Building a Reproducible Model Workflow Cont.

Train, Validation and Experiment Tracking

UFRN UNIVERSIDADE FEDERAL DO RIO GRANDE DO NORTE

DCA

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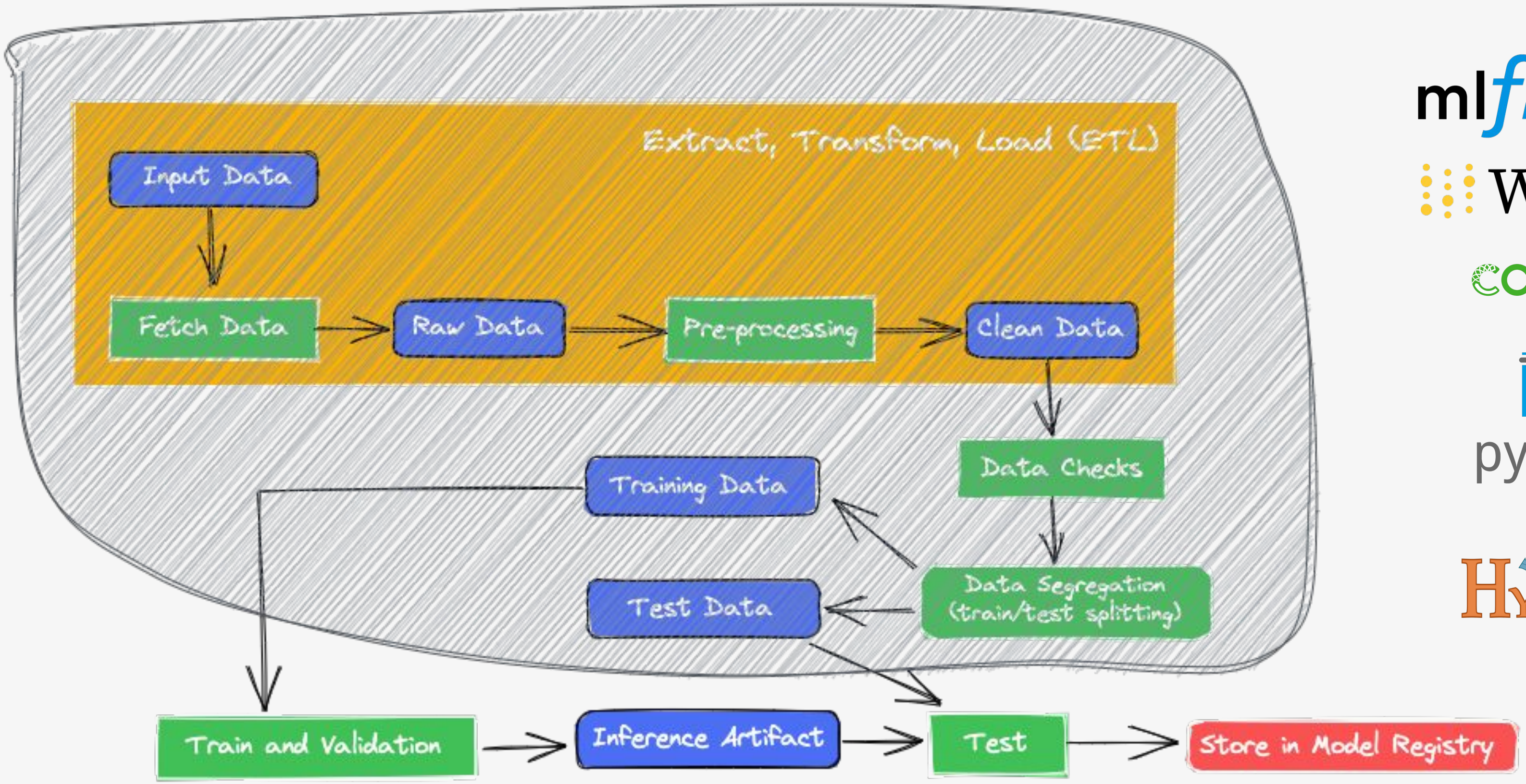
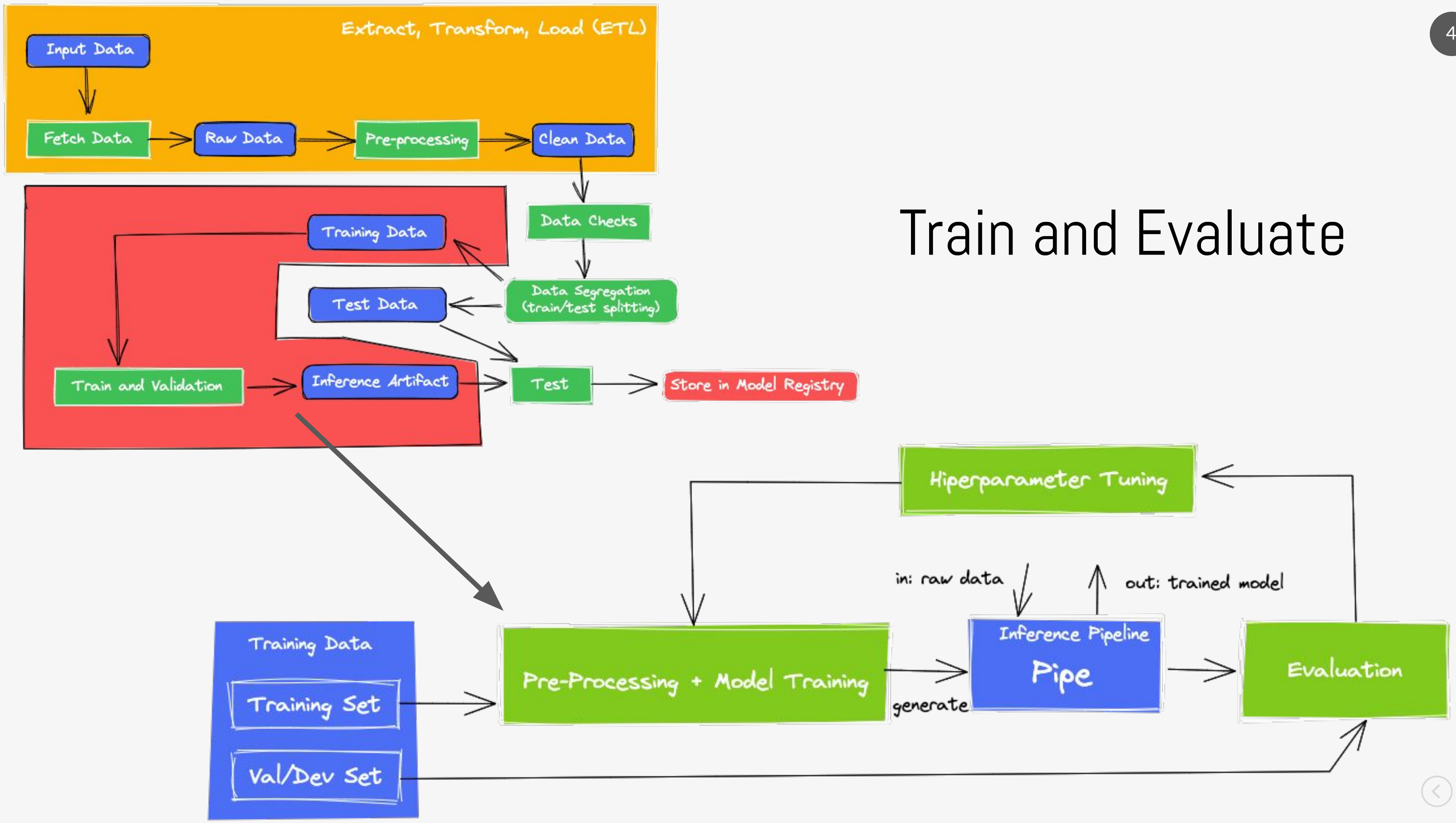
An inference pipeline is an ML pipeline that contains everything that needs to run in production at inference time: a pre-processing step that transforms the data input to the data expected by the model, and then the model

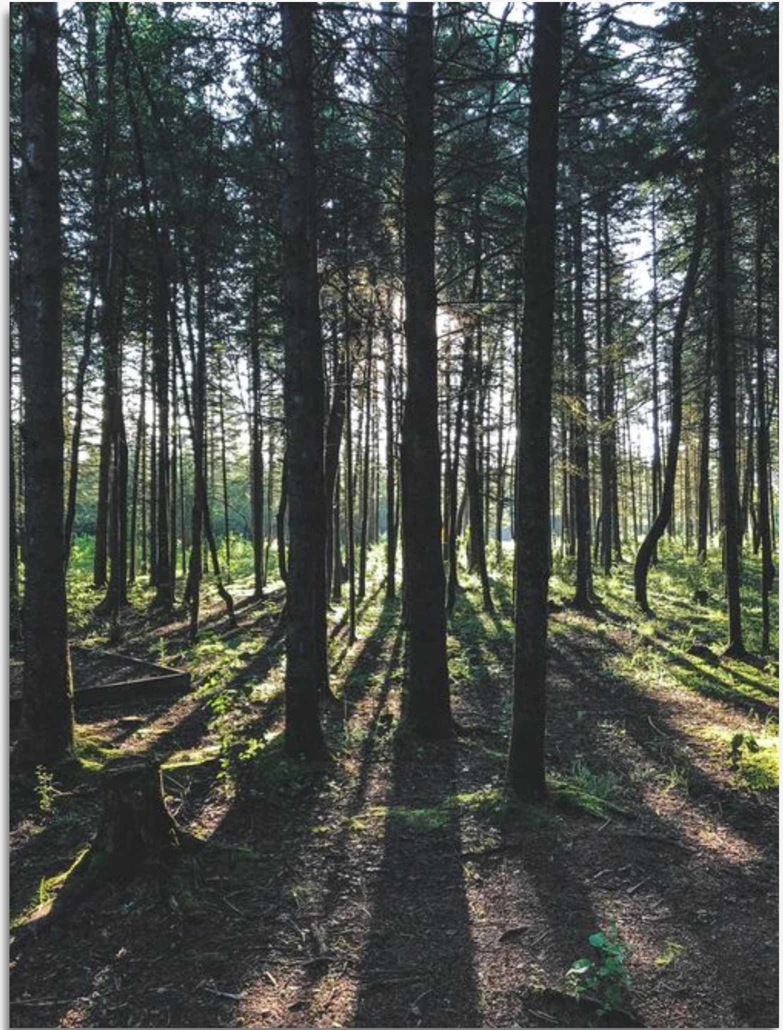
Previously on lessons



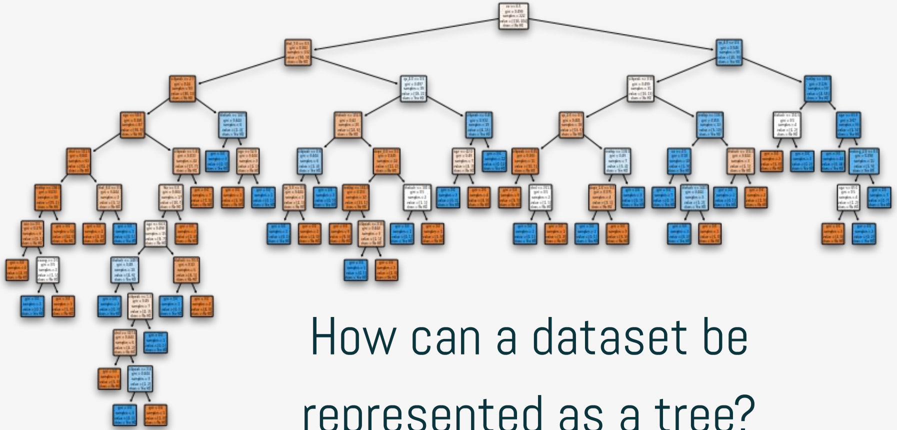
mlflow
W&B
CONDA
pytest
HYDRA

Train and Evaluate





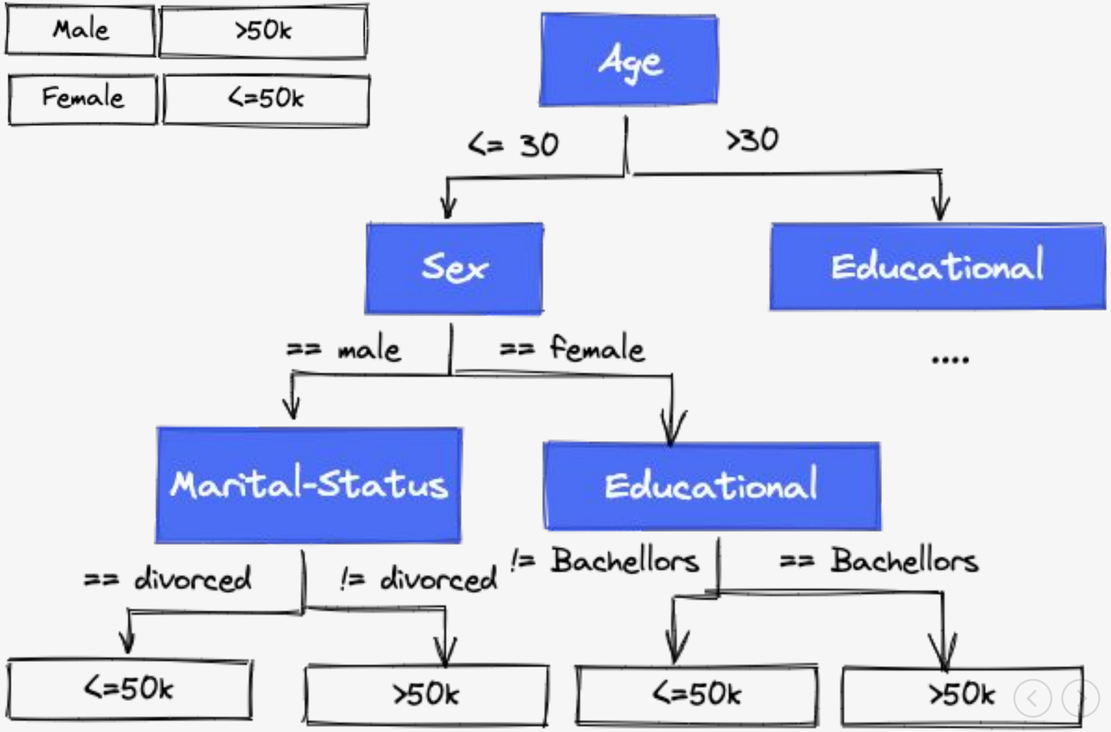
Decision Trees



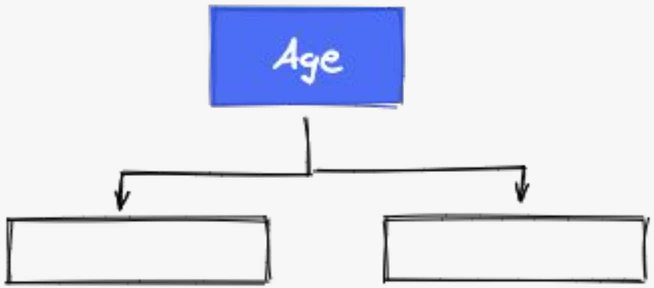
How can a dataset be represented as a tree?

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?

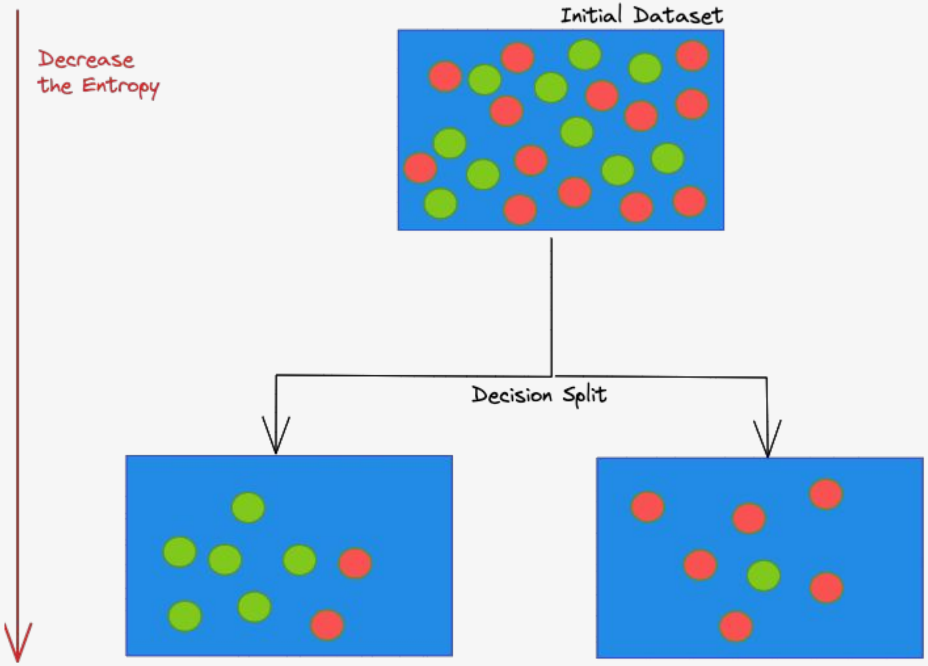


Algorithm used in Decision Trees

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

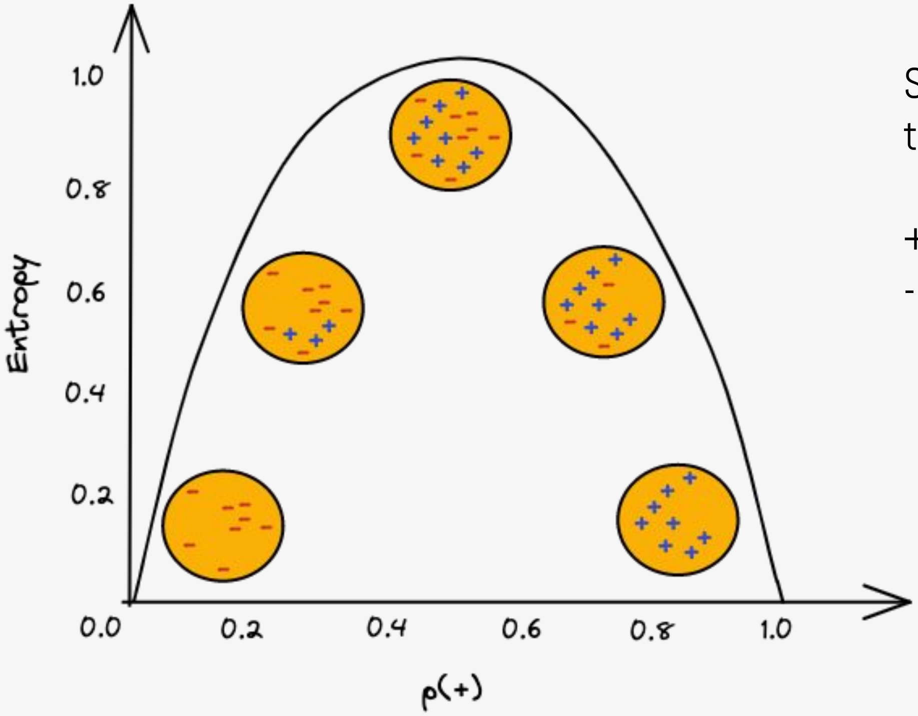
Entropy is an indicator of how messy your data is.

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%)

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

```
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.

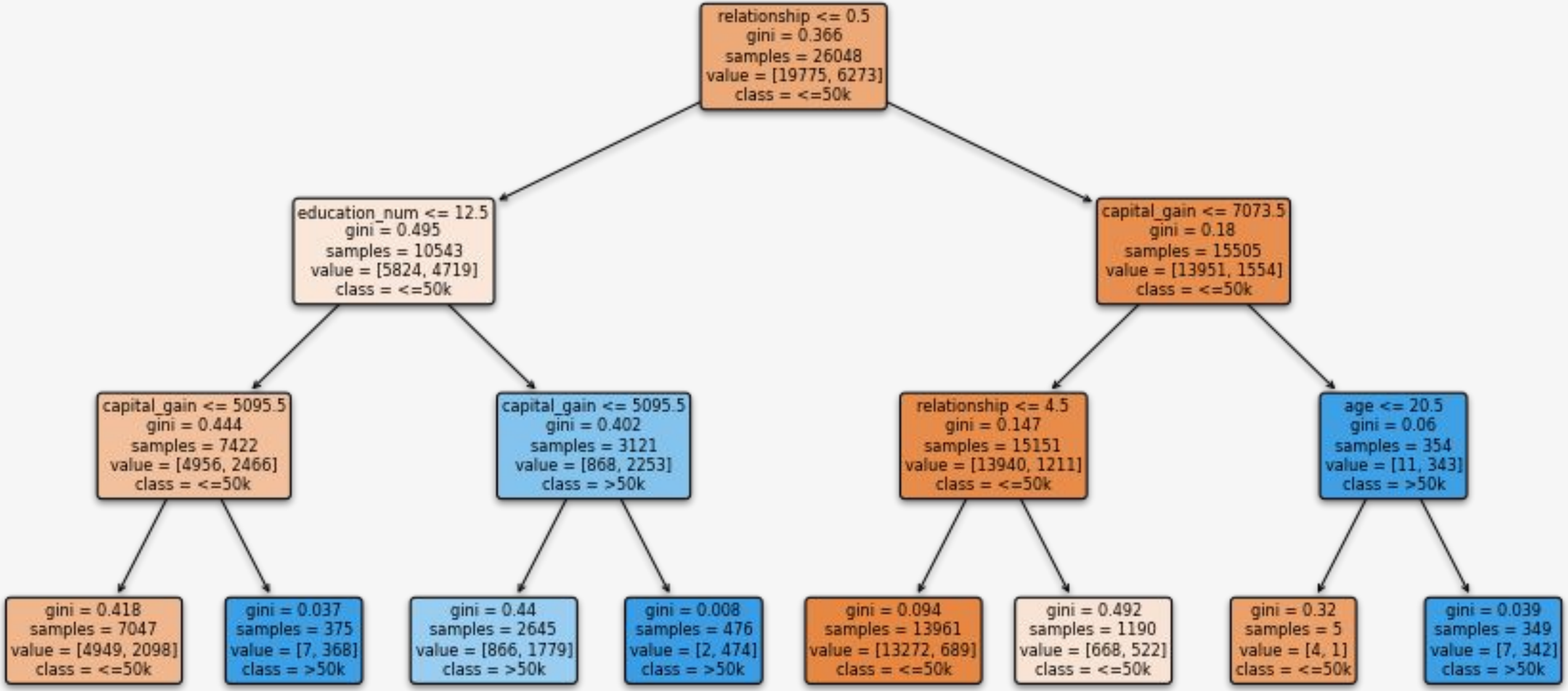
Constructing a decision tree is all about finding attribute that returns the **highest information gain** (i.e., the most homogeneous branches).

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

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

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

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



Taxonomy of Classifier Evaluation Metrics

Threshold Metrics

Ratio when a predicted class does not match

Accuracy, Error, Sensitivity, Specificity, G-mean, precision, recall, fbeta-measure

Ranking Metrics

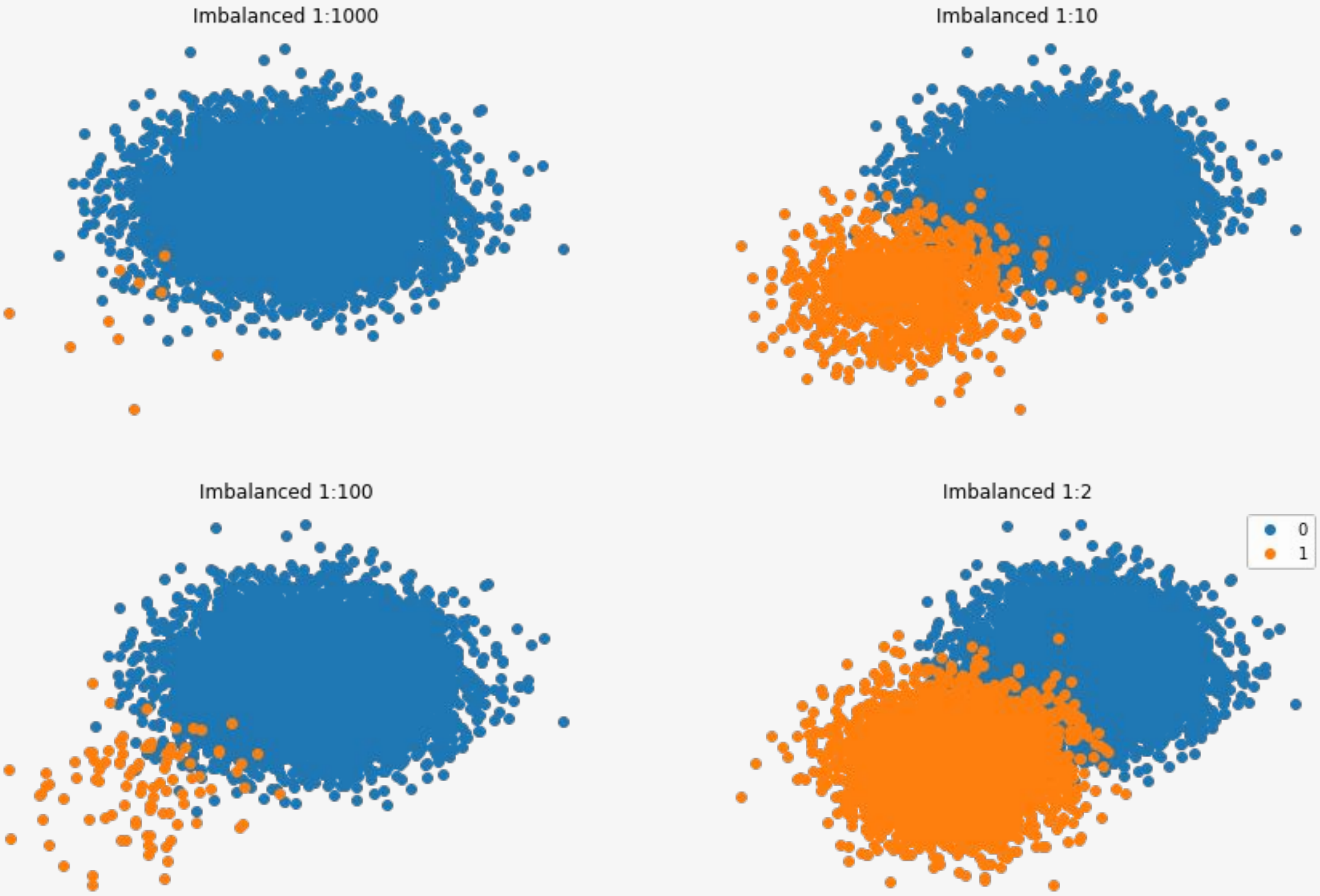
Based on score of class membership and variatons of thresholds to measure the effectiveness of classifiers.

ROC Curve, ROC AUC, Precision-Recall Curve

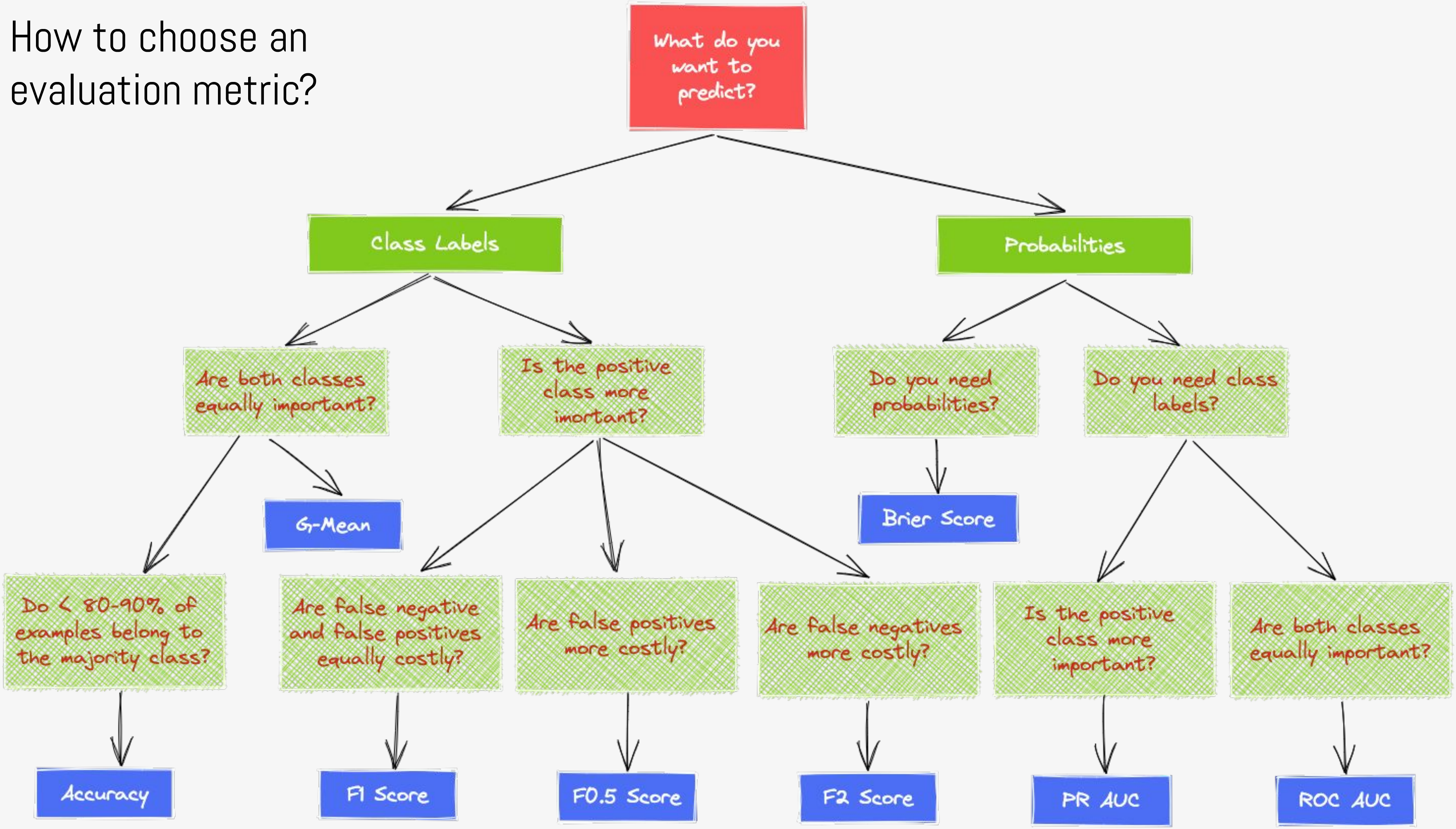
Probability Metrics

Quantify the uncertainty in a classifier's prediction

Log-Loss
Brier Score

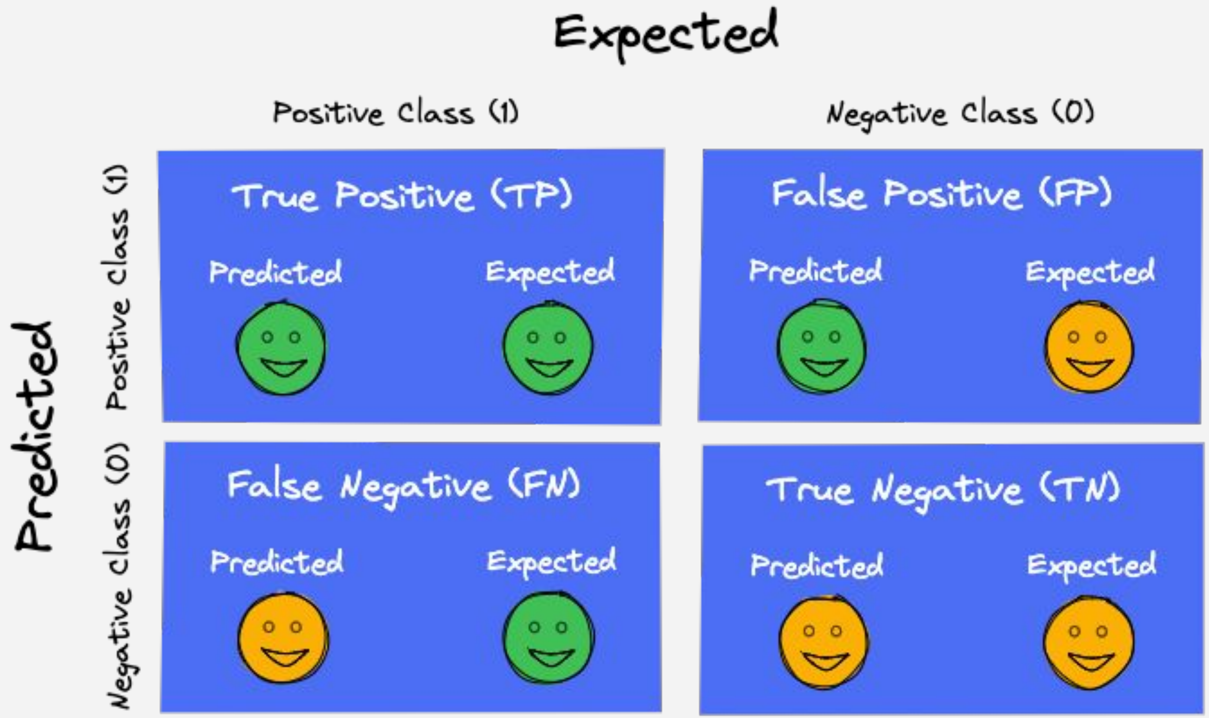

Imbalanced 1:1000
Imbalanced 1:10
Imbalanced 1:100
Imbalanced 1:2
0
1

How to choose an evaluation metric?



@Brownlee, Jason. Imbalanced classification with python.

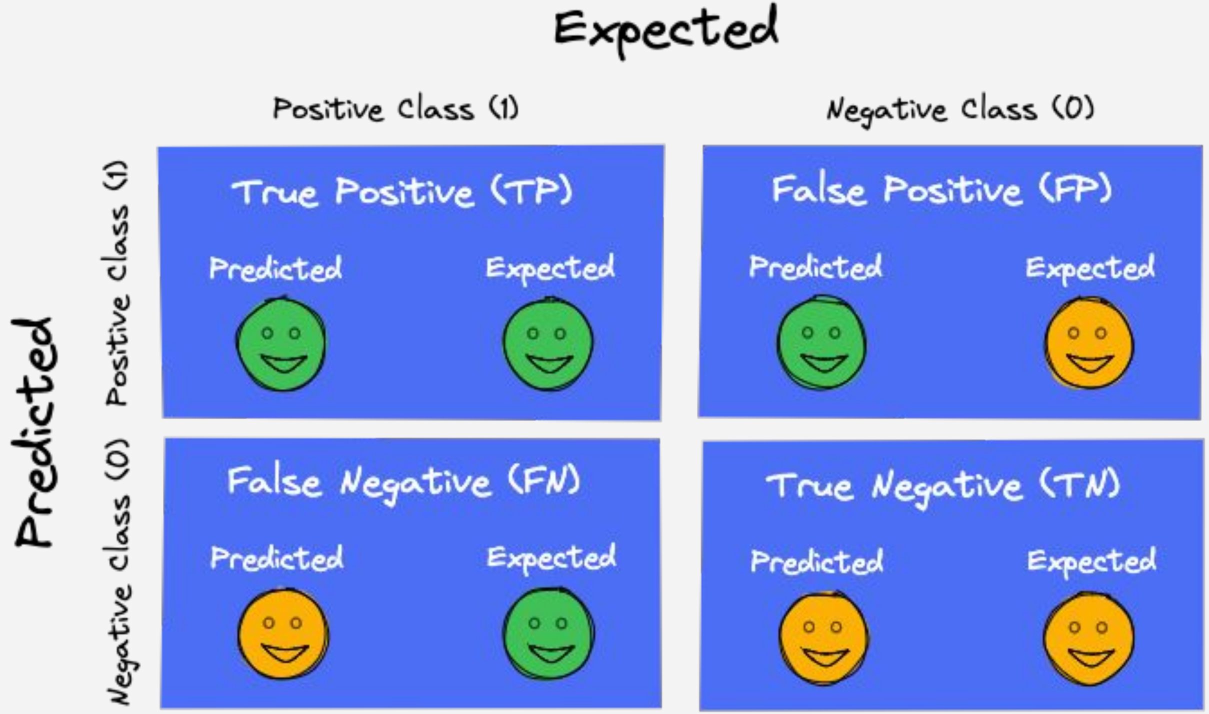
Confusion Matrix



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

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

Confusion Matrix

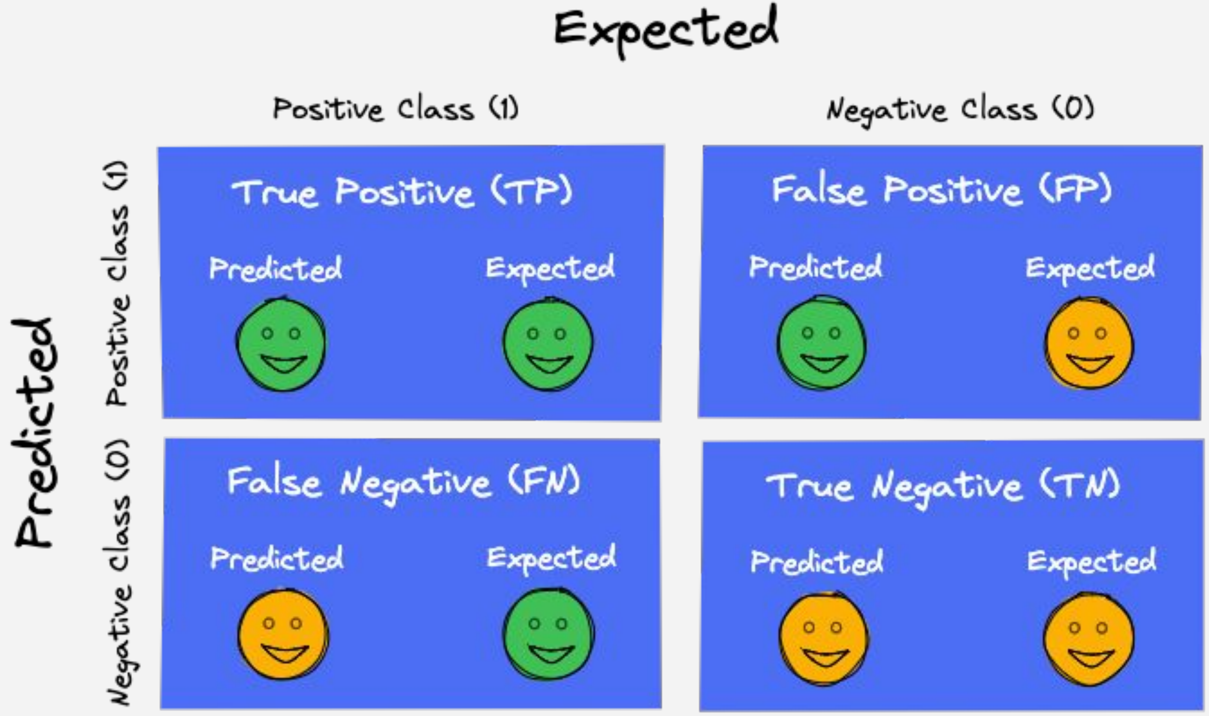


$$\text{Sensitivity} = \frac{TP}{TP + FN}$$

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

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

Confusion Matrix

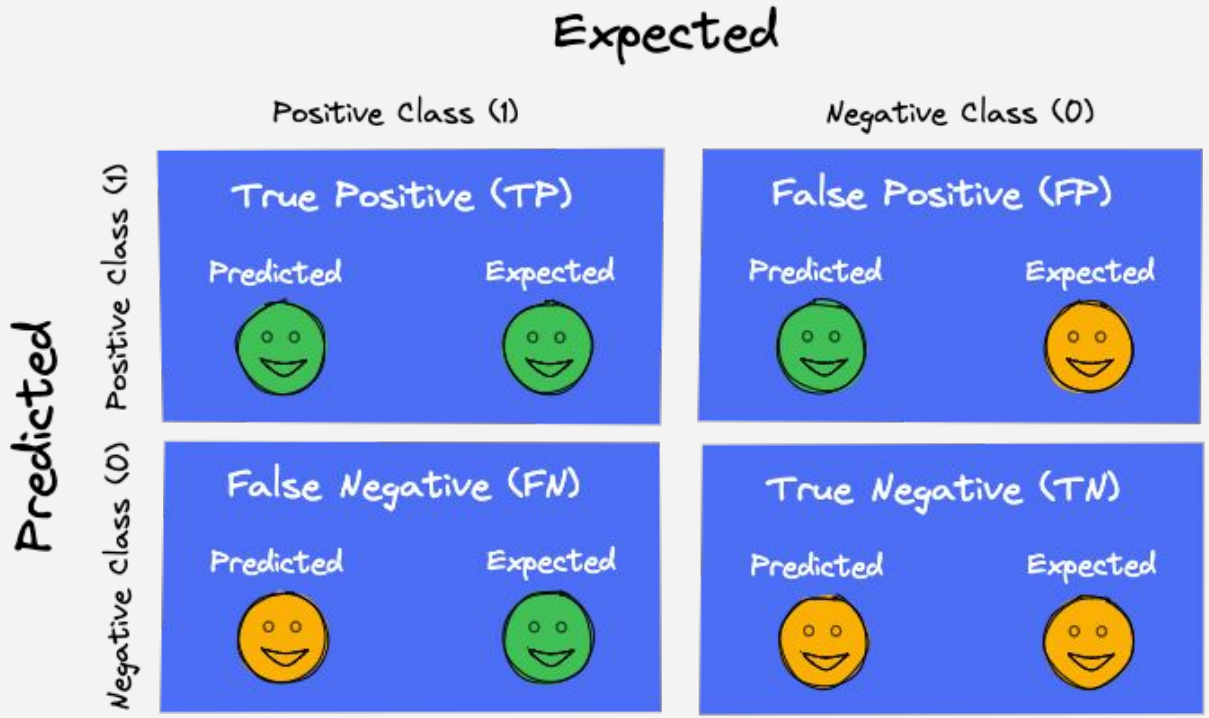


Precision (positive predicte value - PPV) $= \dfrac{TP}{TP + FP}$

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

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

Confusion Matrix



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

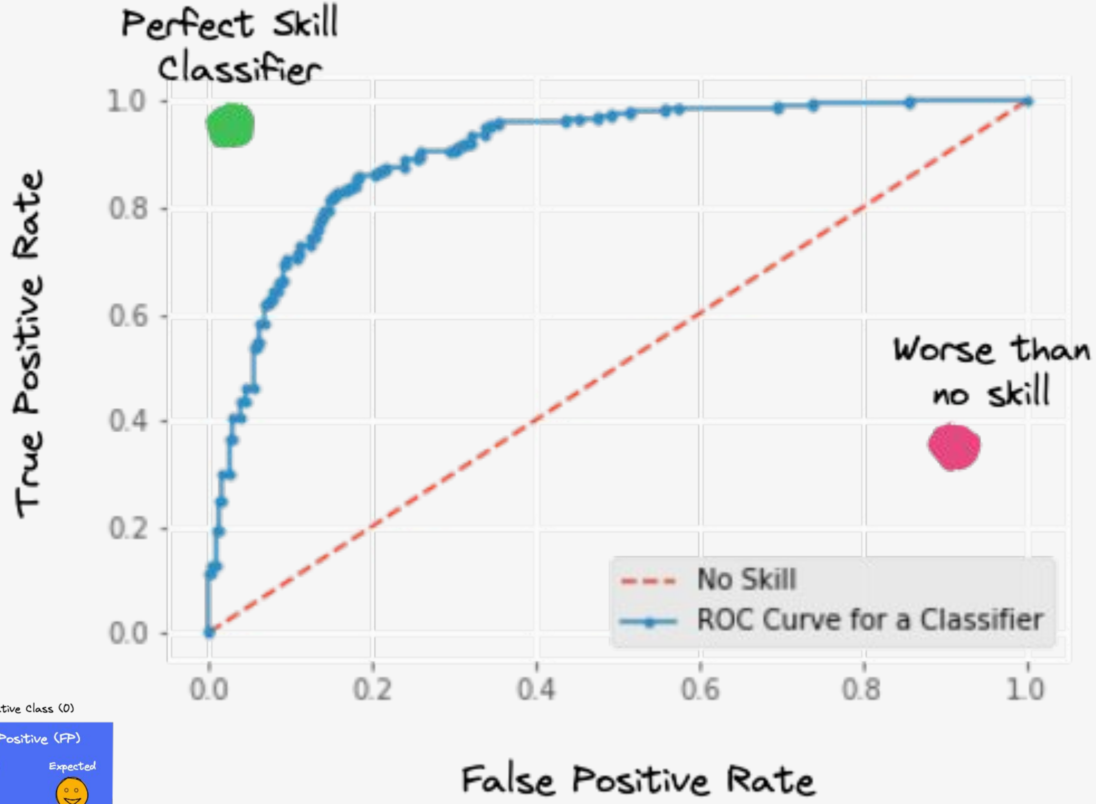
$$\beta == \begin{cases} 0.5, & \text{more weight on precision} \\ 1.0, & \text{balance on weight PR and RE} \\ 2.0, & \text{less weight on precision} \end{cases}$$

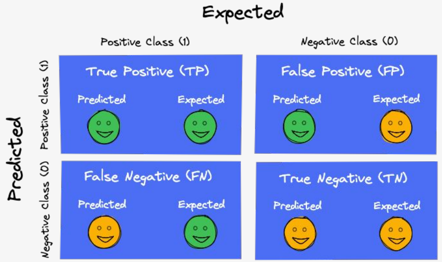
Rank metrics are more concerned with evaluating classifiers based on **how effective** they are at separating classes.

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)

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

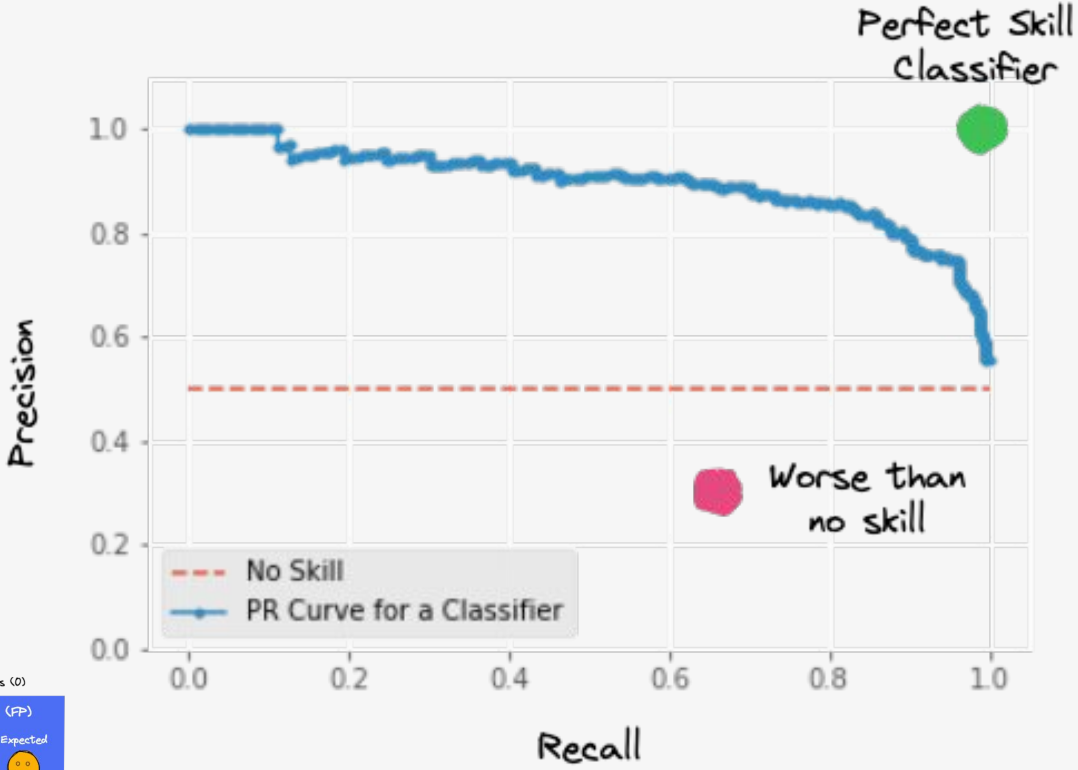


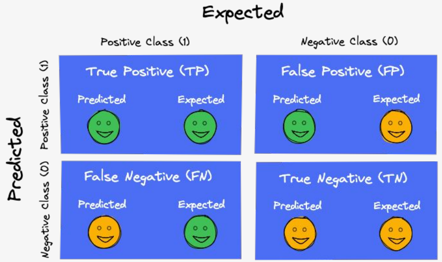


$$FPR = \frac{FP}{FP + TN}$$

Precision-Recall (PR) Curve

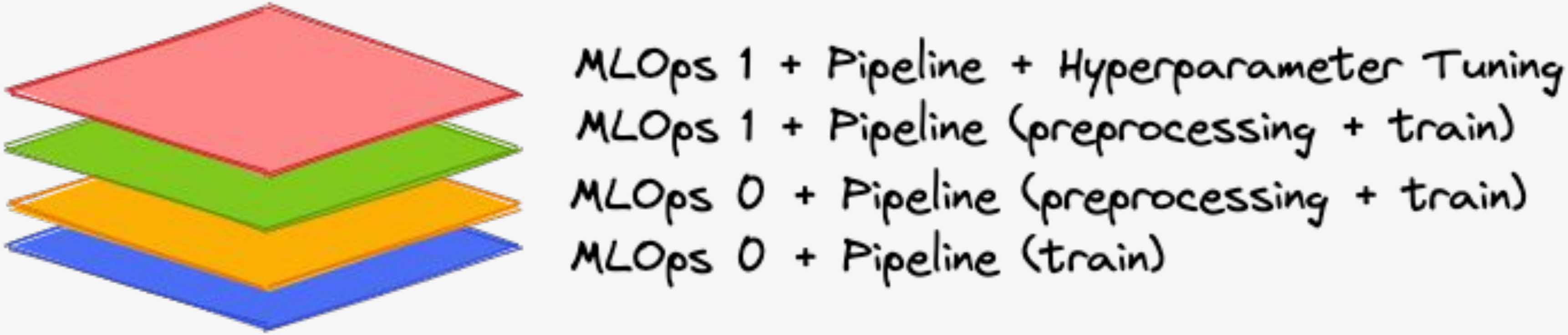
$$\text{Precision} = \frac{TP}{TP + FP}$$



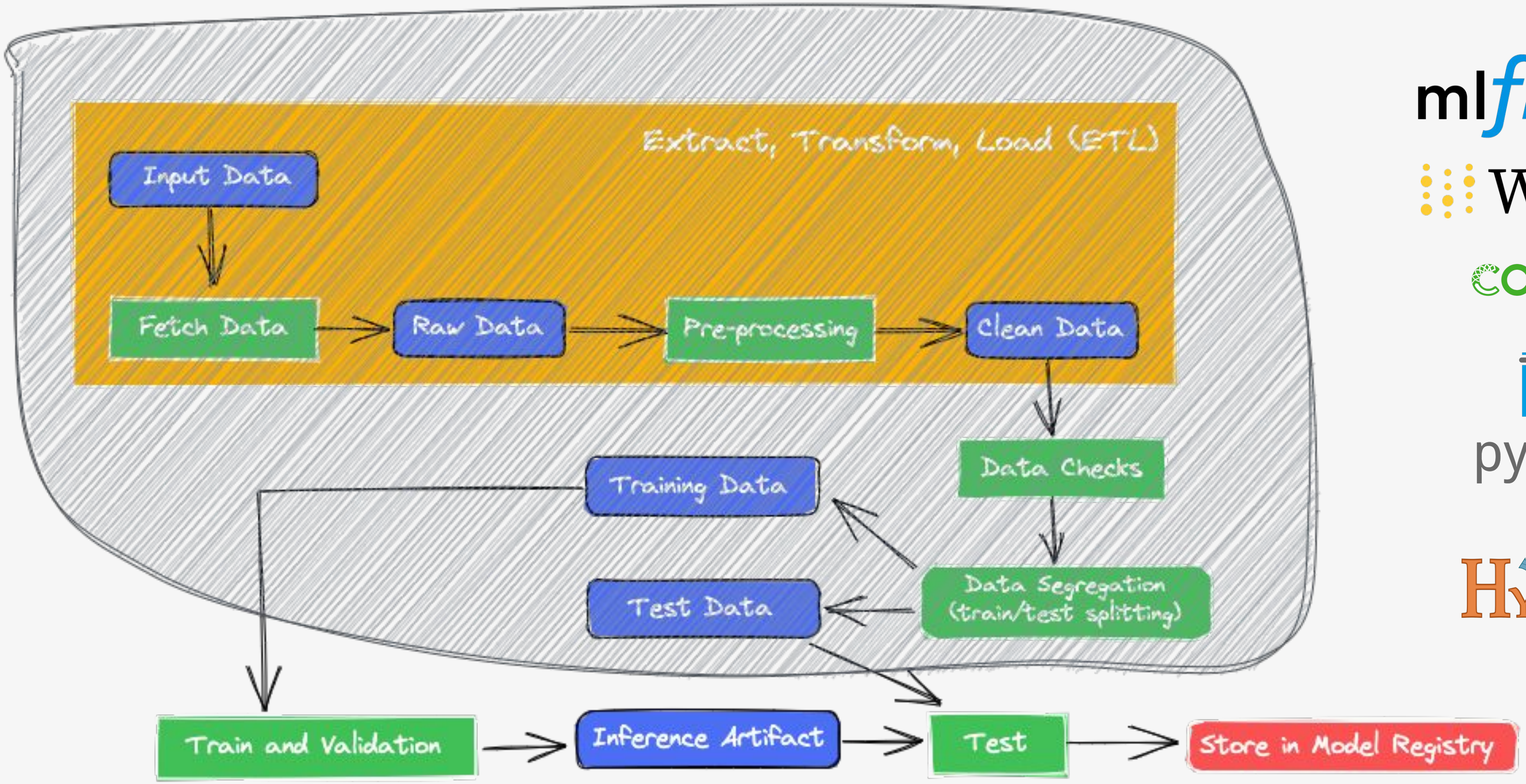


$$\text{Recall} = \frac{TP}{TP + FN}$$

Case Study - Hands on



Final Stage


Extract, Transform, Load (ETL)
Input Data
Fetch Data
Raw Data
Pre-processing
Clean Data
Data Checks
Training Data
Data Segregation (train/test splitting)
Test Data
Train and Validation
Inference Artifact
Test
Store in Model Registry