UNIVERSIDADE FEDERAL DO RIO GRANDE DO NORTE

PPgEEC
Machine Learning
Fundamentals of ML and Decision Trees

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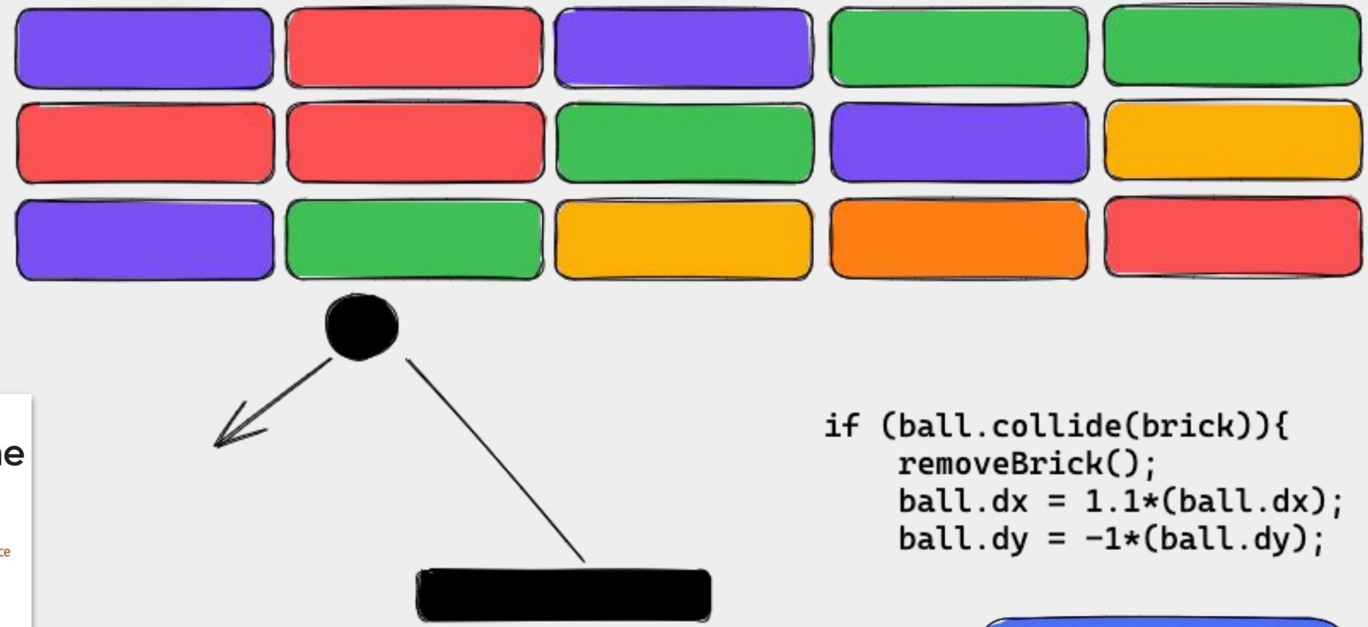
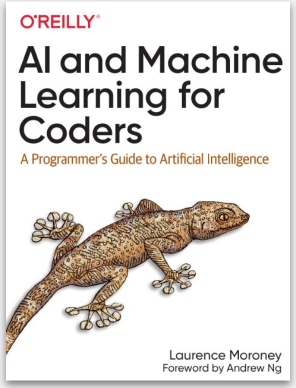
"A reproducible Pipeline is all you need"

What is Machine Learning?



```
if (ball.collide(brick)){
    removeBrick();
    ball.dx = 1.1*(ball.dx);
    ball.dy = -1*(ball.dy);
```



Limitations of traditional programming

<activity detection>

```
if (speed < 4){
    status = WALKING;
}
```

```
if (speed < 4){
    status = WALKING;
} else {
    status = RUNNING;
}
```

```
if (speed < 4){
    status = WALKING;
} else if (speed < 12) {
    status = RUNNING;
} else {
    status = BIKING;
}
```

```
// ????
```

From coding to ML

<gathering and label data>

```
010111100001110101
111010101010111000
111010101010101010
000000000111001111
```

Label = WALKING

```
010111100011101110
000111010101011011
000111101010111000
000000000000001111
```

Label = RUNNING

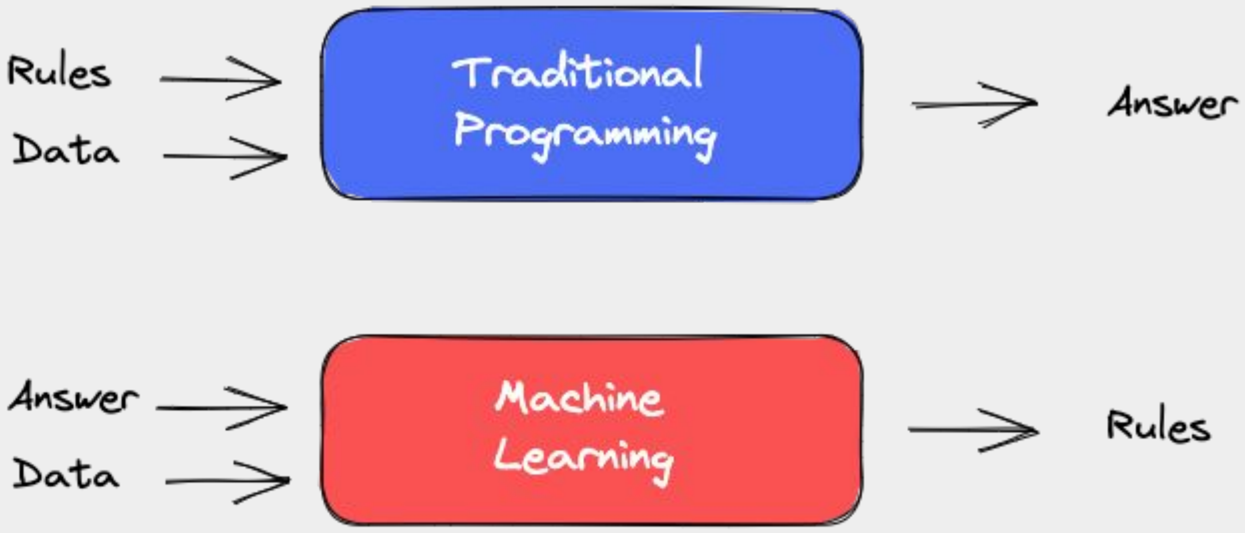
```
111101110010101011
110101110101011011
111110101110010101
000111111001101111
```

Label = BIKING

```
100000000010101011
111111111000011001
000000011100111101
111111111100000001
```

Label = GOLFING

From programming to learning



What is Machine Learning?

Machine Learning (ML): a subset of AI that often uses statistical techniques to give machines the ability to "learn" from data without begging explicitly given the instructions for how to do so. This process is known as "training" a "model" using a learning "algorithm" that progressively improves models performance on a specific task.

Computer Vision

- **Semantic Segmentation** — 203 benchmarks — 2300 papers with code
- **Image Classification** — 279 benchmarks — 1989 papers with code
- **Object Detection** — 264 benchmarks — 1737 papers with code
- **Image Generation** — 169 benchmarks — 771 papers with code
- **Denoising** — 100 benchmarks — 739 papers with code

Time Series

- **Time Series** — 2 benchmarks — 1127 papers with code
- **EEG** — 8 benchmarks — 177 papers with code
- **Imputation** — 10 benchmarks — 160 papers with code

Natural Language Processing

- **Language Modelling** — 27 benchmarks — 1513 papers with code
- **Machine Translation** — 73 benchmarks — 1366 papers with code
- **Question Answering** — 103 benchmarks — 1307 papers with code
- **Sentiment Analysis** — 69 benchmarks — 836 papers with code
- **Text Generation** — 84 benchmarks — 649 papers with code

Speech

- **Speech Recognition** — 121 benchmarks — 575 papers with code
- **Speech Synthesis** — 3 benchmarks — 142 papers with code
- **Dialogue Generation** — 10 benchmarks — 108 papers with code

Medical

- **Medical Image Segmentation** — 86 benchmarks — 244 papers with code
- **Drug Discovery** — 14 benchmarks — 151 papers with code
- **Lesion Segmentation** — 6 benchmarks — 104 papers with code
- **Brain Tumor Segmentation** — 10 benchmarks — 69 papers with code
- **COVID-19 Diagnosis** — 4 benchmarks — 59 papers with code

Playing Games

- **Continuous Control** — 76 benchmarks — 242 papers with code
- **Atari Games** — 65 benchmarks — 213 papers with code
- **OpenAI Gym** — 9 benchmarks — 112 papers with code

Graphs

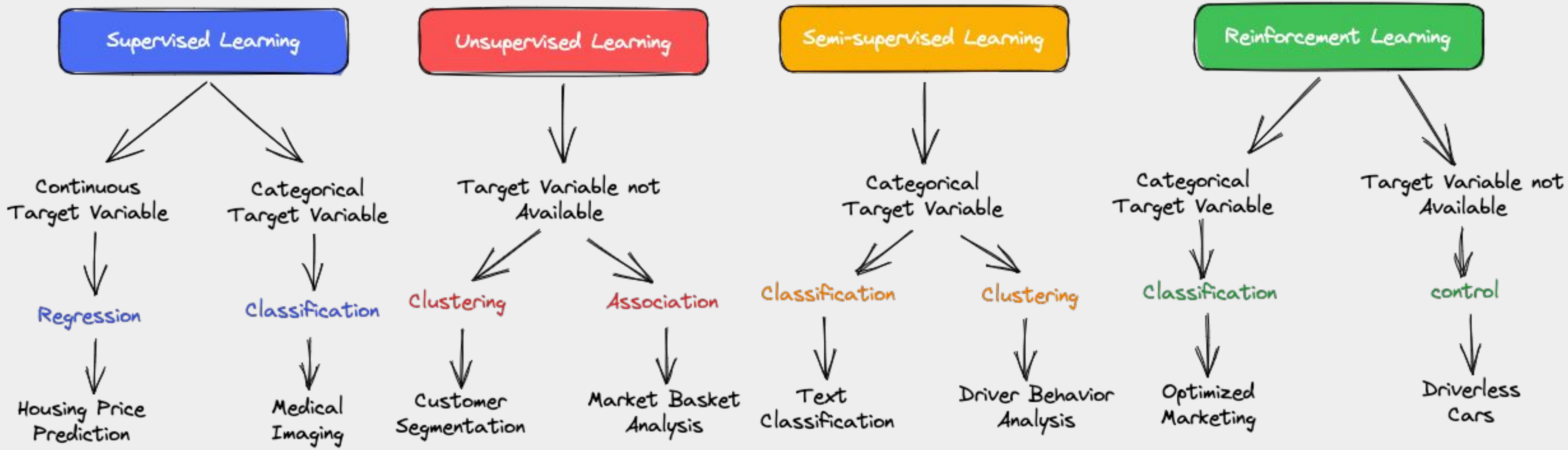
- **Link Prediction** — 69 benchmarks — 463 papers with code
- **Node Classification** — 77 benchmarks — 370 papers with code
- **Graph Embedding** — 2 benchmarks — 252 papers with code
- **Graph Classification** — 54 benchmarks — 209 papers with code
- **Community Detection** — 11 benchmarks — 156 papers with code

Music

- **Music Generation** — 60 papers with code
- **Music Information Retrieval** — 55 papers with code
- **Music Source Separation** — 3 benchmarks — 31 papers with code

https://paperswithcode.com/sota

Machine Learning Types



Supervised Learning

Classification Problem

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
Yes	Yes	205	Yes
No	Yes	180	Yes
Yes	No	210	Yes
Yes	Yes	167	Yes
No	Yes	156	No
No	Yes	125	No
Yes	No	168	No
Yes	Yes	172	No

Chest Pain	Blocked Arteries	Patient Weight
Yes	No	200

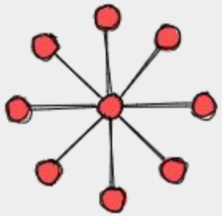
Supervised Learning

Regression Problem

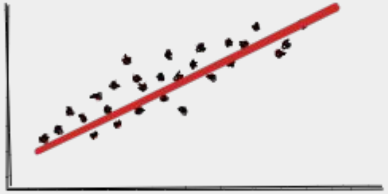
Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	88
1.6	Green	Famale	76
1.5	Blue	Female	56
1.8	Red	Male	73
1.5	Green	Male	77
1.4	Blue	Female	57

Height (m)	Favorite Color	Gender
1.83	Yellow	Male

K-Neighrest Neighbors (KNN)



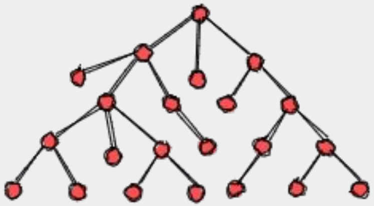
Linear Regression



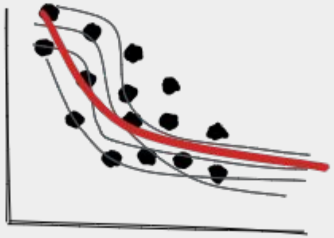
Logistic Regression

Support Vector Machines (SVM)

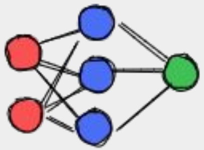
Decision Trees



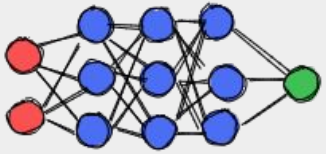
Ensemble



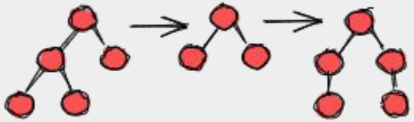
Neural Networks



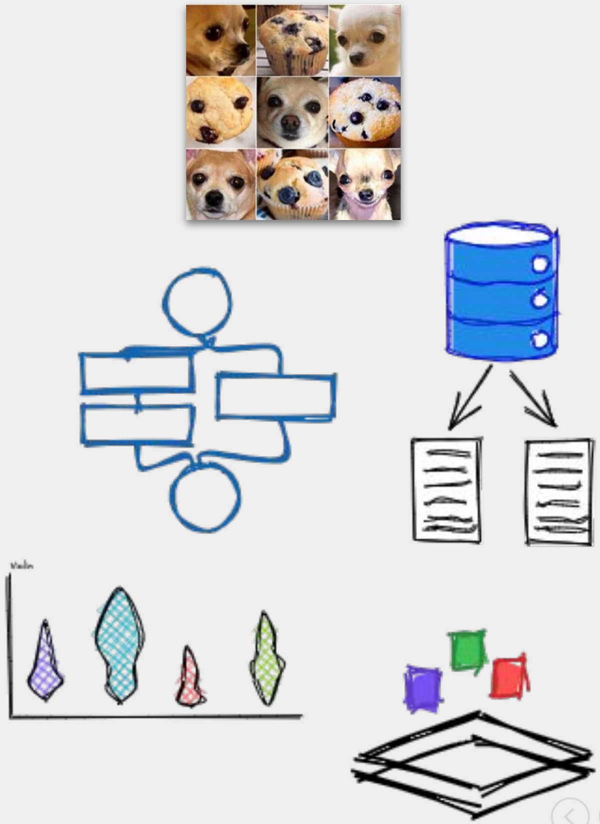
Deep Learning



Bosting

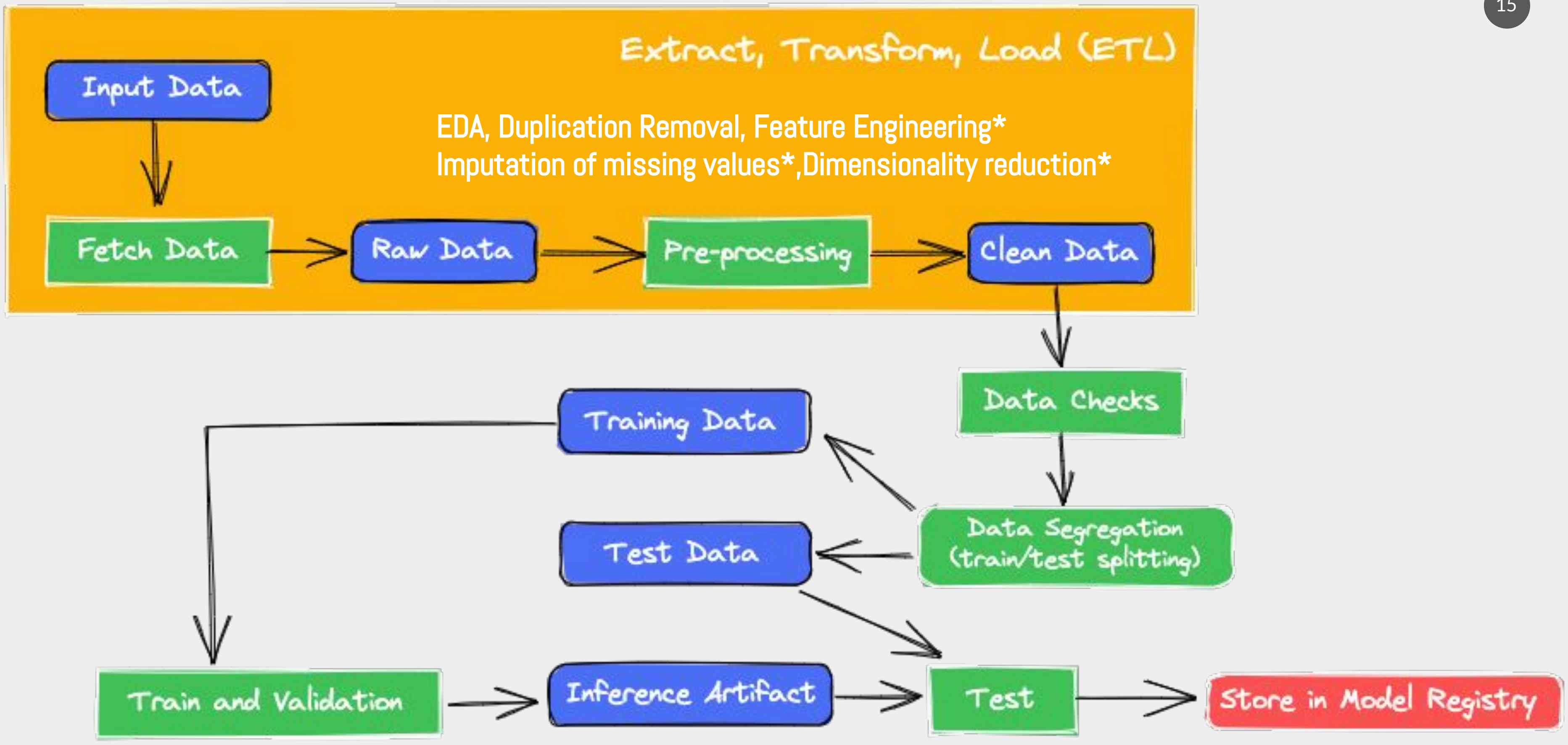


Main Challenges Of Machine Learning

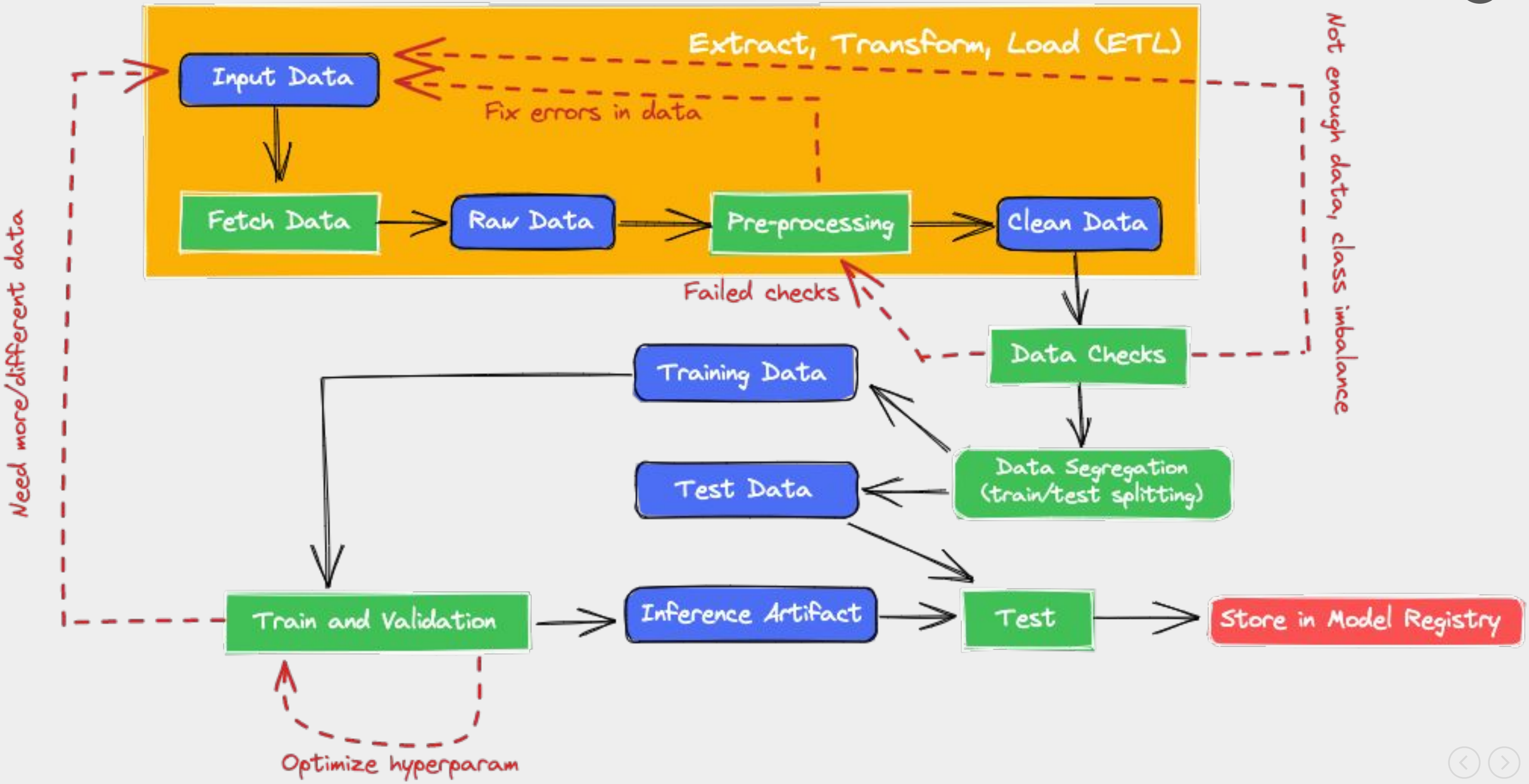


Titanic: Machine Learning from Disaster

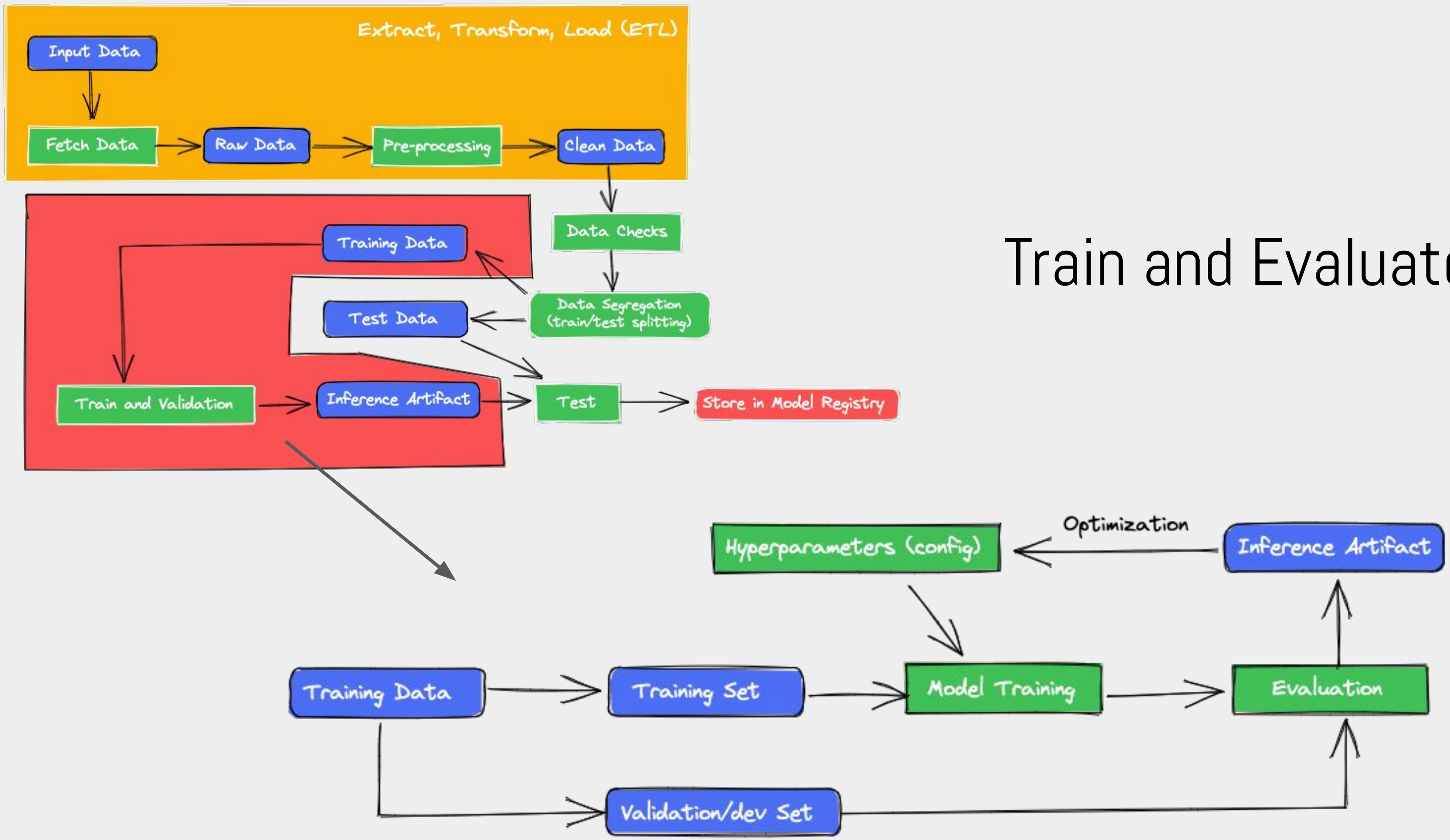
Survived	Pclass	Name	Sex	Age	Ticket	Cabin	Embarked
0	3	Braund, Mr. Owen	Male	22	A/5 21171	NaN	S
1	1	Cummings, Mrs John	Female	38	PC 17599	C85	C
1	3	Heikkinen, Ms Laina	Female	26	STON/02	NaN	S
1	1	Futrelle, Mrs Jacques	Female	35	113803	C123	S
0	3	Allen, Mr. William	Male	35	373450	NaN	S



Feature Store, Categorical encoding missing values imputation, Dimensionality Reduction


Extract, Transform, Load (ETL)
Input Data
Fix errors in data
Fetch Data
Raw Data
Pre-processing
Clean Data
Not enough data, class imbalance
Failed checks
Data Checks
Need more/different data
Training Data
Data Segregation (train/test splitting)
Test Data
Train and Validation
Inference Artifact
Test
Store in Model Registry
Optimize hyperparam

Train and Evaluate



Controlled Chaos

Assume you are going to iterate A LOT

Give yourself time within the project deadlines

Be systematic
Normaly, change one thing at the time

Nothing is lost
You learn something with every experiment

Perfection is the enemy of good
Be clear on your objective and stop once you reach it

Nothing is fixed
data, code and hyperparameters

Train - Dev - Test Sets

Making good choices in how you set up your training, development, and test sets can make a huge difference in helping you quickly find a good high performance neural network.

Previous ML era

- 70/30
- 60/20/20

Big Data era

- 98/1/1
- 99.5/0.25/0.25
- 99.5/0.4/0.1

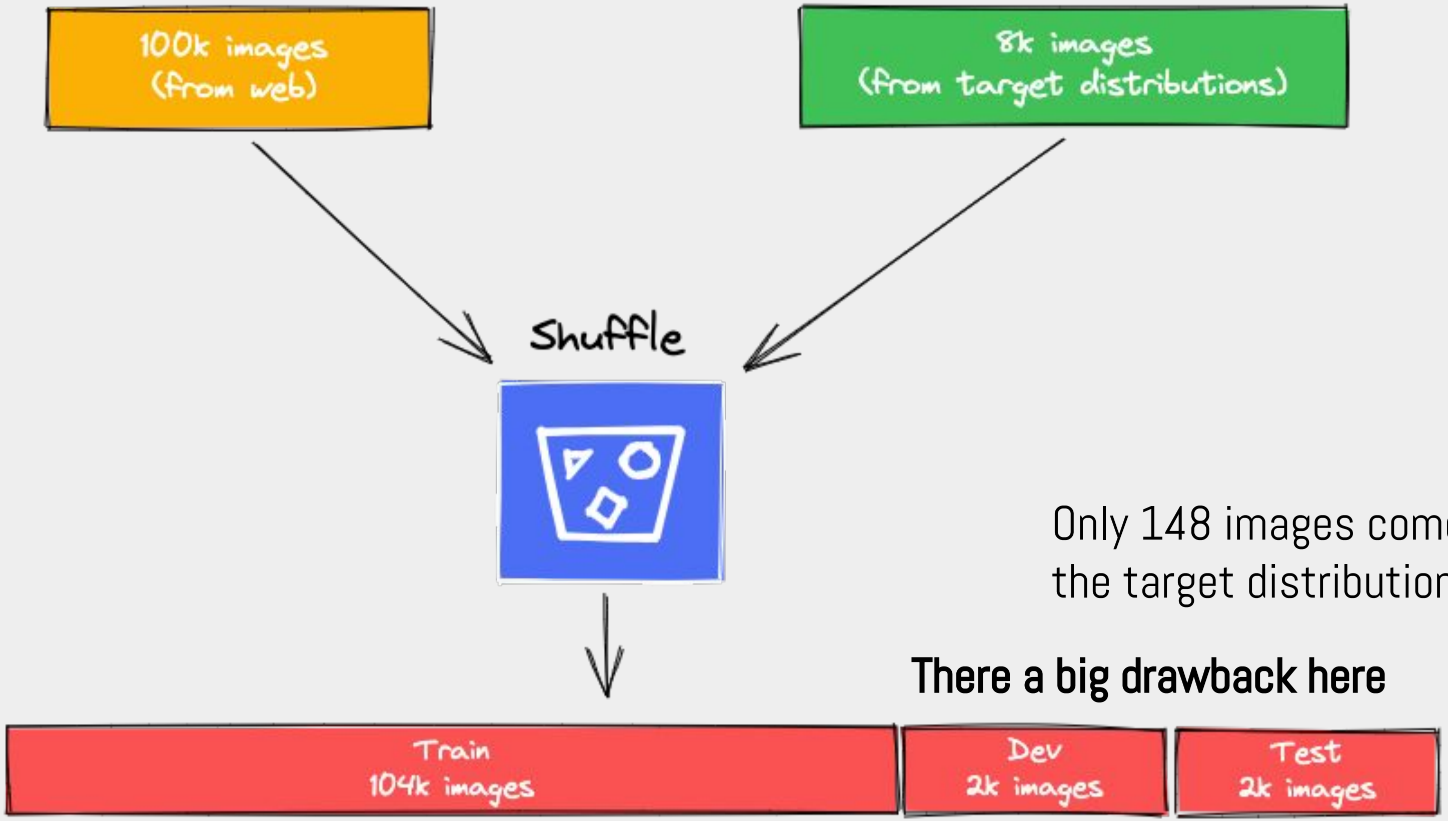
Mismatched train/test distribution

Scenario: say you are building a cat-image classifier application that determines if an image is of a cat or not. The application is intended for users in rural areas who can take pictures of animals by their mobile devices for the application to classify the animals for them.

Scraped from Web Pages
100k images

Collected from Mobile Devices
<<target distribution>>
8k images

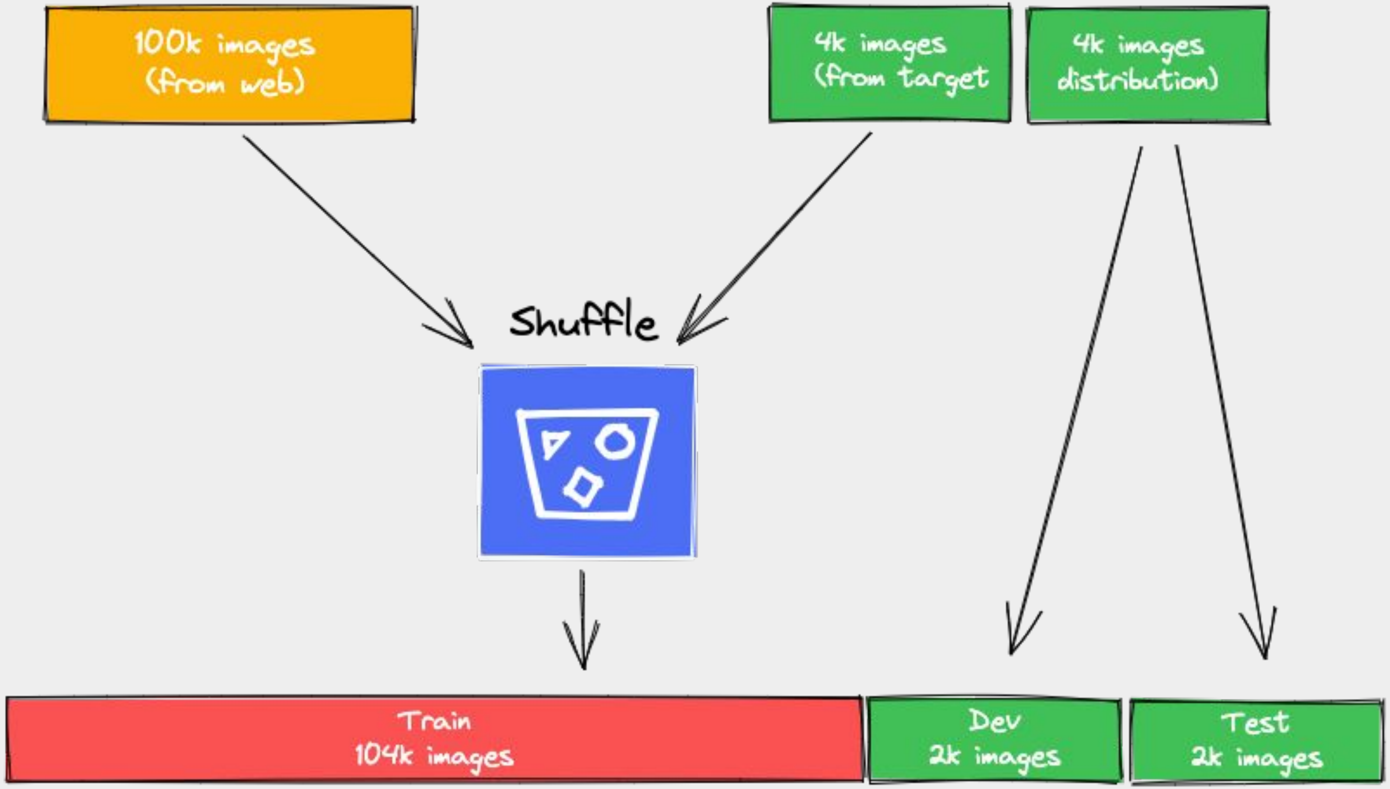
A possible option: shuffling the data



Only 148 images come from the target distribution

There a big drawback here

A better option

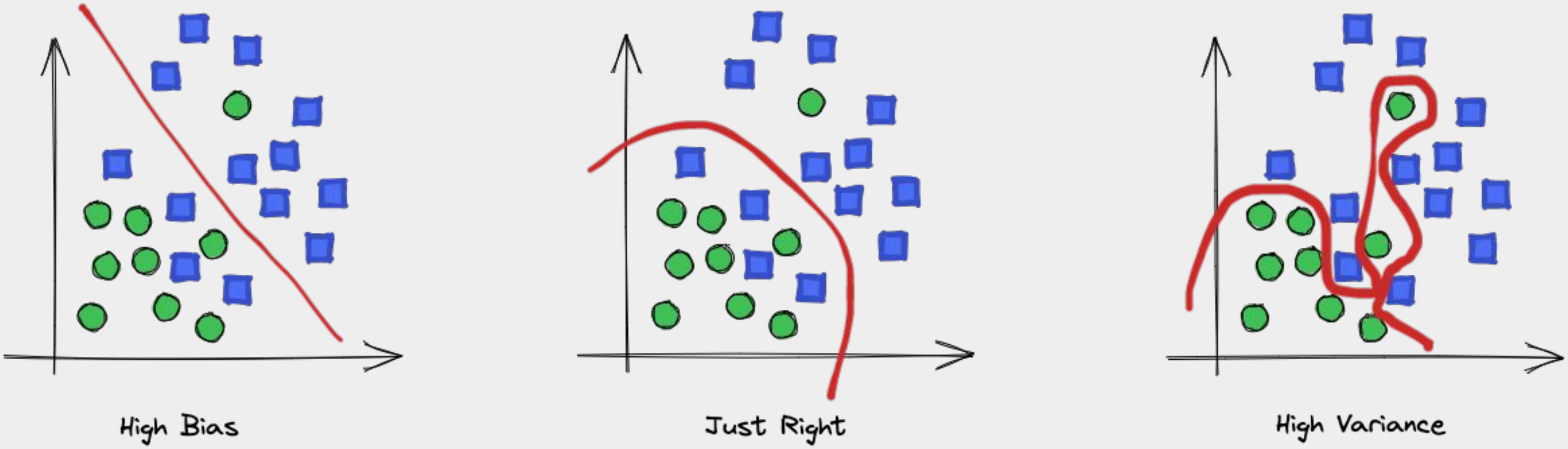


Rule of the thumb

>> make sure that the dev and test sets come from the same distribution

Not having a test set might be okay. (Only dev set)

Bias vs Variance



Underfitting

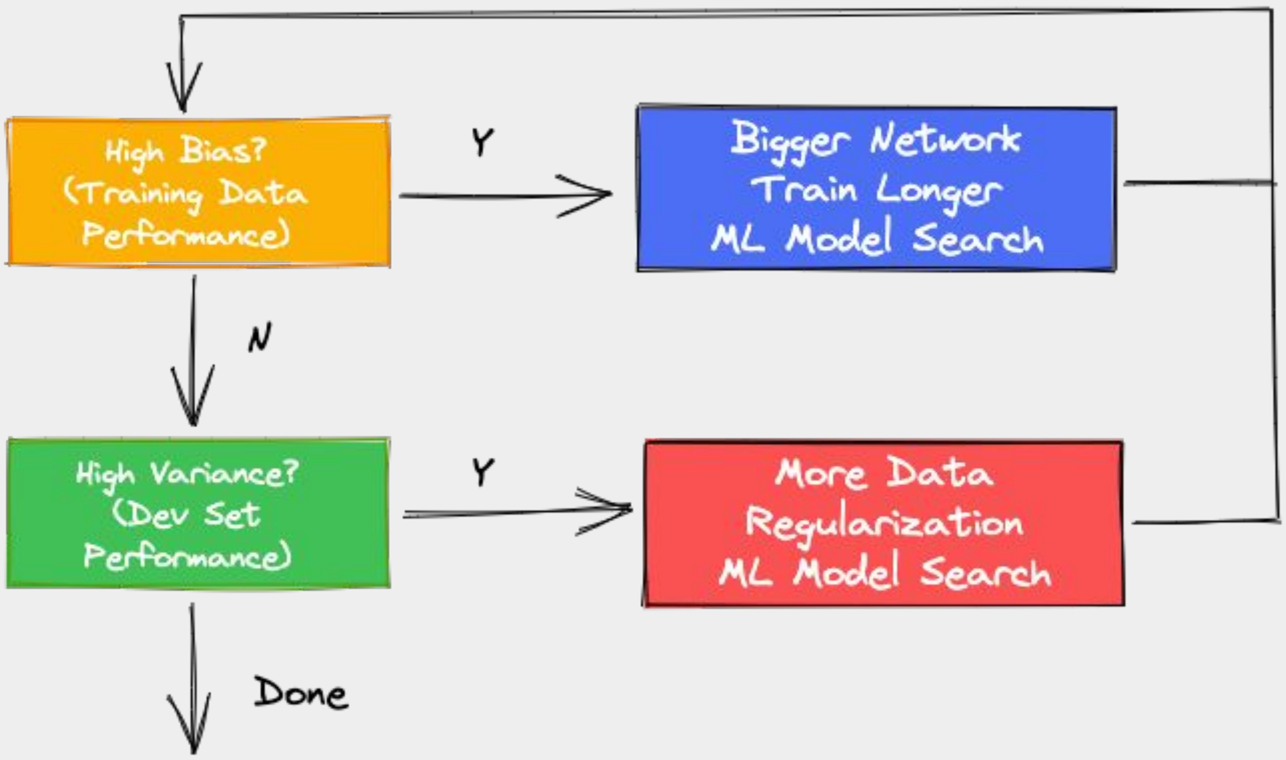
Overfitting

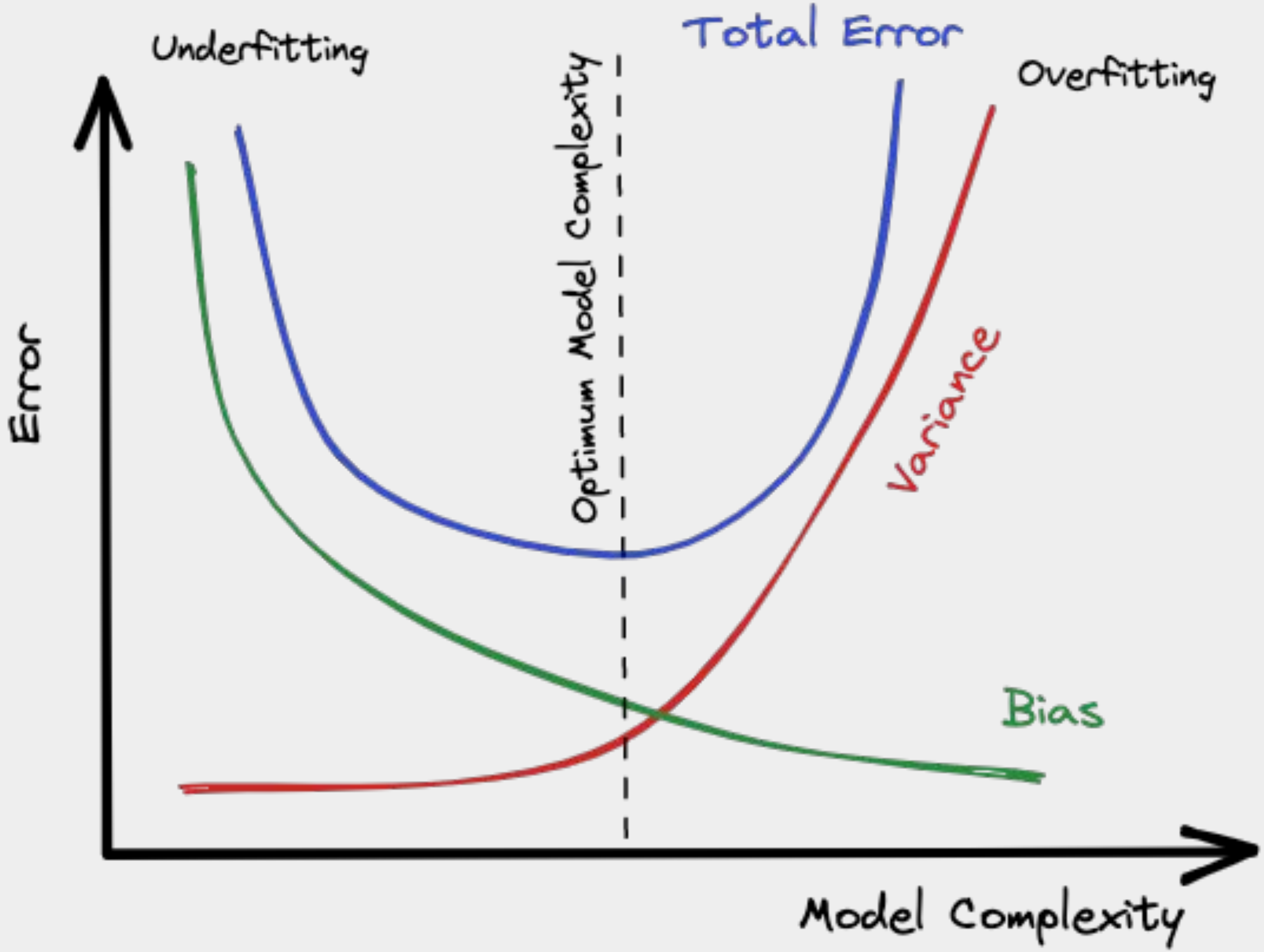
Bias vs Variance

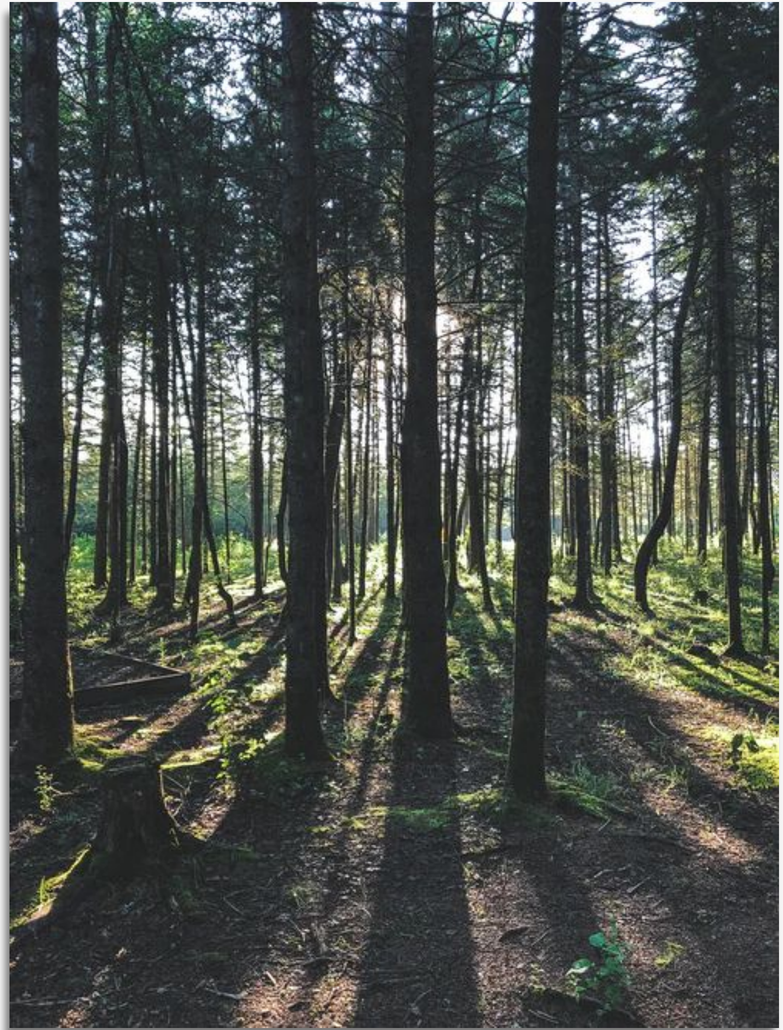
Cat Classification

	Scenario #01	Scenario #02	Scenario #03	Scenario #04
Train Set Error	1%	15%	15%	0.5%
Dev Set Error	16%	16%	30%	1%
	Low Bias High Variance	High Bias Low Variance	High Bias High Variance	Low Bias Low Variance

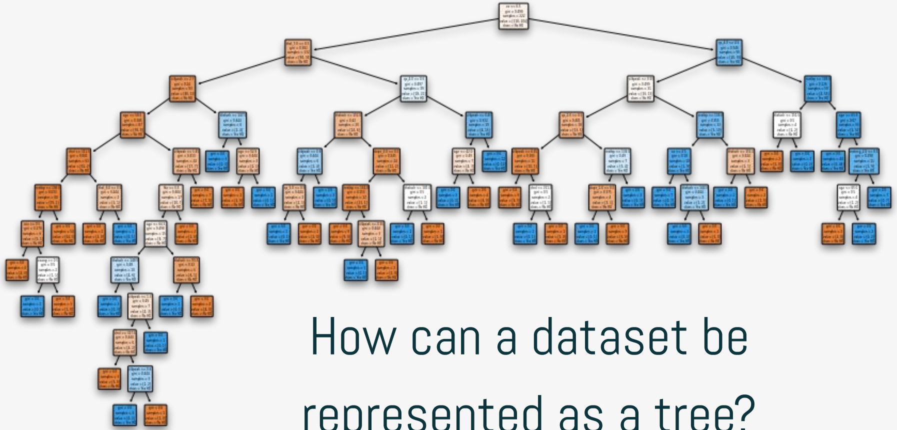
Basic Recipe for Machine Learning




Underfitting
Total Error
Overfitting
Optimum Model Complexity
Error
Variance
Bias
Model Complexity



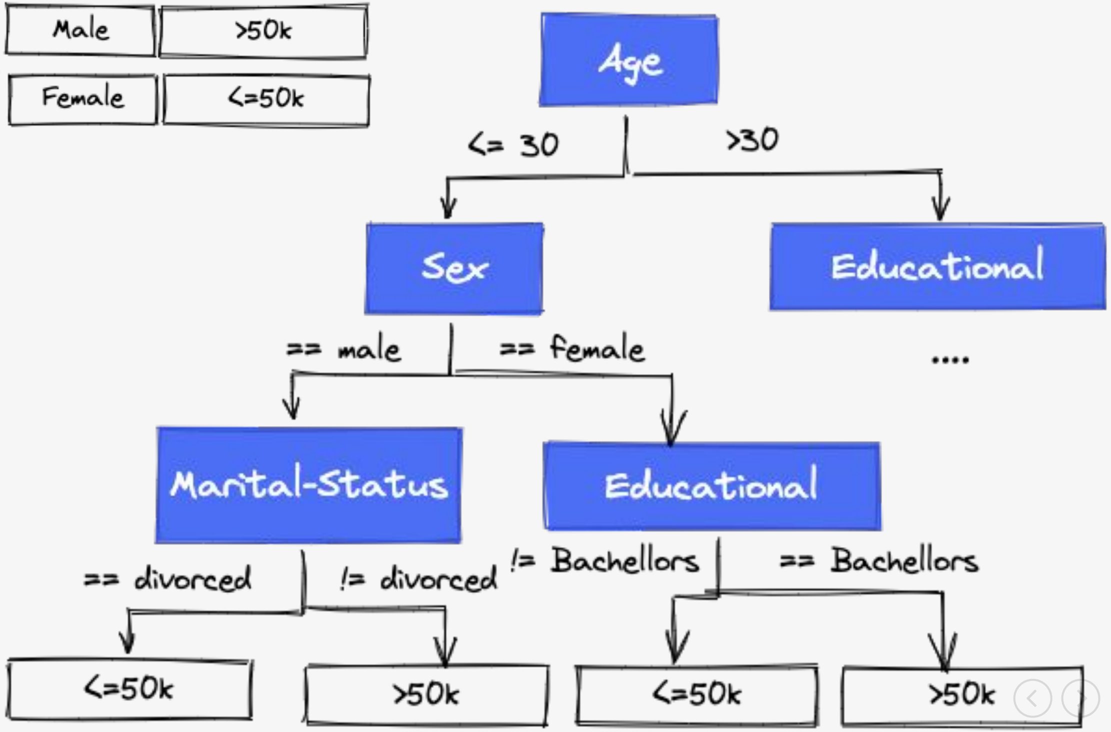
Decision Trees



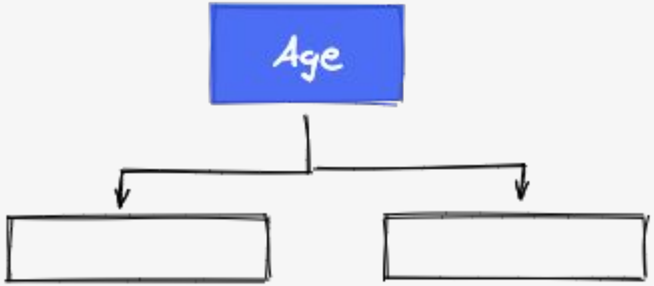
How can a dataset be represented as a tree?

Age	Marital-Status	Educational	Sex	High-Income
28	Never-Married	Bachelors	Female	<=50k
46	Never-Married	Assoc-acdm	Female	<=50k
35	Married-civ-spouse	Some-college	Male	<=50k
27	Married-civ-spouse	Bachelors	Male	>50k
59	Divorced	Some-college	Female	<=50k

Decision Tree (classification)



How can we split the tree?

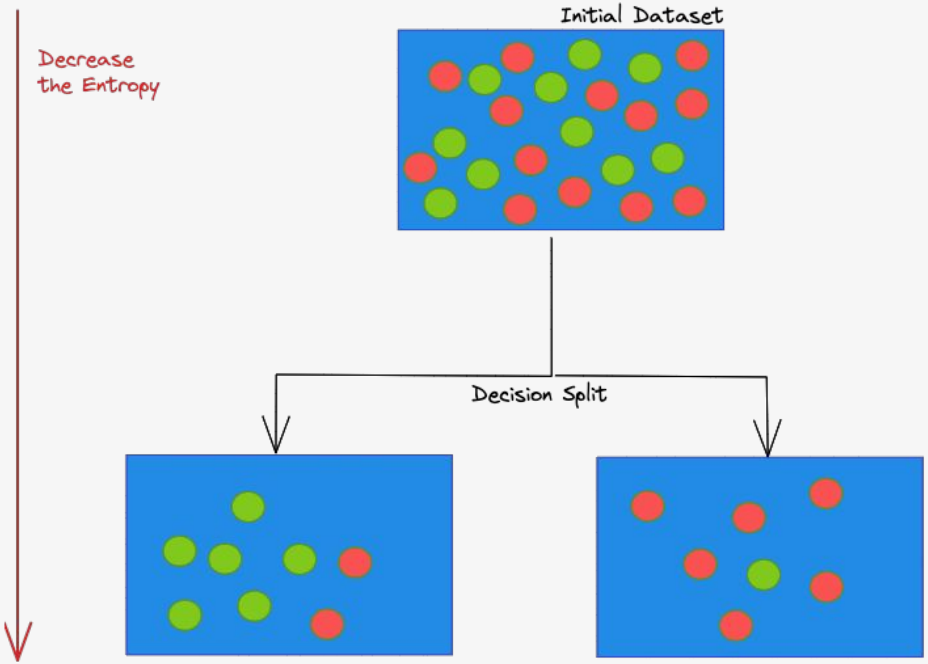


Algorithm used in Decision Trees

1. ID3 (Entropy)
2. Gini Index
3. Chi-Square
4. Reduction in Variance
   a. C4.5, pruning
5. ...

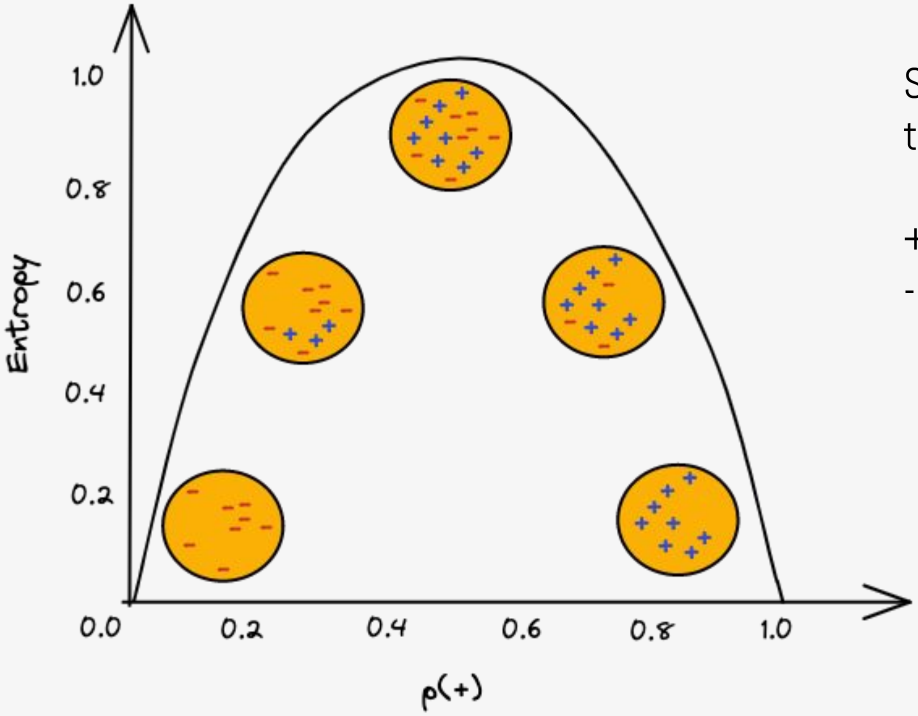
Entropy is an indicator of how messy your data is.

Why Entropy in Decision Trees?



- The goal is to tidy the data.
- You try to separate your data and group the samples together in the classes they belong to.
- You maximize the purity of the groups as much as possible each time you create a new node of the tree
- Of course, at the end of the tree, you want to have a clear answer.

Mathematical Definition of Entropy



Suppose a set of N items, these items fall into two categories:

+ gain > 50k (k)
- gain <= 50k (m)

$$p = \frac{k}{N}, q = \frac{m}{N}$$
$$Entropy = -p\log p - q\log q$$

Generalization

Feature X

$$E(X) = -\sum_{i=1}^{c} P(x_i) \log_b P(x\ )$$

$P(x_i)$ is the fraction of examples in a given class i

<= 50k.	17288
> 50k.	5487

```
from scipy.stats import entropy
entropy(df_train.high_income.value_counts(), base=2)
0.7965702796015677
```

Entropy using the frequency table of two attributes

		High Income		
		<= 50k	> 50k	
Age	<=37	7206	3883	11089 (48%)
	>37	10082	1604	11686 (52%)

$$E(T|X) = \sum_{c \in X} \frac{|X_c|}{|X|} E(T|X_c)$$

```
cross = pd.crosstab(
          df_train.age <= df_train.age.median(),
          df_train.high_income)
```

```
0.486894 * entropy(cross.iloc[0], base=2) \
+ 0.513106 * entropy(cross.iloc[1], base=2)
0.7509335429830957
```

Information Gain

$$IG(T,X) = E(T) - E(T|X)$$

Information Gain from X on T

The information gain is based on the **decrease in entropy after a dataset is split** on an attribute.

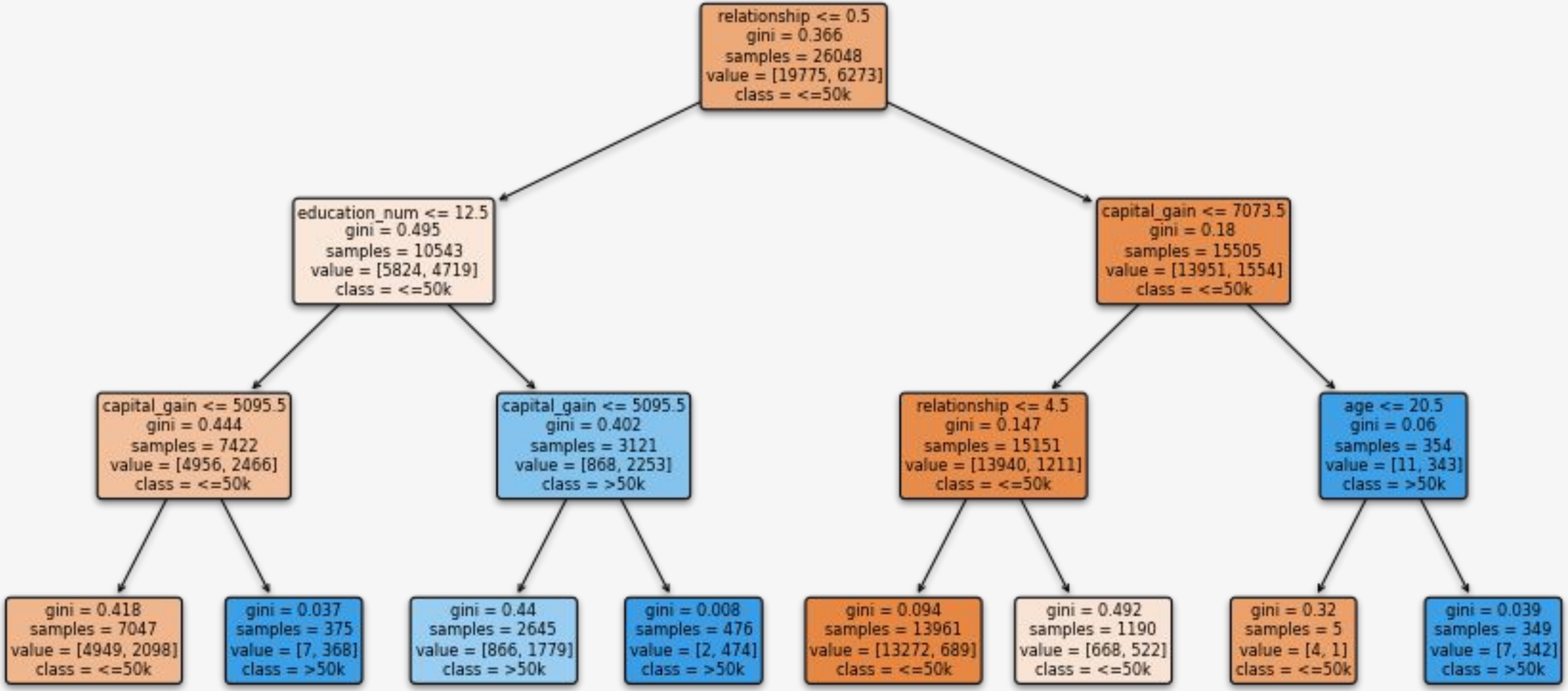
Constructing a decision tree is all about finding attribute that returns the **highest information gain** (i.e., the most homogeneous branches).

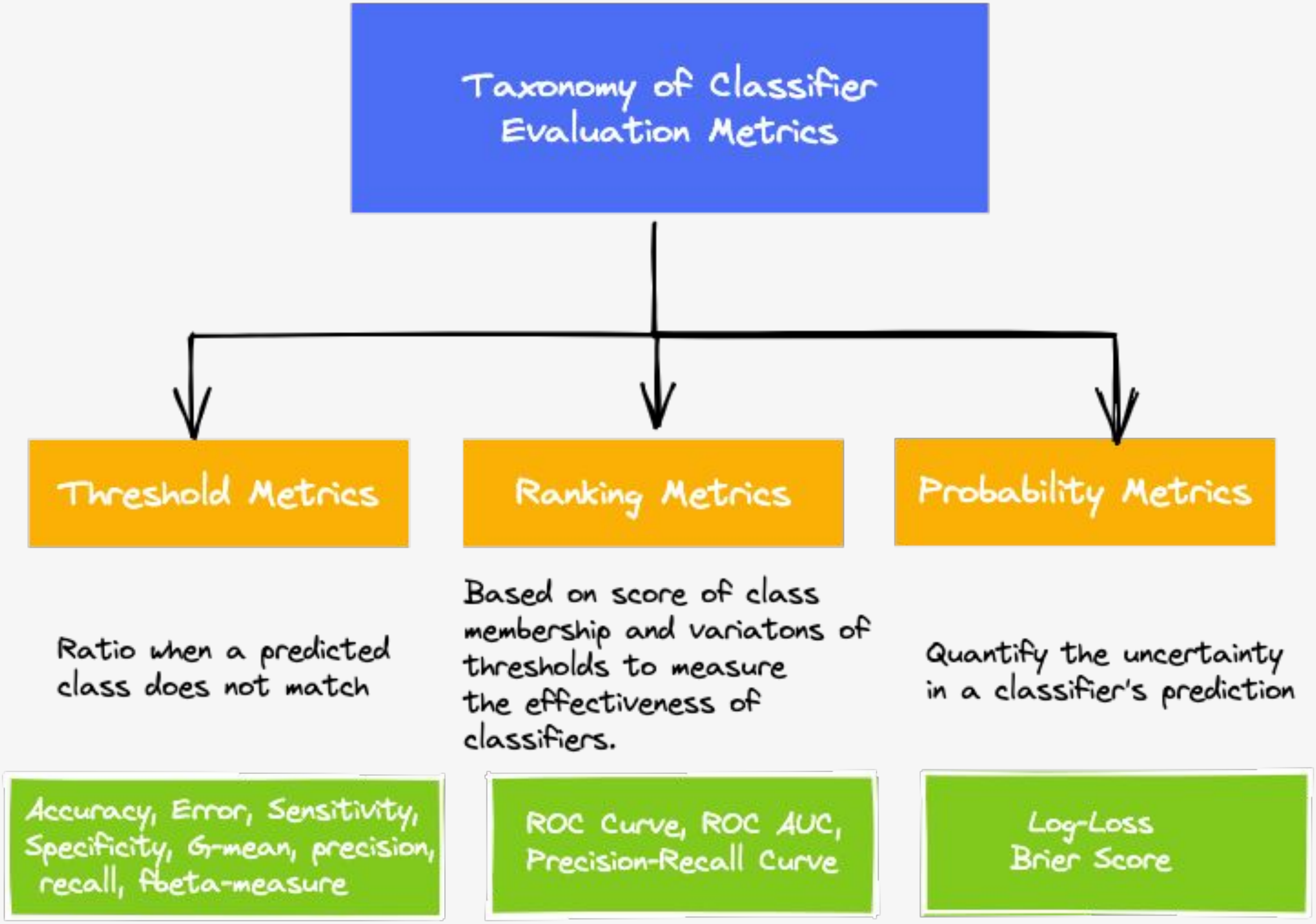
$$Gini(x) = 1 - \sum_{i=1}^{c} P(x_i)^2$$

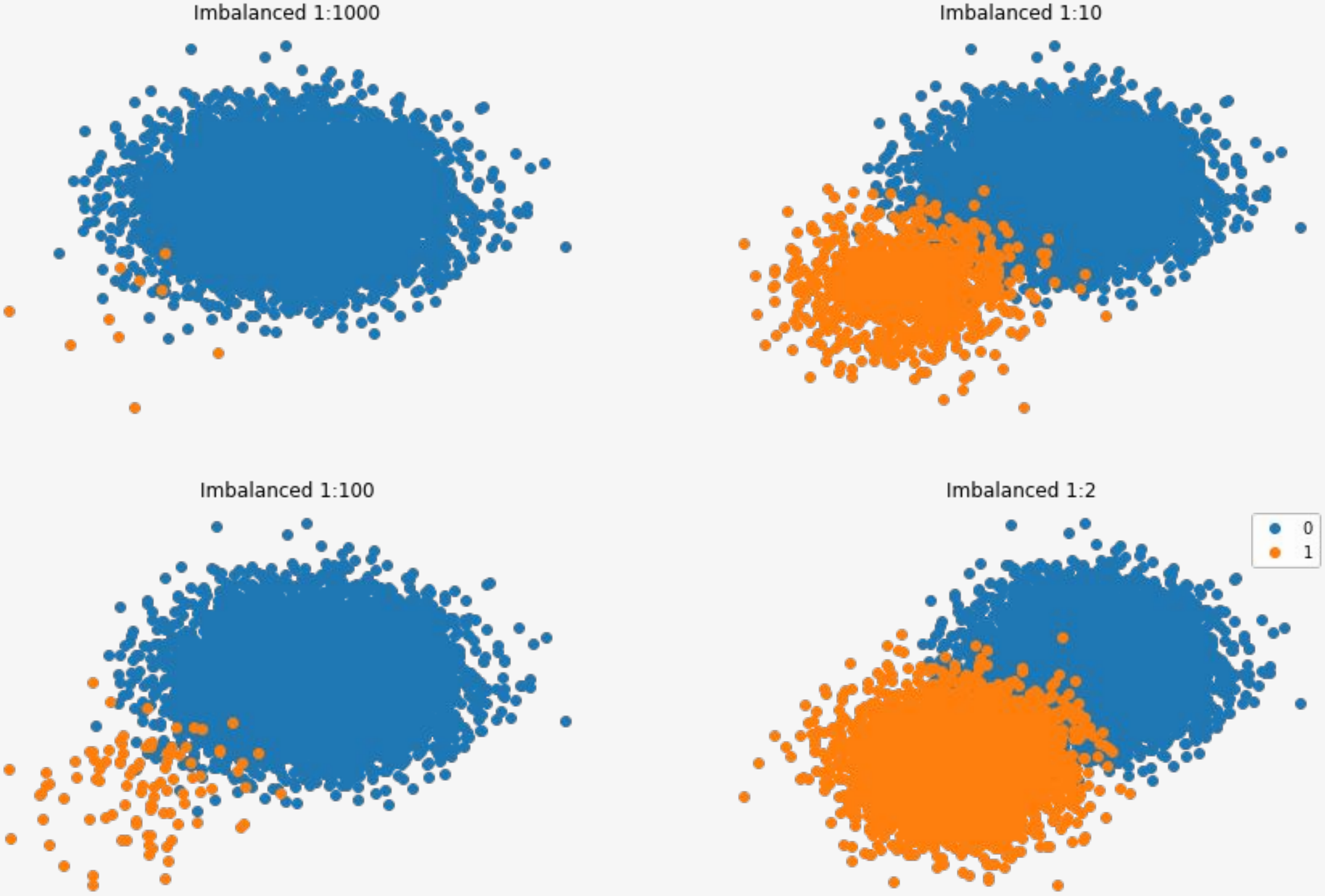
$$Entropy(x) = -\sum_{i=1}^{c} P(x_i) \log_b P(x_i)$$

Gini index or Entropy is the criterion for calculating **Information Gain**. Both of them are measures of impurity of a node.

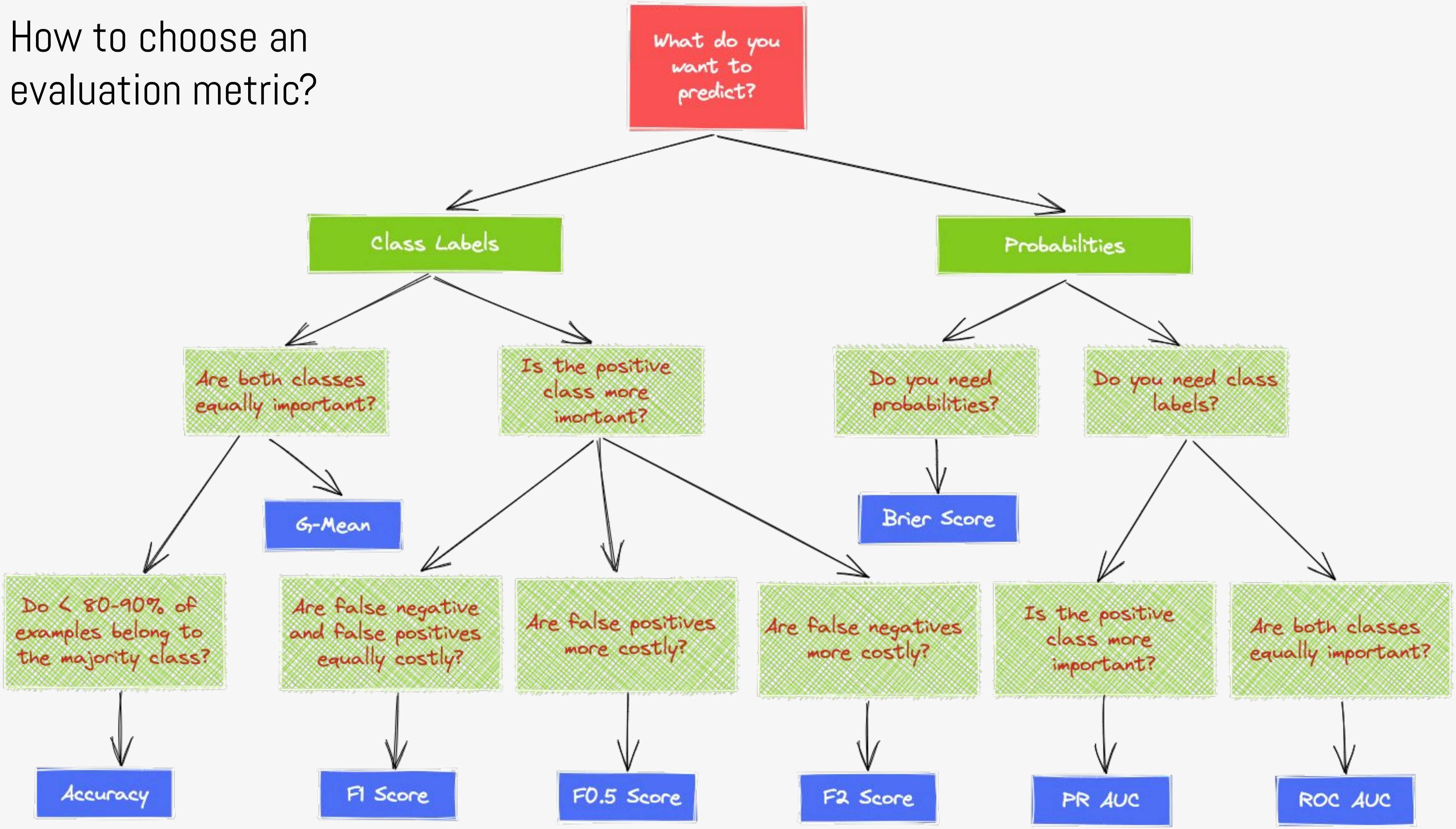
```python
from sklearn.tree import plot_tree
```




Taxonomy of Classifier Evaluation Metrics
Threshold Metrics
Ranking Metrics
Probability Metrics
Ratio when a predicted class does not match
Based on score of class membership and variatons of thresholds to measure the effectiveness of classifiers.
Quantify the uncertainty in a classifier's prediction
Accuracy, Error, Sensitivity, Specificity, G-mean, precision, recall, fbeta-measure
ROC Curve, ROC AUC, Precision-Recall Curve
Log-Loss
Brier Score

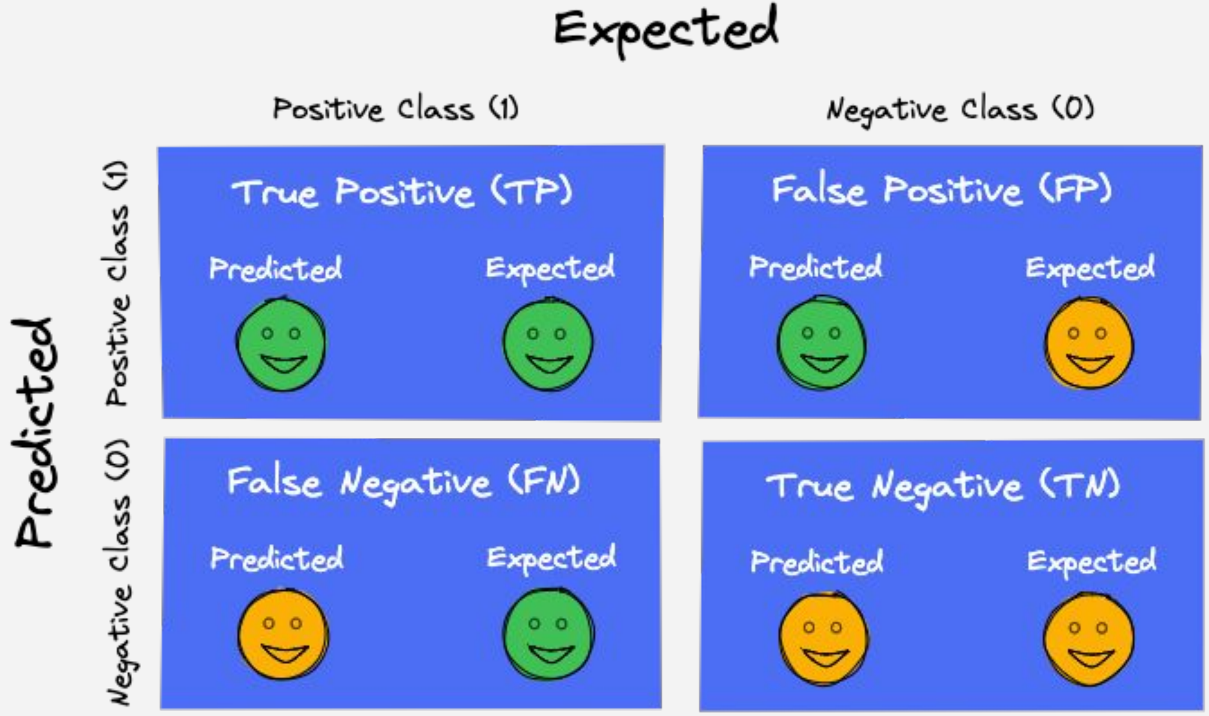

Imbalanced 1:1000
Imbalanced 1:10
Imbalanced 1:100
Imbalanced 1:2
0
1

How to choose an evaluation metric?



@Brownlee, Jason. Imbalanced classification with python.

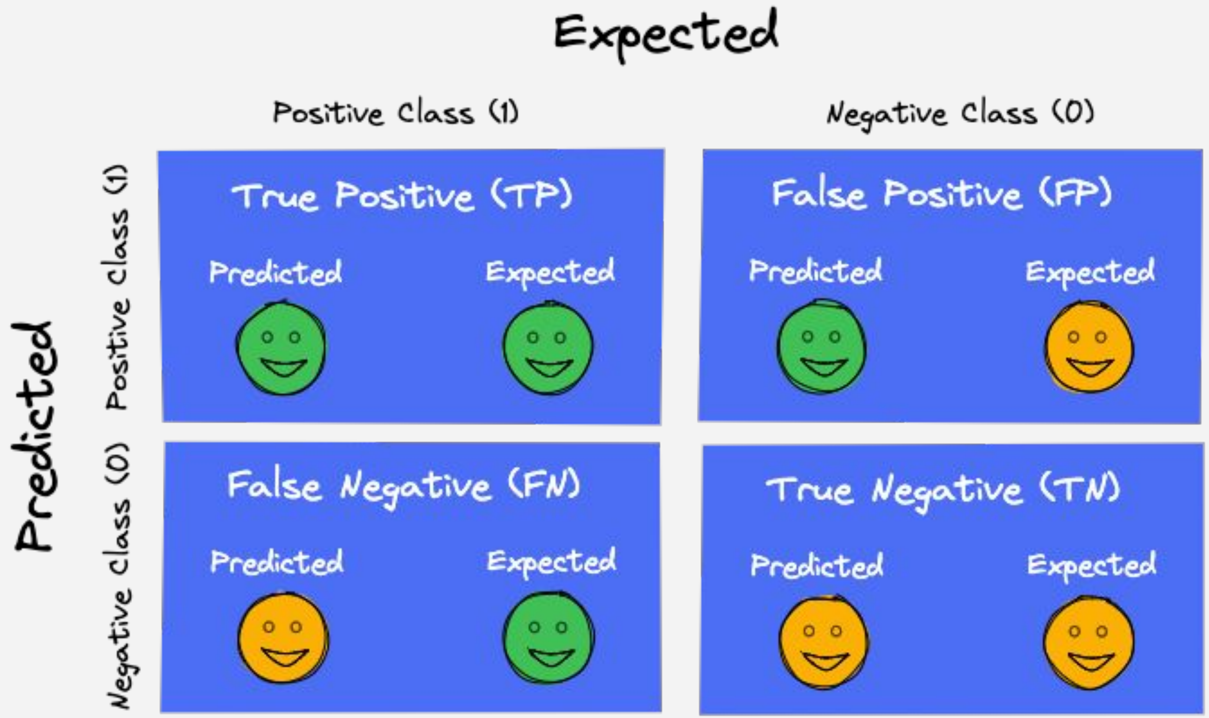
Confusion Matrix



$$\text{Accuracy} = \frac{TP + TN}{TP + FN + FP + TN}$$

$$\text{Error} = 1 - \text{Accuracy}$$

Confusion Matrix

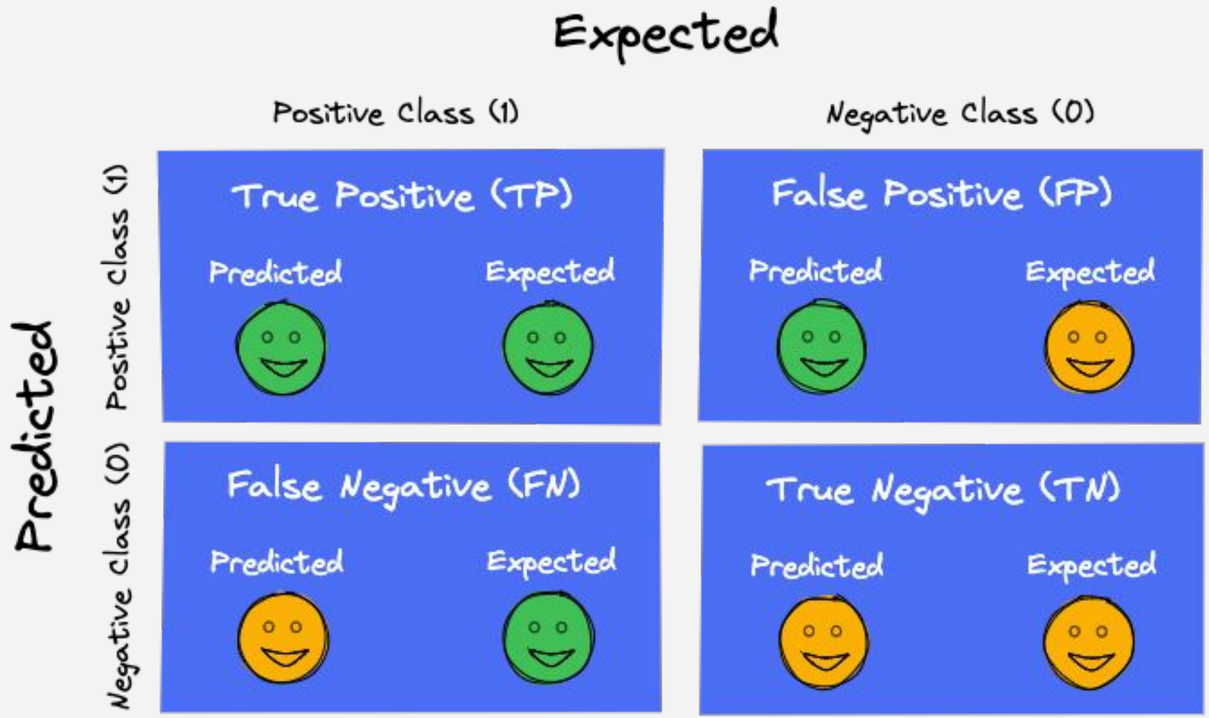


$$\text{Sensitivity} = \frac{TP}{TP + FN}$$

$$\text{Specificity} = \frac{TN}{FP + TN}$$

$$\text{G-mean} = \sqrt{\text{Sensitivity} \times \text{Specificity}}$$

Confusion Matrix

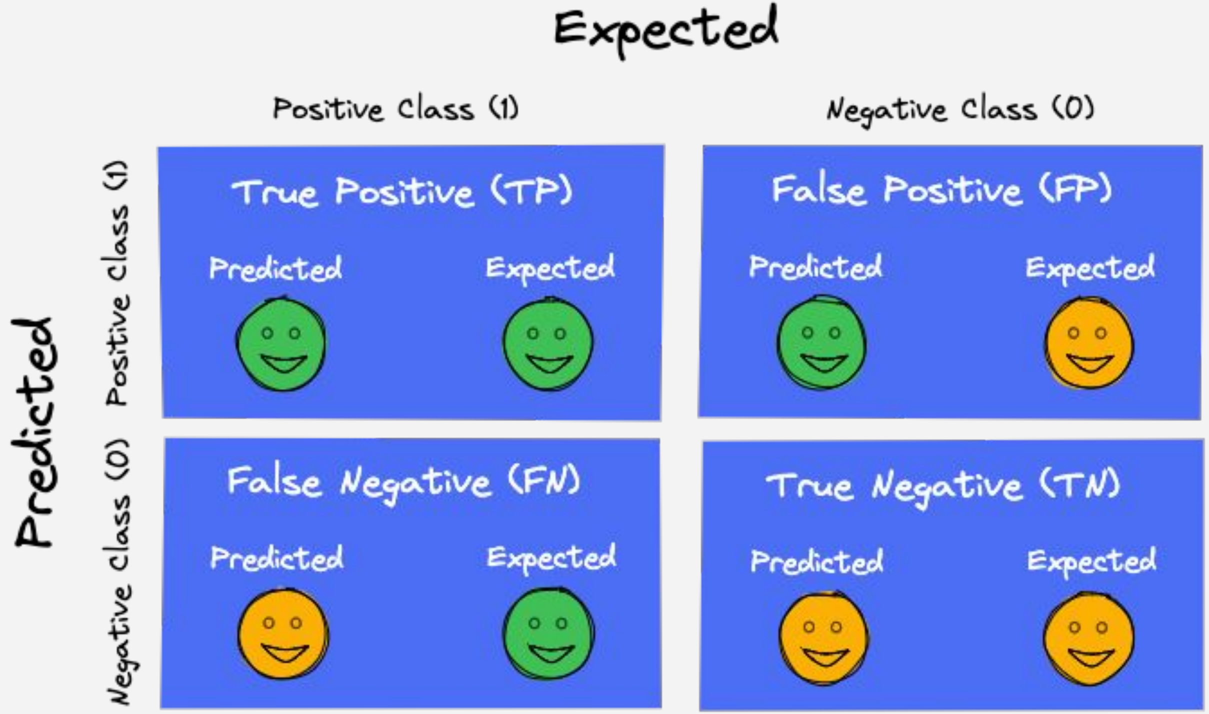


Precision (positive predicte value - PPV) $= \dfrac{TP}{TP + FP}$

Precision (negative predicte value - NPV) $= \dfrac{TN}{TN + FN}$

Recall $= \dfrac{TP}{TP + FN}$

Confusion Matrix



$$\text{Fbeta-measure} = \frac{(1 + \beta^2) \times \text{Precision} \times \text{Recall}}{\beta^2 \times \text{Precision} + \text{Recall}}$$

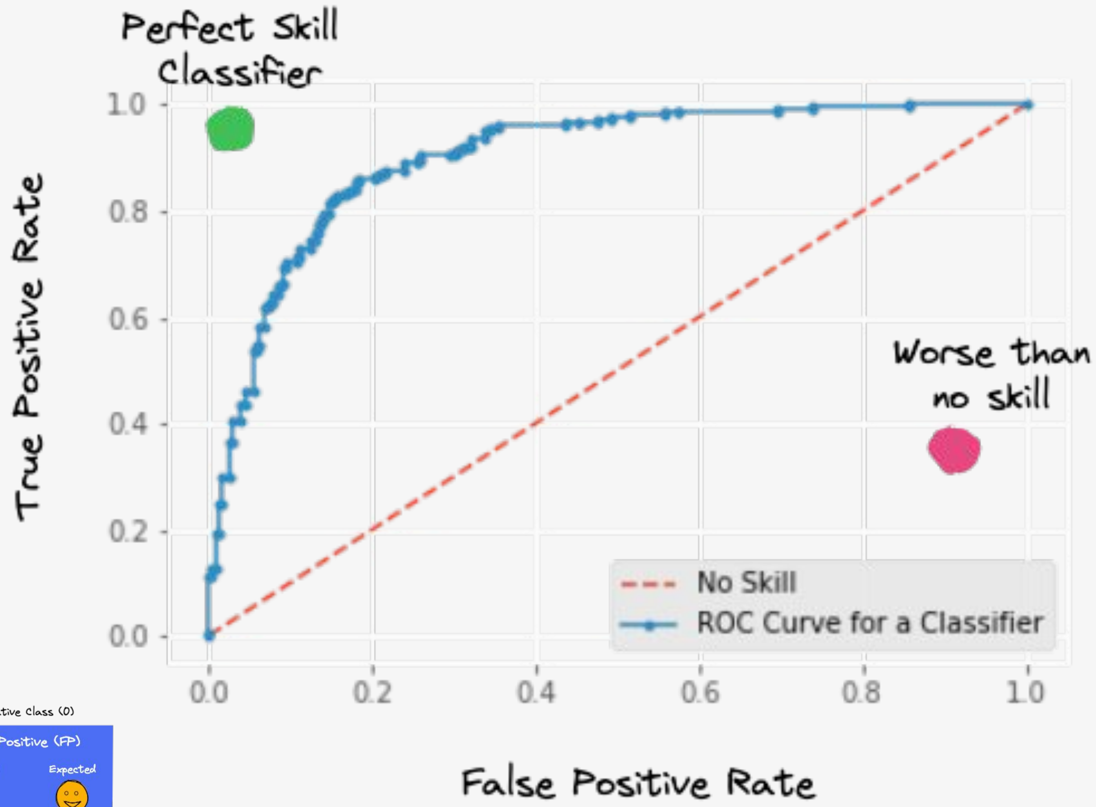
$$\beta == \begin{cases} 0.5, & \text{more weight on precision} \\ 1.0, & \text{balance on weight PR and RE} \\ 2.0, & \text{less weight on precision} \end{cases}$$

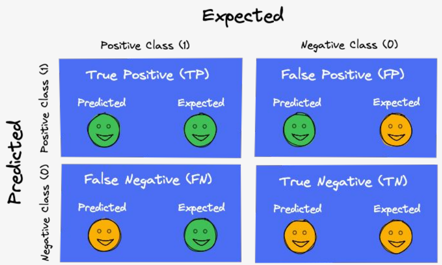
Rank metrics are more concerned with evaluating classifiers based on **how effective** they are at separating classes.

These metrics require that a **classifier predicts a score** or a probability of class membership. From this score, **different thresholds** can be applied to **test the effectiveness of classifiers**. Those models that maintain a good score across a range of thresholds will have good class separation and will be ranked higher.

Receiver Operating Characteristic (ROC)

$$TPR = \frac{TP}{TP + FN}$$



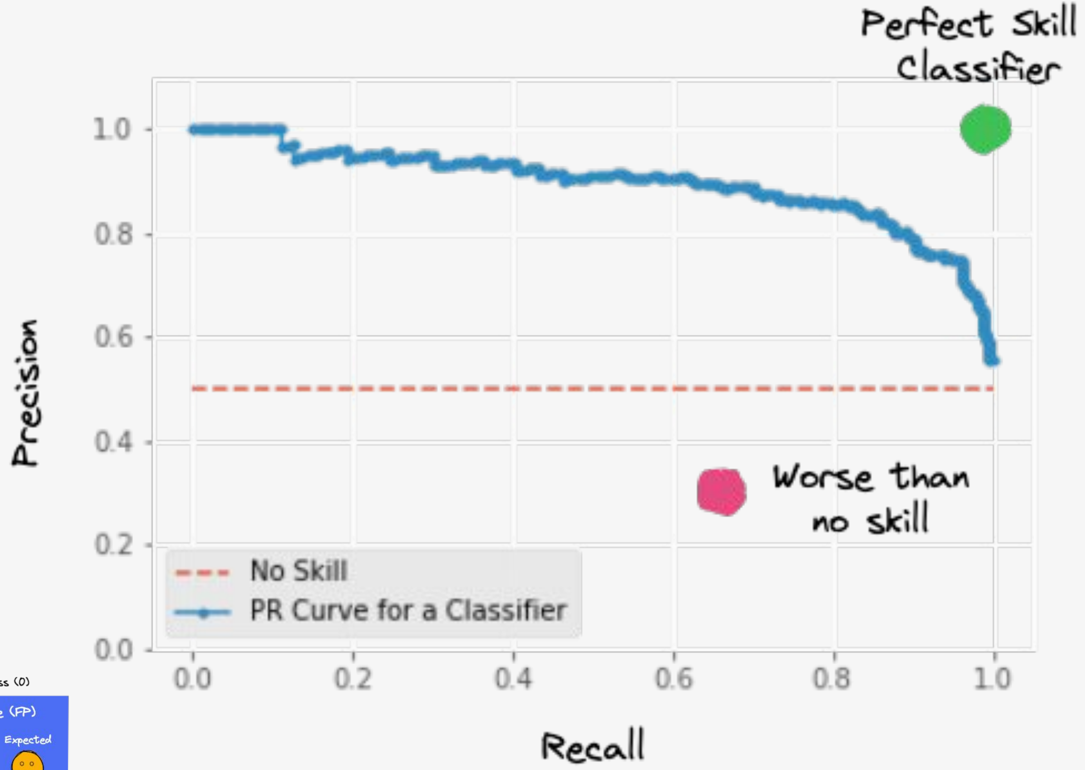


$$FPR = \frac{FP}{FP + TN}$$

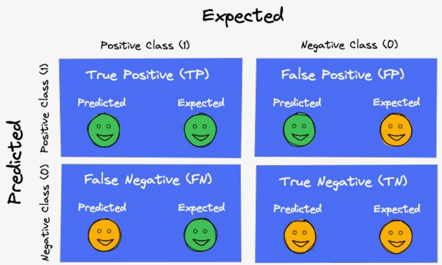
Ranking Metrics

Precision-Recall (PR) Curve

$$\text{Precision} = \frac{TP}{TP + FP}$$



$$\text{Recall} = \frac{TP}{TP + FN}$$



Hands ON

Python

scikit learn

W&B

Jupyter

Streamlit ANACONDA CONDA

Optional

matplotlib

pandas

seaborn

plotly

UCI

Machine Learning Repository

Center for Machine Learning and Intelligent Systems

Adult Data Set

Download: Data Folder, Data Set Description

Abstract: Predict whether income exceeds $50K/yr based on census data. Also known as "Census Income" dataset.

Data Set Characteristics:	Multivariate	**Number of Instances:**	48842	**Area:**	Social
Attribute Characteristics:	Categorical, Integer	**Number of Attributes:**	14	**Date Donated**	1996-05-01
Associated Tasks:	Classification	**Missing Values?**	Yes	**Number of Web Hits:**	2437279

Source:

Donor:

Ronny Kohavi and Barry Becker
Data Mining and Visualization
Silicon Graphics.
e-mail: ronnyk '@' live.com for questions.

Exploratory Data Analysis