Artificial Intelligence I: Introduction to Data Science and Machine Learning

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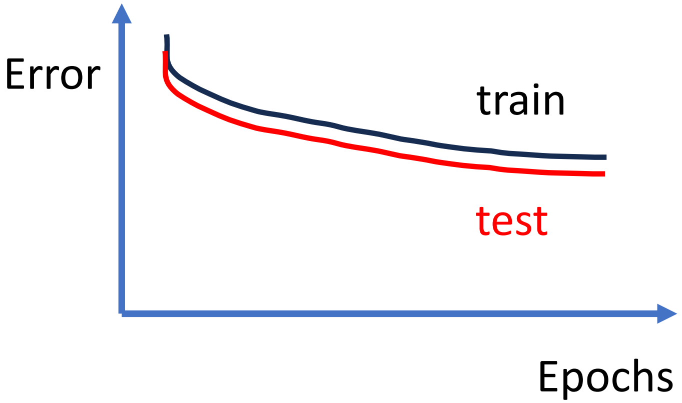
Train/Test Split

- The dataset is divided into two subsets: the training set and the testing set
- Training set:
  - Used to train the machine learning model
  - The model learns patterns and relationships within this set
- Test set:
  - Not used during training
  - Used to test the model's performance on new, unseen data
- **Generalization: Evaluate how well the model generalizes to new, unseen data**
- K-Fold Cross-Validation: multiple train/test subsets

Underfitting, Overfitting

- **Overfitting:**
  - Model that performs exceptionally well on the training data **but poorly on new, unseen data (not generalized)**
  - Typically characterized by a complex model with too many parameters relative to the amount of available training data
- **Underfitting:**
  - Model is too simple to capture the underlying patterns in the training data
  - Model performs poorly on both the training and new data
  - Model is too basic or lacks the necessary complexity to represent the underlying relationships

Underfitting, Overfitting (Visualized)

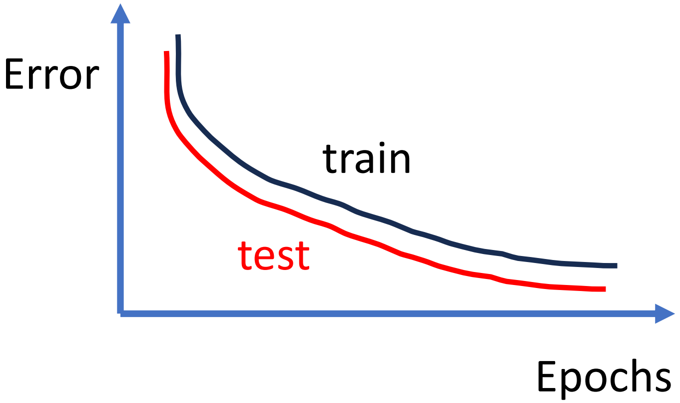


Underfitting

Both train and test error is high

Model is too basic to learn the data

More complex model is required

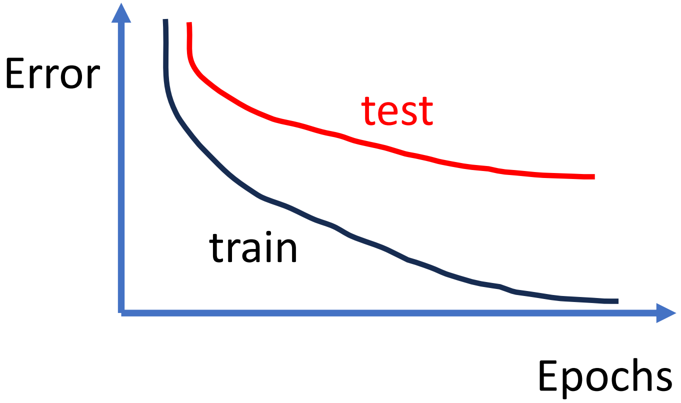


Optimal Fitting

Both train and test error is low

Model learns data well and generalizes

Best results



Overfitting

Train error is low, but test error is high

Model learns data well but can't generalize

Model is too complex or not enough data to generalize

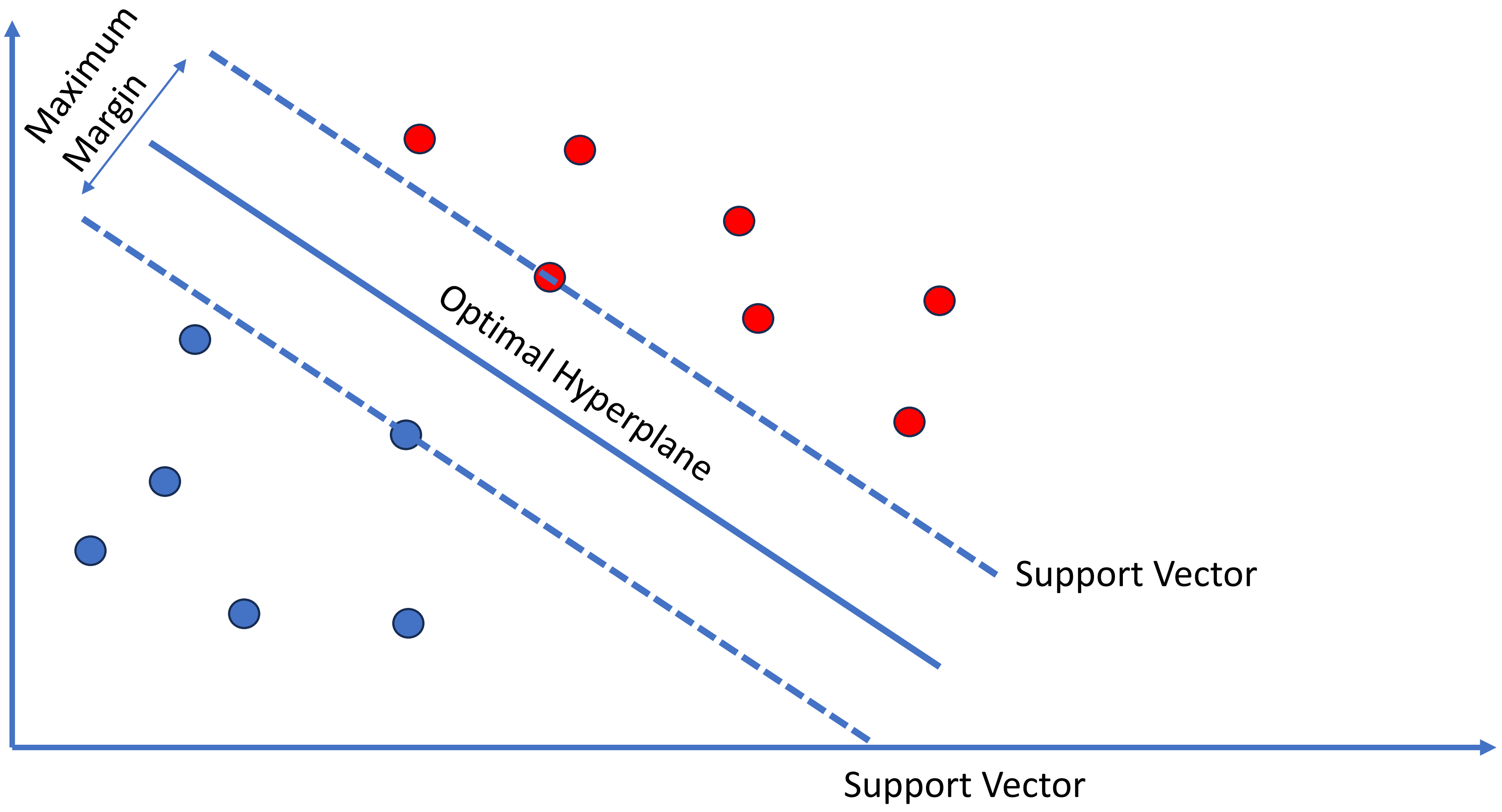
Naïve Bayes Classifier

- Used in classification
- Bayes' Theorem: $P(y|x) = \frac{P(x|y)P(y)}{P(x)}$
  - $P(y|x)$: Probability of class y given features x
  - $P(x|y)$: Probability of features x given class y
  - $P(y)$: Prior probability of class y
  - $P(x)$: Prior probability of features x
- Naïve assumption: features are independent
  - $P(y|x_1, x_2, x_3, \ldots, x_n) = P(y|x_1)P(y|x_2) \ldots P(y|x_n)$
- Sklearn:
  - GaussianNB

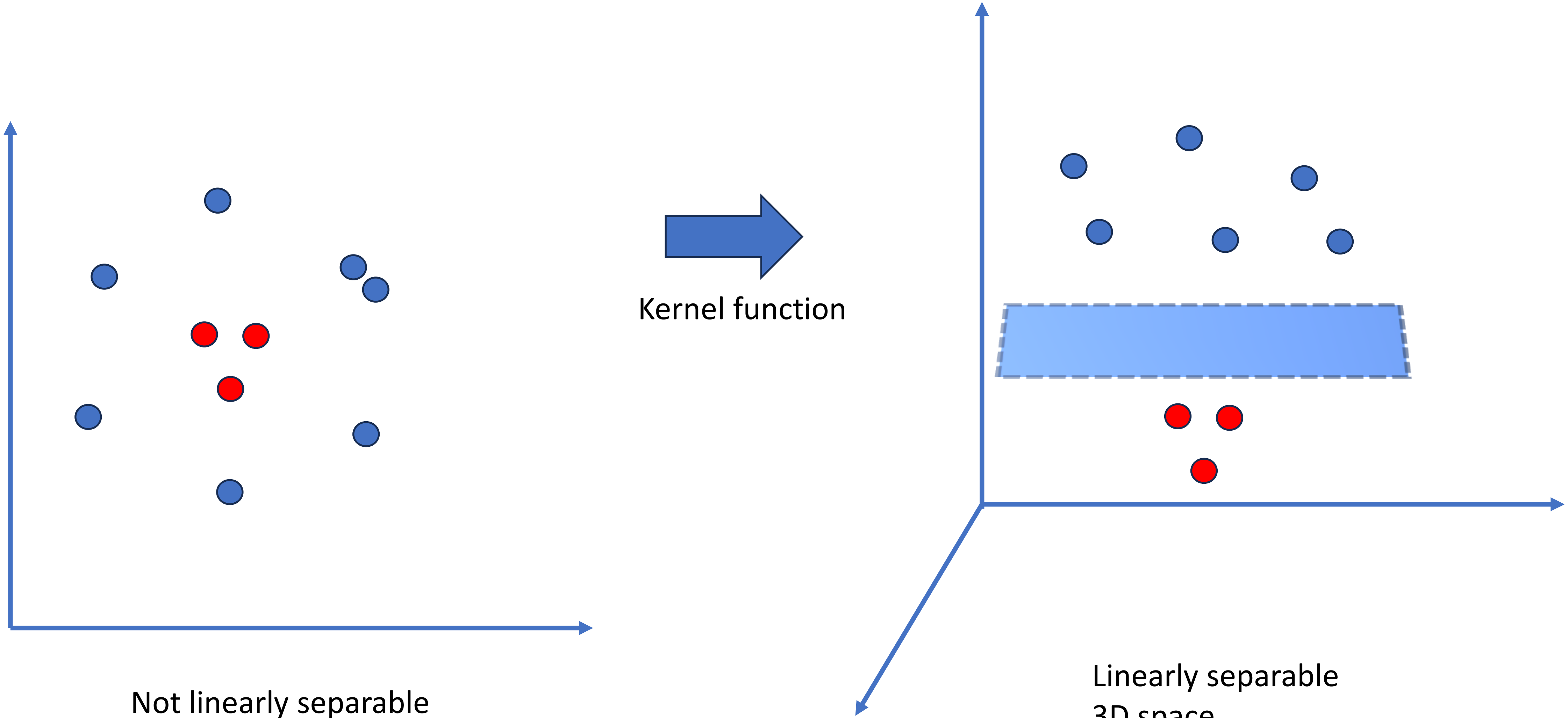
Support Vector Machine (SVM)

- SVM is invented for binary classification tasks, where the goal is to separate data points into two classes using a hyperplane
- **SVM focuses on maximizing the margin**, which is the distance between the hyperplane and the nearest data points of each class
- Kernel Trick: can handle non-linear decision boundaries by transforming the input features using a kernel function
    - polynomial, radial basis function (RBF), sigmoid, etc.
- Sklearn:
    - SVC (Support Vector Classifier)
    - SVR (Support Vector Regressor)

SVM Visualized



SVM Kernel Trick



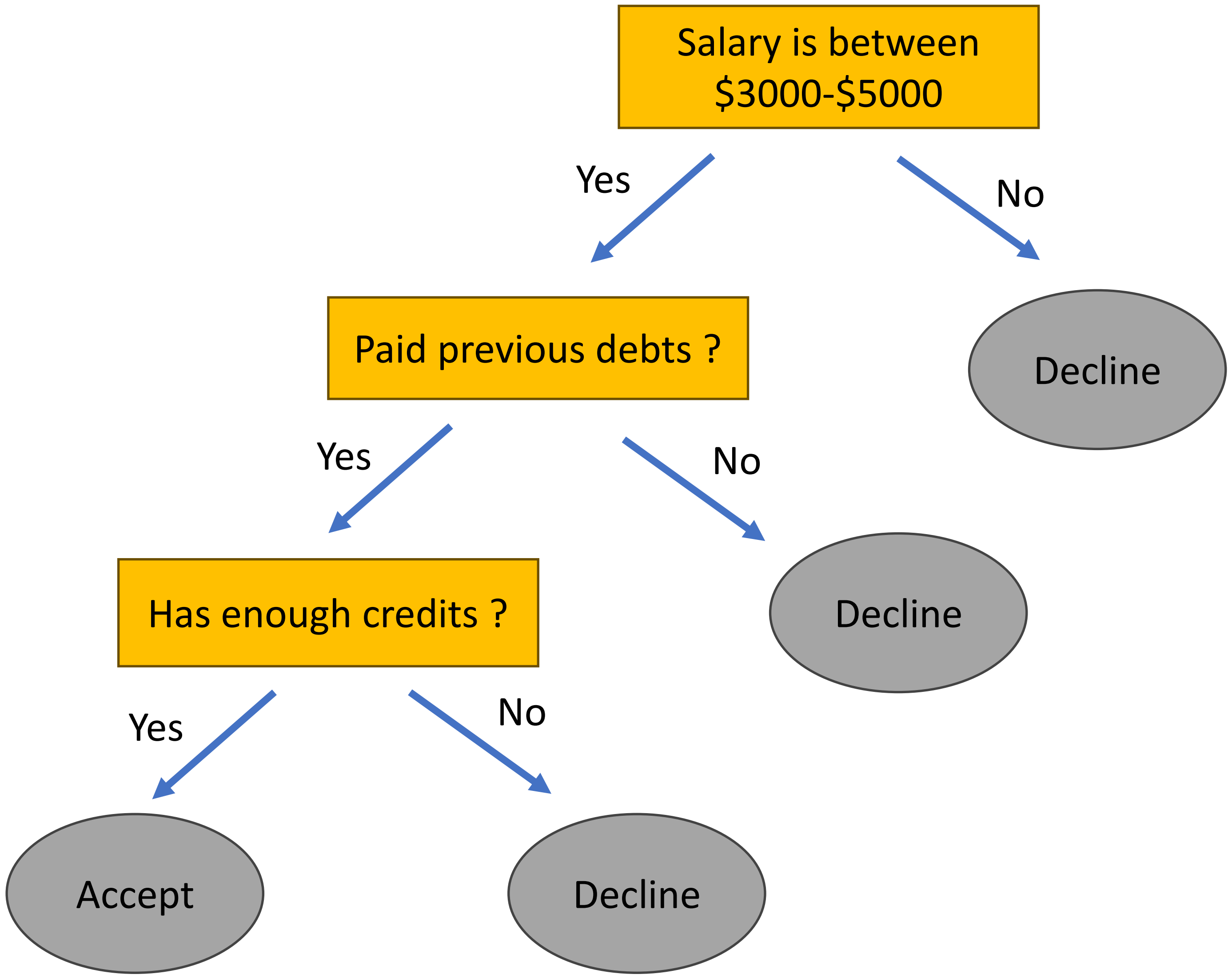
Not linearly separable
2D space

Linearly separable
3D space
2D hyperplane

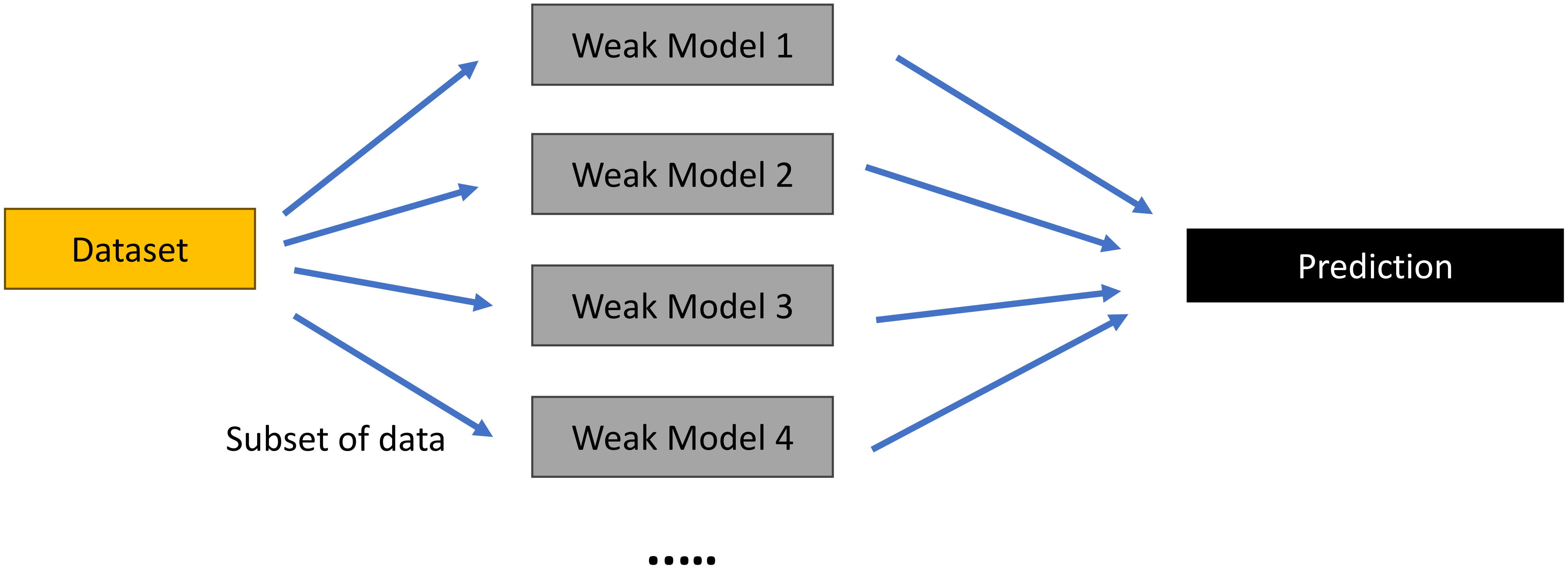
Decision Trees

- Decision Trees are hierarchical structures with nodes representing decisions or test conditions and branches representing possible outcomes
- Uses a splitting criterion to determine the best feature and threshold to split the data at each node
  - Gini impurity for classification
  - mean squared error for regression
- Sklearn:
  - DecisionTreeClassifier
  - DecisionTreeRegressor

Decision Trees Visualized

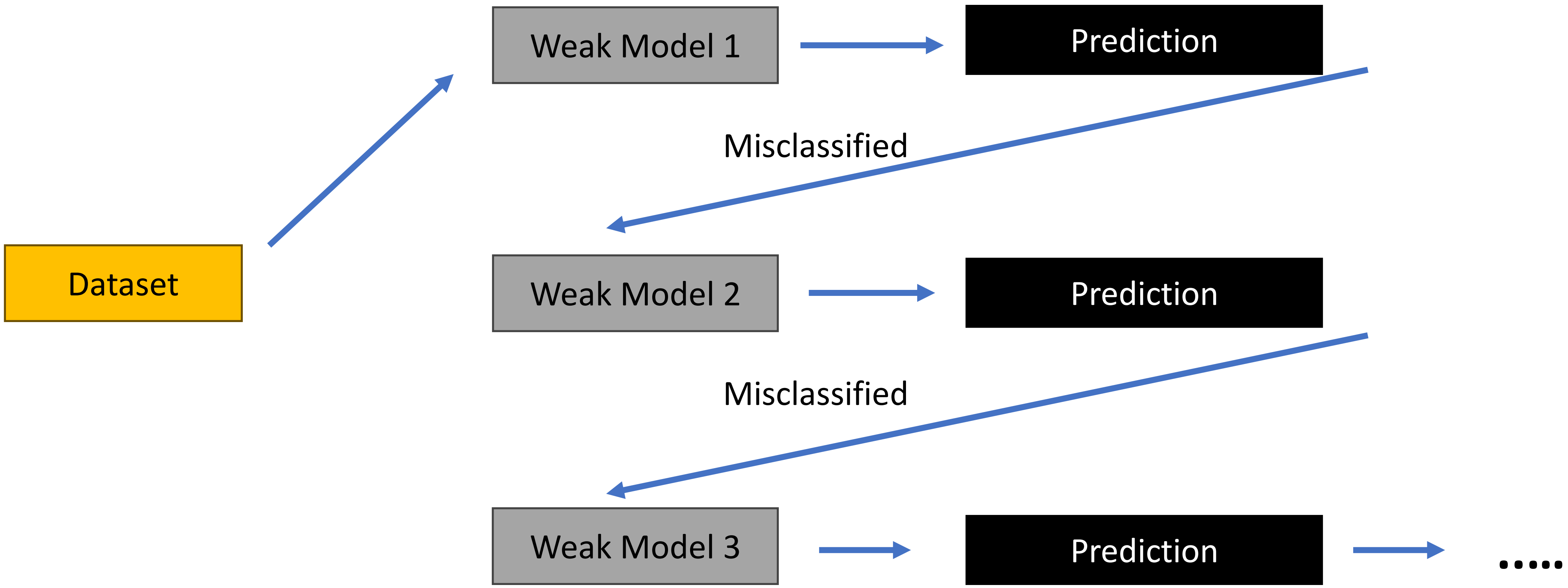


Ensemble Models



Bagging (Bootstrap Aggregating)

Ensemble Models

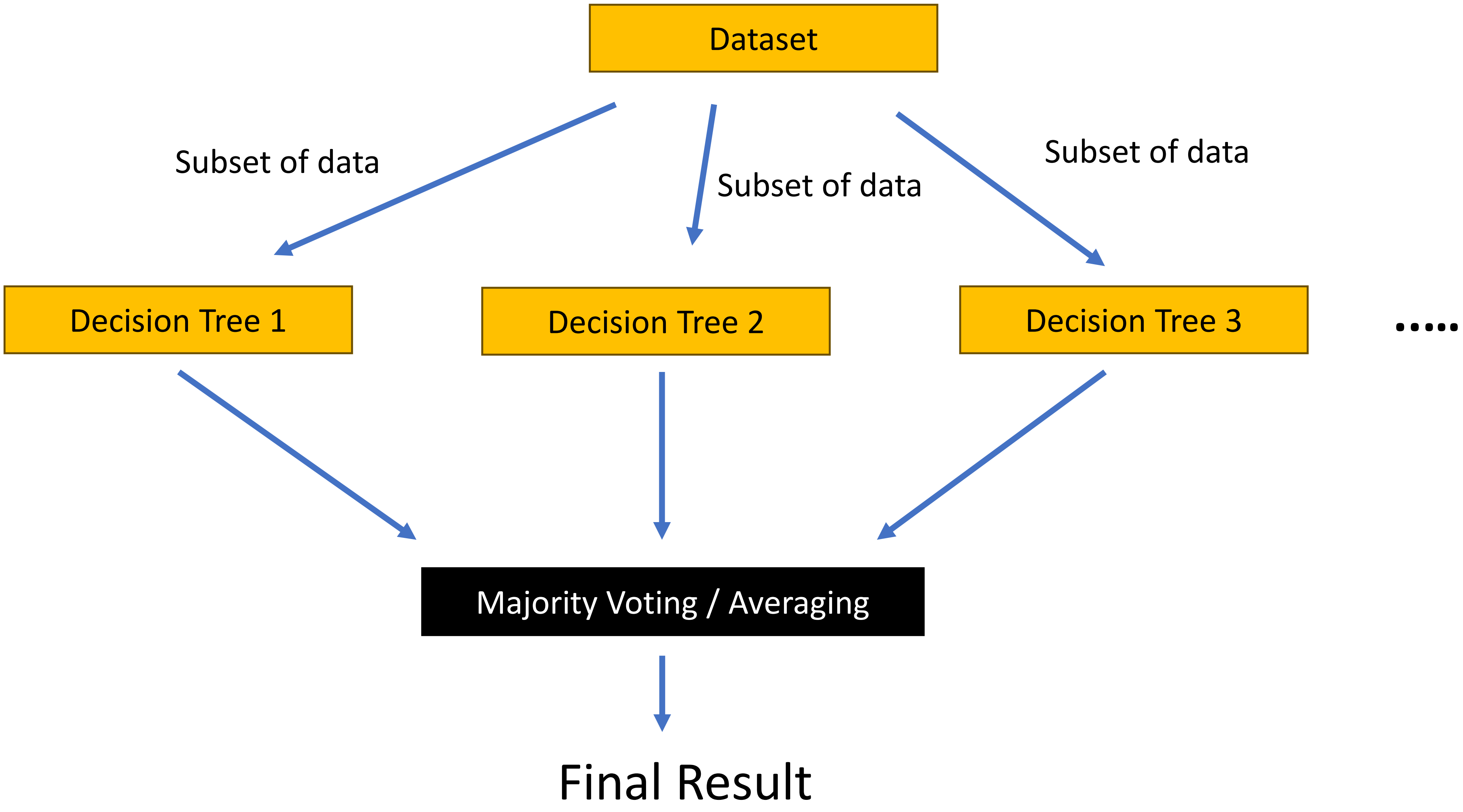


Boosting

Random Forest

- Random Forest is an ensemble learning technique that builds multiple decision trees
- Each tree is trained independently on a random subset of the data using bootstrap sampling (bagging ensemble model)
- Can do feature selection with feature importance
- Sklearn:
  - RandomForestClassifier
  - RandomForestRegressor

Random Forest



Binary Classification

- In binary classification task, we have labels 0 and 1. Actual values comes from dataset and prediction values comes from the model
- **TP (true positive):** Actual is 1 and we predict as 1
- **TN (true negative):** Actual is 0 and we predict as 0
- **FP (false positive):** Actual is 0 and we predict as 1
  - Type I Error
- **FN (false negative):** Actual is 1 and we predict as 0
  - Type II Error

Classification Metrics

- $precision = \frac{TP}{TP + FP}$ Positive Predictive Value (PPV)
- $recall = sensitivity = \frac{TP}{TP + FN}$ True Positive Rate (TPR)
- $F1\ score = 2 * \frac{precision * recall}{precision + recall}$ Harmonic Mean of PPV and TPR
- $specificity = \frac{TN}{TN + FP}$ True Negative Rate (TNR)
- $accuracy = \frac{TP + TN}{TP + TN + FP + FN}$

Confusion Matrix

	Predicted 0	Predicted 1
Actual 0	TN	FP
Actual 1	FN	TP

Confusion Matrix

	Predicted 0	Predicted 1
Actual 0	TN	FP
Actual 1	FN	TP

Recall

Precision

Oversampling, Undersampling

- **Oversampling:** A method to balance class distribution by increasing the number of instances in the minority class
  - SMOTE (Synthetic Minority Oversampling Technique)

- **Undersampling:** A method that addresses imbalanced class distribution by reducing the number of instances in the majority class
  - If dataset is small, we don’t usually prefer this

General Workflow For Data Science & Machine Learning

- Collect / generate data
- Read and visualize the data (EDA)
- Preprocess the data (scaling, missing/imbalanced data etc.)
- Select features (dimentionality reduction, etc.)
- Select model (Linear regression, Random forest, SVM, etc.)
- Select the best hyperparameters for your model (Grid search, etc.)
- Select the evaluation metrics for your task (F1, etc)
- Train (fit) your model to training data, predict on test data
- Evaluate and discuss the results