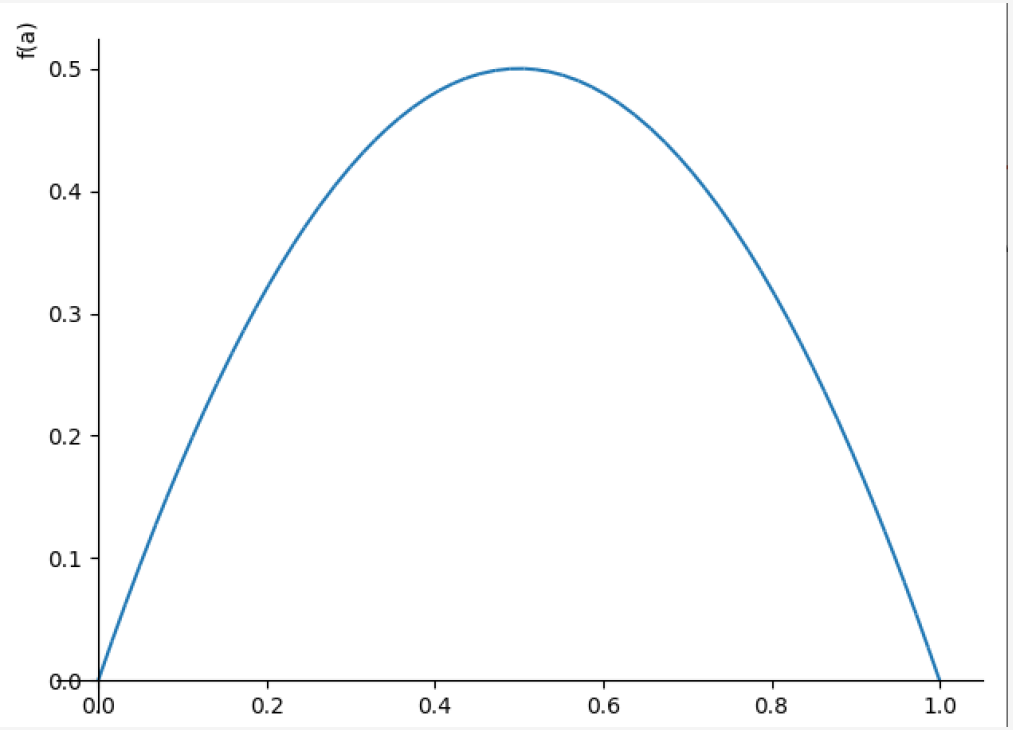
$$1 - \left(\frac{6}{6+3}\right)^2 - \left(\frac{3}{6+3}\right)^2 = .44444$$

Gini Impurity – Plotting for the Curious

The Gini impurity can never exceed 0.5, and this makes sense because having something 100% mixed (1.0) doesn't make sense.

To the right we use SymPy to plot the gini impurity function.

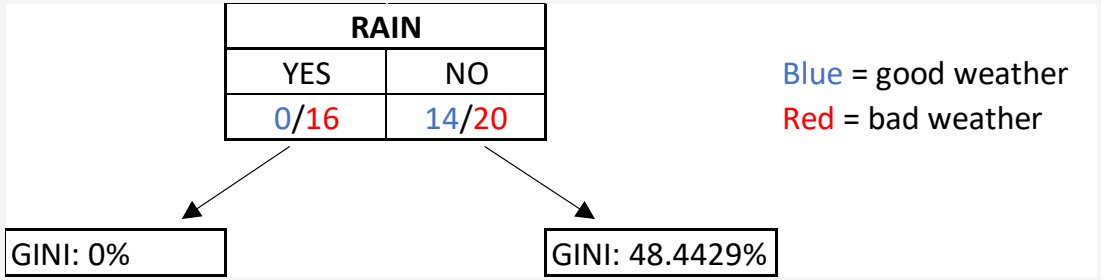
```
from sympy import *

a = symbols('a')
b = 1.0 - a
gini_impurity_f = 1 - a**2 - b**2
plot(gini_impurity_f, (a, 0, 1))
```



Gini Impurity

Going back to the weather example, here's how we look at Gini impurity for ***RAIN***.

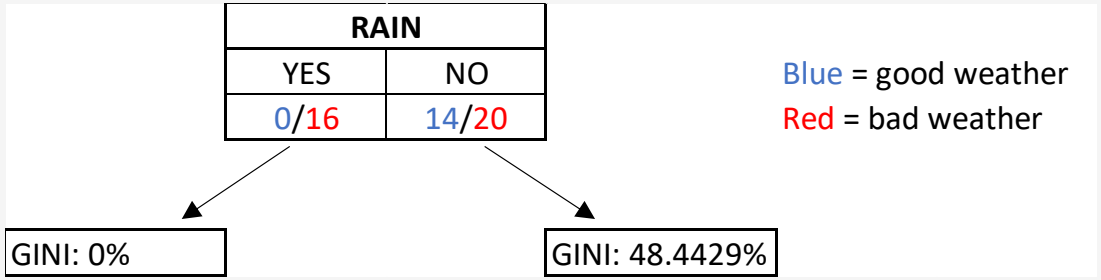
Notice how the impurity for "good/bad weather" on the YES side is 0% meaning it is pure.



$$1 - \left(\frac{0}{0+16}\right)^2 - \left(\frac{16}{0+16}\right)^2 = 0$$

Gini Impurity

Going back to the weather example, here's how we look at Gini impurity for ***RAIN***.



Notice how the impurity for "good/bad weather" on the YES side is 0% meaning it is pure.

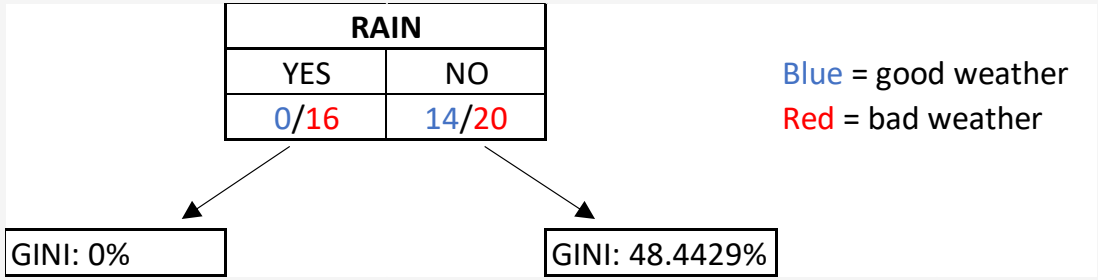
$$1 - \left(\frac{0}{0+16}\right)^2 - \left(\frac{16}{0+16}\right)^2 = 0$$

On the NO side we got an impurity of 48.4429%

$$1 - \left(\frac{14}{14+20}\right)^2 - \left(\frac{20}{14+20}\right)^2 = .484429$$

Weighing Gini Impurities

To calculate the entire impurity of using the ***RAIN*** property for a split, we weight these two impurities together.



$$0\ \frac{0+16}{0+16+14+20} + 0.484429\frac{14+20}{0+16+14+20} = .32941172$$

This is known as the **weighted average Gini impurity**, and it can be used as a measure of quality for splitting with that property. *Lowest impurity is best!*

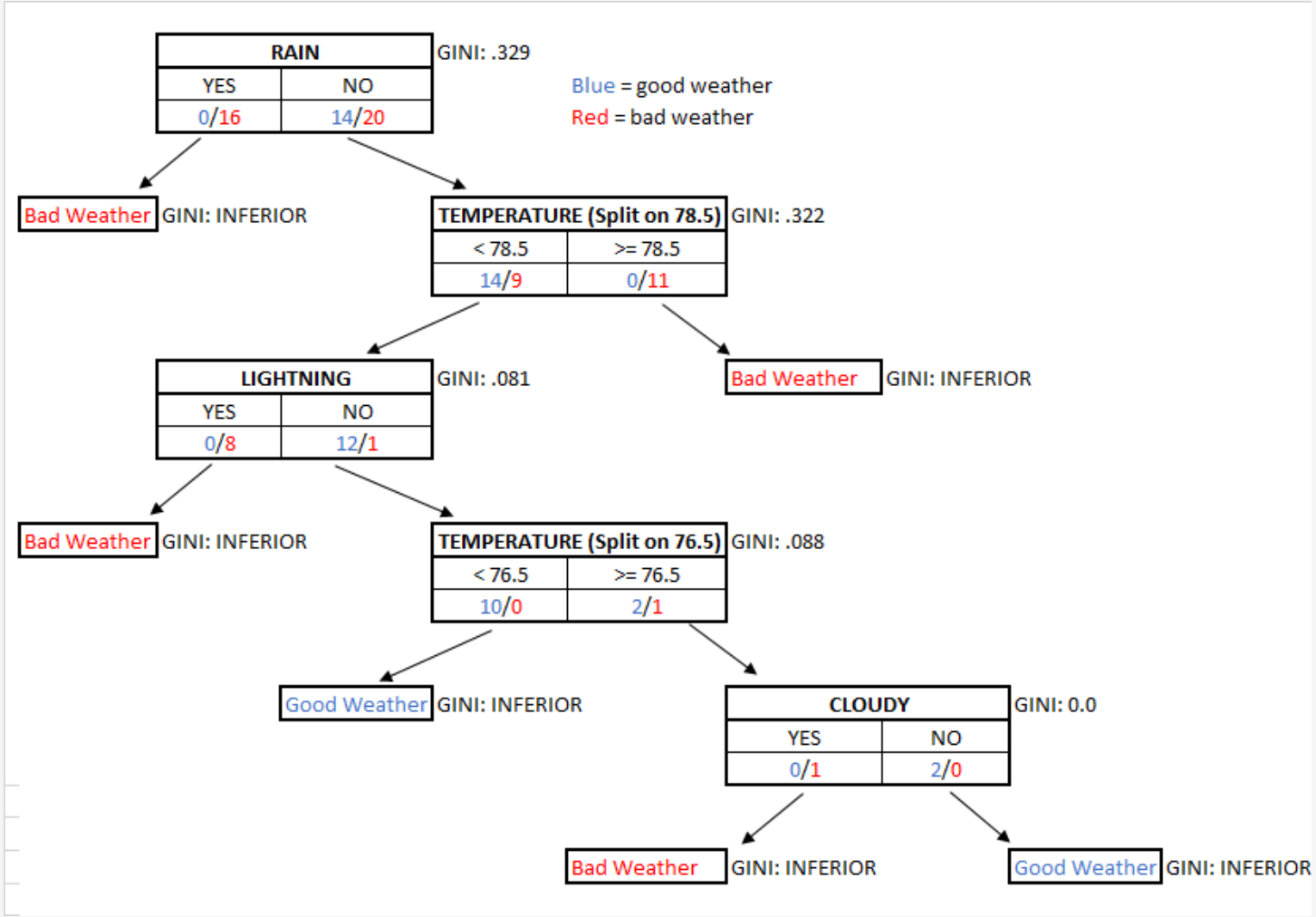
At every step we choose the property that provides the least weighted average Gini impurity.

Building a Decision Tree with GINI

At each decision, we choose the next property with the best GINI impurity and split on it

EXAMPLE: After ***RAIN,*** the property ***TEMPERATURE*** has the next best GINI for those 34 items on the "NO" side.

When the next property's weighted GINI is inferior to the previous GINI, we stop the branch there.



How to Split Continuous Variables?

Once you got the GINI and weighted GINI down, implementing a decision tree becomes relatively simple.

The goal always is to do a split that reduces the GINI impurity until it cannot be reduced anymore.

The only remaining question is how to split on continuous variables, which is not as straightforward as binary (true/false) or discrete (dog/cat/bird) variables.

Observe the following temperatures on the right. Any guesses on what is the best way to find the optimal split?

TEMERATURE
74
76
77
80
81
83
84

TEMPERATURE (Split on 78.5)	
< 78.5	>= 78.5
14/9	0/11

How to Split Continuous Variables?

Continuous variables extend the GINI concept further.

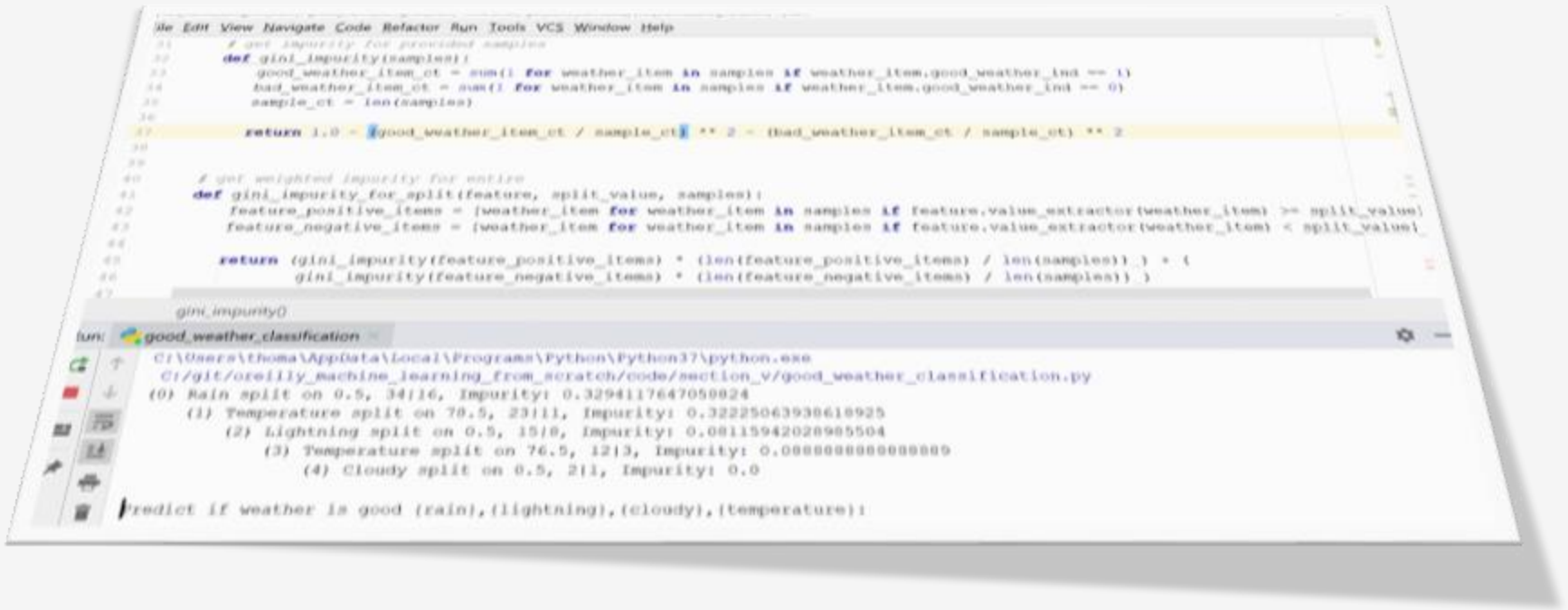
When you evaluate a continuous variable for its GINI, first sort the data for that variable then produce the rolling 2-value averages, each of which is a candidate for the split value.

Then choose the 2-value average that produces the best GINI impurity that splits on that value, which for the Temperature node we saw previously was 78.5.

TEMERATURE	ROLLING 2-VALUE AVG
74	
76	75
77	76.5
80	**78.5**
81	80.5
83	82
84	83.5

TEMPERATURE (Split on 78.5)	
< 78.5	>= 78.5
14/9	0/11

Hands On: Decision Trees



Decision Trees and Overfitting

Decision trees work well, so much they are notorious for overfitting.

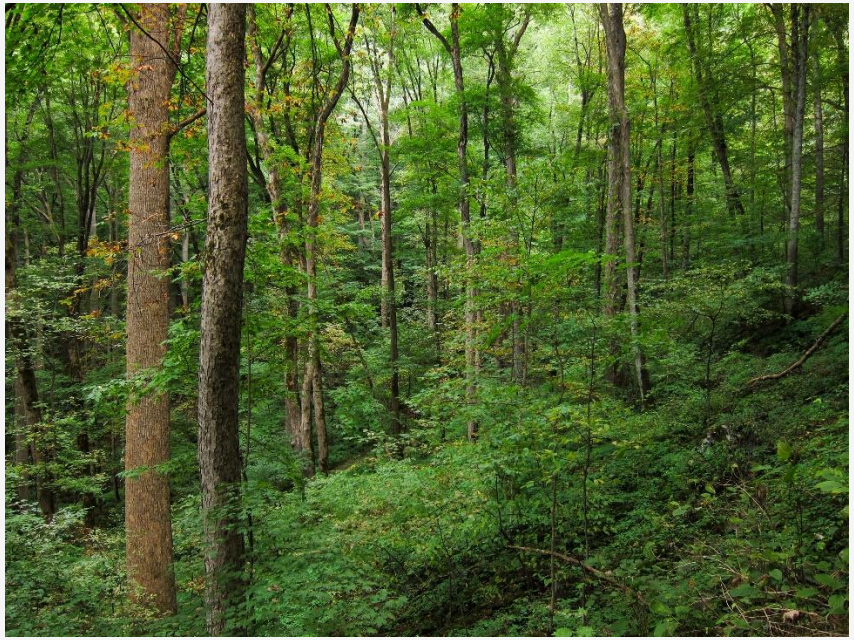
Overfitting again means the model fits to the training data too exactly, and therefore becomes unreliable for predicting new data.

One way to adapt decision trees to not overfit is to utilize random forests, which generates hundreds of decision trees with randomly sampled data and features.

This forces the model to use different subsets of data and properties, and therefore not overfit to the data set.

Random Forests

Random Forests are a machine learning technique that generates hundreds of decision trees, where each one builds off partial random data and properties, rather than all the data.



- Typically each decision tree will train with only 2/3 of the randomly sampled data, which is known as **bootstrapping**.
- You should also only consider a subset of variables when evaluating each node, forcing your decision tree to utilize other variables.
- You can use the other 1/3 of the data (known as the **"out-of-bag" data**) as the test data to evaluate prediction performance.

With these hundreds of decision trees built, you then have each tree "vote" on a prediction. The prediction with the highest votes wins.

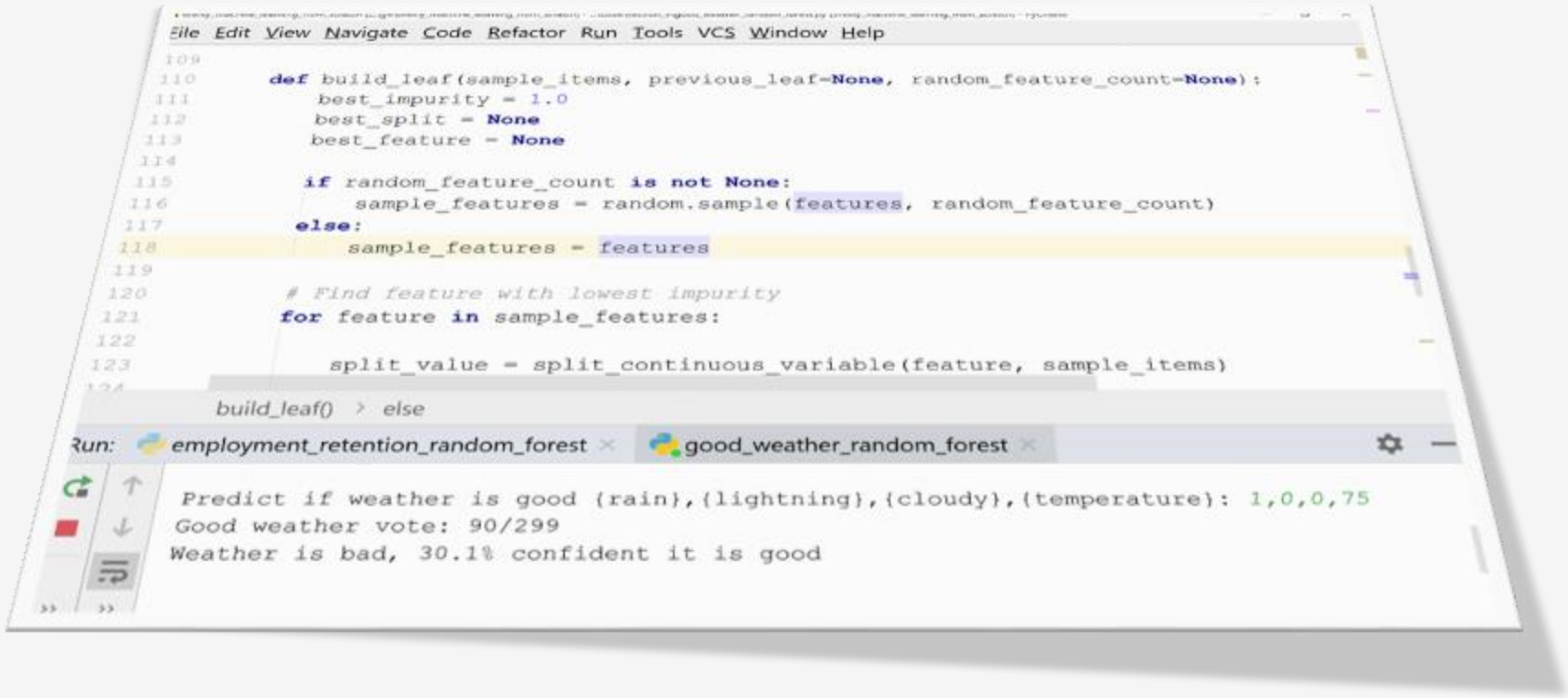
Fine-Tuning Random Forests

Because each decision tree in a random forest uses only 2/3 of the data for training, you can use the other 1/3 as test data.

You can choose the number of variables that yields the best accuracy on that test data.

For this exercise, I'm just going to randomly sample 2-3 properties for each node and call it a day.

Hands-On: Random Forests



Going Forward

Decision trees and random forests are a powerful and flexible tool in machine learning, and together work quite well for a lot of problems.

Decision trees can also be adapted to do regression with regression trees and enhanced with techniques like gradient boosting.

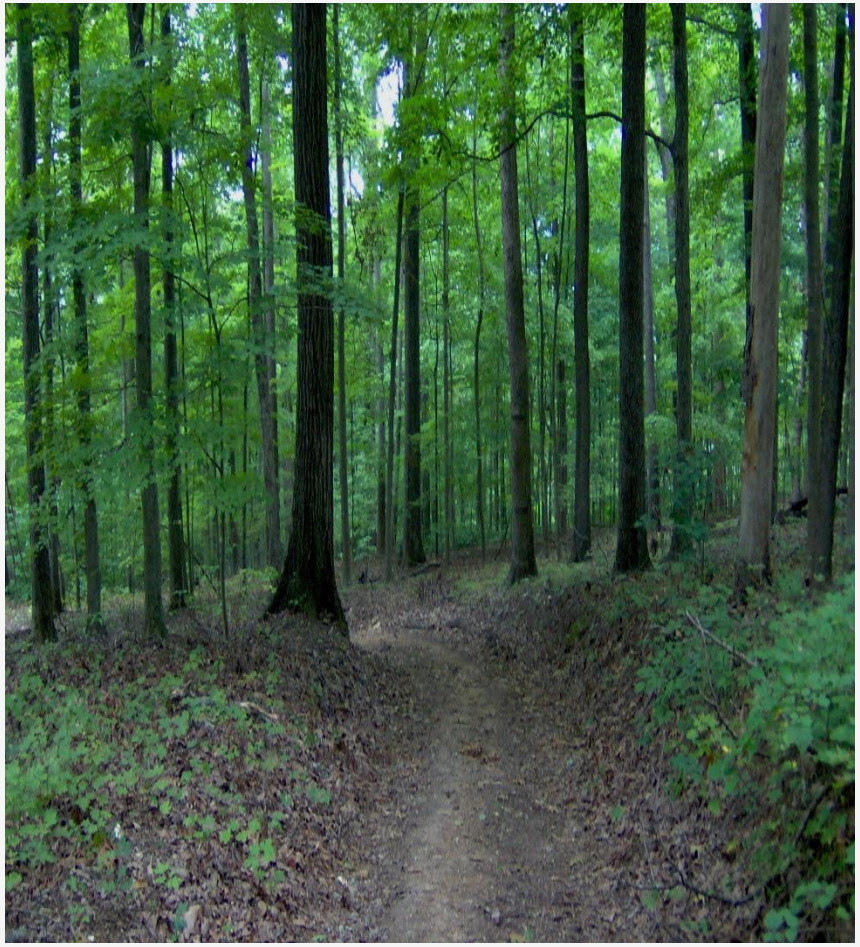
If I were to take one machine learning algorithm with me, it would be decision trees and all of its variants.

Quiz Time!

Decision trees are effective because they do not overfit.

A) True

B) False



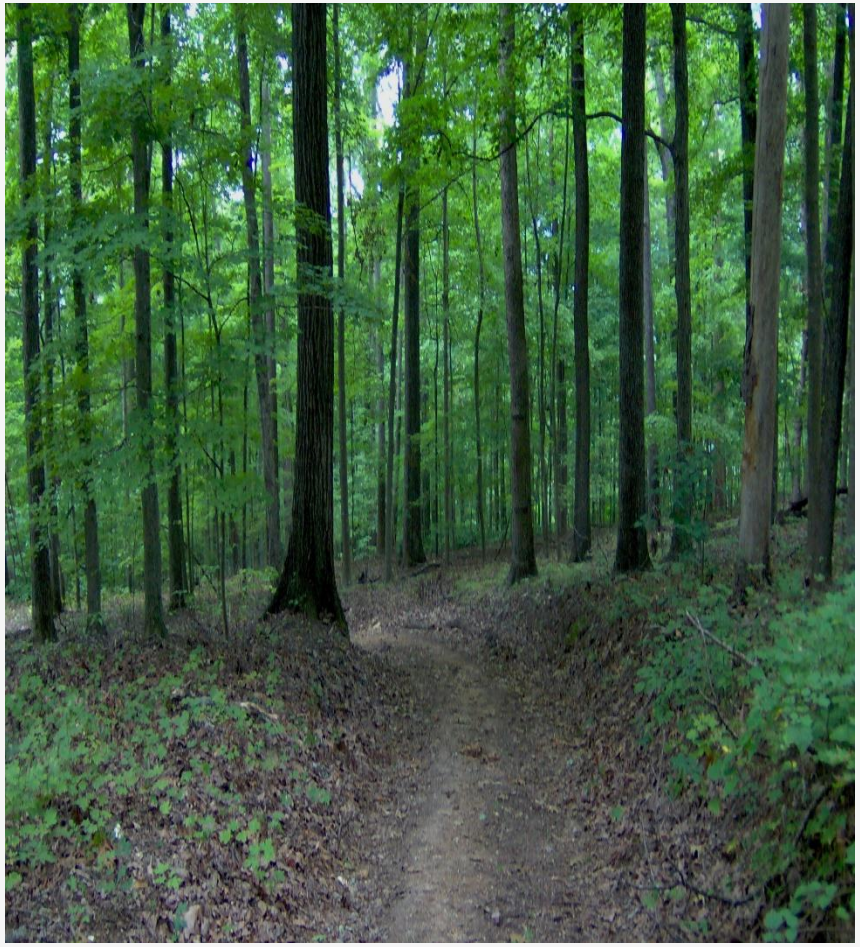
Quiz Time!

Decision trees are effective because they do not overfit.

A) True

B) False

Decision trees are so effective at fitting to data that they often overfit. Random forests and other techniques can be used to prevent overfitting



Quiz Time!

You have 100 patients. 44 have Celiac disease, 56 do not.

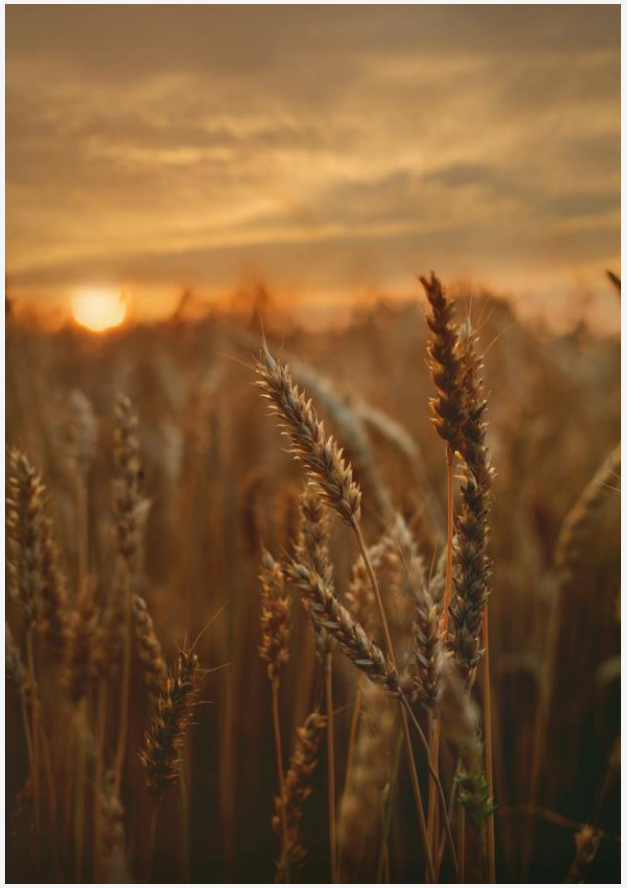
What is the GINI impurity of Celiac to non-Celiac patients?

A) .4928

B) .44

C) .56

D) .4720



Quiz Time!

You have 100 patients. 44 have Celiac disease, 56 do not.

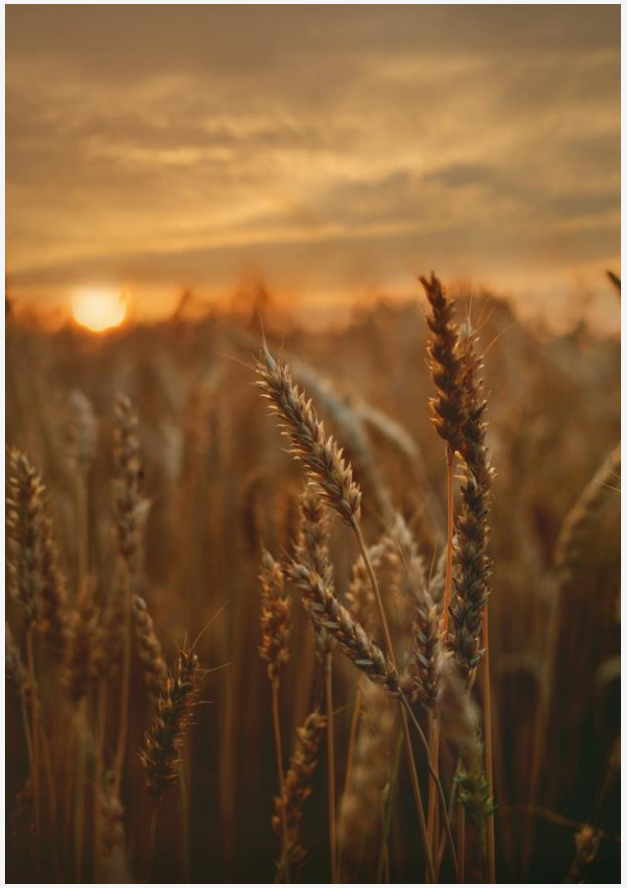
What is the GINI impurity of Celiac to non-Celiac patients?

A) .4928 $1 - \left(\frac{44}{100}\right)^2 - \left(\frac{56}{100}\right)^2 = .4928$

B) .44

C) .56

D) .4720



Quiz Time!

You have 100 patients. 45 complained of stomach pain after drinking beer, the other 55 did not.

Of the 45 patients with stomach pain, 37 have Celiac disease.

Of the 55 patients without stomach pain, 7 have Celiac disease.

What is the weighted GINI impurity for using post-beer stomach pain to determine whether a patient has Celiac disease?

A) .50 B) .2537 C) .4506 D) .45

Quiz Time!

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What is the weighted GINI impurity for using post-beer stomach pain to determine whether a patient has Celiac disease?

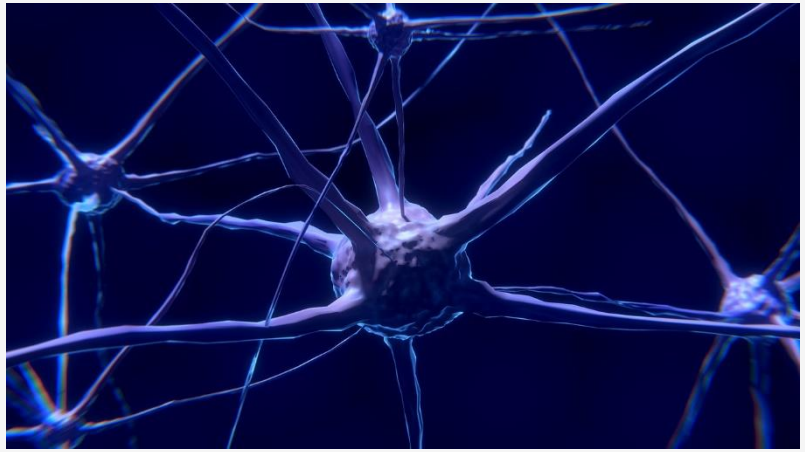
A) .50 B) .2537 C) .4506 D) .45

$$\left(\frac{45}{100}\right)\left(1-\left(\frac{37}{45}\right)^2-\left(\frac{8}{45}\right)^2\right)+\left(\frac{55}{100}\right)\left(1-\left(\frac{7}{55}\right)^2-\left(\frac{48}{55}\right)^2\right)=.2537$$

Section VI
Neural Networks

What Are Neural Networks?

A neural network is a multilayered regression containing layers of weights, biases, and nonlinear functions that reside between input variables and output variables.



- **Deep learning** is a popular variant of neural networks that utilizes multiple “hidden” (or middle) layers of nodes containing weights and biases.
- Each node resembles a linear function before being passed to a nonlinear function (called an activation function).
- Practical applications of neural networks include recognition and generation of image, audio, video, and language.

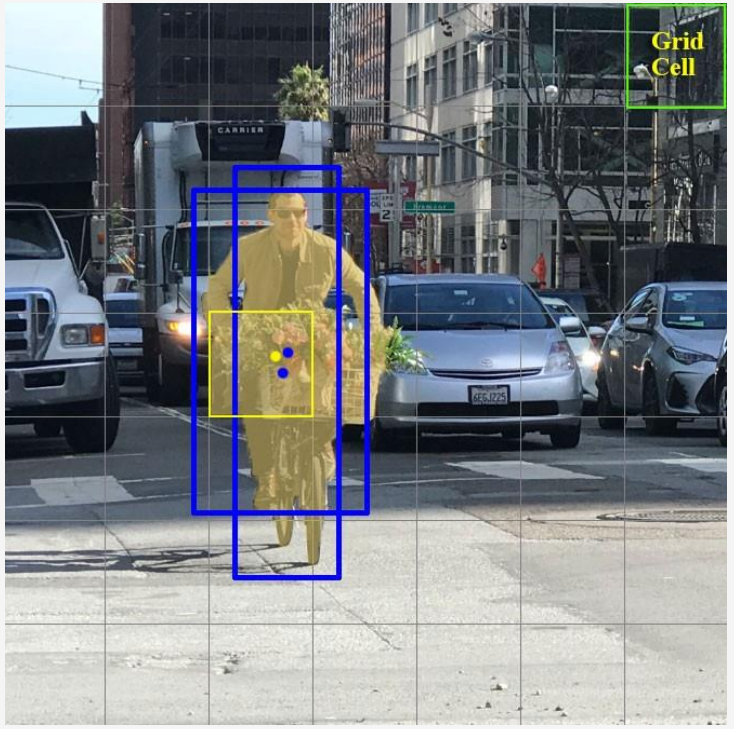
Neural networks are loosely inspired by the biological brain but are by no means a replication of them.

Why Learn About Neural Networks?

Neural networks offer exciting solutions to problems previously difficult for computers to solve.

Some applications that have been used with a degree of success.

- Virtual assistants like Siri and Alexa
- Recognizing road objects in advanced driving systems (ADS)
- Pushing advertisements on social media
- Photo and video tools on the iPhone and Android



YOLO (you only look once) detects and classifies simultaneously by using fixed dimensions of grid cells.

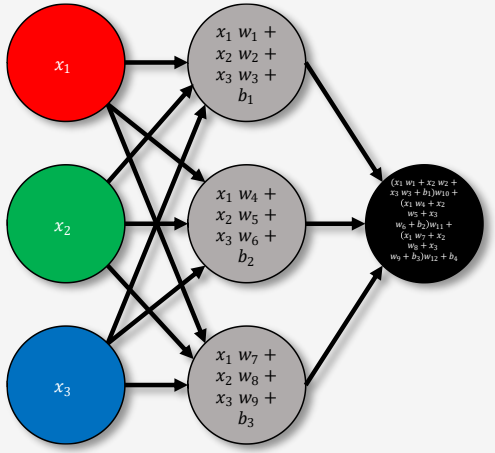
[1] https://zhanghanduo.github.io/post/yolo1/

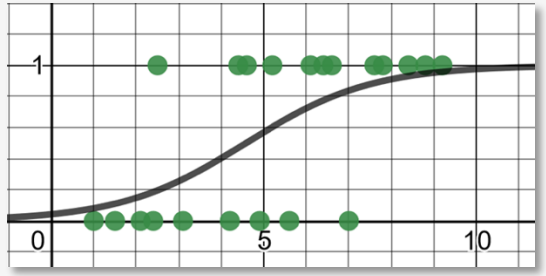
When to Use Neural Networks/Deep Learning?

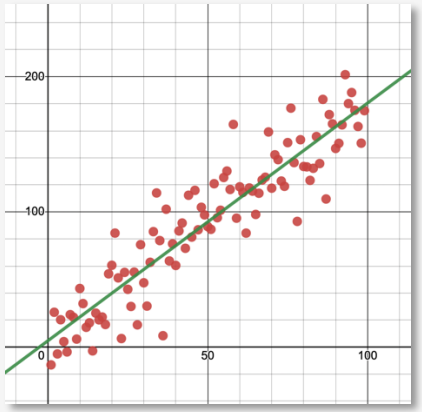
Linear regression, logistic regression, decision trees, and other machine learning models can perform regression and classification.

When do we use those instead of neural networks?

- Typically, you want to use those simpler models for structured problems, meaning that the data is tabular and has rows and columns.
- Perceptual problems that are fuzzier, like recognizing objects in images or predicting the next 4-5 words being typed, are better done by neural networks and its variants.







A Simple Neural Network

Suppose you wanted to take any background color (example: salmon pink) and predict whether you should use a light or dark font for it.

LIGHT DARK

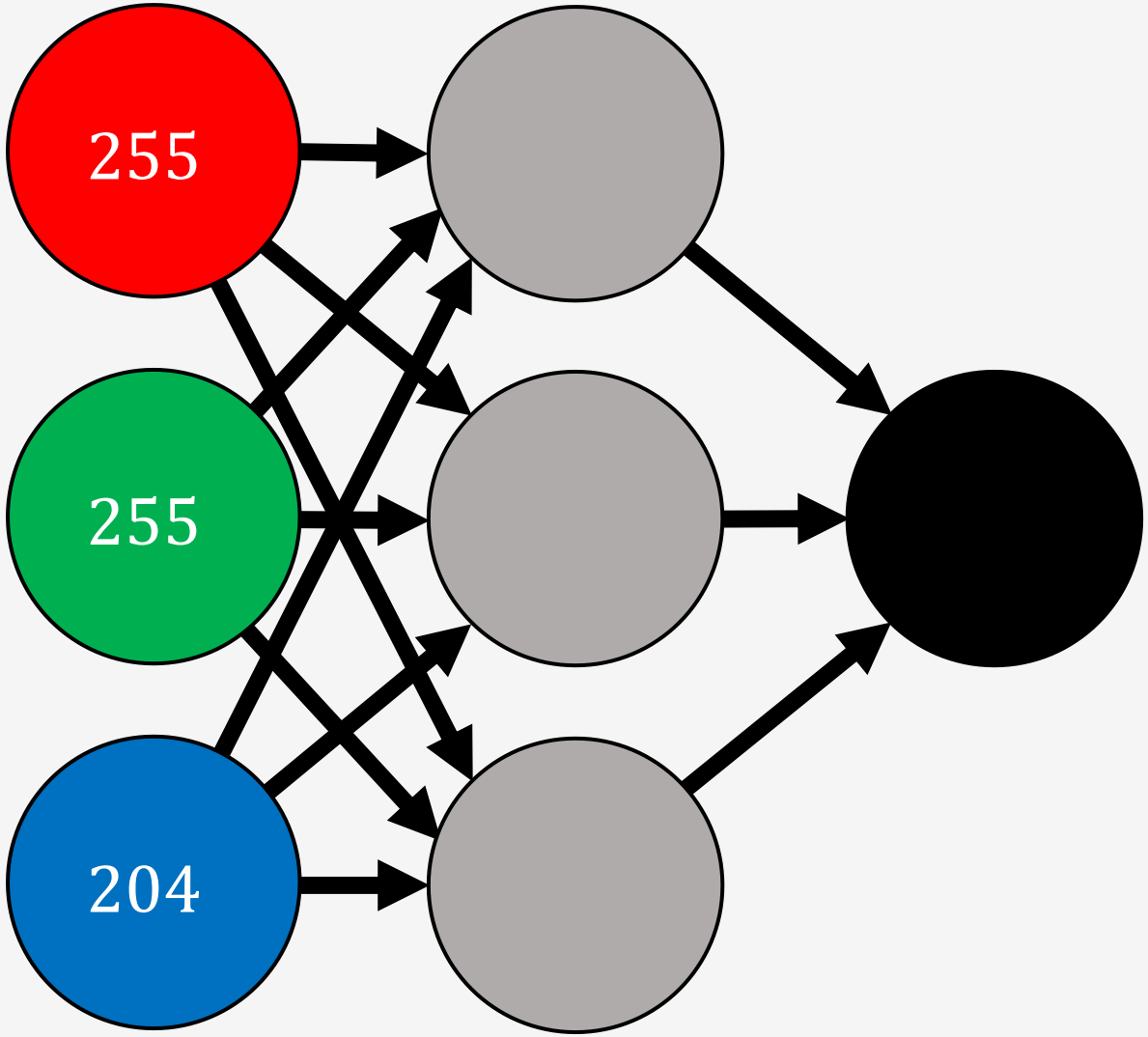
There are deterministic ways to do this, as well as simpler regression models like logistic regression, but we will use a neural network.

In code, a color can be composed out of three colors (**red**, **green**, and **blue**) each expressed as a value between 0-255.

For example, the salmon pink above is expressed as (**255**, **255**, **204**).

Anatomy of a Neural Network

Note the neural network structure to the right accepts those three R,G,B values as inputs into the first layer.

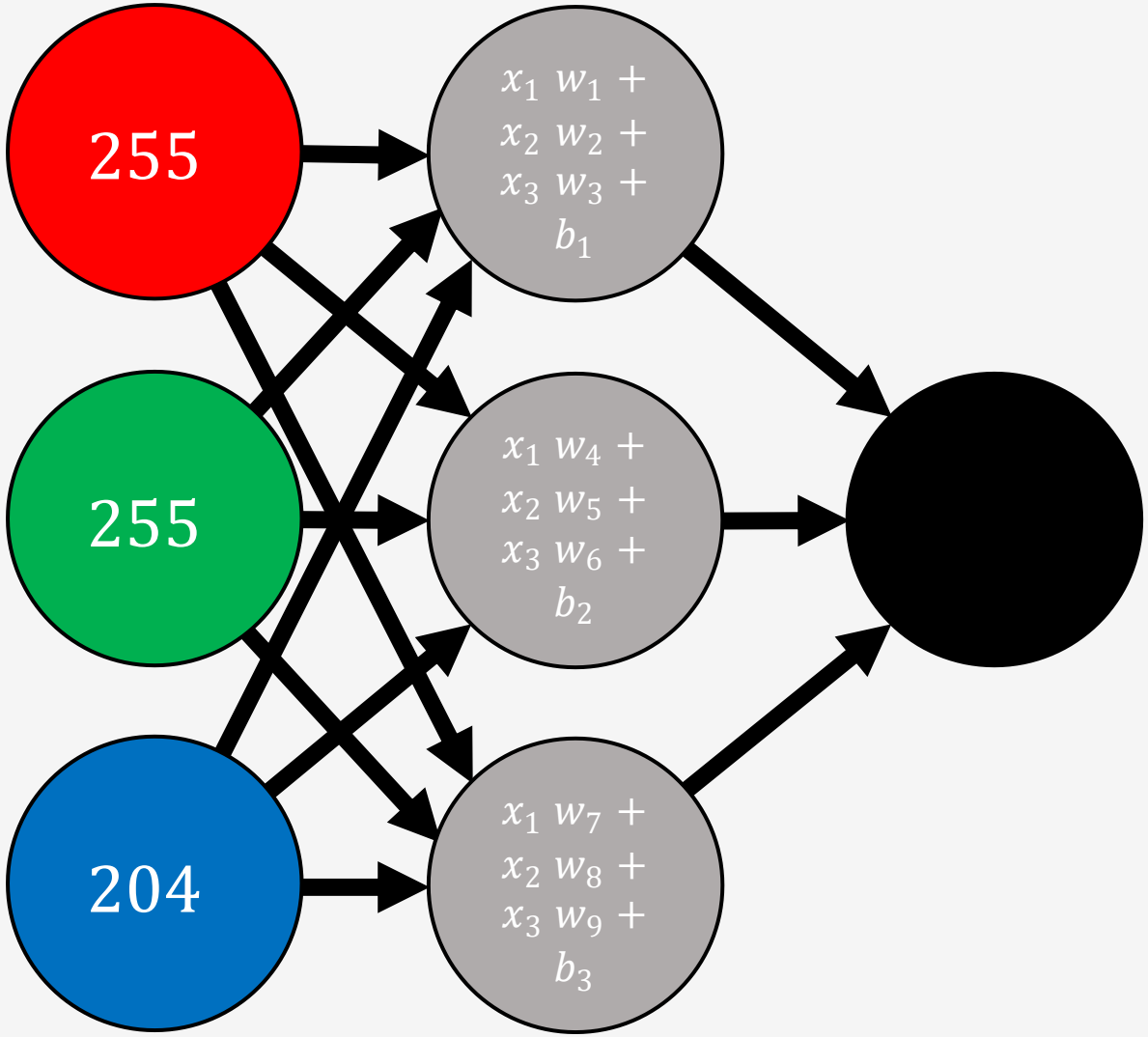


Anatomy of a Neural Network

Those three values are then scaled and passed to three nodes in the **hidden layer**, each with a set of **weights** w_x and a **bias** b_x .

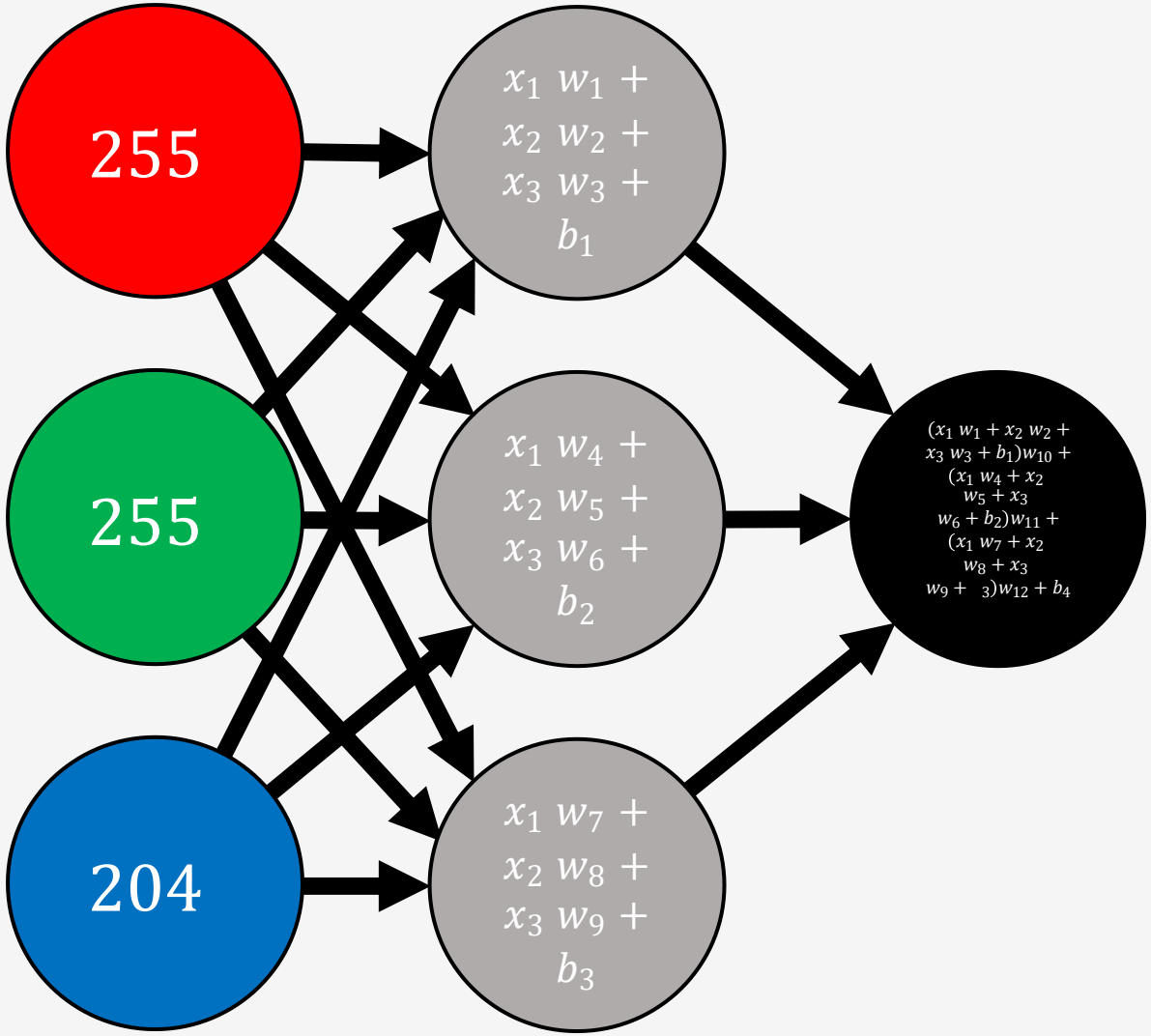
Those weights and biases are then multiplied and added to each respective input.

Notice how each node resembles a linear function!



Anatomy of a Neural Network

Then those output values from the middle nodes are passed to the final node(s) in the **output layer**, which makes a prediction after applying another set of weights and biases.



Anatomy of a Neural Network

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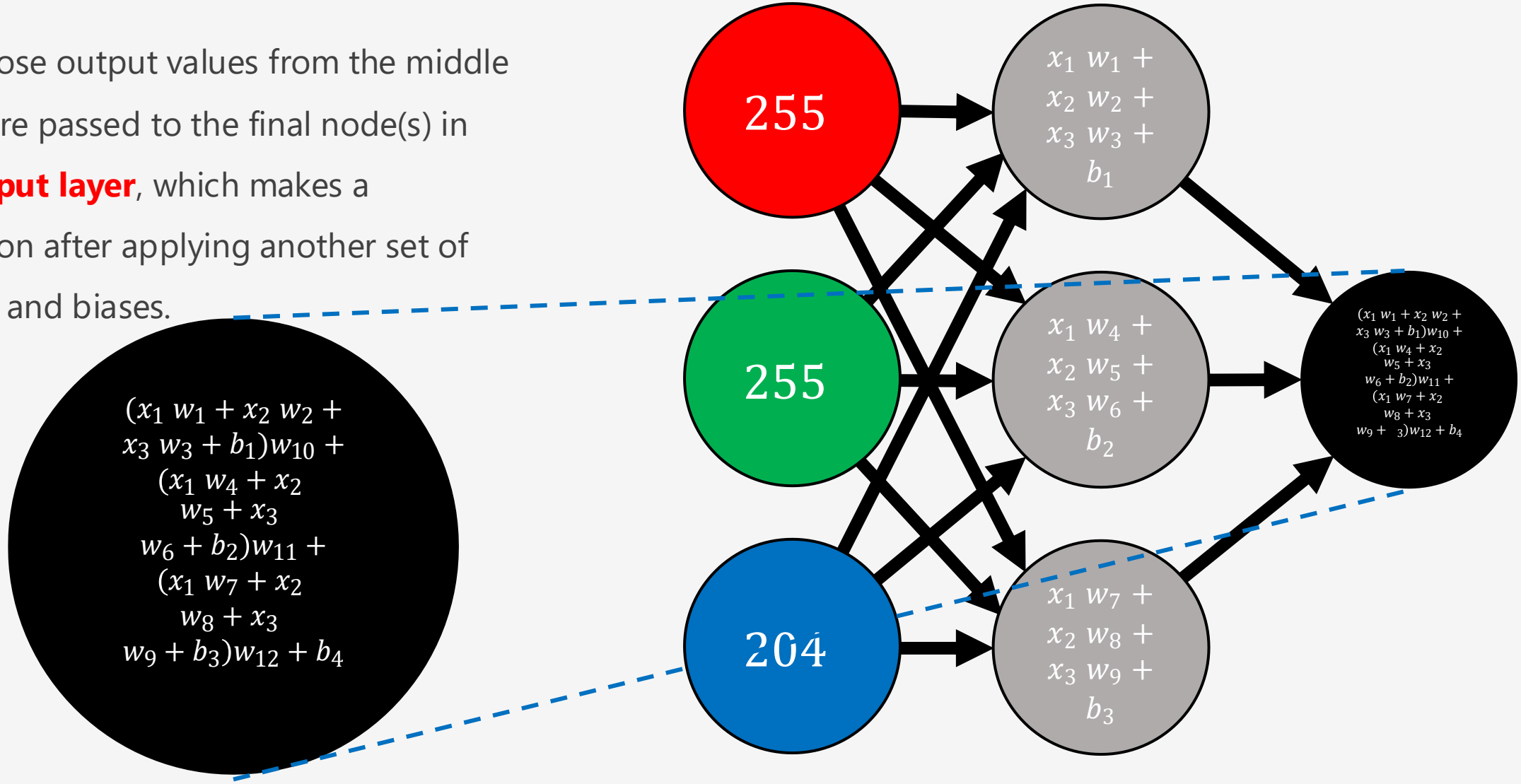
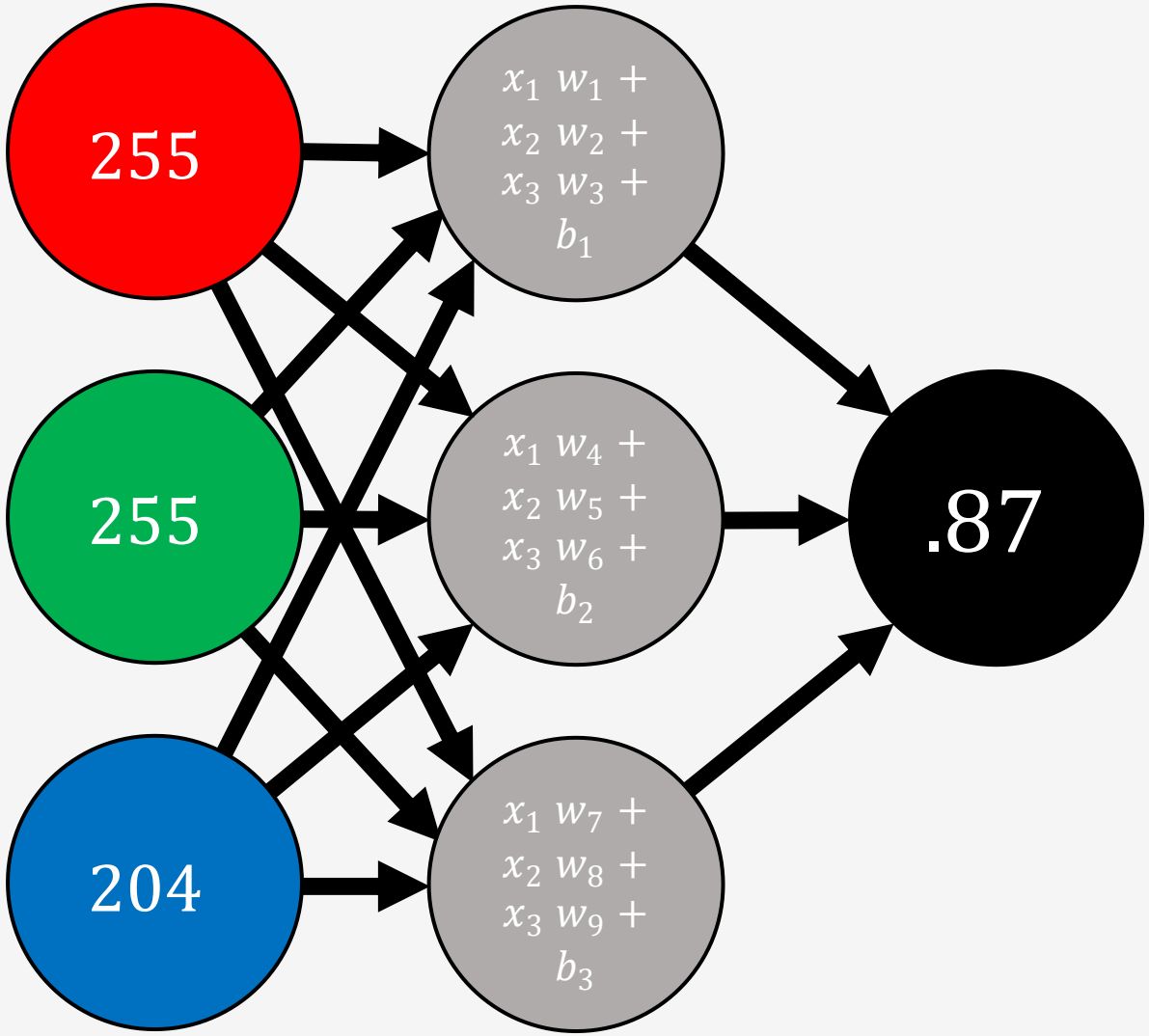


Anatomy of a Neural Network

Then those output values from the hidden nodes are passed to the final node(s) in the **output layer**, which makes a prediction after applying another set of weights and biases.

For a simple binary classification (light/dark font) we will output a single probability of predicting dark font.

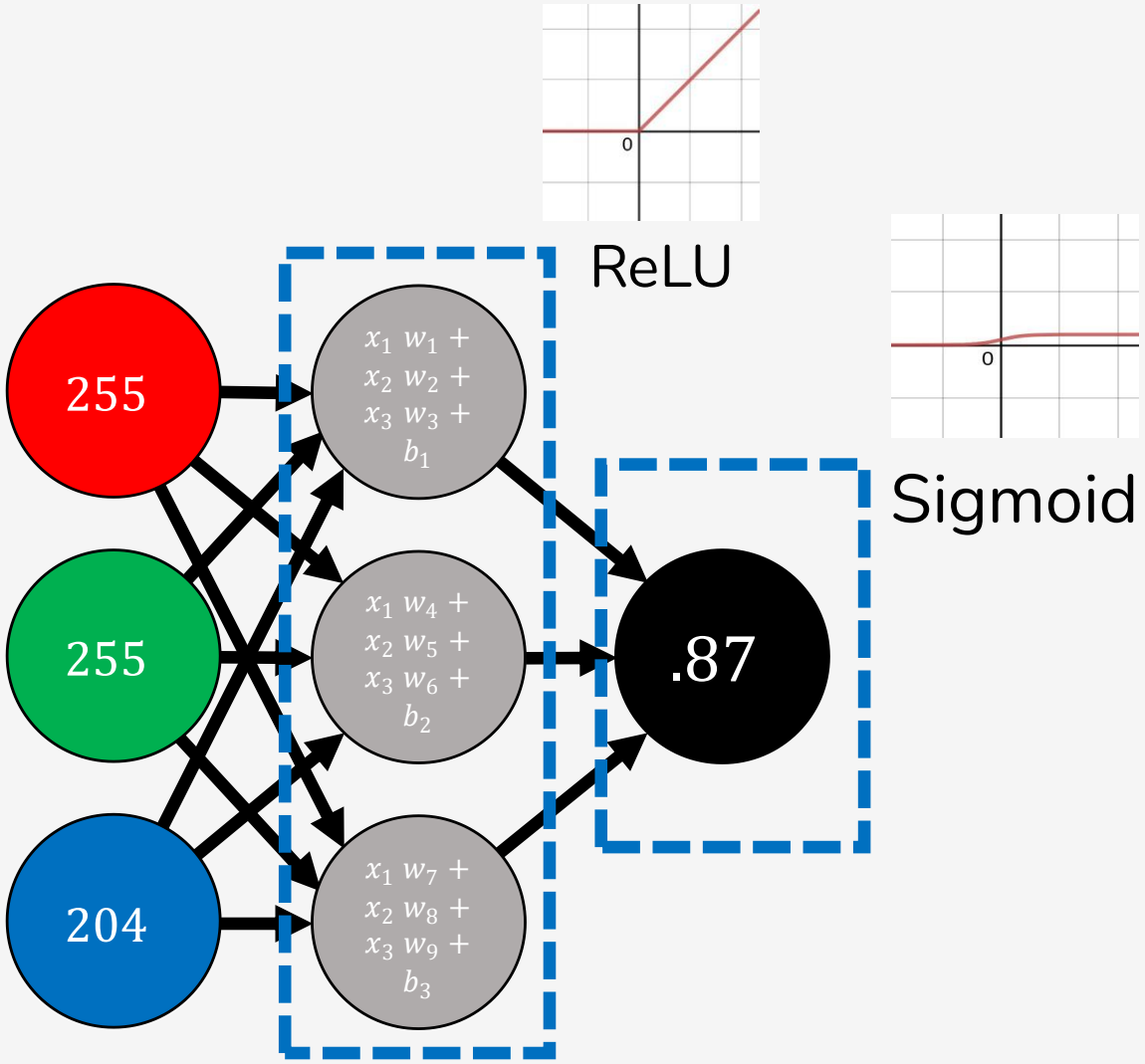
If it's less than .5 it will categorize as LIGHT, and if it is greater than/equal to .5 it will be DARK.

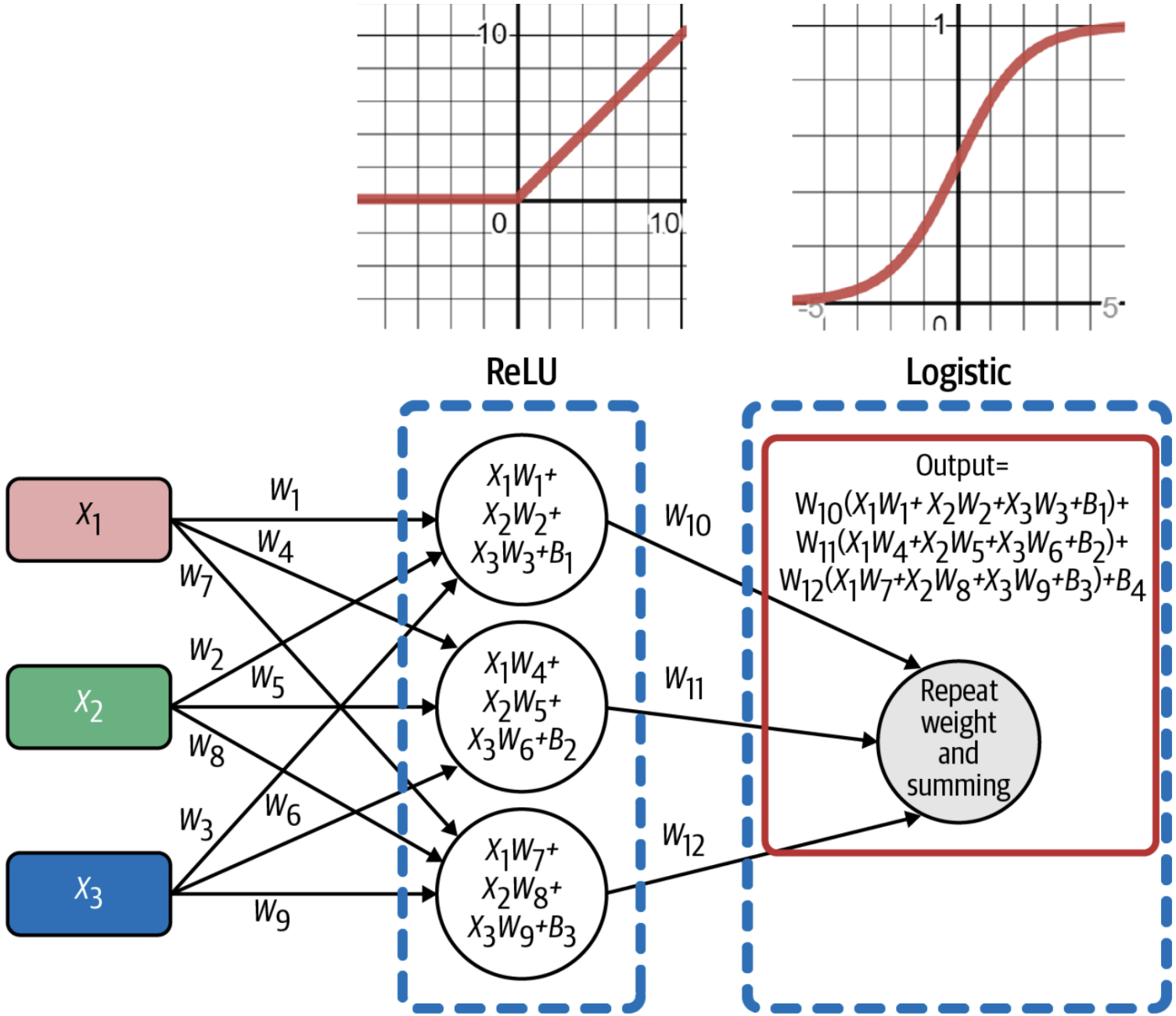


Anatomy of a Neural Network

We also have **activation functions** which are nonlinear functions applied to the output of each layer.

To the right we apply the ReLU and sigmoid (logistic) functions to the hidden and output layers respectively.



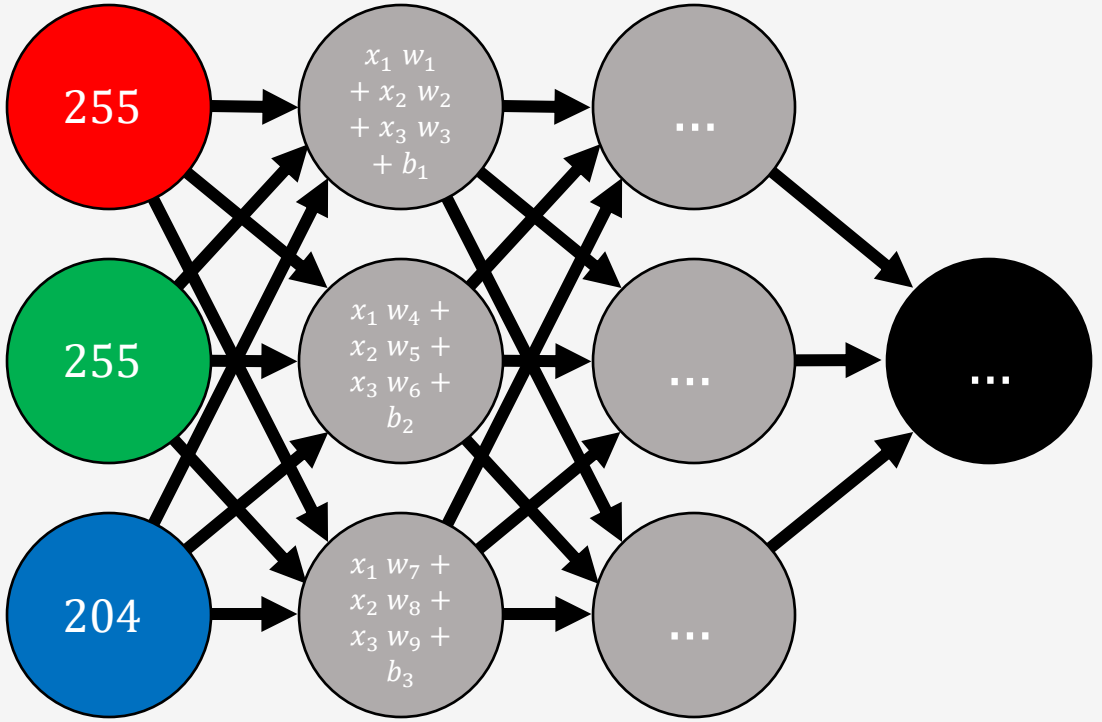

10
0
10
1
0
5
ReLU
Logistic
X_1
X_2
X_3
W_1
W_2
W_3
W_4
W_5
W_6
W_7
W_8
W_9
X_1W_1+ X_2W_2+ $X_3W_3+B_1$
X_1W_4+ X_2W_5+ $X_3W_6+B_2$
X_1W_7+ X_2W_8+ $X_3W_9+B_3$
W_{10}
W_{11}
W_{12}
Output=
$W_{10}(X_1W_1+X_2W_2+X_3W_3+B_1)+$
$W_{11}(X_1W_4+X_2W_5+X_3W_6+B_2)+$
$W_{12}(X_1W_7+X_2W_8+X_3W_9+B_3)+B_4$
Repeat weight and summing

Choosing Number of Layers/Nodes

For a neural network to qualify as "deep learning," there must be more than one hidden layer as shown to the right.

Generally adding more layers to a neural network will give it the ability to discern more features, but this can also lead to overfitting.

Choosing the number of layers, and how many nodes go in each one, is often done through experimentation by practitioners.



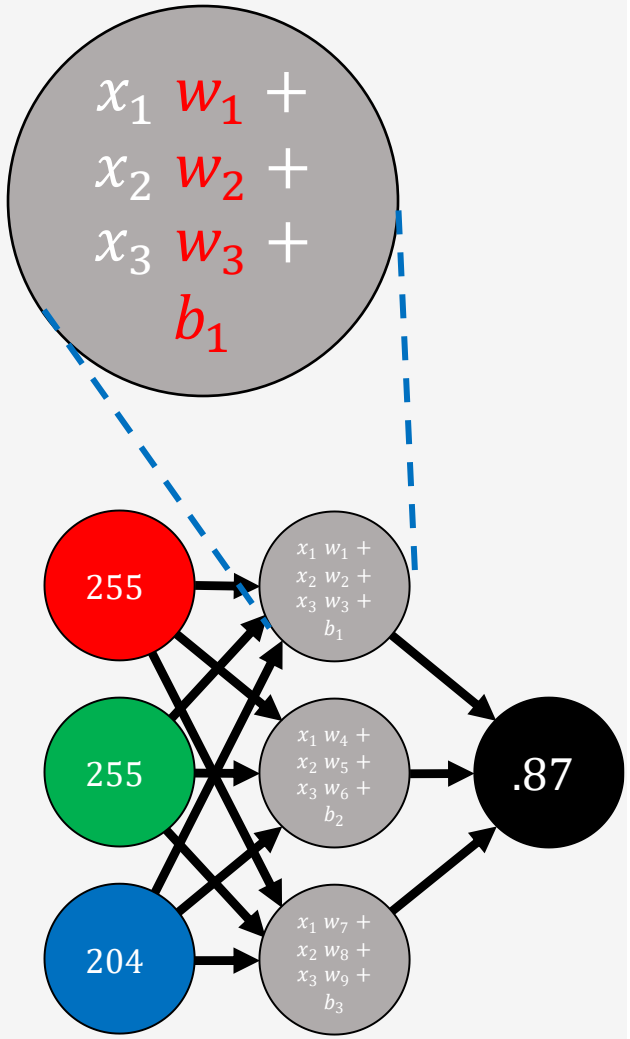
Weights and Biases

Each node in a neural network (in the hidden and output layers) contains weights w_x and biases b_x.

Weights will be between -1 and 1, and the biases between 0 and 1.

The weights and biases are multiplied and added respectively to each incoming value from the previous layer.

The weights and biases are initialized with random values, and then optimized with backpropagation and gradient descent (discussed later).

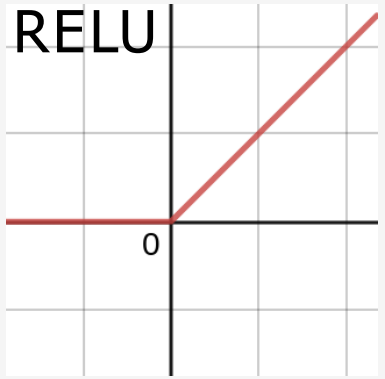


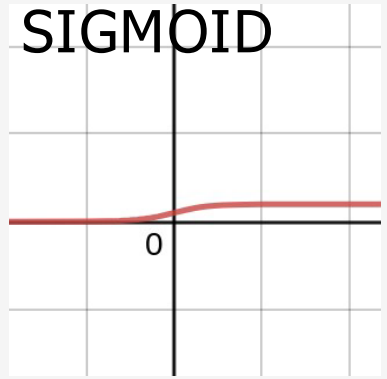
Activation Functions

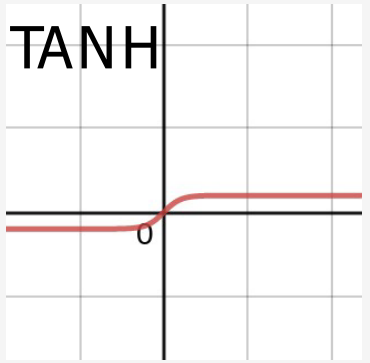
Activation functions will take the results of each node (applying the weights and biases) and pass them through a nonlinear function.

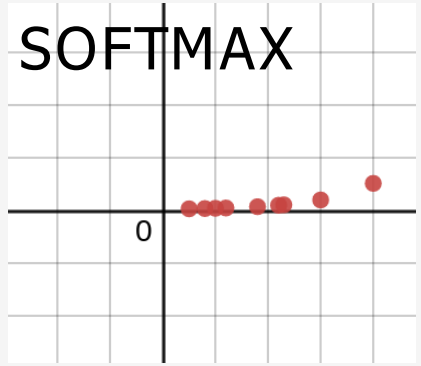
These activation functions make each layer productive separating features out of the input, otherwise the neural network would be no better than a linear model.

Choosing an activation function can be aided with a few best practices (table in next slide).









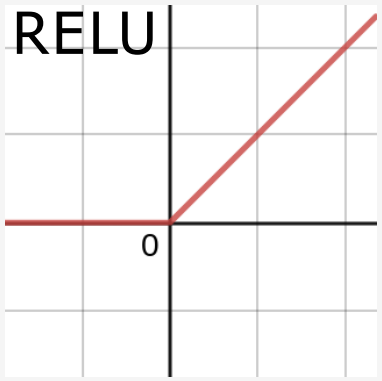
Common Activation Functions

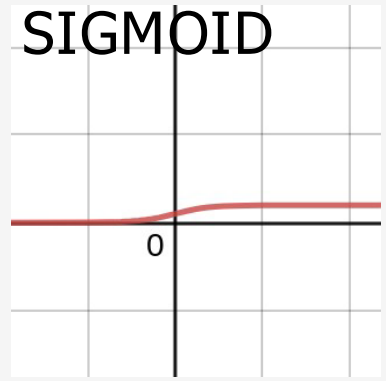
Name	Typical layer used	Description	Notes
Linear	Output	Leaves values as is	Not commonly used
Logistic	Output	S-shaped sigmoid curve	Compresses values between 0 and 1, often assists binary classification
Tangent Hyperbolic	Hidden	tanh, S-shaped sigmoid curve between -1 and 1	Assists in “centering” data by bringing mean close to 0
ReLU	Hidden	Turns negative values to 0	Popular activation faster than sigmoid and tanh, mitigates vanishing gradient problems and computationally cheap
Leaky ReLU	Hidden	Multiplies negative values by 0.01	Controversial variant of ReLU that marginalizes rather than eliminates negative values
Softmax	Output	Ensures all output nodes add up to 1.0	Useful for multiple classifications and rescaling outputs so they add up to 1.0

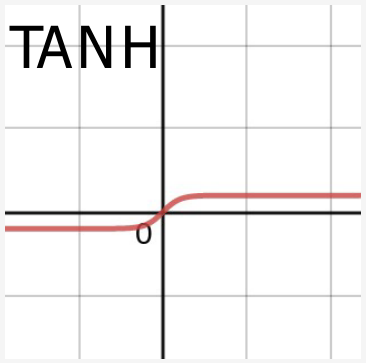
Common Activation Functions

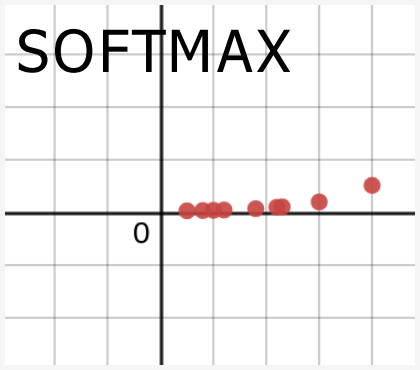
```
import numpy as np
from scipy import special
import math


# Activation functions
def tanh(x):
    return np.tanh(x)


def sigmoid(x):
    return 1 / (1 + math.exp(-x))


def relu(x):
    return np.maximum(x, 0)


def softmax(x):
    return special.softmax(x, axis=0)
```

Four common neural network activation functions implemented in Python.









https://www.desmos.com/calculator/jwjn5rwfy6

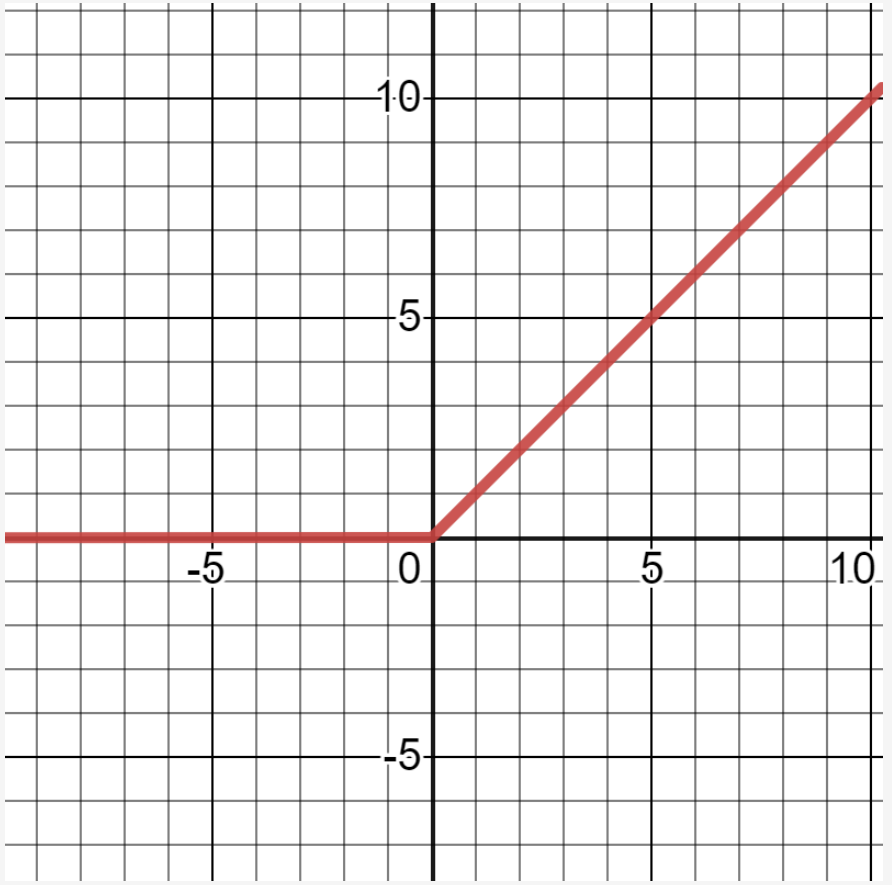
Activation Functions - ReLU

The ReLU activation function will zero out any negative outputs from the hidden nodes. If the weights, biases, and inputs multiply and sum to a negative number, it will be converted to 0.

ReLU is short for “rectified linear unit.”

ReLU has gotten popular for hidden layers in neural networks and deep learning because of its speed and mitigation of the vanishing gradient problem.

Vanishing gradients occur when the partial derivative slopes get so small they prematurely approach 0 and bring training to a screeching halt.

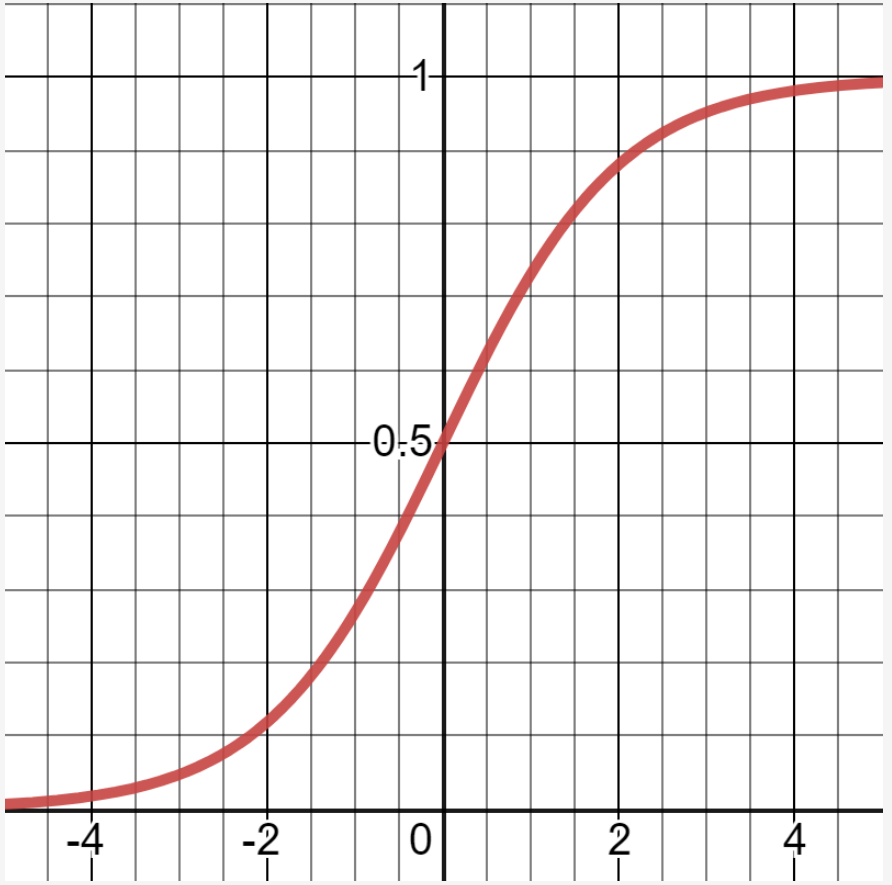


Activation Functions - Sigmoid

The output layer has an important job: it takes the piles of math from the hidden layers of the neural network and turns them into an interpretable result, such as presenting classification predictions.

The output layer for our example uses sigmoid activation function, which scales the output between 0 and 1.

If it is greater than or equal to 0.5, the neural network is suggesting a light font, but less than that will advise a dark font.



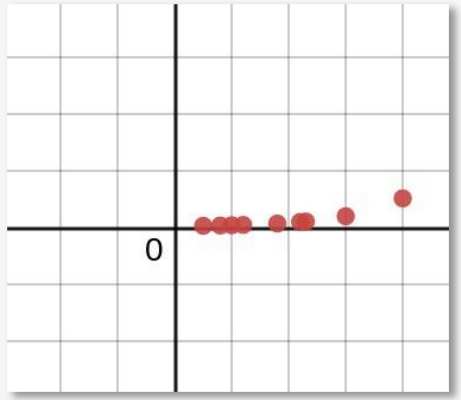
Activation Functions - Softmax

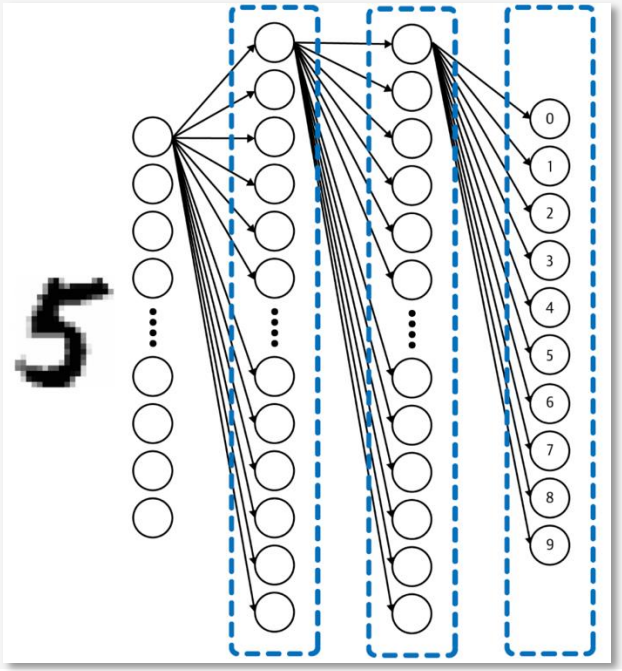
If you want to support multiple classes (and not just LIGHT/DARK or TRUE/FALSE), you could add more output nodes for each class.

You might want to consider using the softmax activation function in this case, which scales each node so they all add up to 1.0.

For instance, if you are trying to recognize handwritten digits 0–9, there would be 10 output nodes representing the probability a given image is each of those numbers.

Each node then represents a probability of the prediction for each corresponding digit.





Training a Neural Network

To the right is a sample of a dataset containing 1345 colors and their correct LIGHT/DARK font labels.

We need to train our neural network off this data so it optimizes the weights and biases to make accurate predictions on colors it has not seen before.

This is beyond the scope of this course, and is covered in *Deep Learning for Beginners* and *Essential Math for Data Science (Chapter 7)*.

RED	GREEN	BLUE	LIGHT_OR_DARK_FONT_IND
178	58	238	0
135	206	235	1
198	113	113	1
197	193	170	1
61	61	61	0
255	130	71	1
0	104	139	0
179	179	26	1
255	153	128	1
204	128	153	1
13	13	13	0
176	176	176	1
165	42	42	0
198	113	113	1
107	142	35	0
132	132	132	1
255	245	238	1
153	102	0	0
128	77	128	0
84	255	159	1

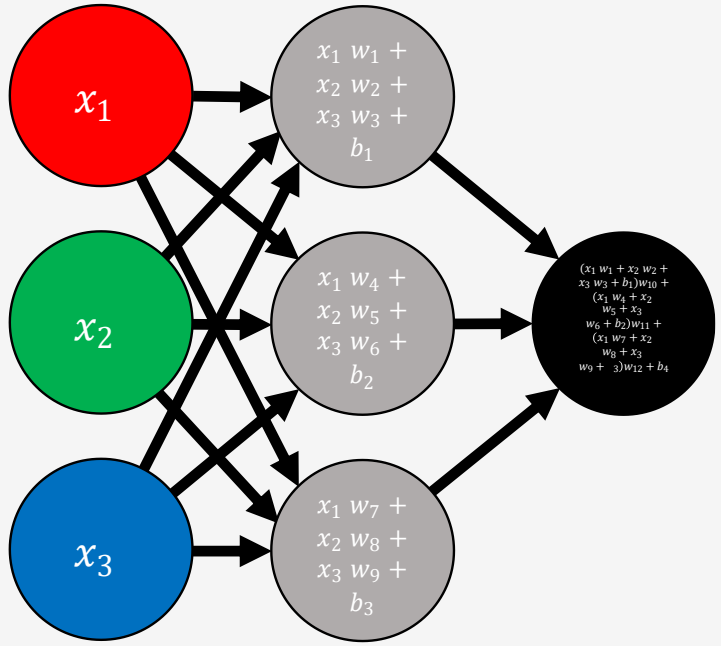
Section III
Forward Propagation

What is Forward Propagation

In this section we are going to learn about forward propagation, which is passing an input through a neural network or deep learning model to get a prediction.

This neural network has not been optimized yet, as that will require backpropagation and gradient descent.

This will be the first step in building a neural network completely from scratch, expressing weights, biases, activation functions, and layers as NumPy operations.



Linear Algebra Basics

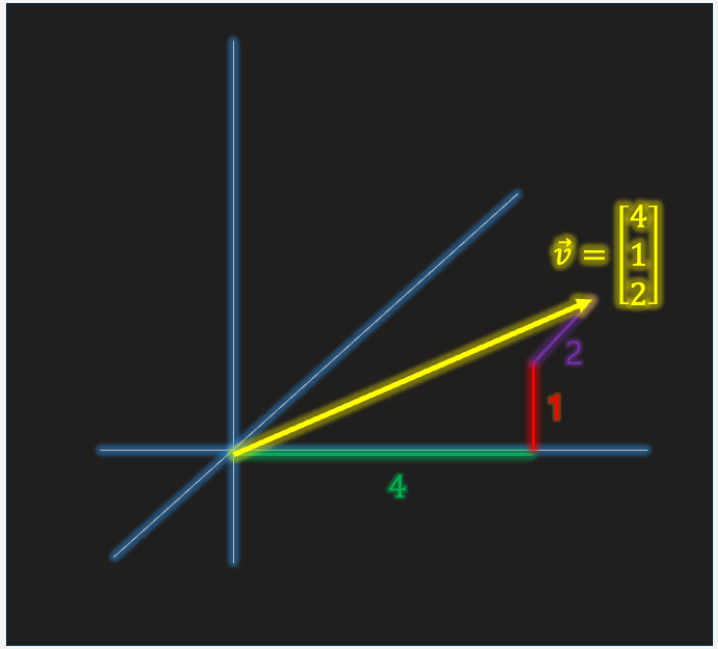
Hopefully, the concept of a matrix is familiar.

A **matrix** is a grid of numbers that can be manipulated, transformed, and combined with other grids of numbers.

A **vector** is a single row or column of a matrix.

We express the weights and biases in a neural network as a matrices, as well as the training/testing data.

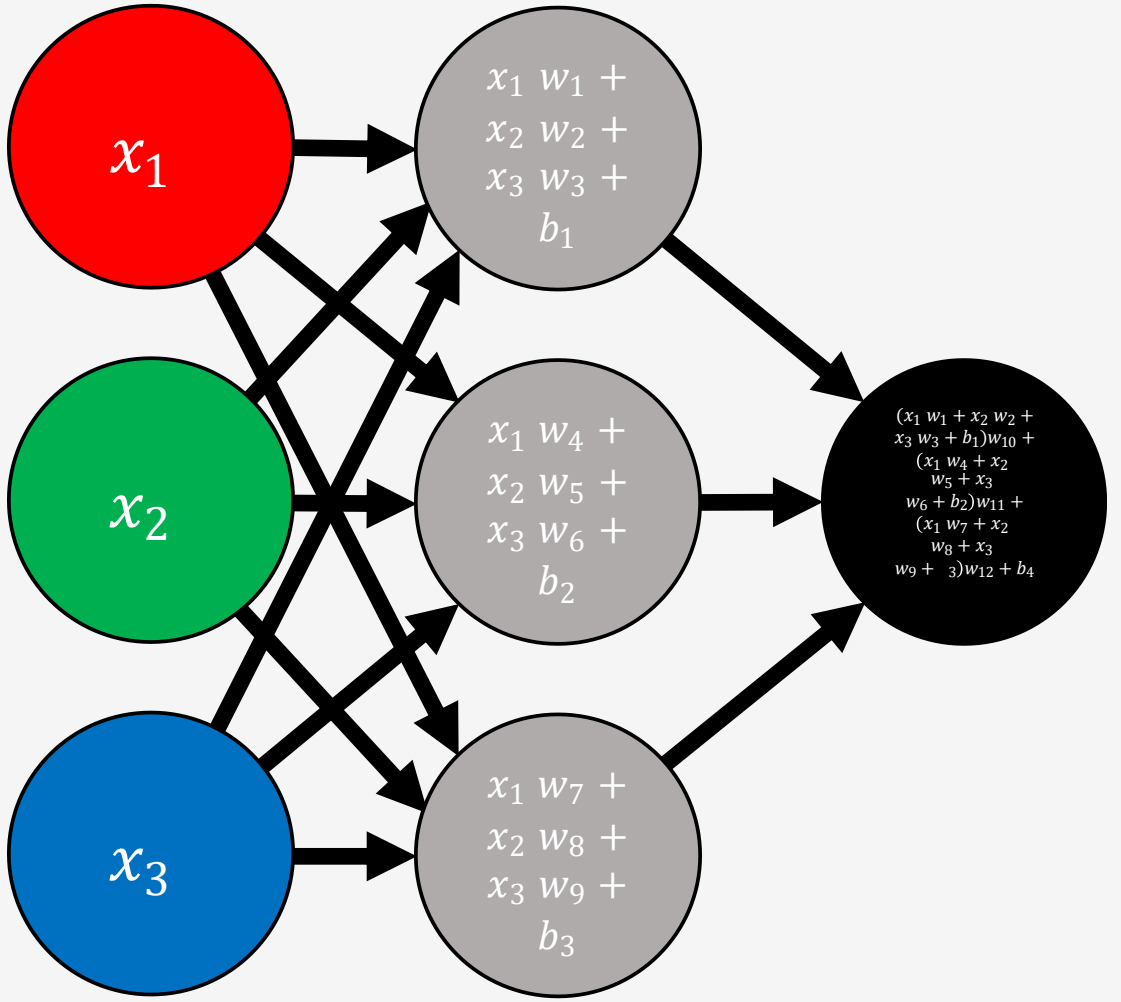
We can then efficiently perform operations to execute our neural network.



Expressing the Weights and Biases

We can express the weights in the hidden layer as a matrix as shown below.

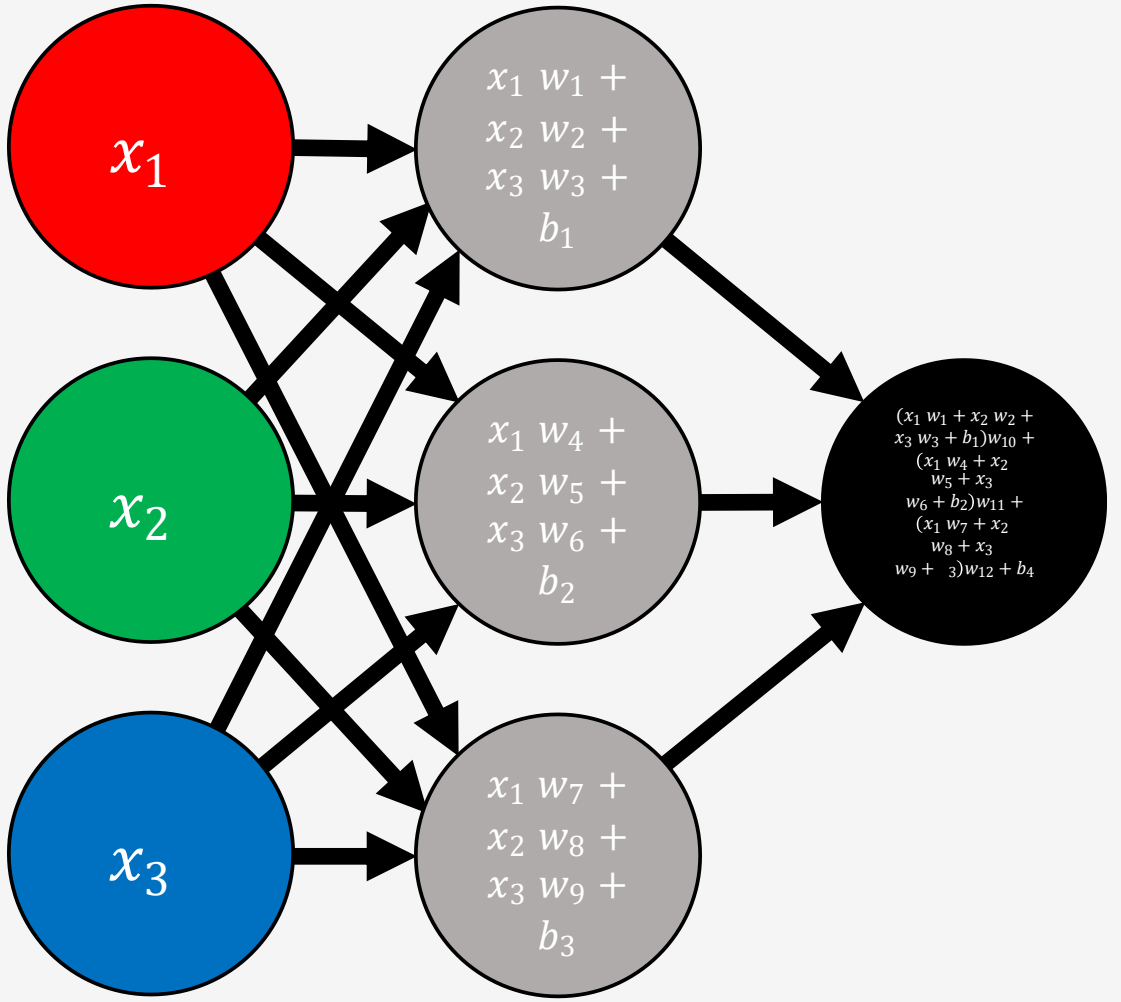
Notice how each row of the matrix corresponds to one node in the hidden layer.



Expressing the Weights and Biases

There are three bias b_x values for each of the three hidden layer nodes.

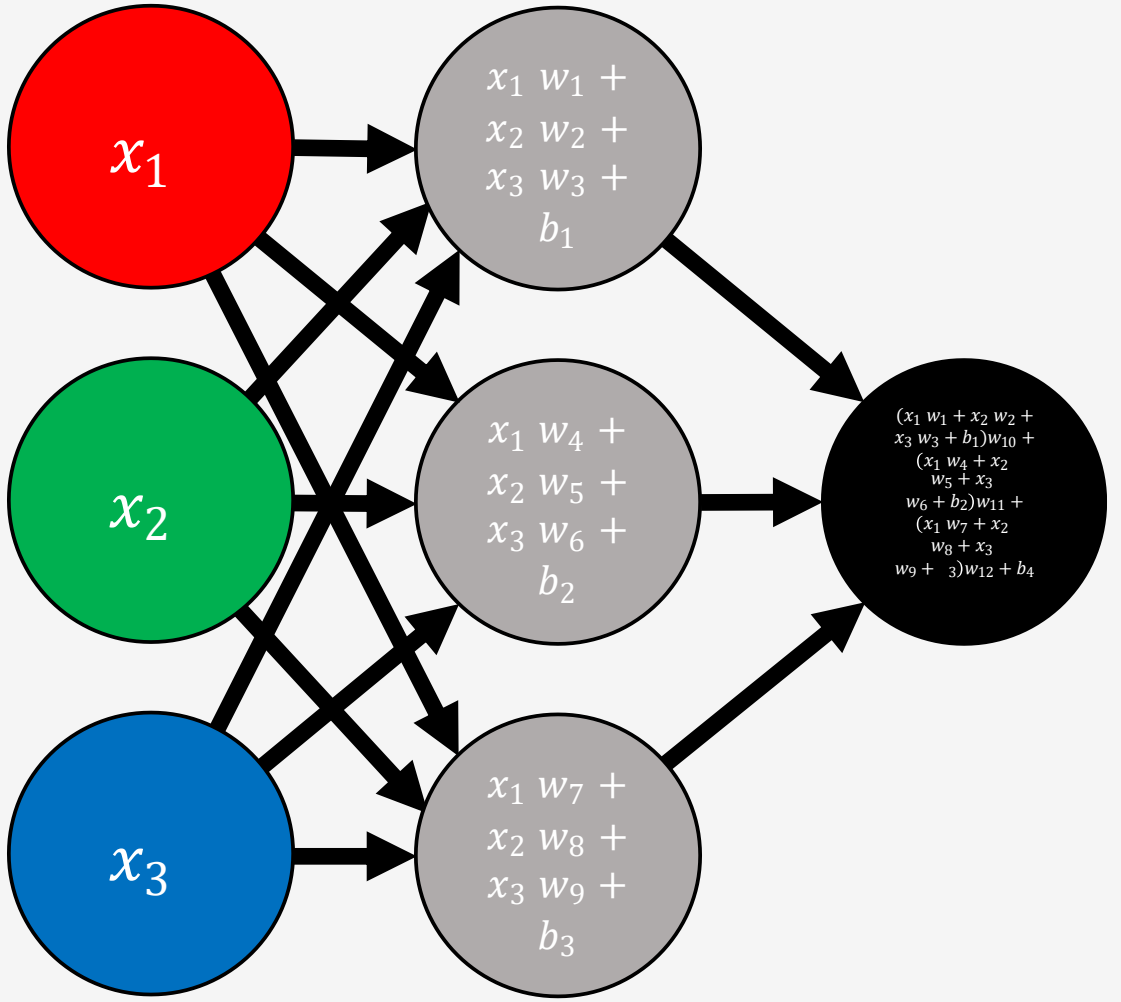
We can express this as a simple vector of three values.



Expressing the Weights and Biases

The output layer will only have three weights w_x, as there are only three feeding nodes from the hidden layer.

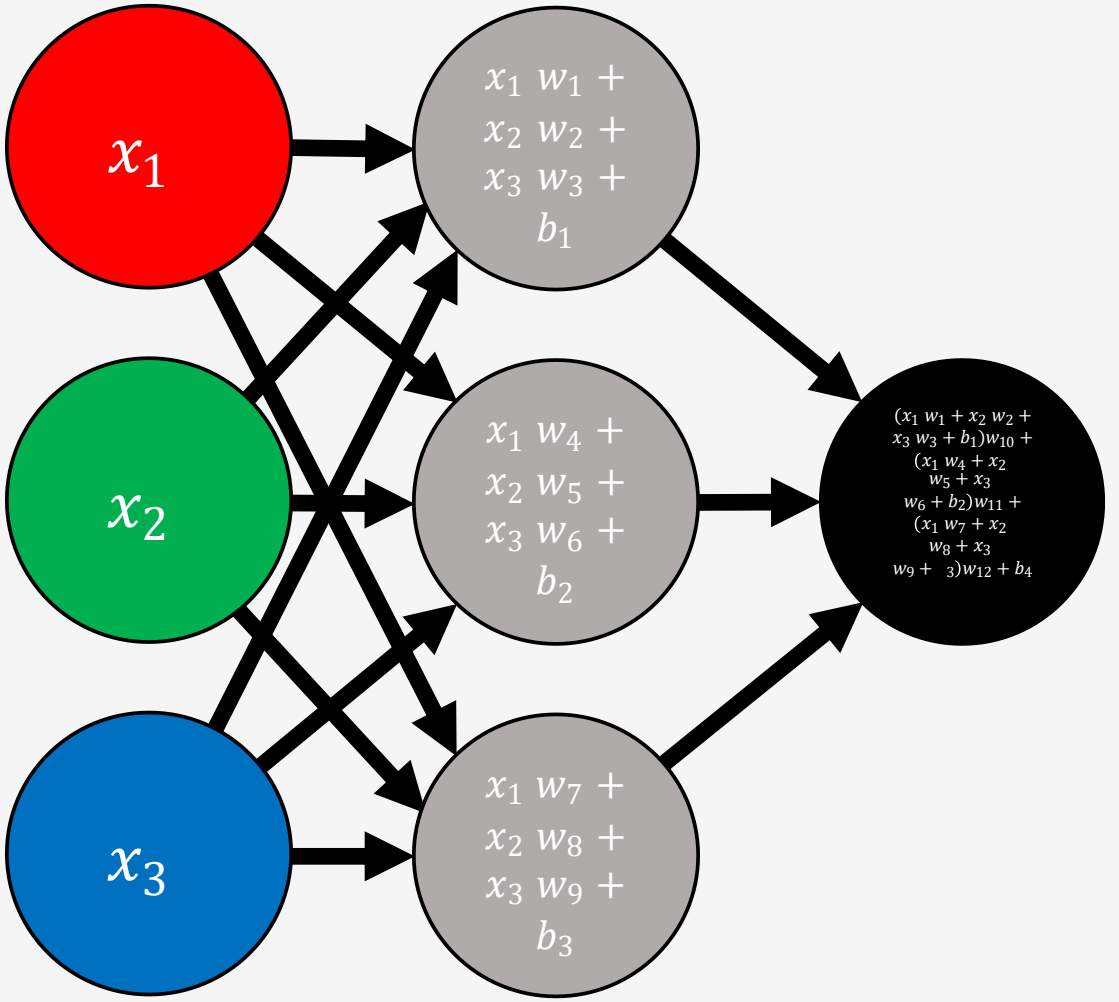
There is only one node in the output layer, so there will only be one row.



Expressing the Weights and Biases

There is only one output node, so there is only one bias value b_4.

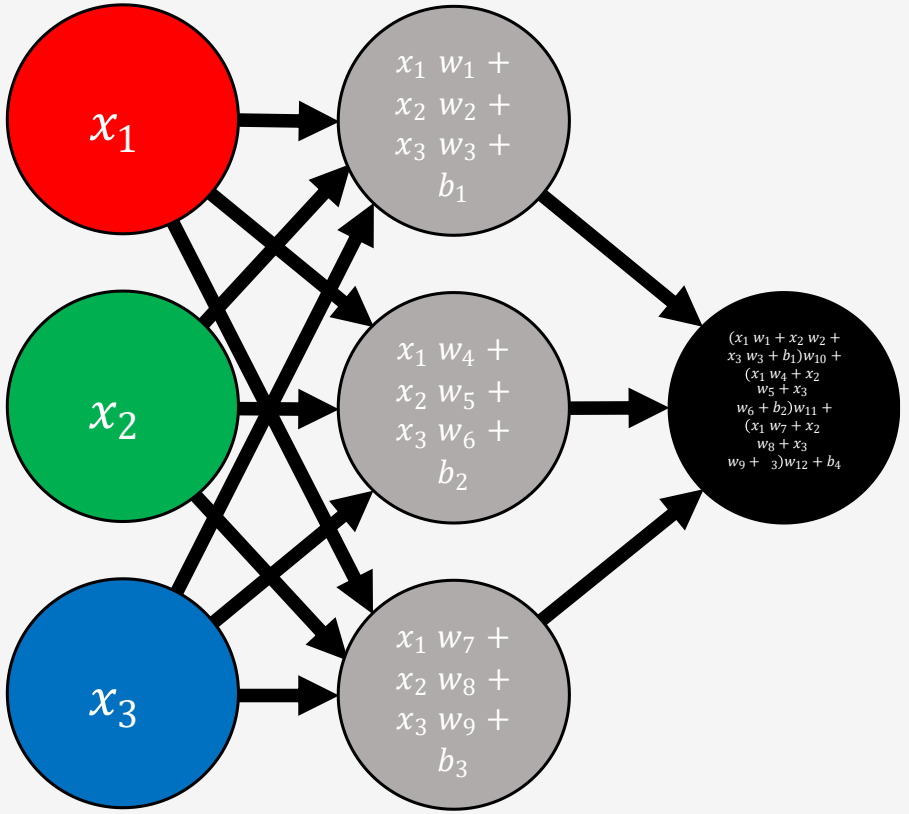
The next slide captures all the matrix/vector components that make our neural network.



Weights and Biases

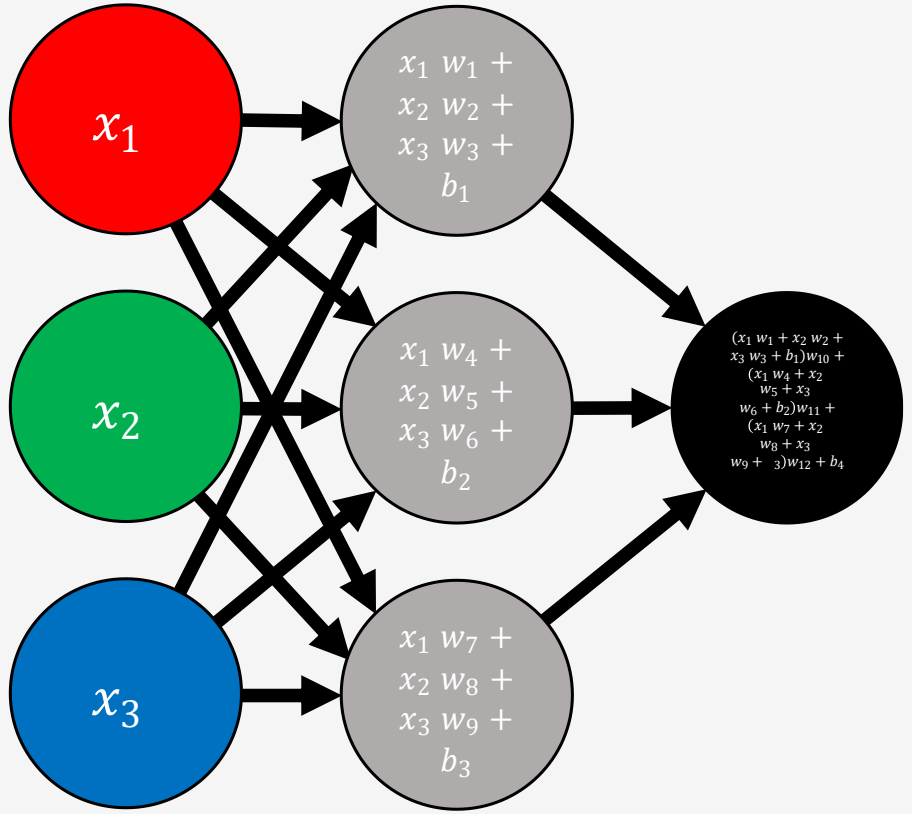
We randomly initialize all these matrices using NumPy.

Each weight w_x will be between -1 and 1, and each bias b_x will be between 0 and 1.



Weights and Biases

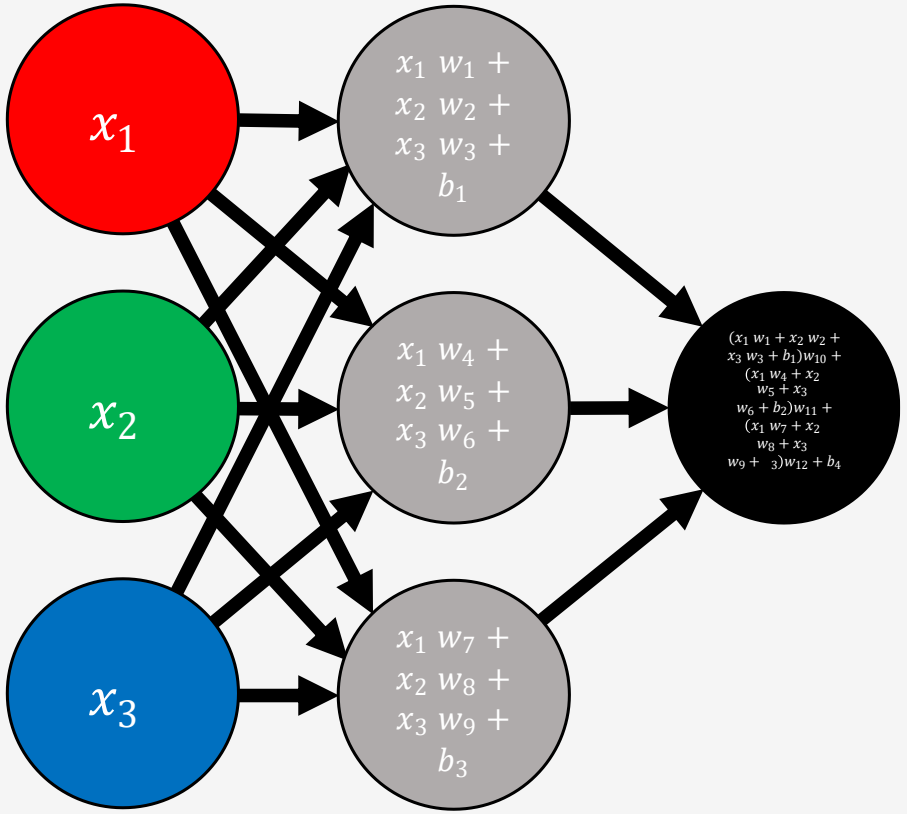
```
import numpy as np

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)
```



Weights and Biases

```
import numpy as np

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)
```

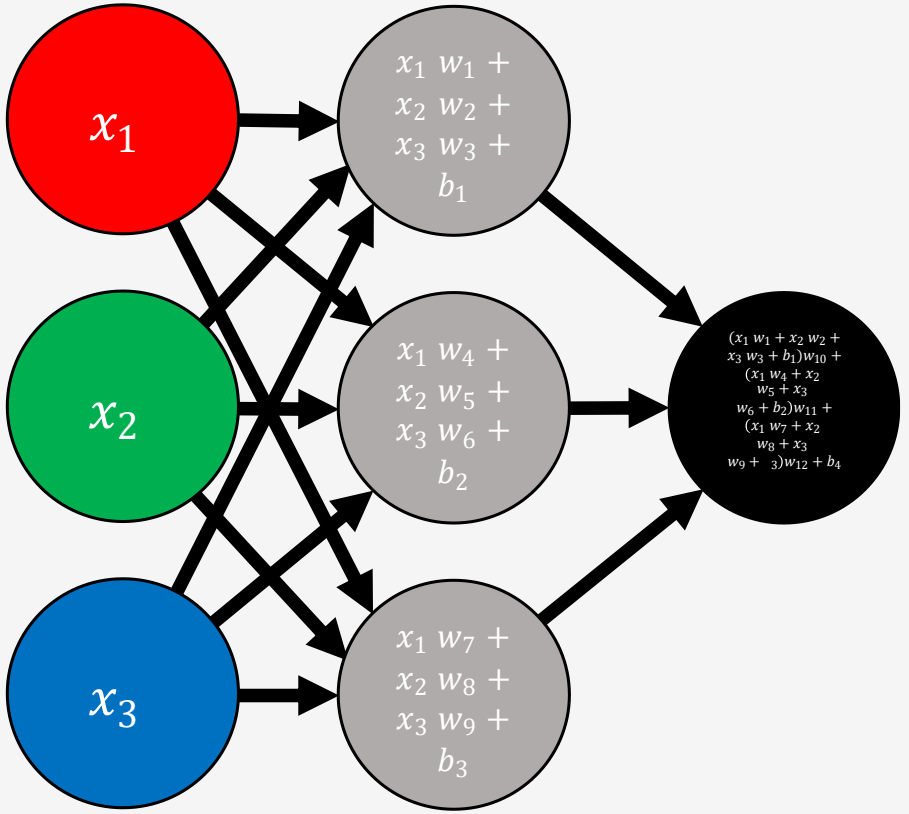
Rows



Weights and Biases

```
import numpy as np

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3
w_output = np.random.rand(1, 3

b_hidden = np.random.rand(3, 1
b_output = np.random.rand(1, 1
```

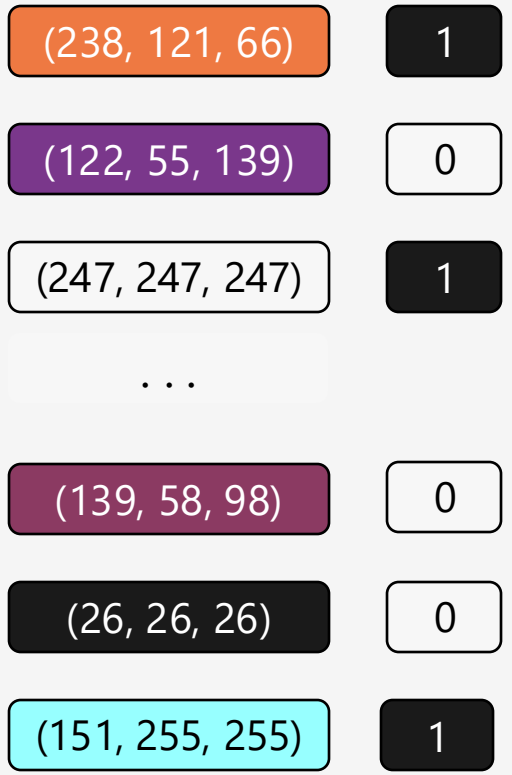
Columns



The Input Data

The input data will separate into X and Y matrices/vectors, where the input X will contain the three R,G,B values for all $1,345$ records.

The output Y will contain the binary $1, 0$ classifications.



The Input Data

We will scale down the R,G,B values by 255 to help the optimization.

$$X = \begin{bmatrix} 238 & 121 & 66 \\ 122 & 55 & 139 \\ 247 & 247 & 247 \\ \dots & \dots & \dots \\ 139 & 58 & 98 \\ 26 & 26 & 26 \\ 151 & 255 & 255 \end{bmatrix} \times \frac{1}{255} \qquad Y = \begin{bmatrix} 1 \\ 0 \\ 1 \\ \dots \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

(238, 121, 66)	1
(122, 55, 139)	0
(247, 247, 247)	1
. . .	
(139, 58, 98)	0
(26, 26, 26)	0
(151, 255, 255)	1

The Input Data

We will scale down the R,G,B values by 255 to help the optimization.

Let's sample this first color and see how we pass it through the neural network.

$$X = \begin{bmatrix} .93 & .47 & .26 \\ .48 & .22 & .55 \\ .97 & .97 & .97 \\ \dots & \dots & \dots \\ .55 & .23 & .38 \\ .10 & .10 & .10 \\ .59 & 1 & 1 \end{bmatrix} \qquad Y = \begin{bmatrix} 1 \\ 0 \\ 1 \\ \dots \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

(238, 121, 66)	1
(122, 55, 139)	0
(247, 247, 247)	1
. . .	
(139, 58, 98)	0
(26, 26, 26)	0
(151, 255, 255)	1

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

We will call the raw output of the first layer Z_1.

It will apply the weights and biases.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Multiply and add each respective row of weights with each respective column of input data, in an element-wise fashion.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ \\ \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Multiply and add each respective row of weights with each respective column of input data, in an element-wise fashion.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ (0.733)(.93) + (0.054)(.47) + (0.49)(.26) \\ \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Multiply and add each respective row of weights with each respective column of input data, in an element-wise fashion.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ (0.733)(.93) + (0.054)(.47) + (0.49)(.26) \\ (0.952)(.93) + (0.635)(.47) + (0.001)(.26) \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Multiply and add each respective row of weights with each respective column of input data, in an element-wise fashion.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

In NumPy, we can achieve this matrix multiplication using the @ operator.

```
Z1 = w_hidden @ X + b_hidden
```

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ (0.733)(.93) + (0.054)(.47) + (0.49)(.26) \\ (0.952)(.93) + (0.635)(.47) + (0.001)(.26) \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ (0.733)(.93) + (0.054)(.47) + (0.49)(.26) \\ (0.952)(.93) + (0.635)(.47) + (0.001)(.26) \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

Finally, add the biases in element-wise fashion.

We have the output of the first layer Z_1.

Raw Output of Hidden Layer

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$Z_1 = \begin{bmatrix} 0.102 & 0.323 & 0.626 \\ 0.733 & 0.054 & 0.49 \\ 0.952 & 0.635 & 0.001 \end{bmatrix} \times \begin{bmatrix} 0.93 \\ 0.47 \\ 0.26 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} (0.102)(.93) + (0.323)(.47) + (0.626)(.26) \\ (0.733)(.93) + (0.054)(.47) + (0.49)(.26) \\ (0.952)(.93) + (0.635)(.47) + (0.001)(.26) \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} 0.40943 \\ 0.83447 \\ 1.18407 \end{bmatrix} + \begin{bmatrix} 0.223 \\ 0.472 \\ 0.768 \end{bmatrix} = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix}$$

Finally, add the biases in element-wise fashion.

We have the output of the first layer Z_1.

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

We will call the activated output of the first layer A_1, which passes Z_1 through the activation function *ReLU*.

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

$$A_1 = Z_1 \times (Z_1 > 0)$$

ReLU **can be implemented by multiplying Z_1 with a binary (1,0) outcome whether it is greater than 0.**

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

$$A_1 = Z_1 \times (Z_1 > 0)$$

$$A_1 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times \begin{bmatrix} 0.63243 > 0 \\ 1.30647 > 0 \\ 1.95207 > 0 \end{bmatrix}$$

ReLU **can be implemented by multiplying Z_1 with a binary (1,0) outcome whether it is greater than 0.**

In this case, all the numbers are positive so each element will be multiplied by 1.

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

$$A_1 = Z_1 \times (Z_1 > 0)$$

$$A_1 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

ReLU **can be implemented by multiplying Z_1 with a binary (1,0) outcome whether it is greater than 0.**

In this case, all the numbers are positive so each element will be multiplied by 1.

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

$$A_1 = Z_1 \times (Z_1 > 0)$$

$$A_1 = \begin{bmatrix} 0.63243 \times 1 \\ 1.30647 \times 1 \\ 1.95207 \times 1 \end{bmatrix}$$

ReLU **can be implemented by multiplying Z_1 with a binary (1,0) outcome whether it is greater than 0.**

In this case, all the numbers are positive so each element will be multiplied by 1.

Activated Output of Hidden Layer

$$A_1 = ReLU(Z_1)$$

$$A_1 = Z_1 \times (Z_1 > 0)$$

$$A_1 = \begin{bmatrix} 0.63243 \times 1 \\ 1.30647 \times 1 \\ 1.95207 \times 1 \end{bmatrix}$$

$$A_1 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix}$$

ReLU **can be implemented by multiplying Z_1 with a binary (1,0) outcome whether it is greater than 0.**

In this case, all the numbers are positive so each element will be multiplied by 1.

Raw Output of Output Layer

$$Z_2 = A_1 \times W_{output} + B_{output}$$

The activated output of the hidden layer now becomes the input for the output layer, which we will call Z_2.

Raw Output of Output Layer

$$Z_2 = A_1 \times W_{output} + B_{output}$$

$$Z_2 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times [0.309 \quad 0.662 \quad 0.007] + [0.06]$$

The activated output of the hidden layer now becomes the input for the output layer, which we will call Z_2.

Raw Output of Output Layer

$$Z_2 = A_1 \times W_{output} + B_{output}$$

$$Z_2 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times [0.309 \quad 0.662 \quad 0.007] + [0.06]$$

The activated output of the hidden layer now becomes the input for the output layer, which we will call Z_2.

$$Z_2 = [0.63243 \times 0.309 + 1.30647 \times 0.662 + 1.95207 \times 0.007] + [0.06]$$

Raw Output of Output Layer

$$Z_2 = A_1 \times W_{output} + B_{output}$$

$$Z_2 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times [0.309 \quad 0.662 \quad 0.007] + [0.06]$$

$$Z_2 = [1.0739685] + [0.06]$$

The activated output of the hidden layer now becomes the input for the output layer, which we will call Z_2.

Raw Output of Output Layer

$$Z_2 = A_1 \times W_{output} + B_{output}$$

$$Z_2 = \begin{bmatrix} 0.63243 \\ 1.30647 \\ 1.95207 \end{bmatrix} \times [0.309 \quad 0.662 \quad 0.007] + [0.06]$$

$$Z_2 = [1.0739685] + [0.06]$$

$$Z_2 = [1.1339685]$$

The activated output of the hidden layer now becomes the input for the output layer, which we will call Z_2.

Activated Output of Output Layer

$$A_2 = sigmoid(Z_2)$$

$$A_2 = sigmoid([1.1339685])$$

$$A_2 = \frac{1}{1 + e^{-1.1339685}}$$

$$A_2 = 0.75657$$

Finally, we can work through the final output value A_2 which is produced by passing Z_2 through the activation function, which in this case is *sigmoid()*.

Summary of Layer Calculations

$$Z_1 = W_{hidden}X + B_{hidden}$$

$$A_1 = ReLU(Z_1)$$

$$Z_2 = A_1 \times W_{output} + B_{output}$$

$$A_2 = sigmoid(Z_2)$$

In summary, we calculate the raw and activated outputs of each layer as shown to the right.

We can use the Python function below to execute these in NumPy.

```
relu = lambda x: np.maximum(x, 0)
logistic = lambda x: 1 / (1 + np.exp(-x))

def forward_prop(X):
    Z1 = w_hidden @ X + b_hidden
    A1 = relu(Z1)
    Z2 = w_output @ A1 + b_output
    A2 = logistic(Z2)
     return Z1, A1, Z2, A2
```

Walkthrough: Forward Propagation in NumPy

```
import numpy as np
import pandas as pd

all_data = pd.read_csv("https://tinyurl.com/y2qmhfsr")

# Extract the input columns, scale down by 255
X = (all_data.iloc[:, 0:3].values / 255.0)
Y = all_data.iloc[:, -1].values

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)

# Activation functions
relu = lambda x: np.maximum(x, 0)
logistic = lambda x: 1 / (1 + np.exp(-x))
```

```
# Runs inputs through the neural network to get predicted
outputs
def forward_prop(X):
    Z1 = w_hidden @ X + b_hidden
    A1 = relu(Z1)
    Z2 = w_output @ A1 + b_output
    A2 = logistic(Z2)
    return Z1, A1, Z2, A2

# Calculate accuracy
test_predictions = forward_prop(X.transpose())[3]

test_comparisons = np.equal((test_predictions >=
.5).flatten().astype(int), Y)
accuracy = sum(test_comparisons.astype(int) / X.shape[0])
print("ACCURACY: ", accuracy)
```

What About Training a Neural Network?

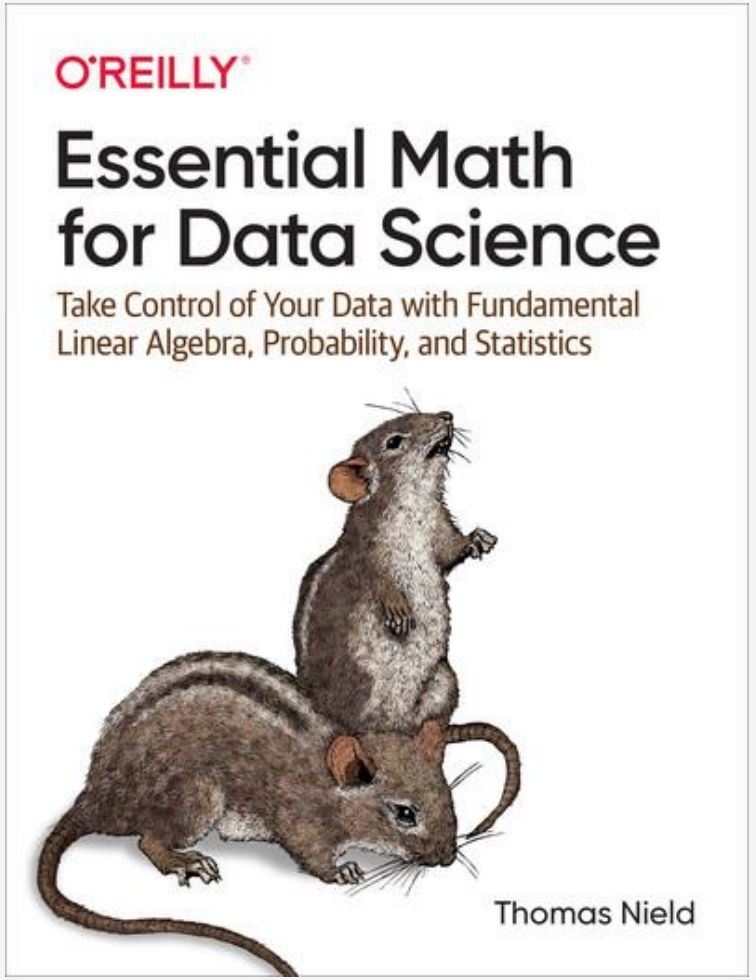
O'Reilly Online Training *Deep Learning for Beginners*

https://learning.oreilly.com/live-events/deep-learning-for-beginners-in-3-weeks/0636920079316/0790145063610/

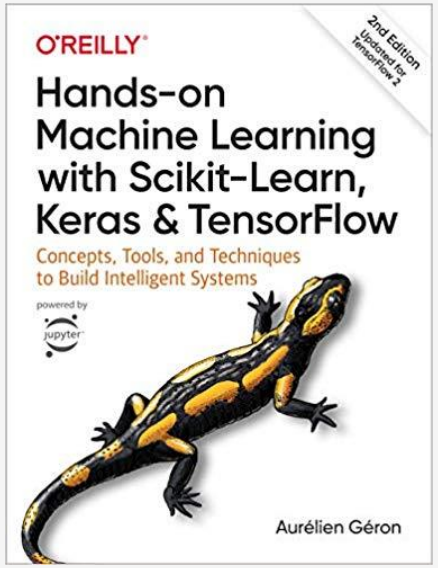
Or check out Chapter 7 of my book…

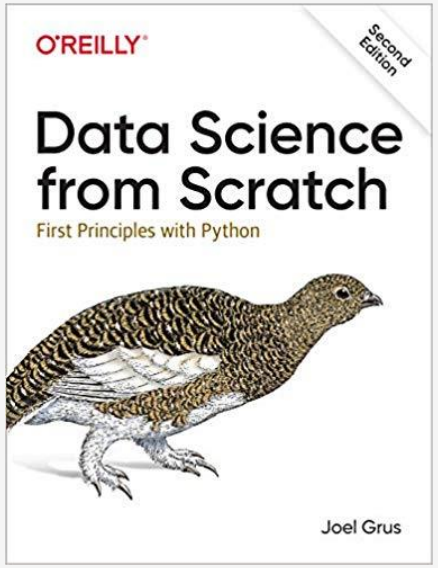
Section VII
Going Forward

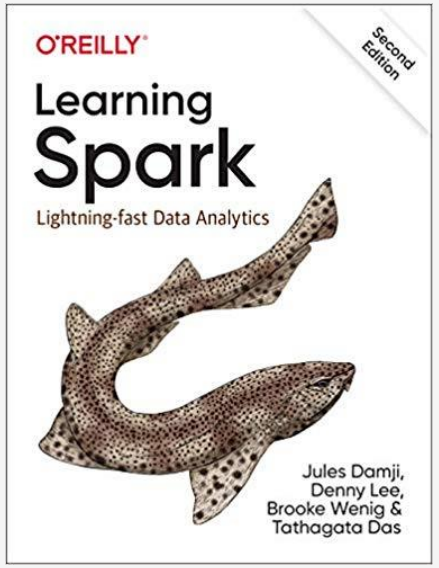
To Learn More…

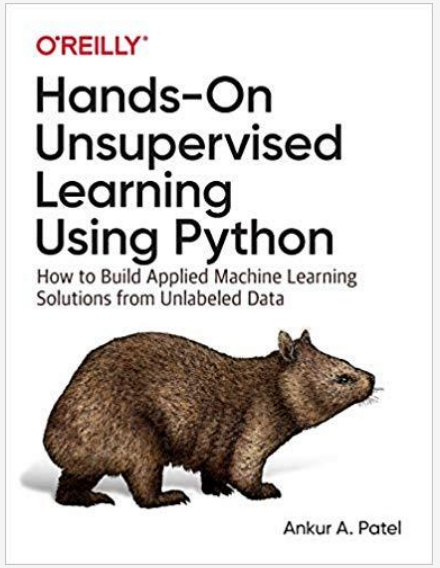


To Learn More…









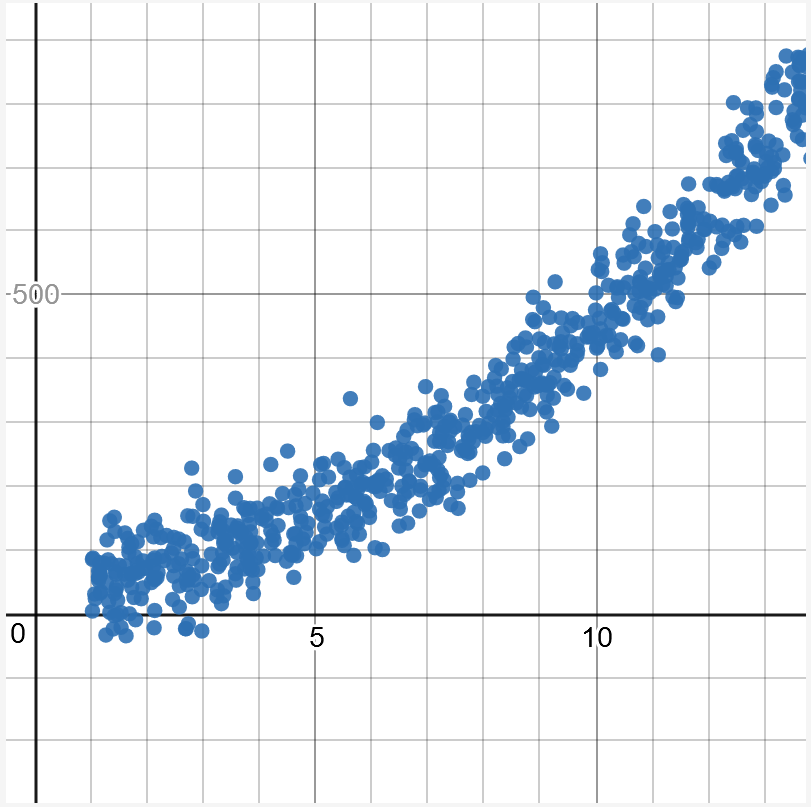
Homework Assignments (Answers Are In “code” Folder)

Homework #1

You notice some data (accessible at https://bit.ly/2UBhrMG) has a familiar shape on a scatterplot, and you believe that the best regression will fit to a function

$$y = ax^2 + b$$

where a and b are some constants. Find the a and b constants for the best fit regression based on sum of squares. I recommend using this Desmos Graph to graph your points and function to eyeball whether a good fit occurred.



https://www.desmos.com/calculator/canygmx67n

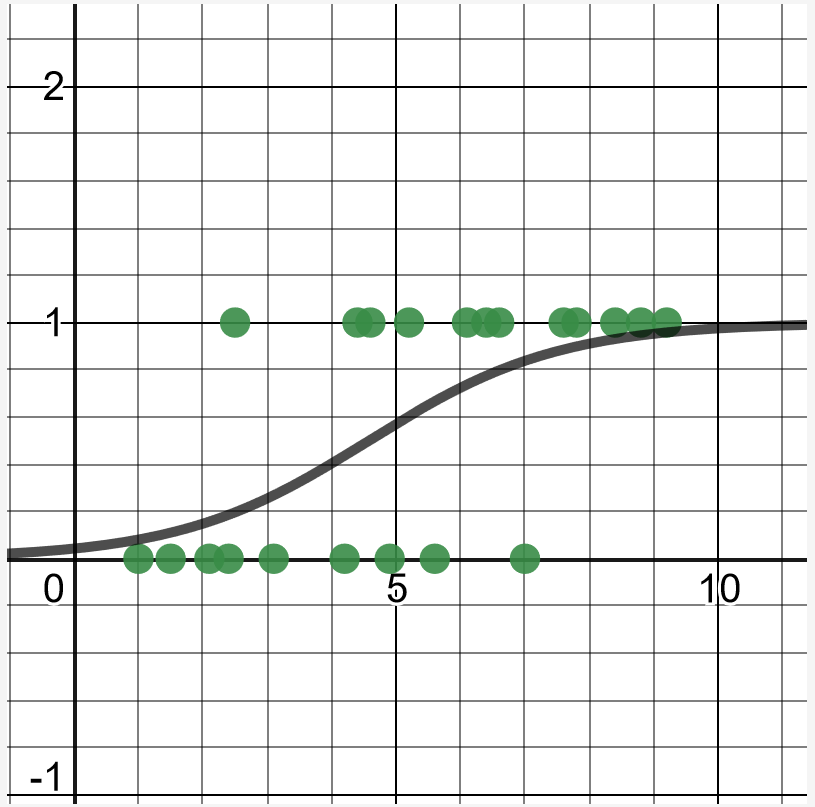
HINT: Think of how you solved a linear regression using hill-climbing, and how it could apply here. Solution is in the folder *code/homework_answers*

Homework #2

Take the RGB background color data (accessible at https://tinyurl.com/y2qmhfsr) that recommends a light (1) or dark (0) font. Create a logistic regression model that trains with that data and predicts a light/dark font for new background colors. Test to make sure a black background (0,0,0) will predict a LIGHT font and a white background (255,255,255) will predict a DARK font.

HINT: Remember the first three columns are the numeric inputs (red, green, blue) and the fourth column is the output ("1" for light, "0" for dark).

Solution is in the folder *code/homework_answers*



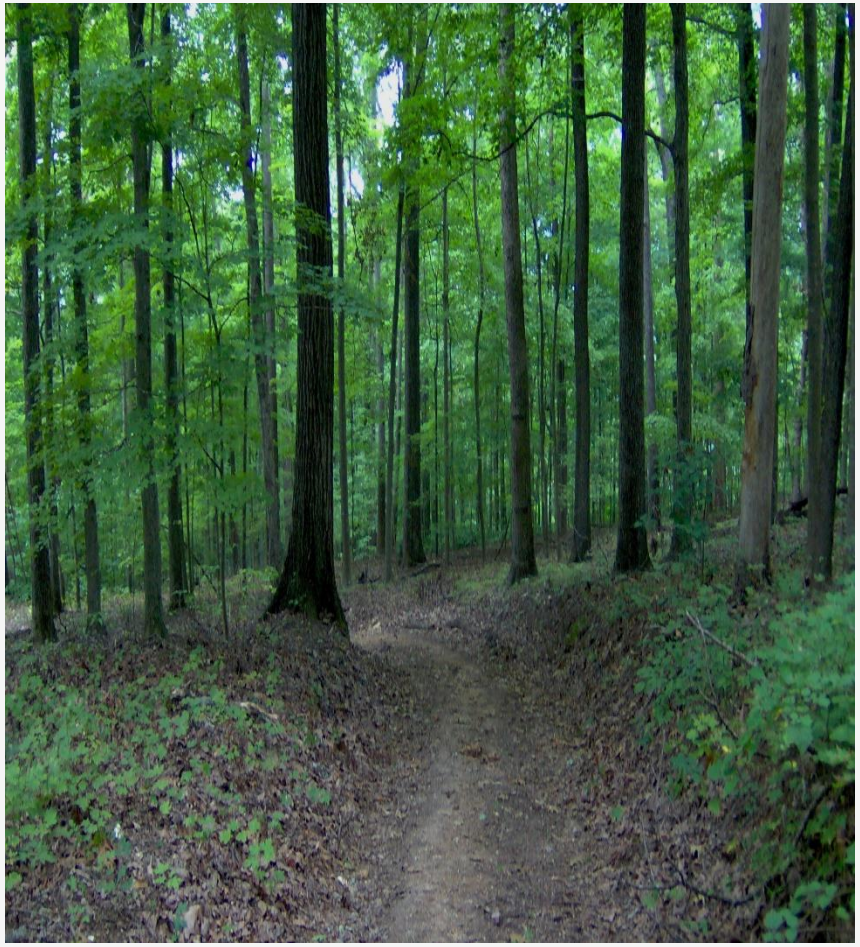
Homework #3

Take the employee retention data (accessible at https://tinyurl.com/y6r7qjrp) and make a decision tree to predict whether the employee will quit (1) or not quit (0).

As a quick and dirty test, check to see if employees who are not promoted for over two years generally quit by putting some in as inputs.

Solution is in the folder *code/homework_answers*

BONUS: Can you convert the model into a random forest with 600 decision trees?



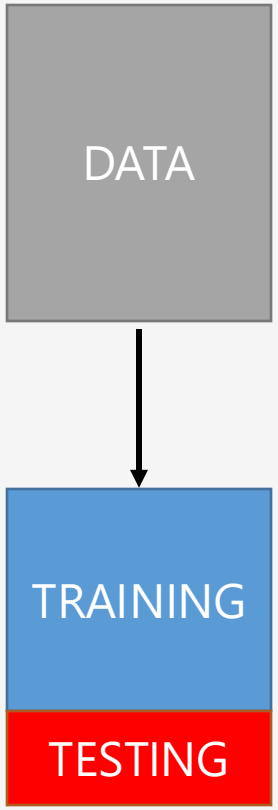
Appendix A:
Classification Validation

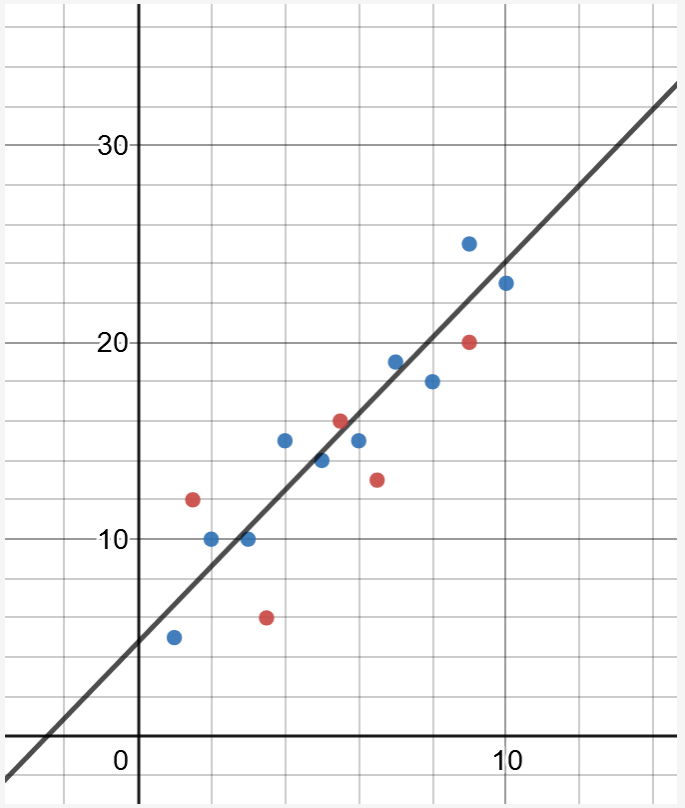
Training and Testing Data

A common practice to proactively prevent overfitting in machine learning is to separate training data and testing data.

- **Training data** is data used to fit a model and is typically 2/3 of the data.
- **Test data** is used to test the model and is the remaining 1/3 of the data.

By omitting the testing data from training, we see how well the model works on data it has not seen before and change our parameters accordingly.





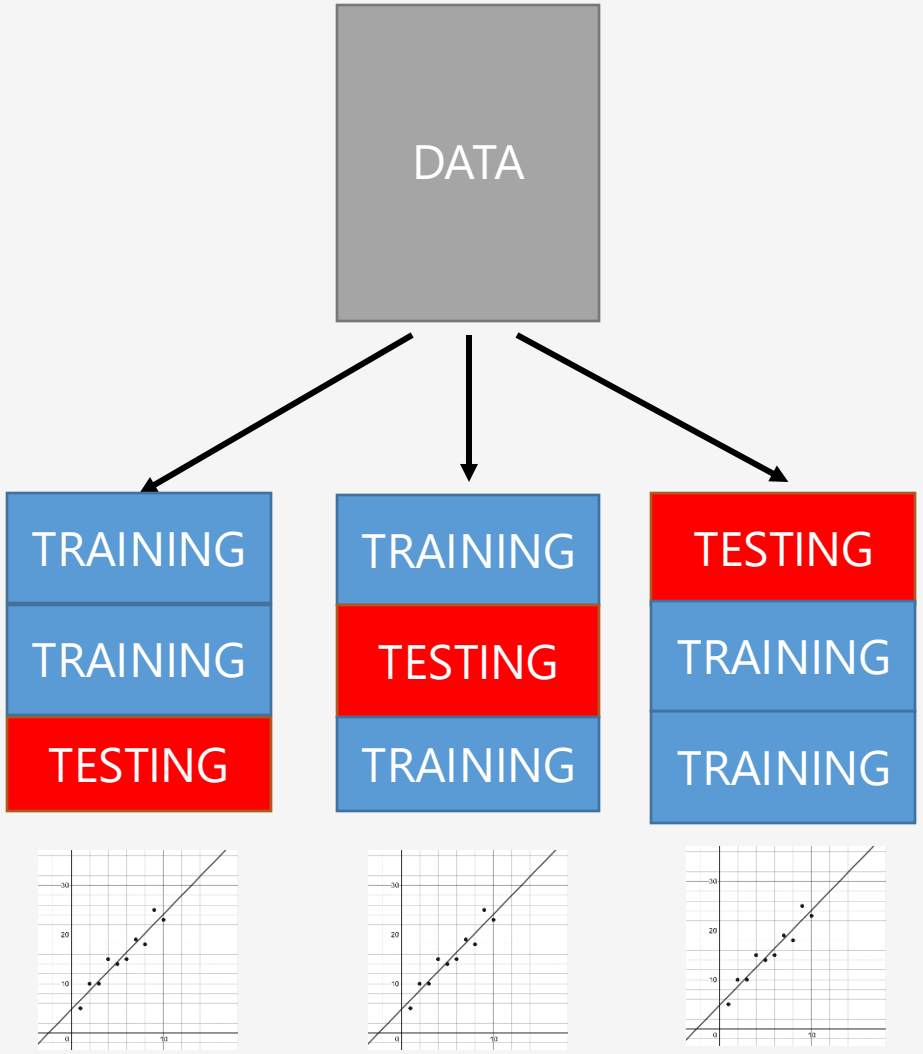
Cross-Validation

We can take this concept of training/testing data a step further, and test different combinations of training and testing data.

This is known as **cross-validation**, the gold standard of validation techniques.

To the right we have **3-fold cross validation** which breaks the data into thirds and uses one of the pieces for testing.

We can then evaluate how well each of these perform, being able to compare different parameters and models (e.g. linear regression vs decision trees) and see which setup produces the best performance.



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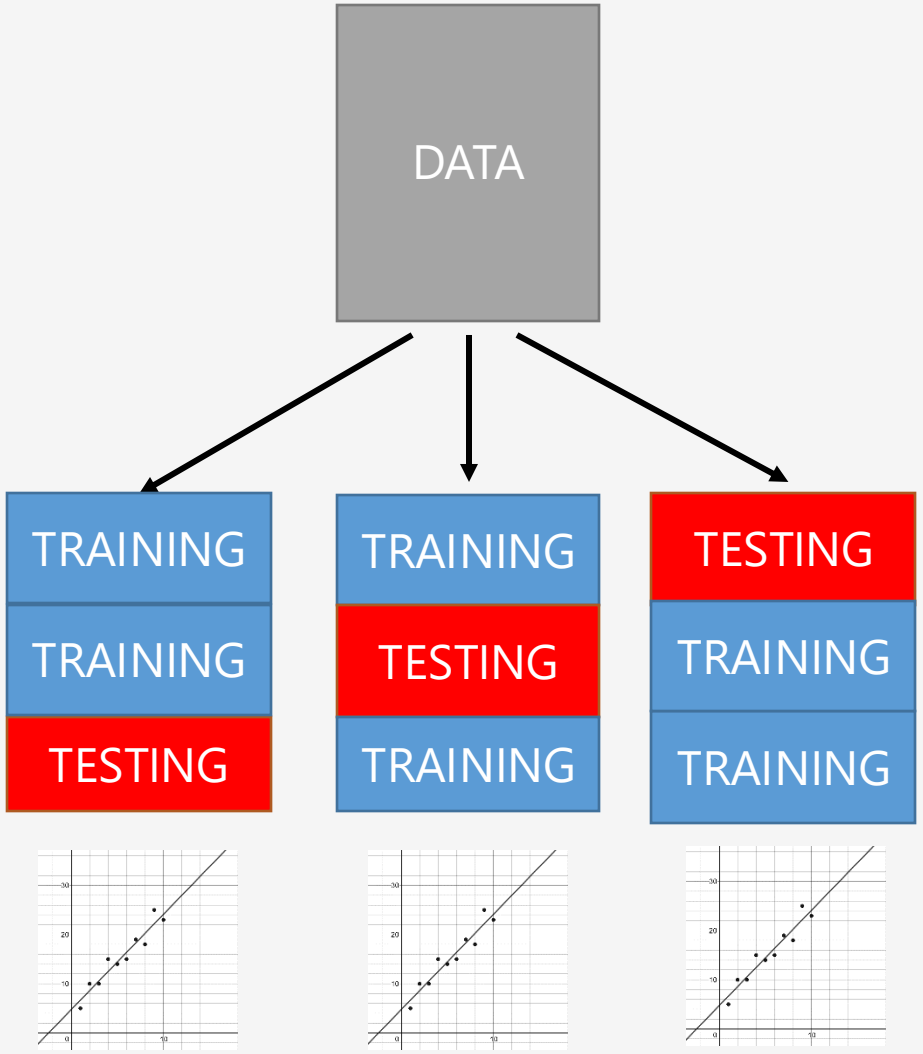
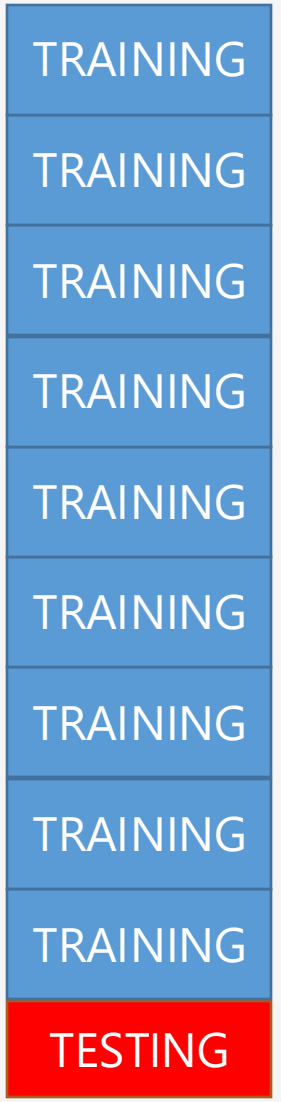


Cross-Validation

Note that **k-fold cross validation** allows us to slice our data into any number and not just 3 (typically 3, 5, or 10).

For example we can do 10-fold cross validation and validate 10 different combinations of training/test data.

The most extreme form of folding is **leave-one-out cross validation**, which omits one data record for testing and uses the remaining records for training, and this is done repeatedly.

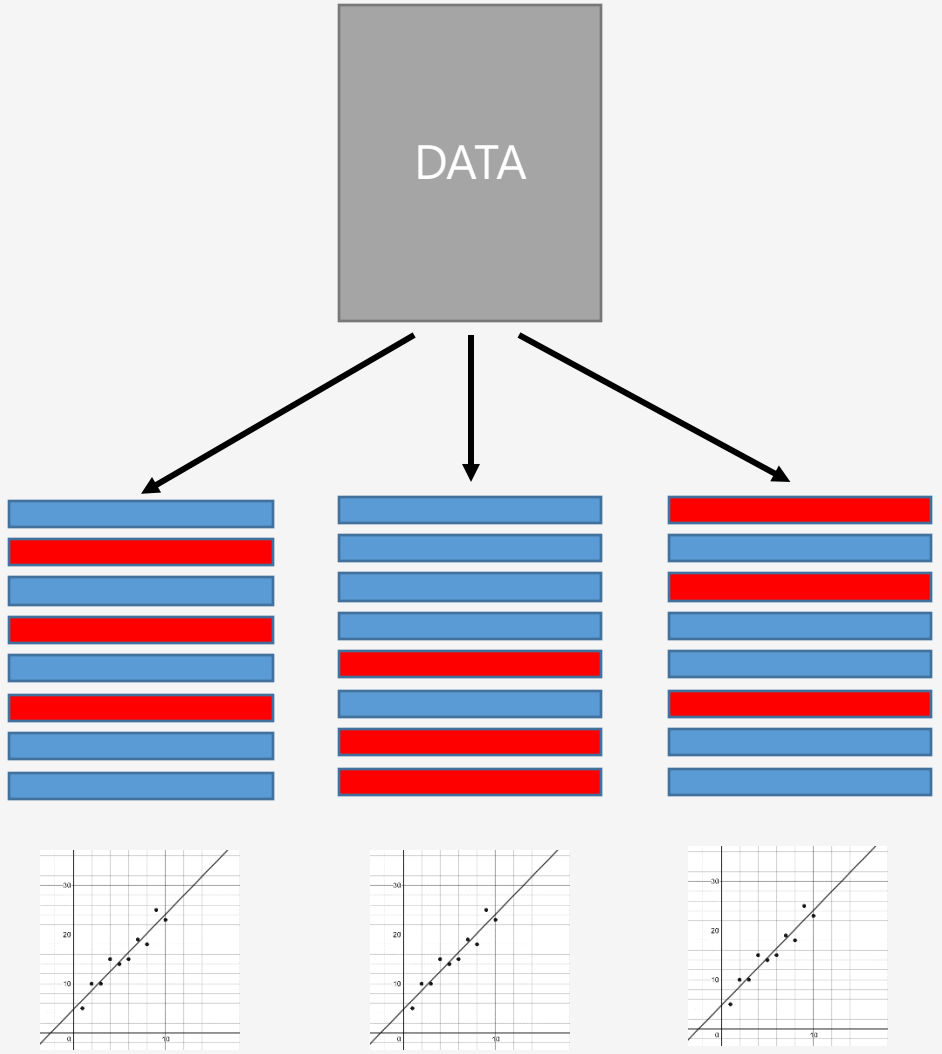


Random Fold Validation

As you may be noticing, machine learning often tries to overcome data variance with randomness.

A variant with fold validation is **repeated random fold validation**, where we randomly shuffle the data and create random train/test folds as many times as desired.

This is helpful when we need to mitigate variance in the model.



Which Validation to Use?

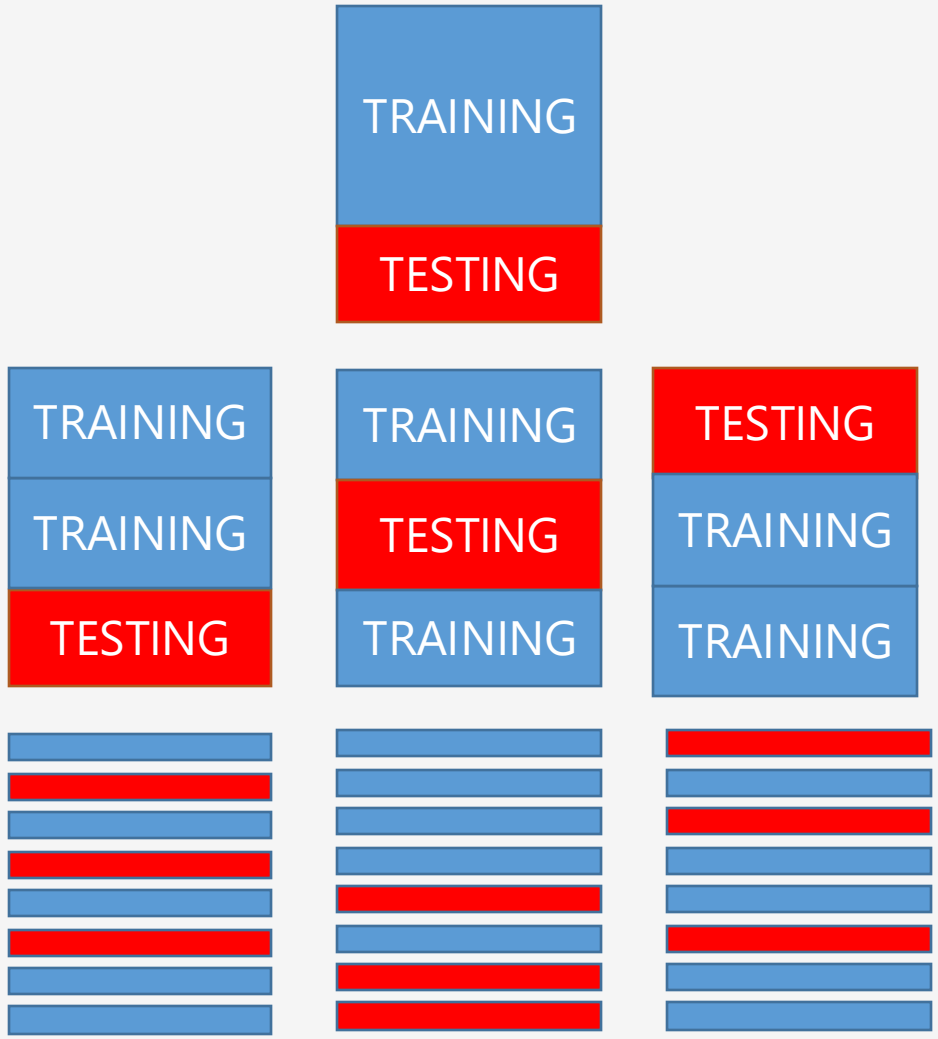
Generally, you will want to prefer k-fold validation as it is the gold standard.

A single train/test split might be warranted if performance of machine learning algorithm is slow and has enough data with lower bias.

Use the random fold split to mitigate variance in the model while balancing training speed and dataset sizes.

We will talk about class imbalance later, but if you do not have an equal number of samples for each class, you might want to consider using stratification in your k-fold validation.

Stratification means an equal proportion of data for each class is sampled for training and testing data (even it is sampled repeatedly), so that no class is neglected.



A Stratified Validation in Scikit-Learn

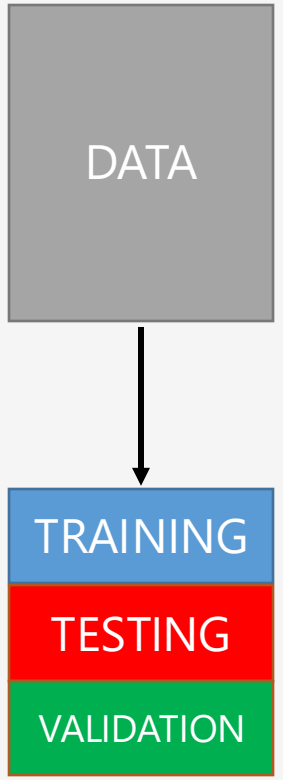
```
import numpy as np
import pandas as pd
# load data
from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPClassifier

df = pd.read_csv("https://tinyurl.com/y6r7qjrp", delimiter=",")

# Extract input variables (all rows, all columns but last column)
# Note we should do some linear scaling here
X = (df.values[:, :-1] / 255.0) + .01

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Get a count of each group to ensure samples are equitably balanced
print(df.groupby(["class"]).agg({"class" : [np.size]}))

# Separate training and testing data
# Note that I use the 'stratify' parameter to ensure
# each class is proportionally represented in both sets
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=.33, stratify=Y)

nn = MLPClassifier(solver='sgd', hidden_layer_sizes=(100, ),
                   max_iter=480, learning_rate_init=.1)

nn.fit(X_train, Y_train)

print("Training set score: %f" % nn.score(X_train, Y_train))
print("Test set score: %f" % nn.score(X_test, Y_test))
```

Validation Data

Validation is a separate type of testing data used to compare performance of different models.

When you are comparing two or more models (e.g. logistic regression versus decision trees), you may hold back one more chunk of data for validation.

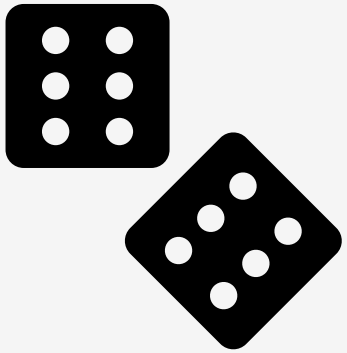
It is different than the testing data, which is used to tune parameters of the individual model, not compare different models altogether.



Random Seeding

Machine learning deals with a lot of random-based operations:

- Randomly sampled training/testing data
- Random-based optimization and training (e.g. stochastic gradient descent, simulated annealing)
- Randomly generated data from simulations



Testing can be challenging as the above operations make outputs nondeterministic, so setting a random seed is common practice to make them deterministic.

This allows tests to be conveniently reproducible, where sequences of randomly generated values are the same.

Be careful to not rely on random seeds too much! They can give the illusion of determinism so test many random seeds, not just one, to ensure they converge towards the same outcome.

Random Seeding a 3-Fold Split for Reproducibility

```
import pandas as pd
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import KFold, cross_val_score

# Load the data
df = pd.read_csv("https://tinyurl.com/y6r7qjrp", delimiter=",")

X = df.values[:, :-1]
Y = df.values[:, -1]

# "random_state" is the random seed, which we fix to 7
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LogisticRegression(solver='liblinear')
results = cross_val_score(model, X, Y, cv=kfold)

print("Accuracy Mean: %.3f (stdev=%.3f)" % (results.mean(), results.std()))
```

Why “Accuracy” is a Bad Measure for Classification

Suppose your machine learning model observed people with the name “Michael” quit their job.

Therefore it simply predicts any employee with the name “Michael” will quit, and everyone else will stay.

If there was one Michael in a company of 100 employees, but a different employee ended up quitting, the machine could still boast 98% accuracy.

Why stop there? If 99% of employees do not quit, you might as well predict every employee *will not quit* and get 99% accuracy.

Machine learning makes shortcuts like this all the time especially when the event of interest is rare (e.g. diseases, security breaches, employee attrition, rare road/highway events).

Confusion Matrix

As seen in the previous example, **accuracy** (the rate of correct labeling) can be a misleading measure of performance, especially in classification problems with class imbalance.

A better way to evaluate classification models is the **confusion matrix**, which keeps track of **false positives** (Type I Error) and **false negatives** (Type II Error).

We want to evaluate how many employees who were predicted to quit actually did quit (**true positives**).

Conversely, we also want to evaluate how many employees who were predicted to stay actually did stay (**true negatives**).

	Actually Quits (True)	Actually Stays (False)
Predicted will quit (True)	0	1
Predicted will stay (False)	1	98

Confusion Matrix

From the confusion matrix, we can derive all sorts of useful metrics beyond just accuracy.

We can easily see that **precision** (how accurate positive predictions were) and **sensitivity** (rate of identified positives) are 0, meaning this machine learning model fails entirely at positive predictions.

	Actually Quits	Actually Stays	
Predicted will quit	0 (TP)	1 (FN)	**Sensitivity** $\frac{TP}{TP+FN} = \frac{0}{0+1} = 0$
Predicted will stay	1 (FP)	98 (TN)	**Specificity** $\frac{TN}{TN+FP} = \frac{98}{98+1} = .989$
	Precision $\frac{TP}{TP+FP} = \frac{0}{0+1} = 0$	**Negative Predicted Value** $\frac{TN}{TN+FN} = \frac{98}{98+1} = .989$	**Accuracy** $\frac{TP+TN}{TP+TN+FP+FN} = \frac{98+0}{0+98+1+1} = .98$

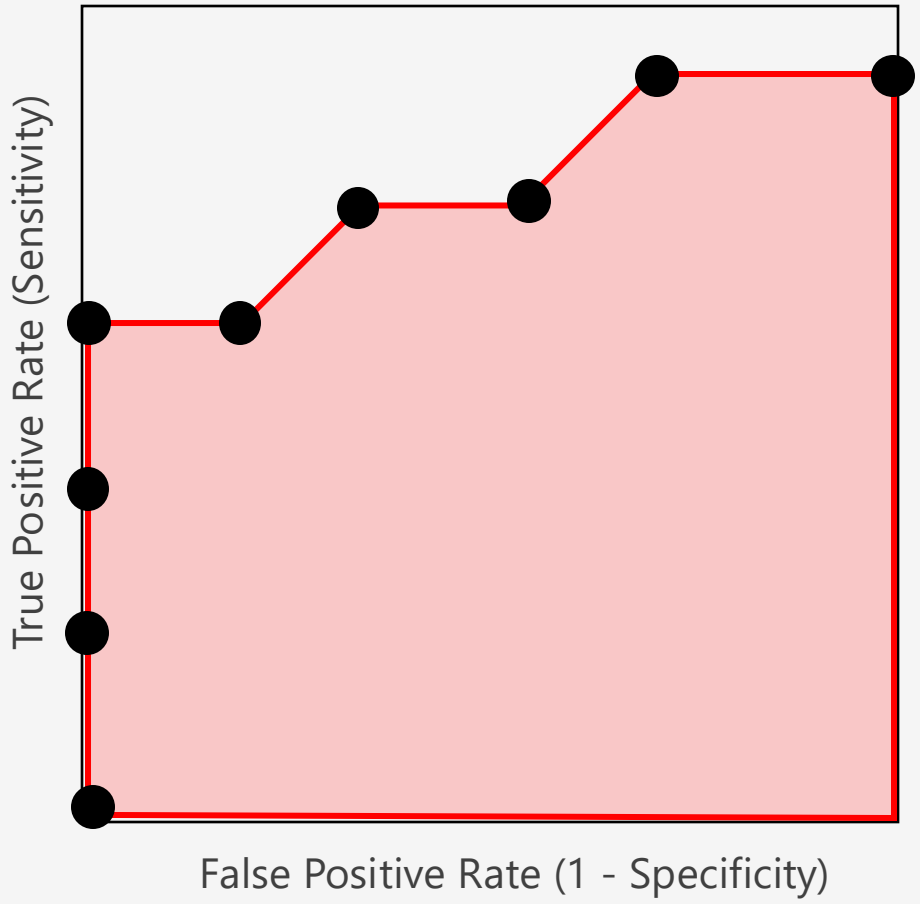
F1 Score $\frac{2*Precision*Recall}{Precision+Recall}$ = Undefined

ROC and AUC

When we are evaluating different machine learning configurations, we may end up with dozens, hundreds, or thousands of confusion matrices.

These can be tedious to review, so we can summarize all of them with a **receiver operator characteristic (ROC)** curve as shown to the right.

This allows us to see each testing instance (each represented by a black dot) and find an agreeable balance between true positives and false positives.

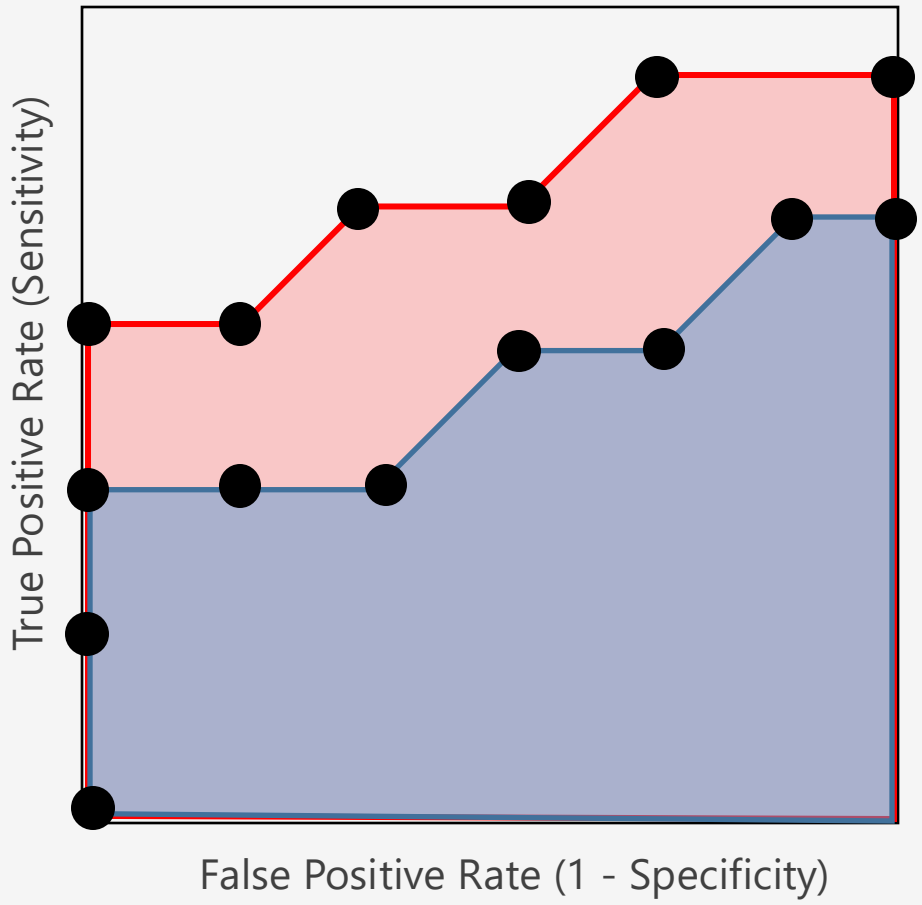


ROC and AUC

We can also compare different machine learning models by creating separate ROC curves for each.

For example, if our red curve represents a logistic regression and the blue curve represents a decision tree, we can see the performance of them side-by-side.

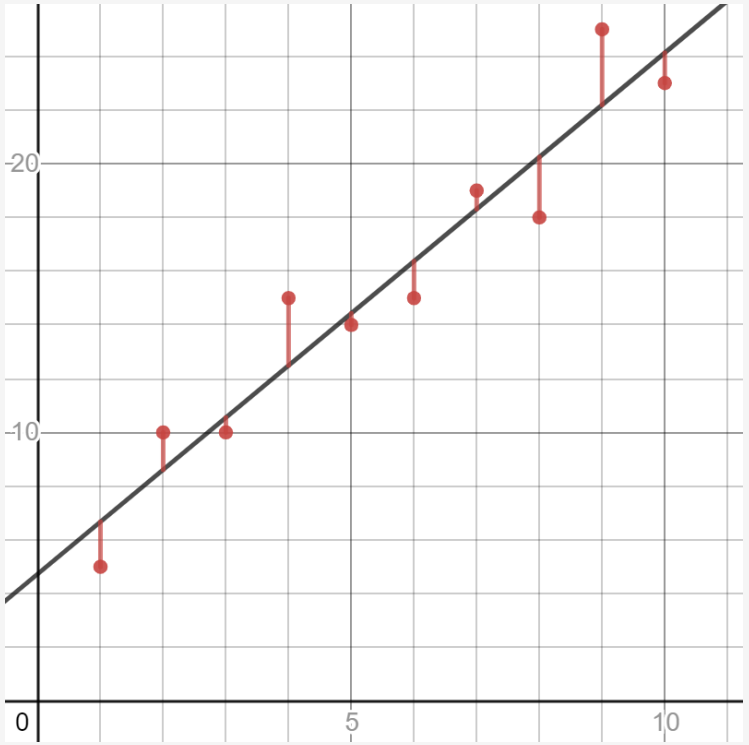
The **area under the curve (AUC)** is a good metric for choosing which model to use. Since the red curve (logistic regression) has a greater area, this suggests it is a superior model.



Appendix B:
Regression Validation

Mean Absolute Error

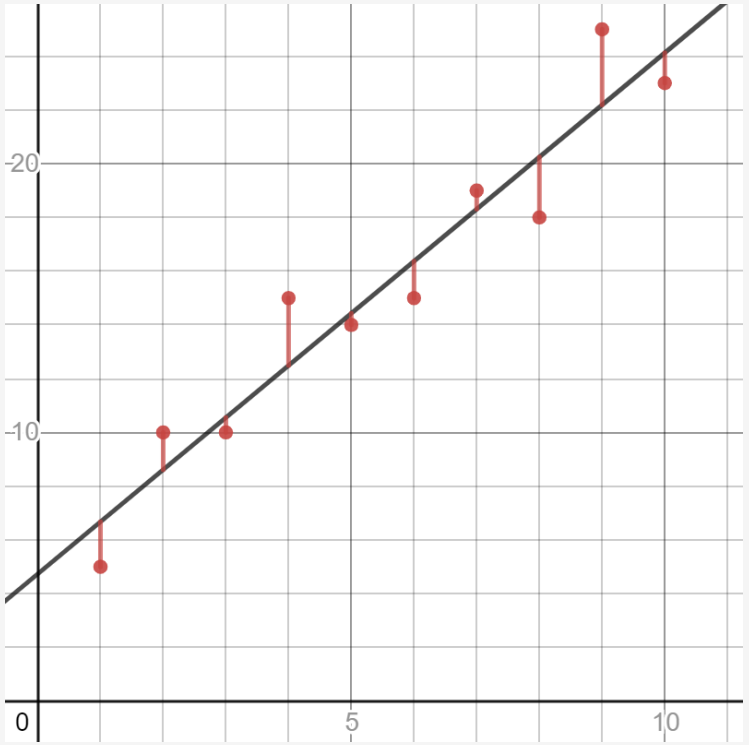
Mean absolute error (MAE) simply measures the sum of absolute values of residuals (difference between predicted values and actual values).




```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score, validation_curve

df = pd.read_csv('https://bit.ly/3cIH97A', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]

# Perform a simple linear regression
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LinearRegression()

# Use negative mean absolute error
# It is negative because it is inverted
results = cross_val_score(model, X, Y, cv=kfold, scoring='neg_mean_absolute_error')

print("MAE: mean=%.3f (stdev-%.3f)" % (results.mean(), results.std()))
# prints MAE: mean=-2.446 (stdev-0.791)
```

Mean Squared Error

Mean squared error (MSE) simply measures the average squared values of residuals (difference between predicted values and actual values).

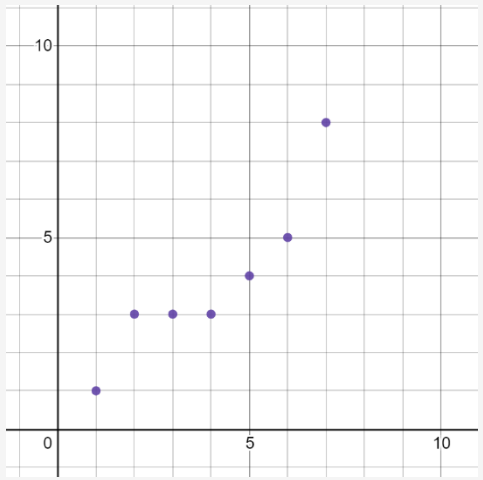



```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score, validation_curve

df = pd.read_csv('https://bit.ly/3nJBdj9', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Perform a simple linear regression
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LinearRegression()

# Use negative mean squared error
# It is negative because it is inverted
results = cross_val_score(model, X, Y, cv=kfold, scoring='neg_mean_squared_error')

print("MAE: mean=%.3f (stdev-%.3f)" % (results.mean(), results.std()))
# prints MSE: mean=-7.664 (stdev-3.110)
```

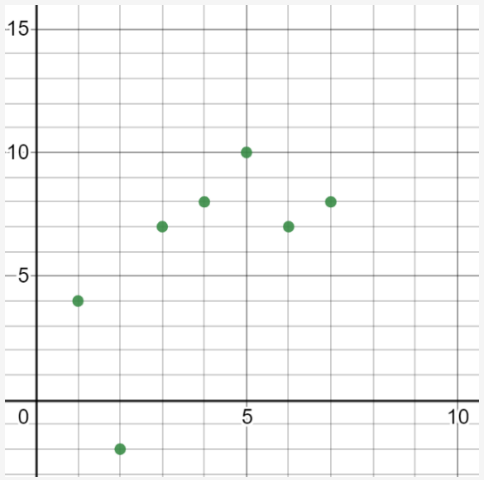
Pearson Correlation

Using a **Pearson correlation**, we can measure the strength of a correlation between two variables (from a range of -1.0 to 1.0).

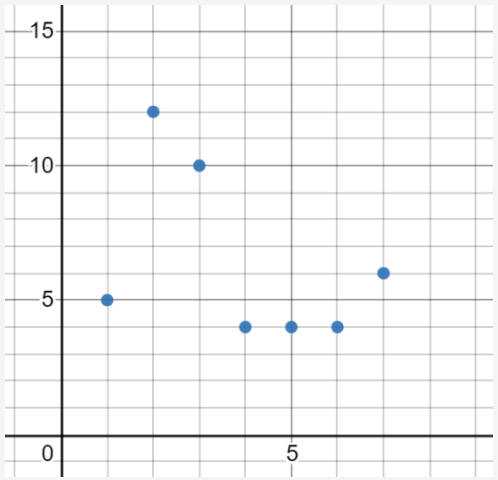
A correlation closer to 1.0 means a strong positive correlation, 0.0 means no correlation, and closer to -1.0 indicates negative correlation.



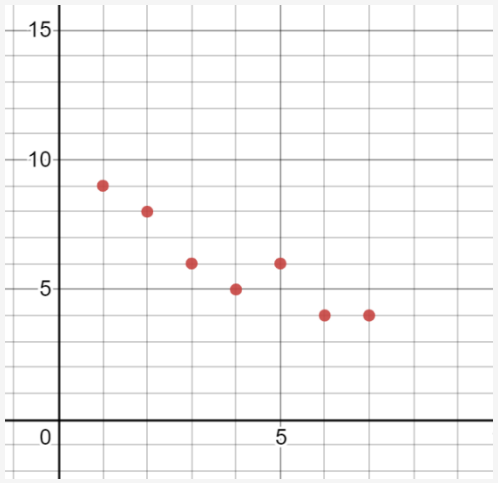
PEARSON CORRELATION: .923133



PEARSON CORRELATION: .643237



PEARSON CORRELATION: -.44984



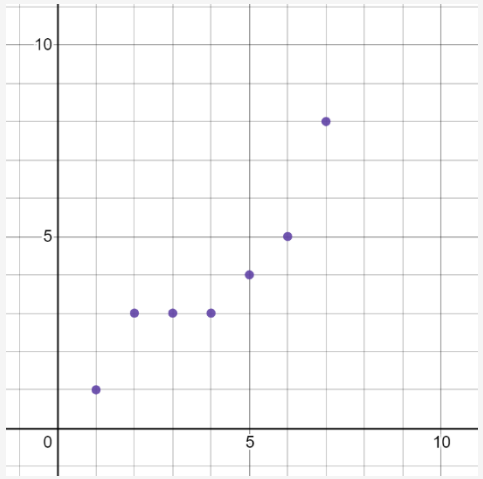
PEARSON CORRELATION: -.9267

Pearson Correlation

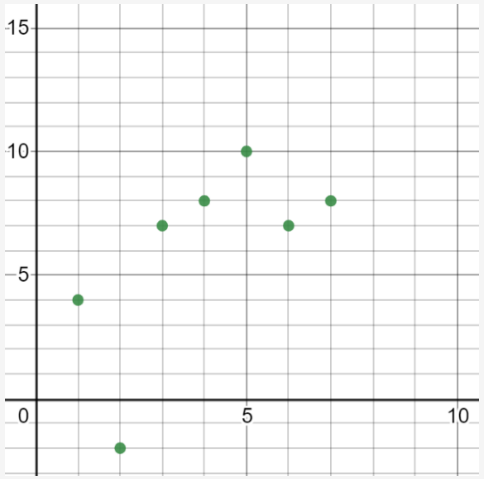
The more data you collect, the more confident you can be in your correlation value.

Having more data decreases the **P-value**, the probability you would observe this correlation randomly by chance.

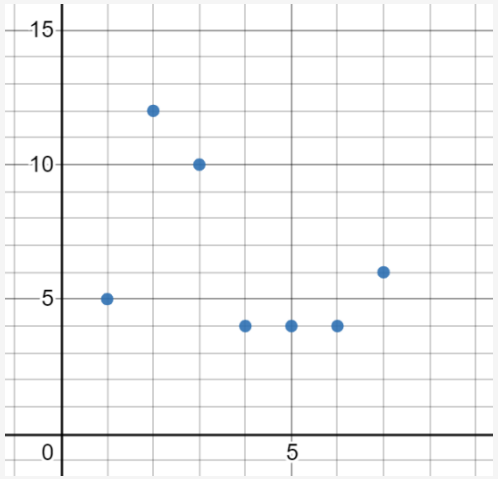
If our correlation is unlikely to have happened at random, that means we are more likely to have discovered something meaningful rather than by chance.



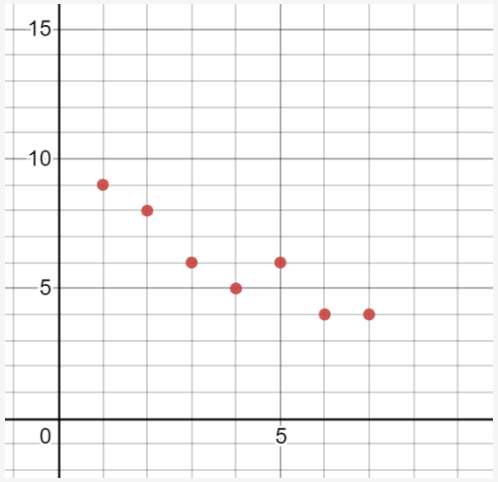
PEARSON CORRELATION: .923133



PEARSON CORRELATION: .643237



PEARSON CORRELATION: -.44984



PEARSON CORRELATION: -.9267

R^2

Probably the most useful performance metric is the R-square (R^2), which ratios the residuals against the average y-value to the average of the residuals.

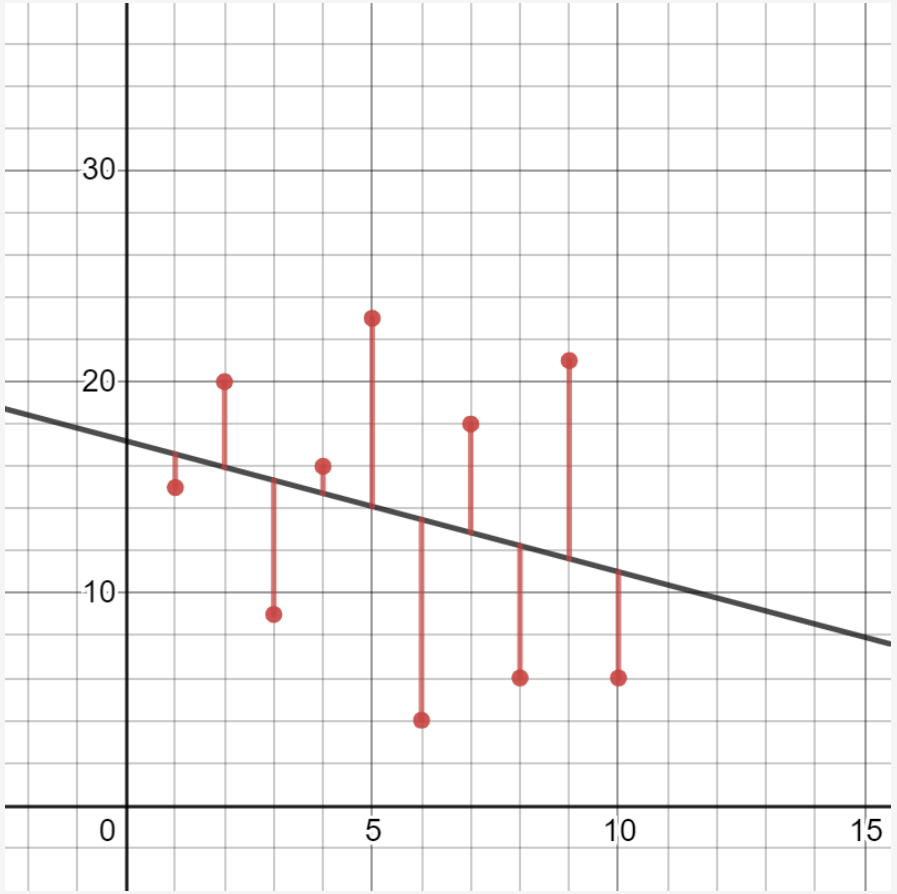
Note R^2 is also called the coefficient of determination and is the square of the Pearson correlation.

It's used to evaluate the quality of a model.

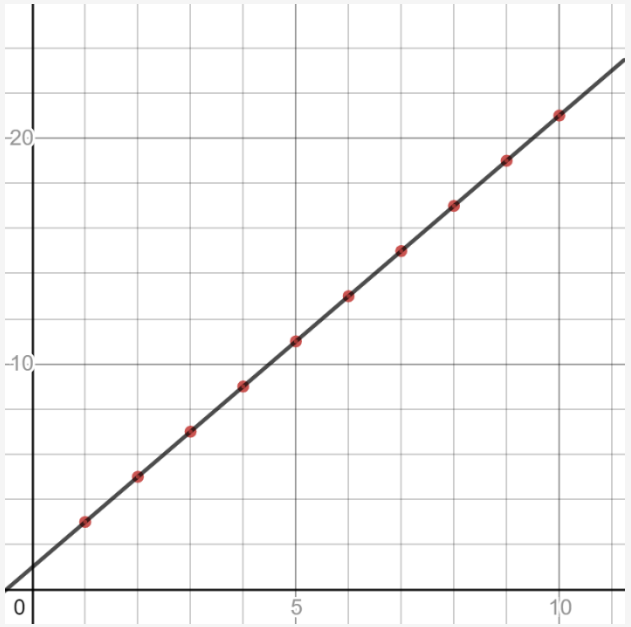
Think of R^2 as a measurement (between 0.0 and 1.0) of how well independent variables explain a dependent variable, rather than predicting with a simple average.

An R^2 of 1.0 indicates a variable perfectly explains a variable while 0.0 indicates there's no explanatory connection at all.

EXAMPLE: If ***x*** was calories consumed and ***y*** was number of pounds gained, and I got an R^2 of .85 on my test data, that means calories explains weight gain 85% better than just predicting with the average weight **y.**

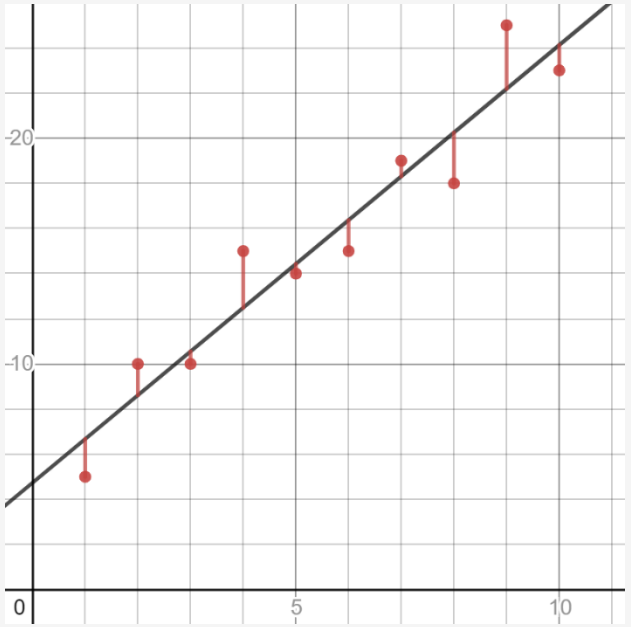


R^2 Visual Examples



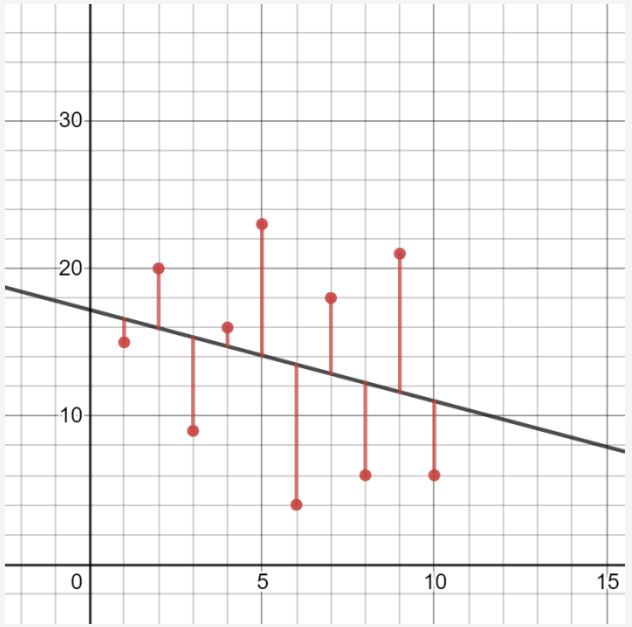
$R^2 = 1.0$

(PERFECT!)



$R^2 = 0.917$

(GOOD!)



$R^2 = 0.071$

(POOR!)

How to Calculate R^2 by Hand

1) Separate training and test data, perform linear regression on training data.

2) **Calculate sum of squares for regression:** using test data, subtract each predicted y value from each actual y value, square and sum

3) **Calculate sum of squares for average:** using test data, subtract the average y value from each actual y value, square and sum

4) Divide the sum of squares for regression by the sum of squares for average, subtract that from 1.0.

Now you calculated R^2 from scratch!

```
# Calculating R-square from scratch

slope = 1.73333333
y_intercept = 5.49999999999999

x_test = [9, 3, 6, 7]
y_test = [25, 10, 15, 19]

y_test_avg = sum(y_test) / len(y_test)
# 17.25

y_test_predict = [(slope * x) + y_intercept for x in x_test]
# [21.099999969999992, 10.699999989999991, 15.899999979999999, 17.633333309999997]

sum_sq_regression = sum((y_test[i] - y_test_predict[i])**2 for i in range(0,len(y_test)))
sum_sq_total = sum((y_test[i] - y_test_avg)**2 for i in range(0,len(y_test)))

r_square = 1.0 - sum_sq_regression / sum_sq_total
# 0.8478030805337009

print(r_square)
```

Scikit-Learn and R^2

Using 3-Fold

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score,
train_test_split

df = pd.read_csv('https://bit.ly/3m20B31', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=.33)

# Perform a simple linear regression
model = LinearRegression()
model.fit(X_train, Y_train)

result = model.score(X_test, Y_test)
print(result) # prints 0.8478030825856914
```

Using Cross Validation

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score

df = pd.read_csv('https://bit.ly/3nJBdj9', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]

# Perform a simple linear regression
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LinearRegression()

# Use R-square to evaluate the performance
# An R-square of 0 is no-fit, and 1 is perfect fit
results = cross_val_score(model, X, Y, cv=kfold, scoring='r2')

print("R^2: mean=%.3f (stdev-%.3f)" % (results.mean(), results.std()))
# prints R^2: mean=0.590 (stdev-0.219)
```

Appendix C
Rescaling Data

Normalization

Normalization is scaling and converting the values of each variable, so they are relatively close together.

- Imagine you had a variable ***age*** whose values typically range in 0-99.
- But you had another variable ***income*** that typically ranges from 30,000 to 1,000,000.
- Because these ranges are so drastically different, fitting a model is not going to be productive until you transform them somehow.

There are a variety of techniques you can employ from linear scaling to fitting to a standard normal distribution.

Rescaling

When you have different fields with varying scales, it can be helpful to rescale, or normalize, the data by compressing it between 0.0 and 1.0.

This can be helpful for optimization algorithms that perform training, making it easier to iterate parameters to fit the data more productively.

Note you do not always have to rescale, but sometimes it can give a better result especially for data with fields that vary in scale.

```
import pandas as pd
from sklearn.preprocessing import MinMaxScaler

df = pd.read_csv('https://bit.ly/33iTfS9', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, 5th column)
Y = df.values[:, 4]

# Rescale all the input variables to be between 0 and 1
scaler = MinMaxScaler(feature_range=(0.0, 1.0))
rescaled_X = scaler.fit_transform(X)

print(rescaled_X)
```

Doing a simple rescale between 0.0 and 1.0 above in scikit-learn

```
[[ 0 25  2  3]
 [ 0 30  2  3]
 [ 0 26  2  3]
 [ 0 25  1  2]
 [ 0 28  1  2]
 [ 0 30  2  4]
 [ 0 49  4  8]]
```

```
[[0.         0.         0.5        0.2       ]
 [0.         0.20833333 0.5        0.2       ]
 [0.         0.04166667 0.5        0.2       ]
 [0.         0.         0.25       0.1       ]
 [0.         0.125      0.25       0.1       ]
 [0.         0.20833333 0.5        0.3       ]
 [0.         1.         1.         0.7       ]]
```

Standardization

Standardization is transforming numeric variables to fit a standard normal distribution (with a mean of 0 and standard deviation of 1) and express each value in standard deviations.

It can be preferable to rescaling, if the data can assume a normal distribution for each variable.

In other words, standardization is finding the z-scores for each variable.

```
import pandas as pd
from sklearn.preprocessing import StandardScaler


df = pd.read_csv('https://bit.ly/3flZJSR', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Rescale all the input variables to be between 0 and 1
scaler = StandardScaler().fit(X)
rescaled_X = scaler.fit_transform(X)

print(rescaled_X)
```

Doing a standardization on all data fields

```
[[  6.    148.     72.    ...  33.6     0.627  50.   ]
 [  1.     85.     66.    ...  26.6     0.351  31.   ]
 [  8.    183.     64.    ...  23.3     0.672  32.   ]
```

```
[[ 0.63994726  0.84832379  0.14964075 ...  0.20401277  0.46849198
   1.4259954 ]
 [-0.84488505 -1.12339636 -0.16054575 ... -0.68442195 -0.36506078
  -0.19067191]
 [ 1.23388019  1.94372388 -0.26394125 ... -1.10325546  0.60439732
  -0.10558415]
```

Unit Vector Normalization

Not to be confused with standardization, unit vector normalization is rescaling each data record to have a vector length of 1.0.

This is probably the most complicated transformation, as it involves some understanding of linear algebra.

It works well for sparse data sets and it compresses the data into a smaller space, which is especially helpful for high-dimension datasets.

It is often used for neural networks, k-nearest neighbors, and a few other ML algorithms.

```
import pandas as pd
from sklearn.preprocessing import Normalizer

df = pd.read_csv('https://bit.ly/3flZJSR', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Rescale all the input variables to be normalized
scaler = Normalizer().fit(X)
rescaled_X = scaler.fit_transform(X)

print(rescaled_X)
```

Doing a normalization on all data fields

```
[[  6.    148.     72.    ...  33.6     0.627  50.   ]
 [  1.     85.     66.    ...  26.6     0.351  31.   ]
 [  8.    183.     64.    ...  23.3     0.672  32.   ]
```

```
[[0.03355237 0.82762513 0.40262844 ... 0.18789327 0.00350622 0.27960308]
 [0.008424   0.71604034 0.55598426 ... 0.22407851 0.00295683 0.26114412]
 [0.04039768 0.92409698 0.32318146 ... 0.11765825 0.00339341 0.16159073]
```