Introduction to Machine Learning

Introduction to Data Science

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Outline

Outline

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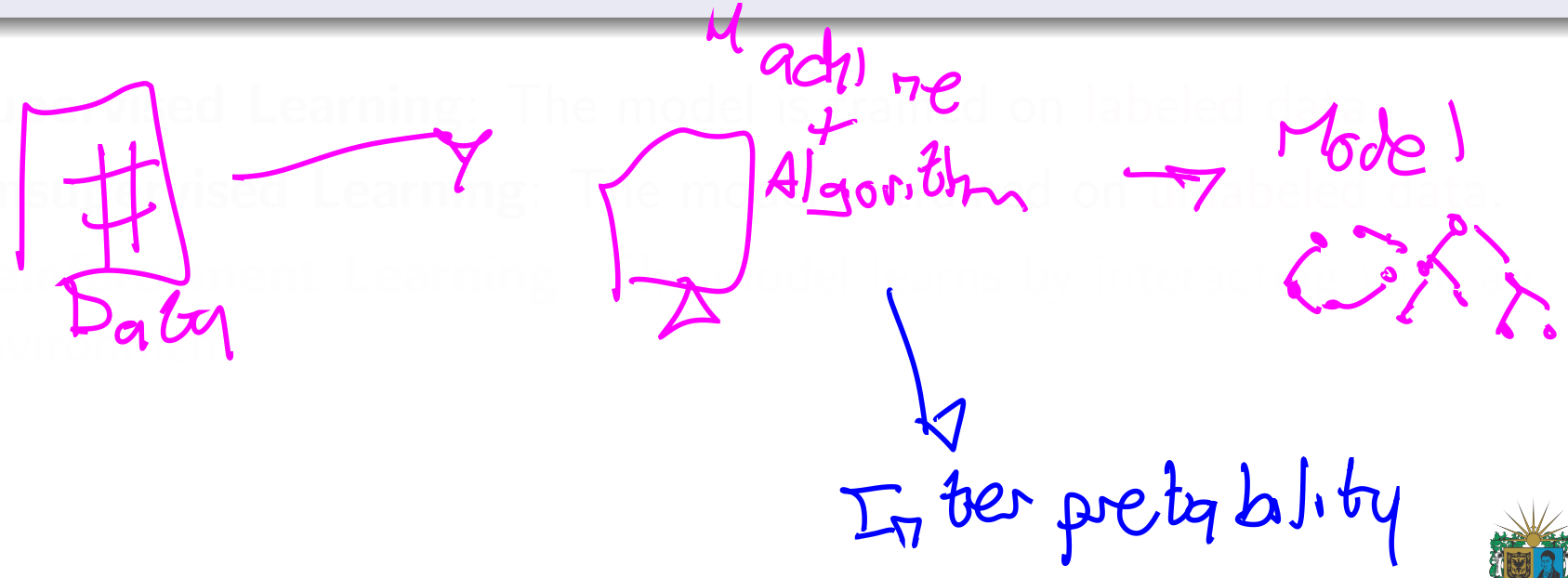
Key Concepts in Machine Learning

Machine Learning

- **Machine learning** is a method of data analysis that automates analytical model building.
- It is a **branch** of artificial intelligence based on the idea that systems can learn from data, identify patterns and make decisions with `minimal human intervention`.



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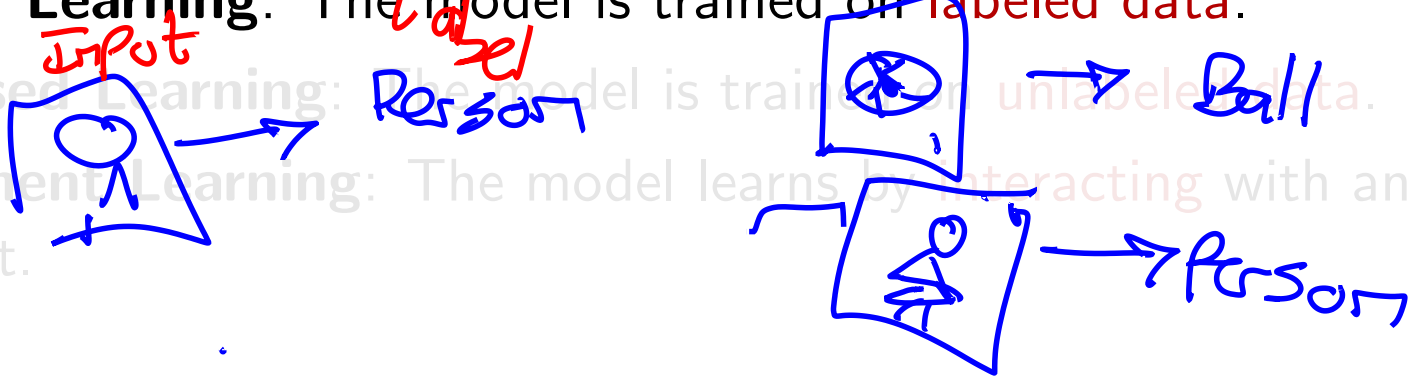
- **Supervised Learning**: The model is trained on labeled data.
- **Unsupervised Learning**: The model is trained on unlabeled data.
- **Reinforcement Learning**: The model learns by interacting with an environment.



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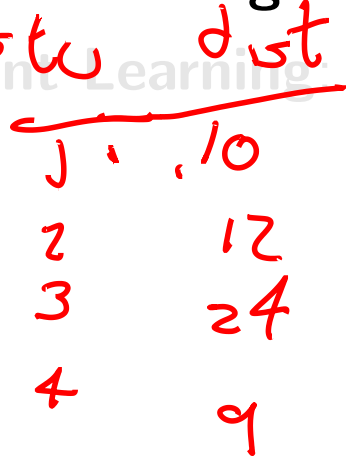

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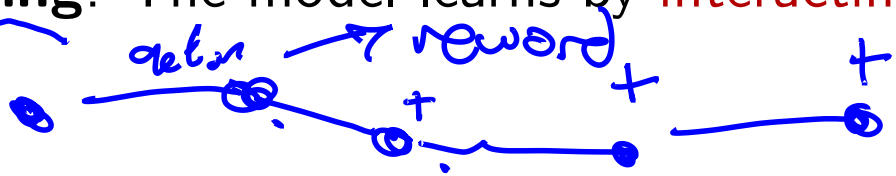

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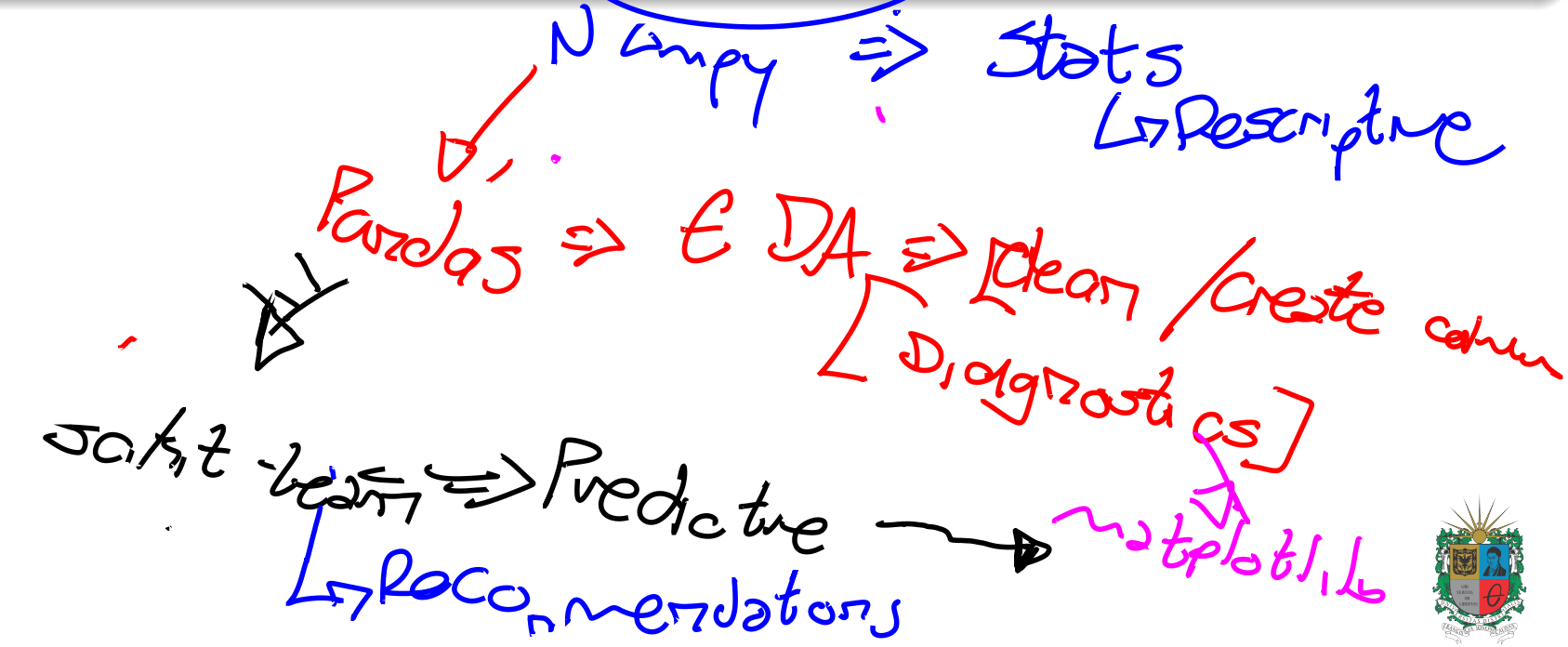
Python Tools for Machine Learning

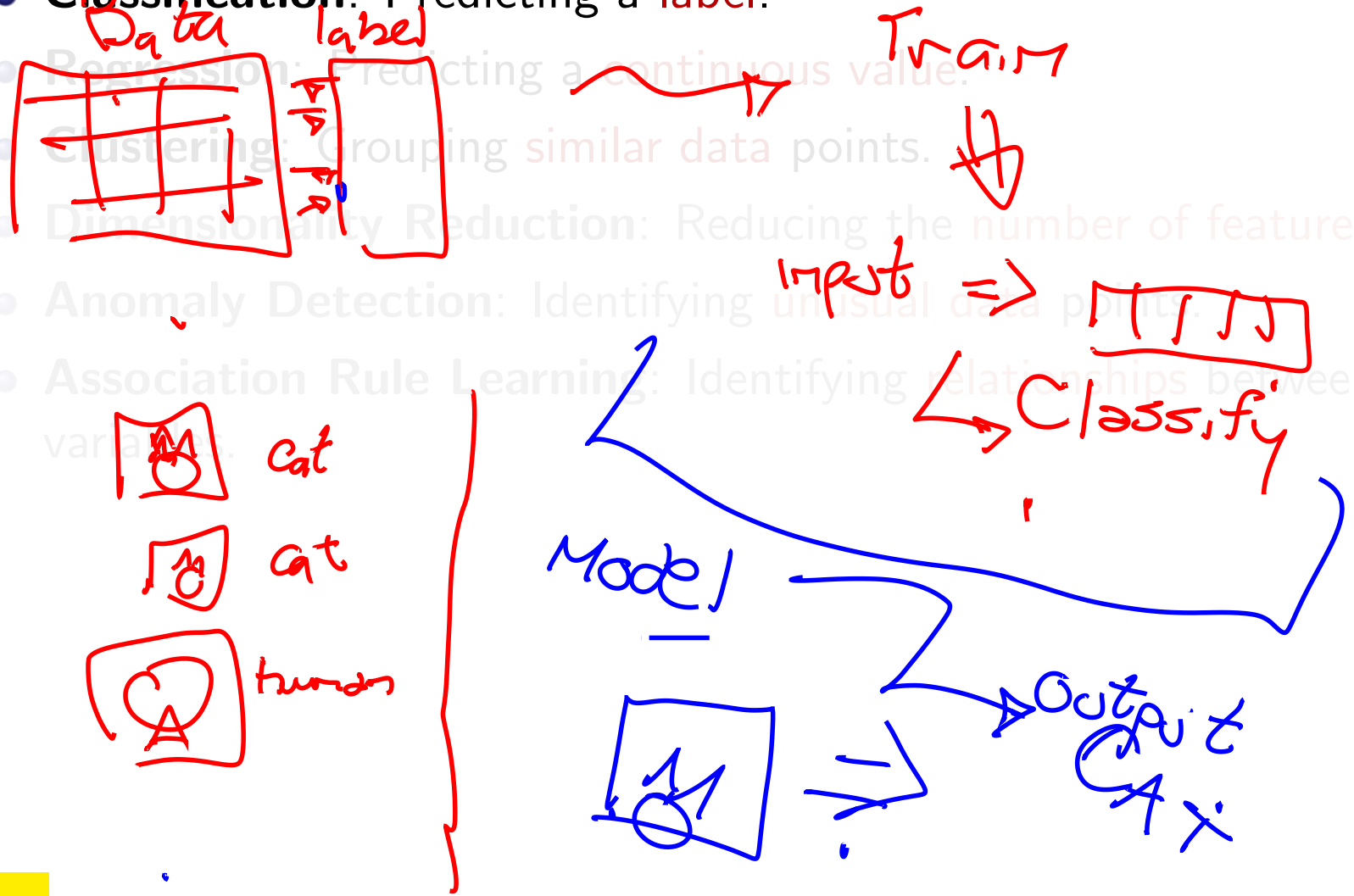
Python Tools

- **NumPy**: A library for numerical computing.
- **Pandas**: A library for data manipulation and analysis.
- **Matplotlib**: A library for data visualization.
- **Scikit-learn**: A library for machine learning.



Typical Machine Learning Problems

- **Classification**: Predicting a label.
- **Regression**: Predicting a continuous value.
- **Clustering**: Grouping similar data points.
- **Dimensionality Reduction**: Reducing the number of features.
- **Anomaly Detection**: Identifying unusual data points.
- **Association Rule Learning**: Identifying relationships between variables.



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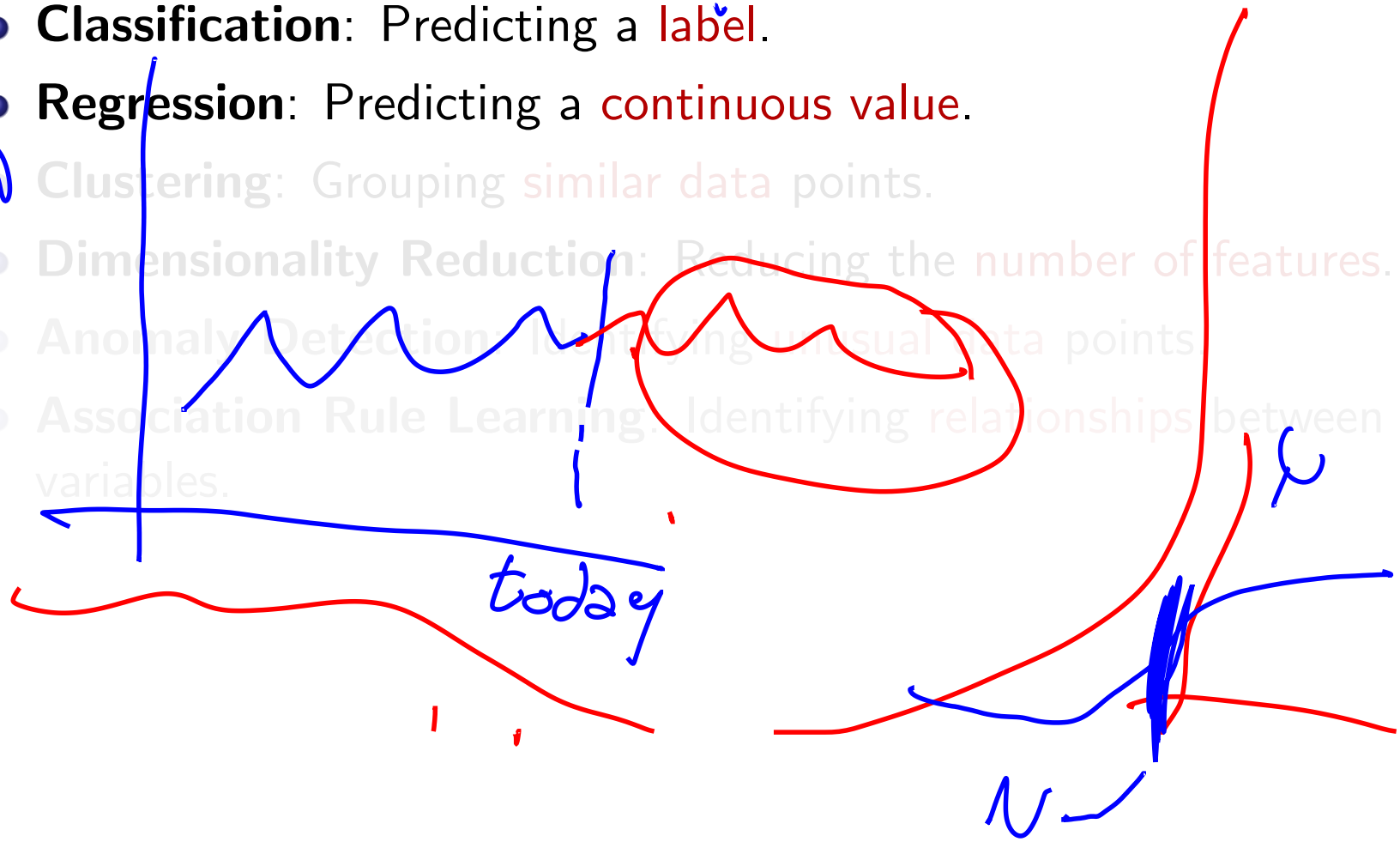

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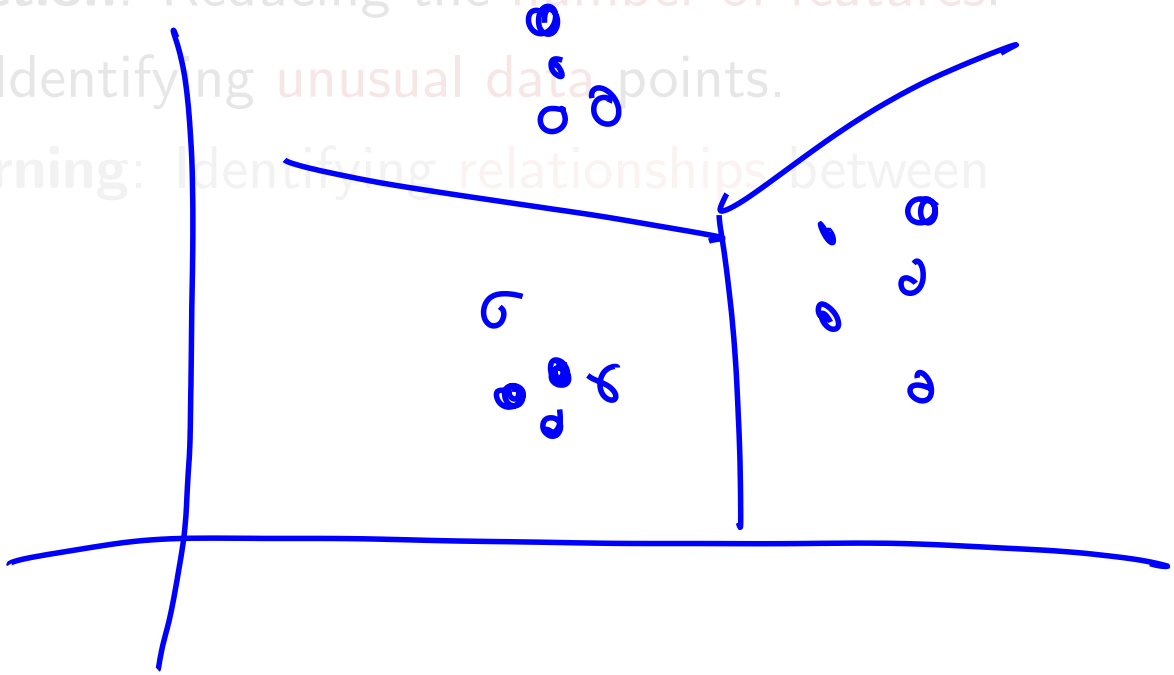

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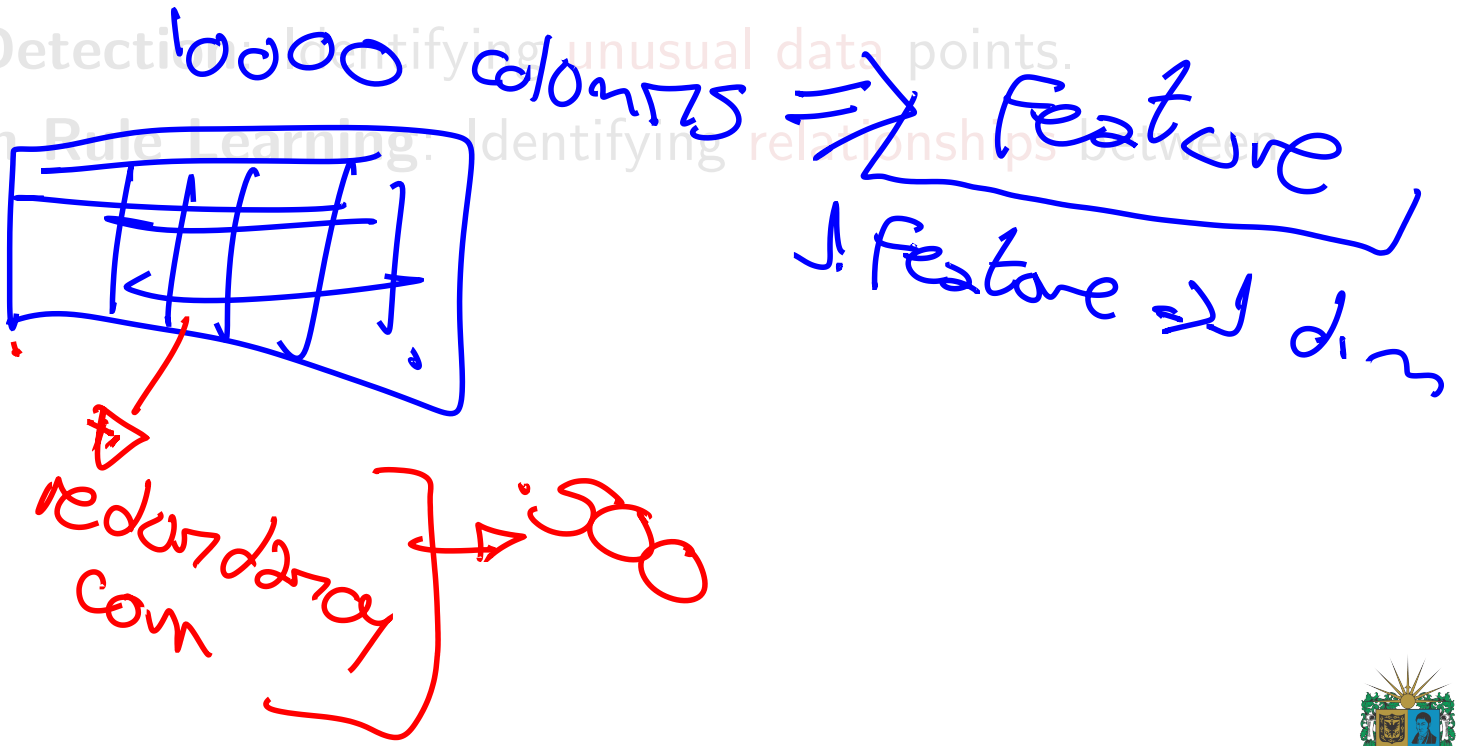

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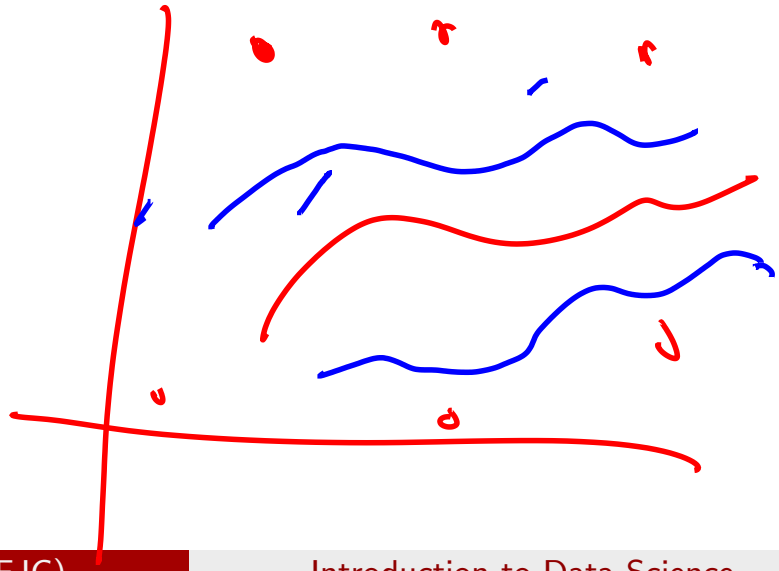

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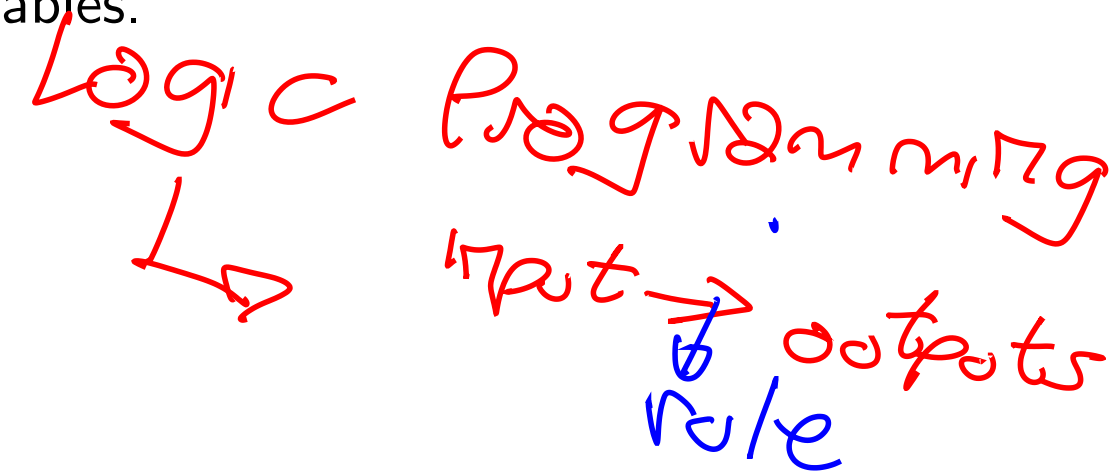

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The Machine Learning Workflow

- **Data Collection**: Gathering the data.
- **Data Preprocessing**: Cleaning and preparing the data.
- **Feature Engineering**: Creating new features.
- **Model Selection**: Choosing the best model.
- **Model Training**: Training the model on the data.
- **Model Evaluation**: Assessing the model's performance.
- **Model Deployment**: Putting the model into production.

Data Raw
Multiple Data Sources
Data lake

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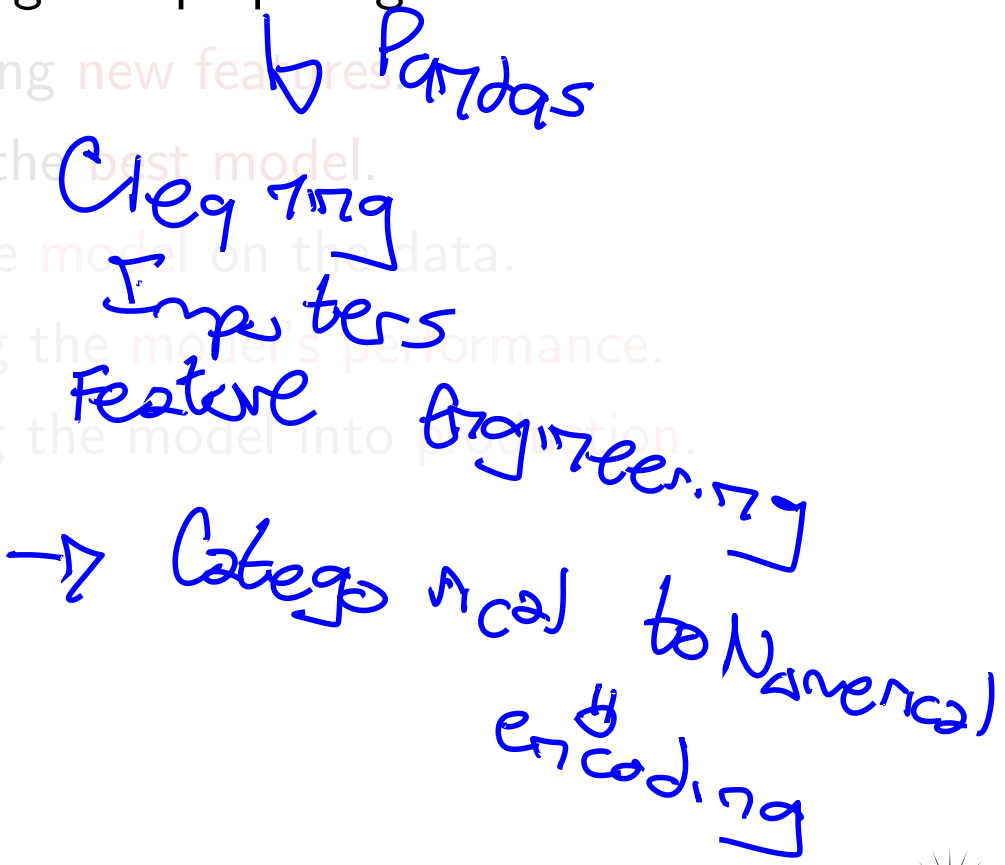

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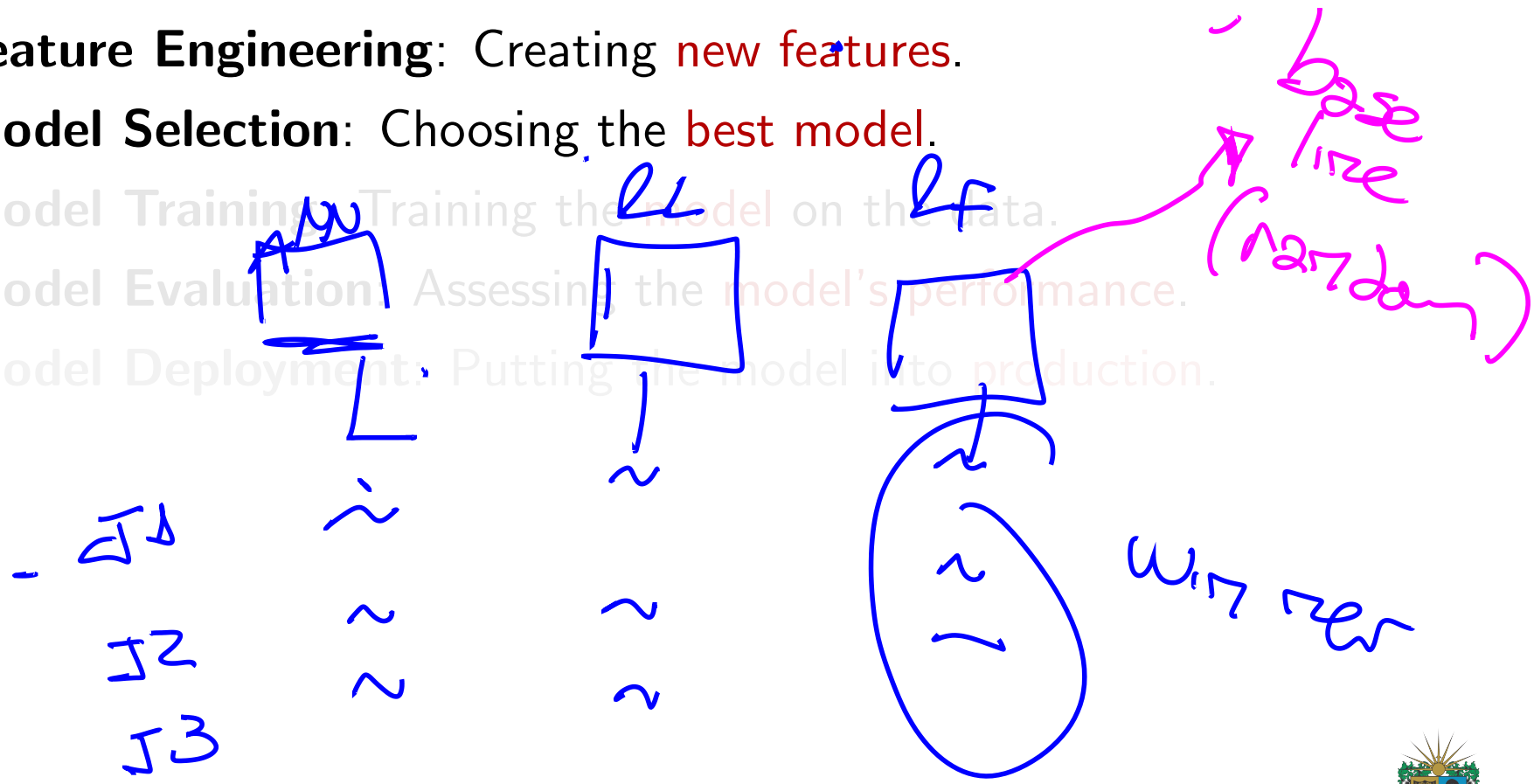

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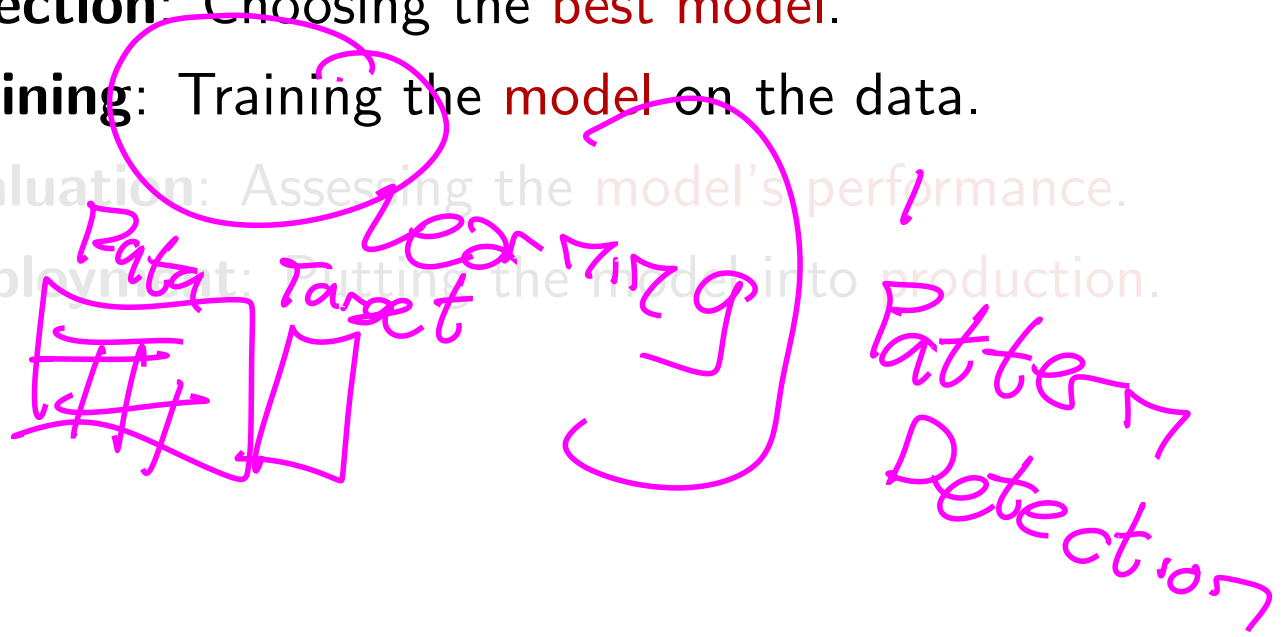

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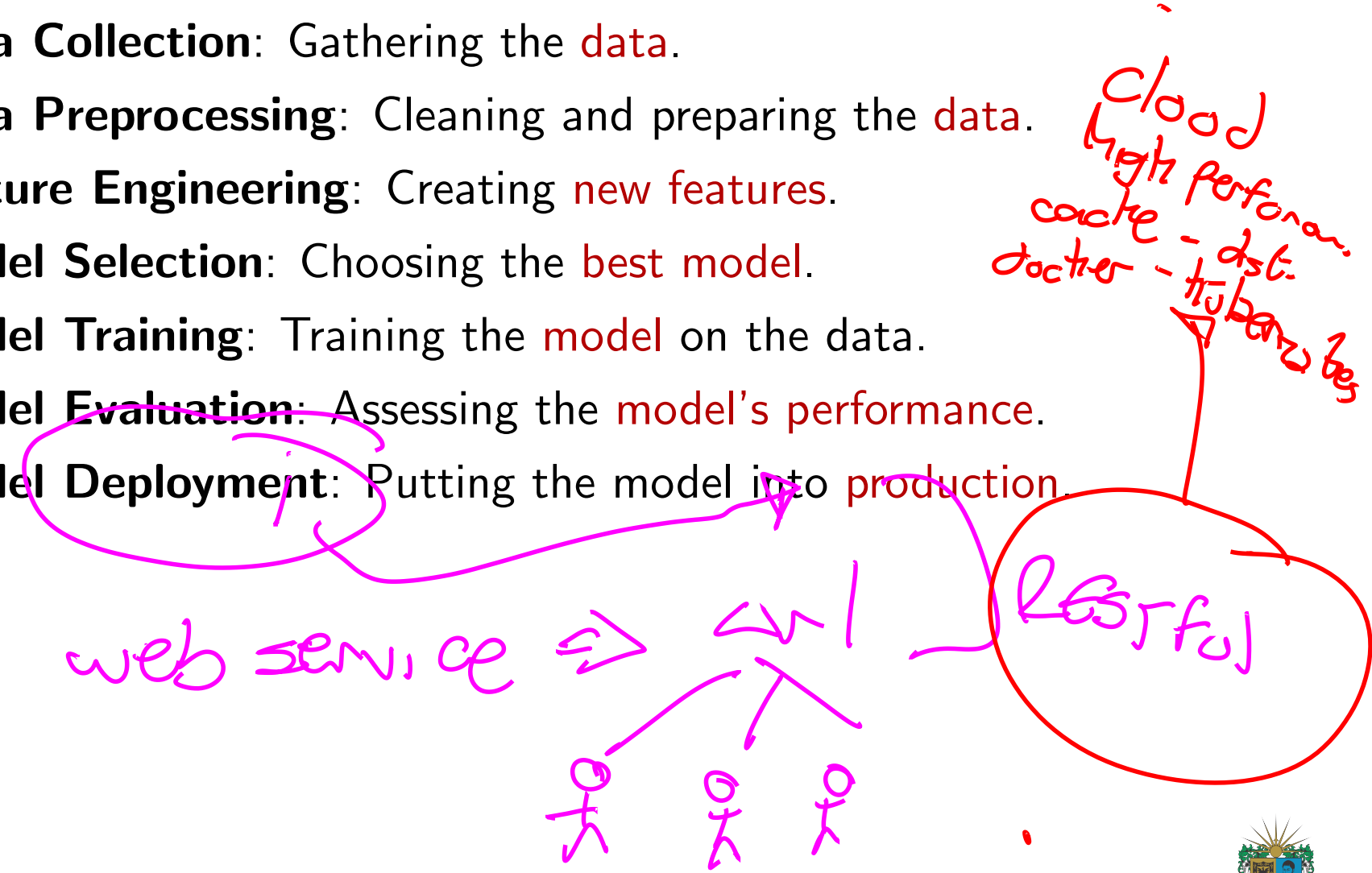
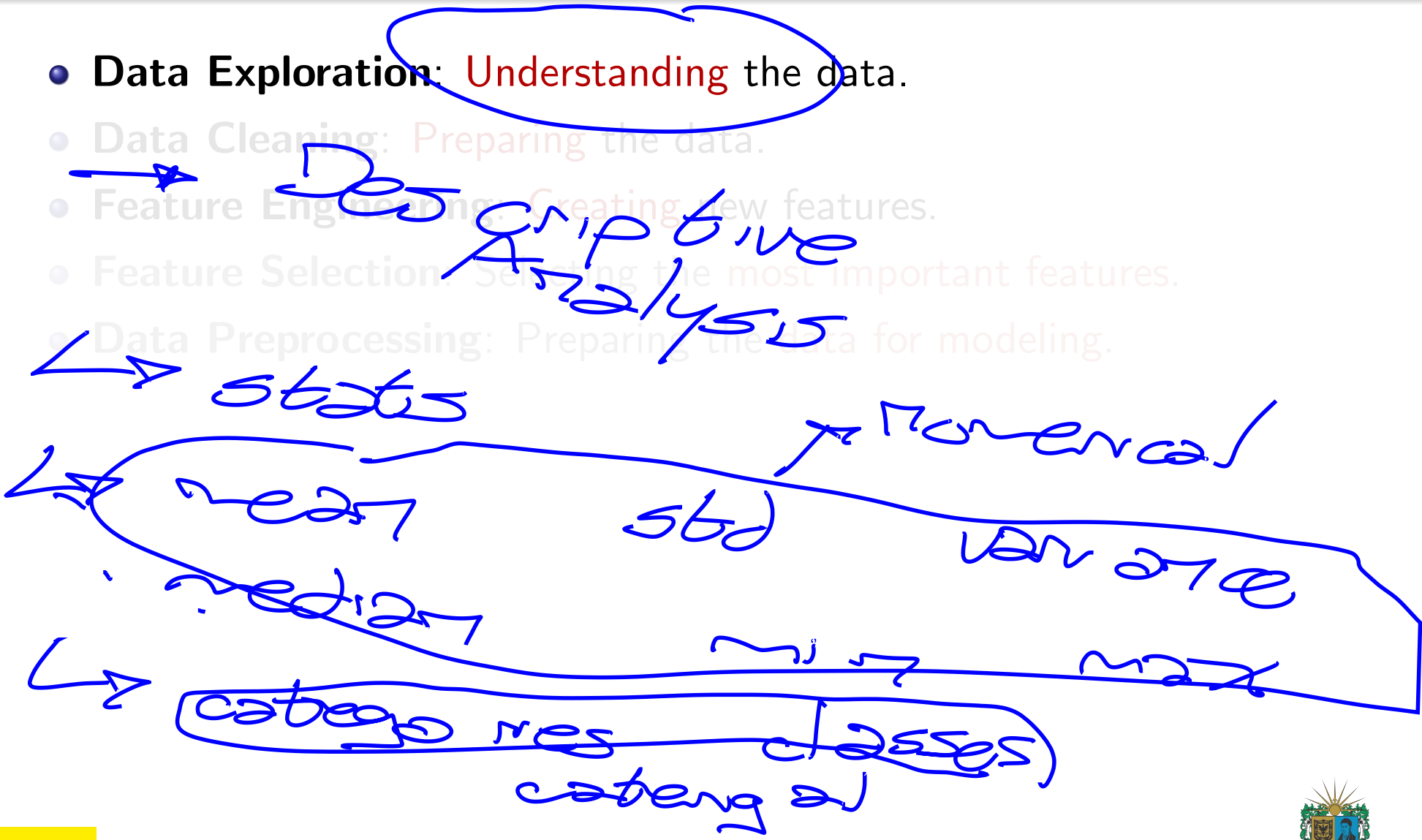


Examining the Data

- **Data Exploration**: Understanding the data.
- **Data Cleaning**: Preparing the data.
- **Feature Engineering**: Creating new features.
- **Feature Selection**: Selecting the most important features.
- **Data Preprocessing**: Preparing the data for modeling.



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- **Data Exploration**: Understanding the data.
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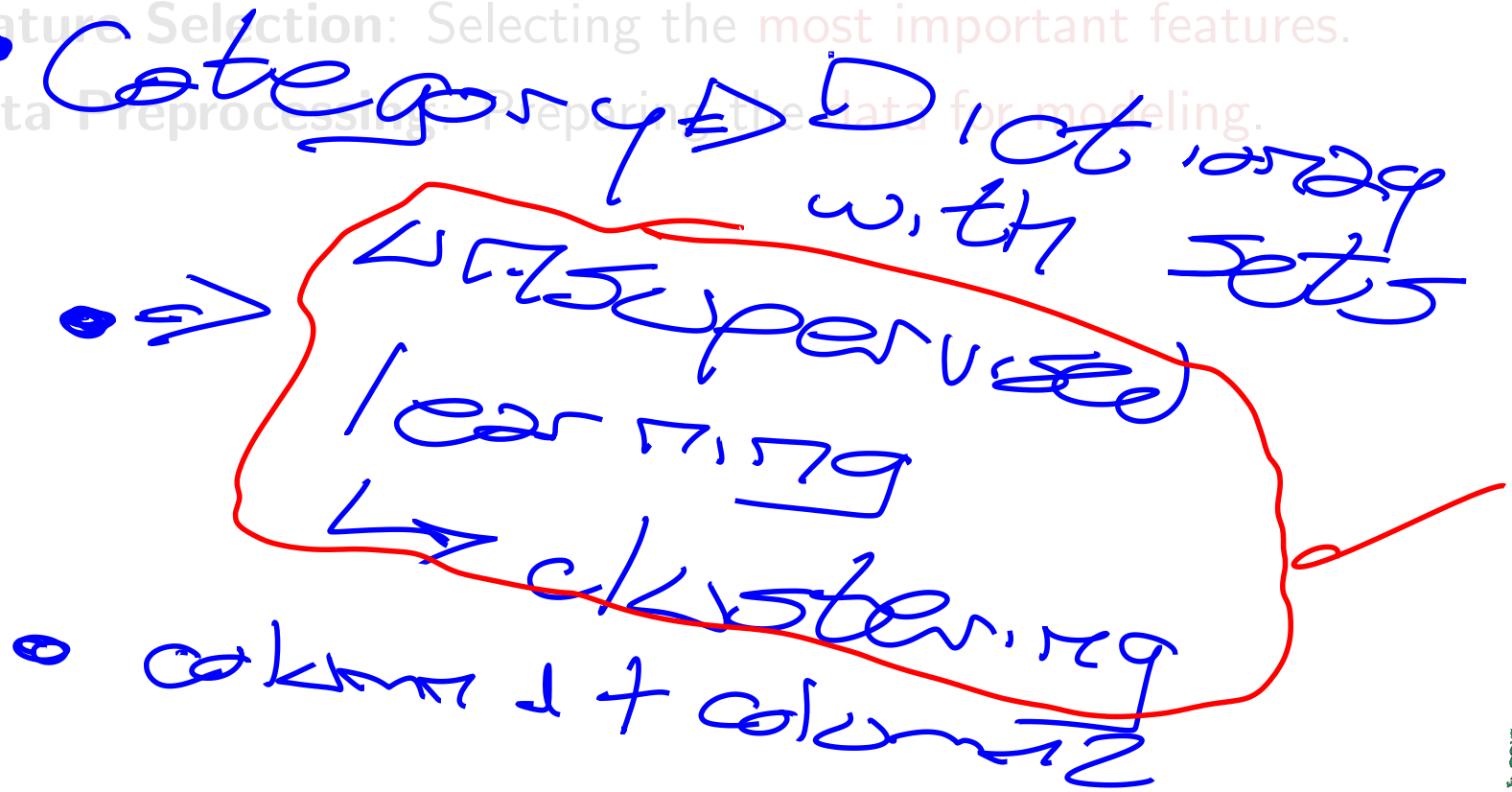

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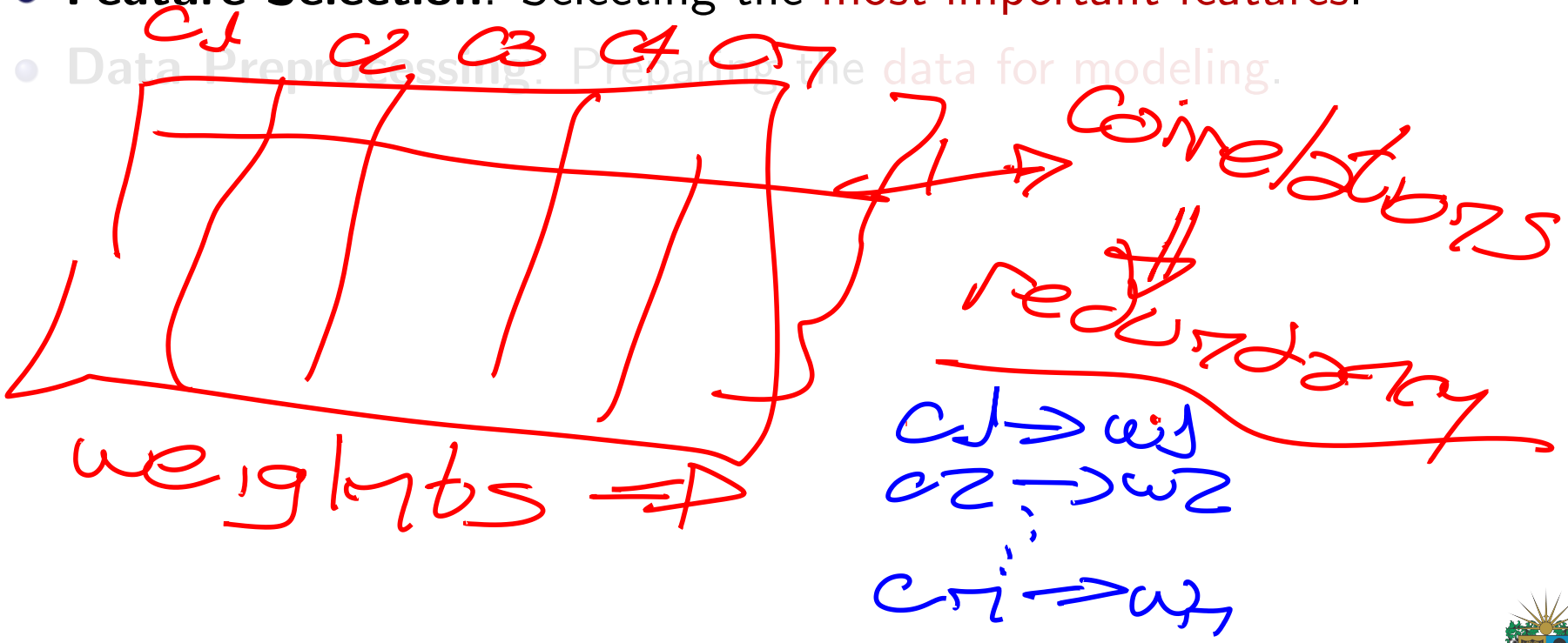

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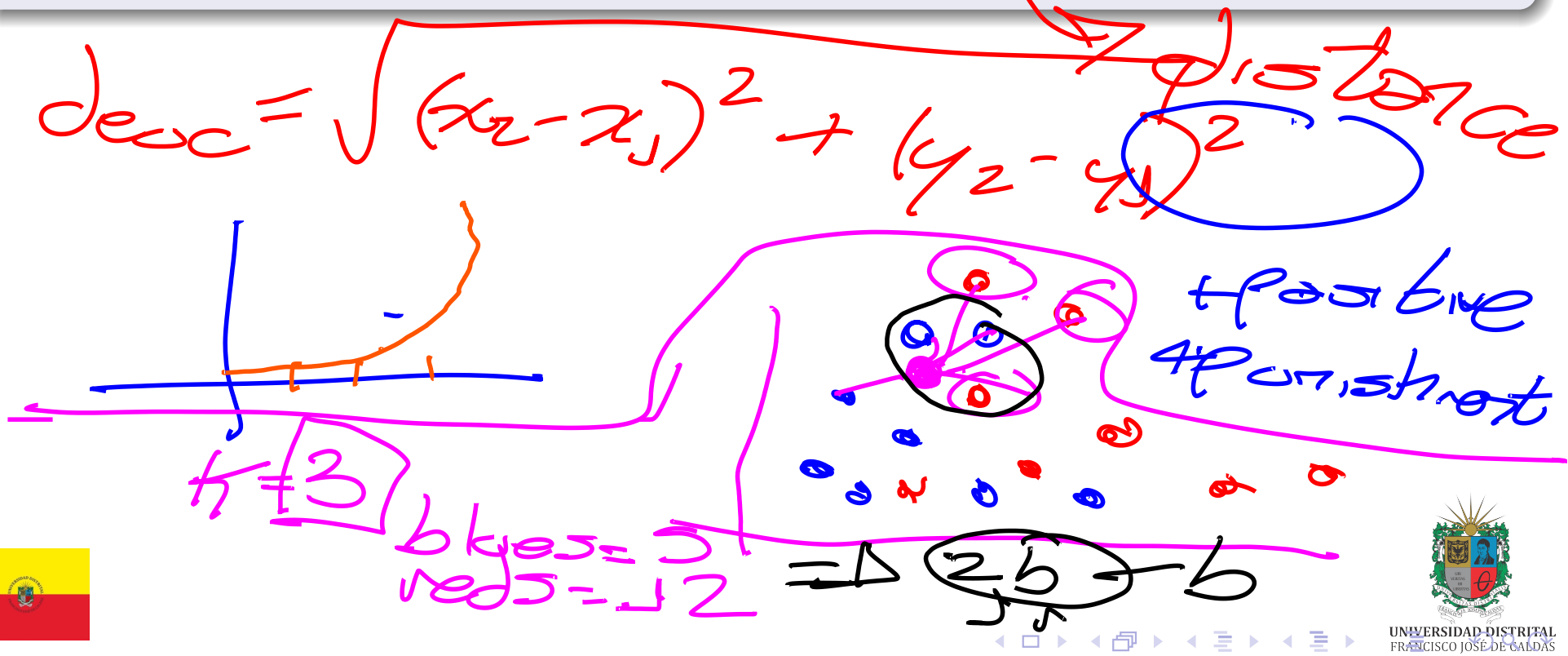
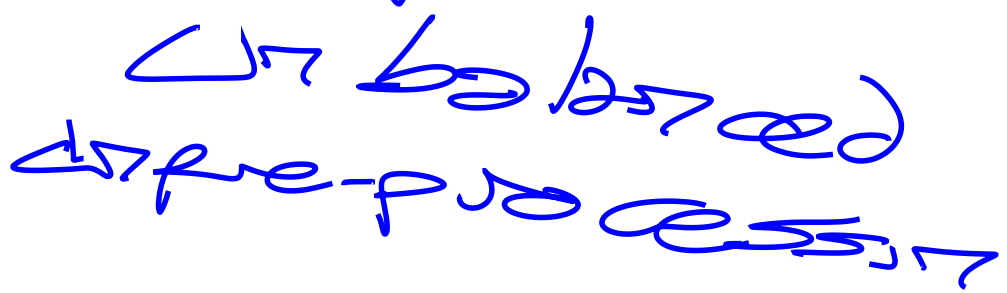
K-Nearest Neighbors Classification

- **K-Nearest Neighbors** is a simple algorithm that stores all available cases and classifies new cases based on a similarity measure.
- It is a type of instance-based learning, or lazy learning, where the function is only approximated locally and all computation is deferred until function evaluation.



Algorithmic Bias

- **Algorithmic bias** is a systematic error in a model that results in unfair outcomes.
- It can be caused by biased training data, biased algorithms, or biased decision-making.

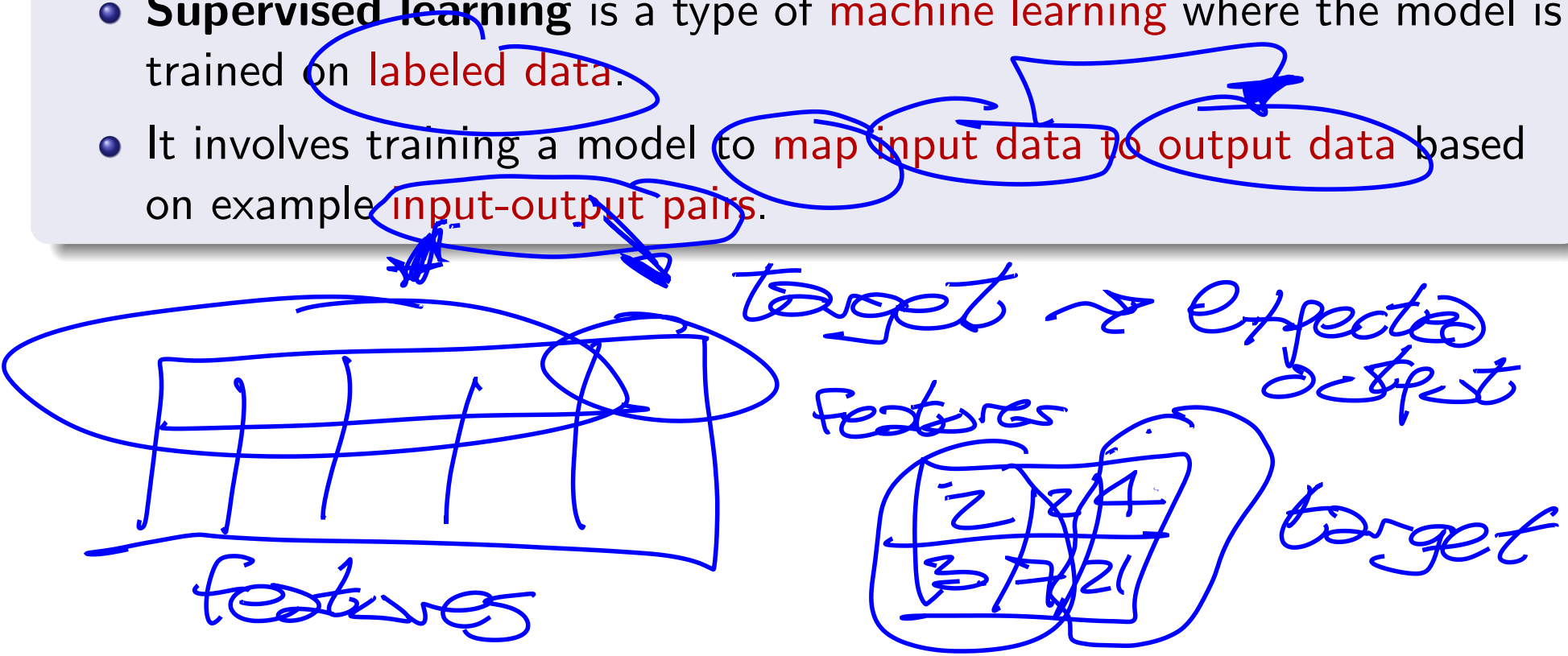


Outline

Introduction to Supervised Machine Learning

Definition

- **Supervised learning** is a type of machine learning where the model is trained on labeled data.
- It involves training a model to map input data to output data based on example input-output pairs.



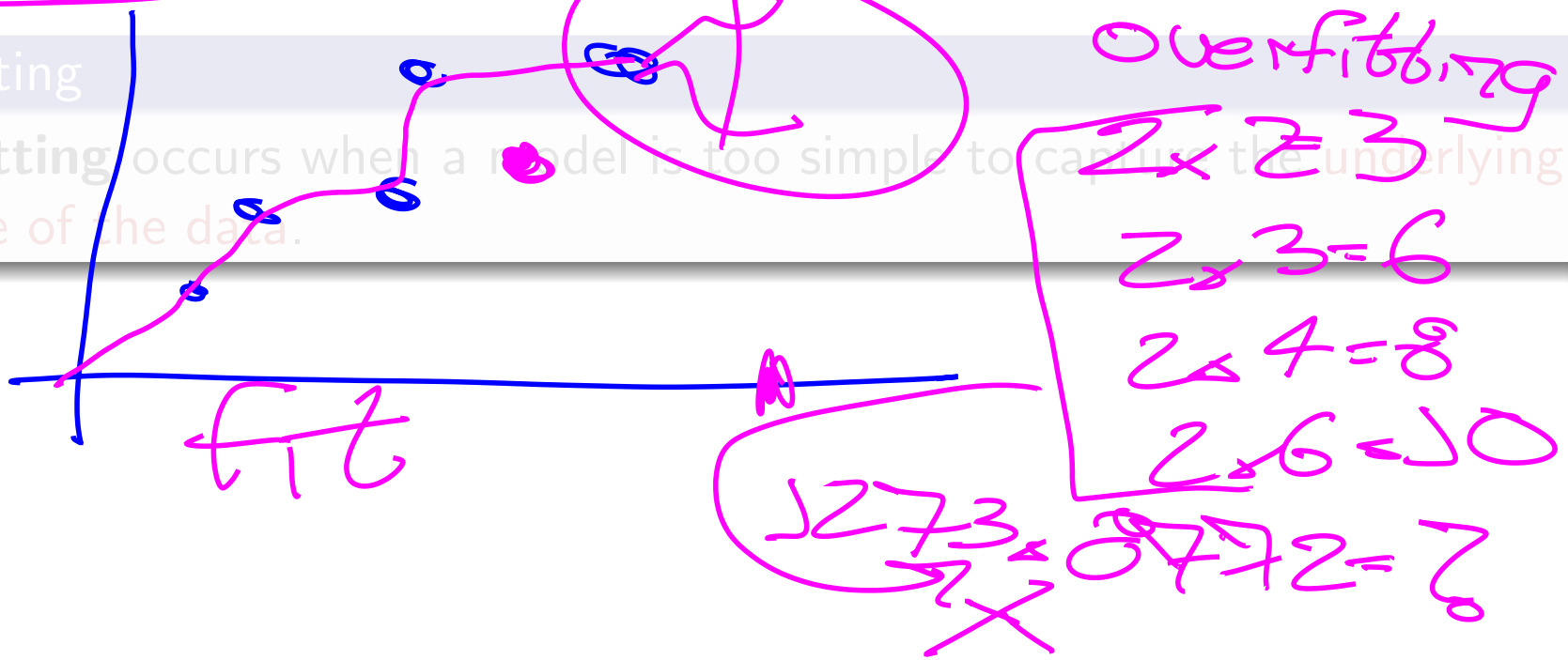
Overfitting and Underfitting

Overfitting

Overfitting occurs when a model learns the training data too well and performs poorly on new data.

Underfitting

Underfitting occurs when a model is too simple to capture the underlying structure of the data.



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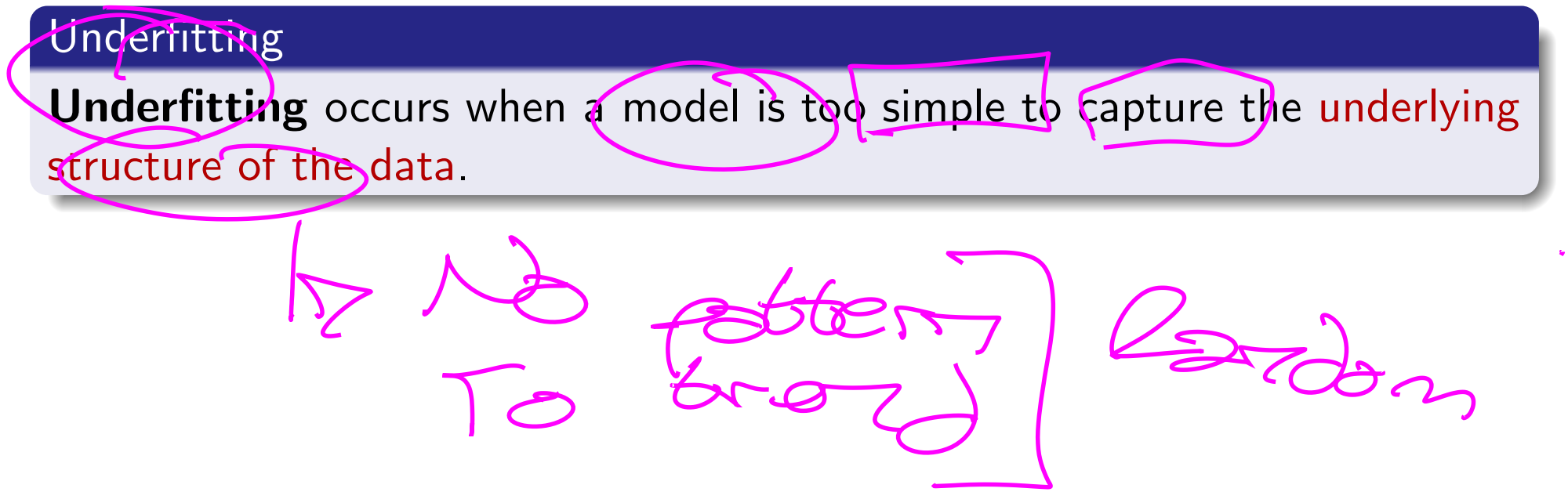

Supervised Learning Datasets

- **Training Dataset**: The data used to train the model.
- **Validation Dataset**: The data used to tune the model hyperparameters.
- **Test Dataset**: The data used to evaluate the model performance.

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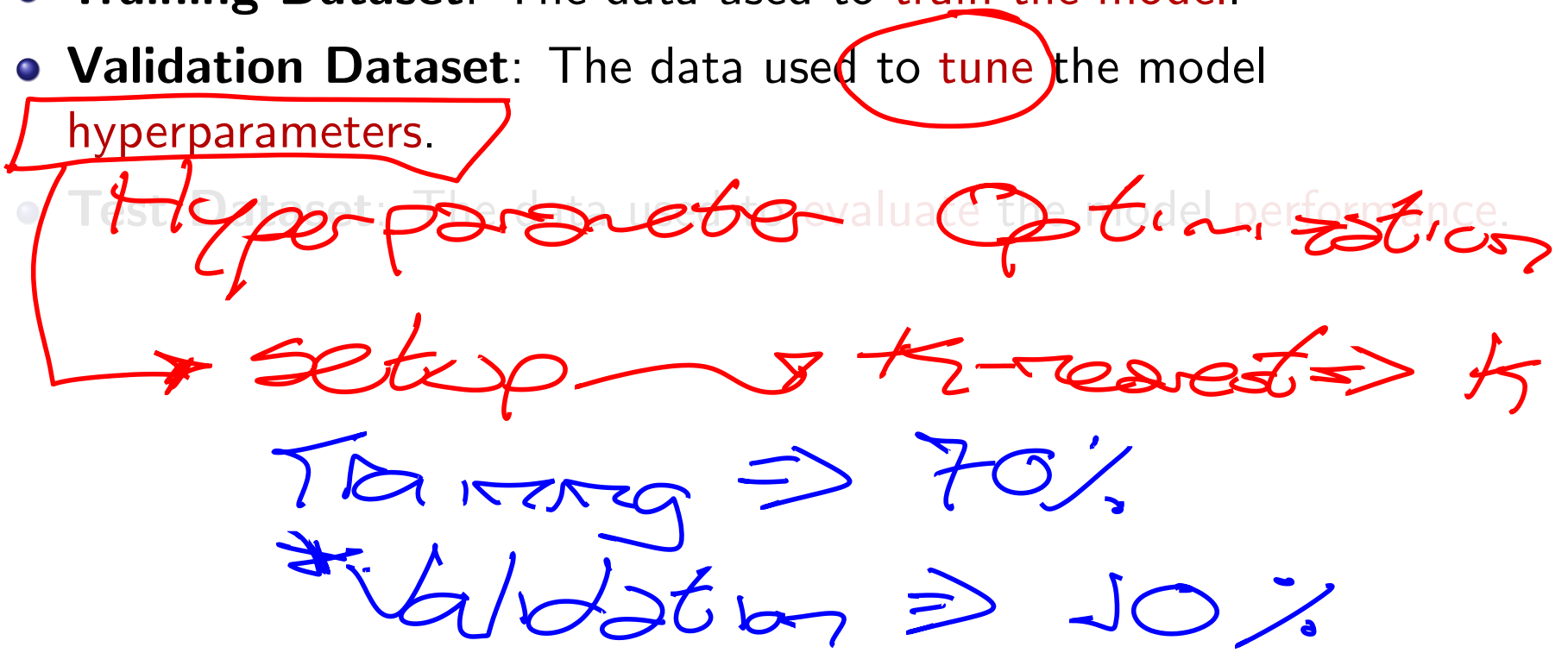

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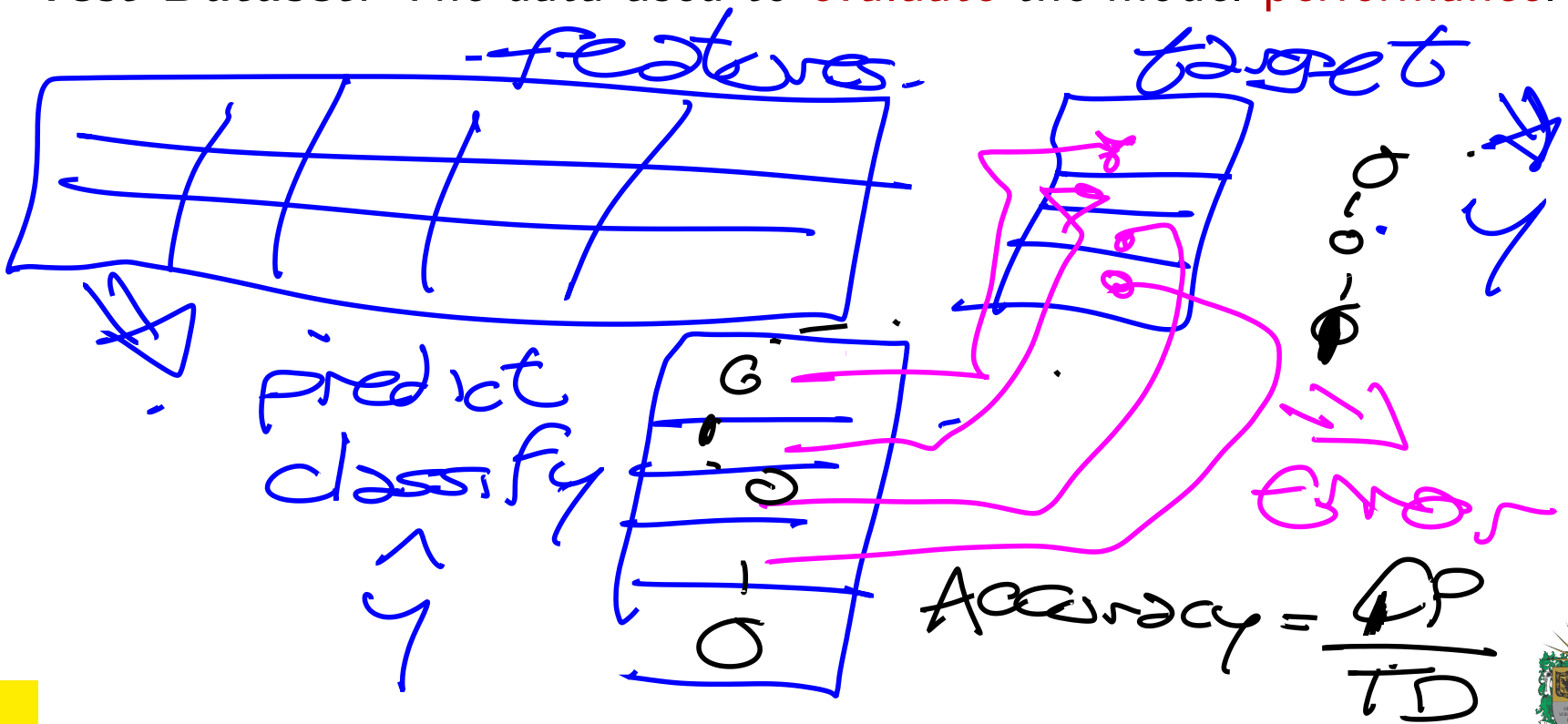
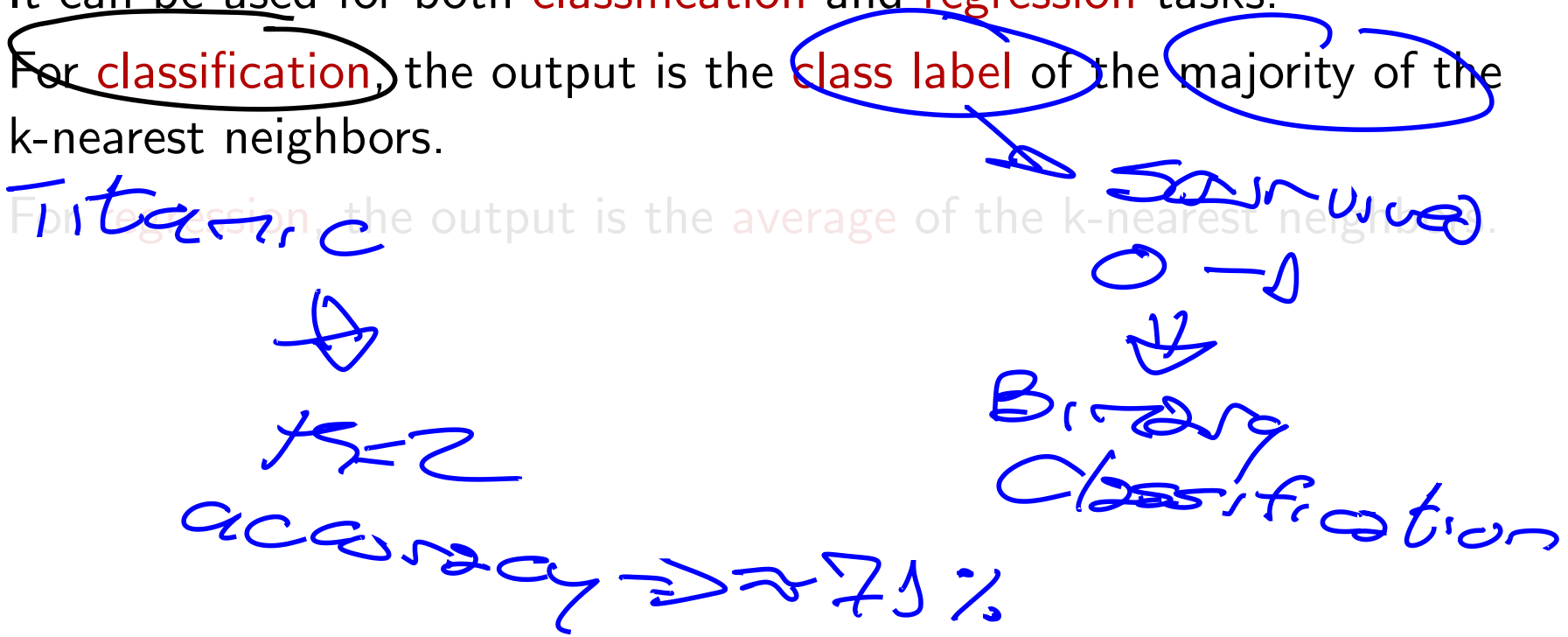


K-Nearest Neighbors: Classification and Regression

- **K-Nearest Neighbors (KNN)** is a simple algorithm that stores all available cases and classifies new cases based on a similarity measure.
- It can be used for both classification and regression tasks.
- For classification, the output is the class label of the majority of the k-nearest neighbors.
- For regression, the output is the average of the k-nearest neighbors.



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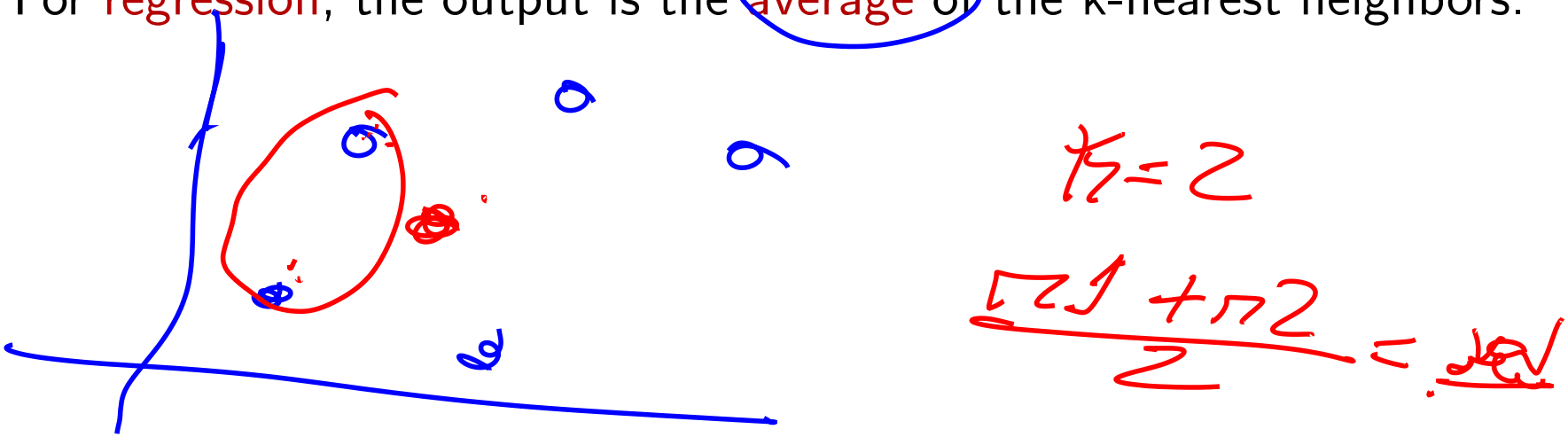


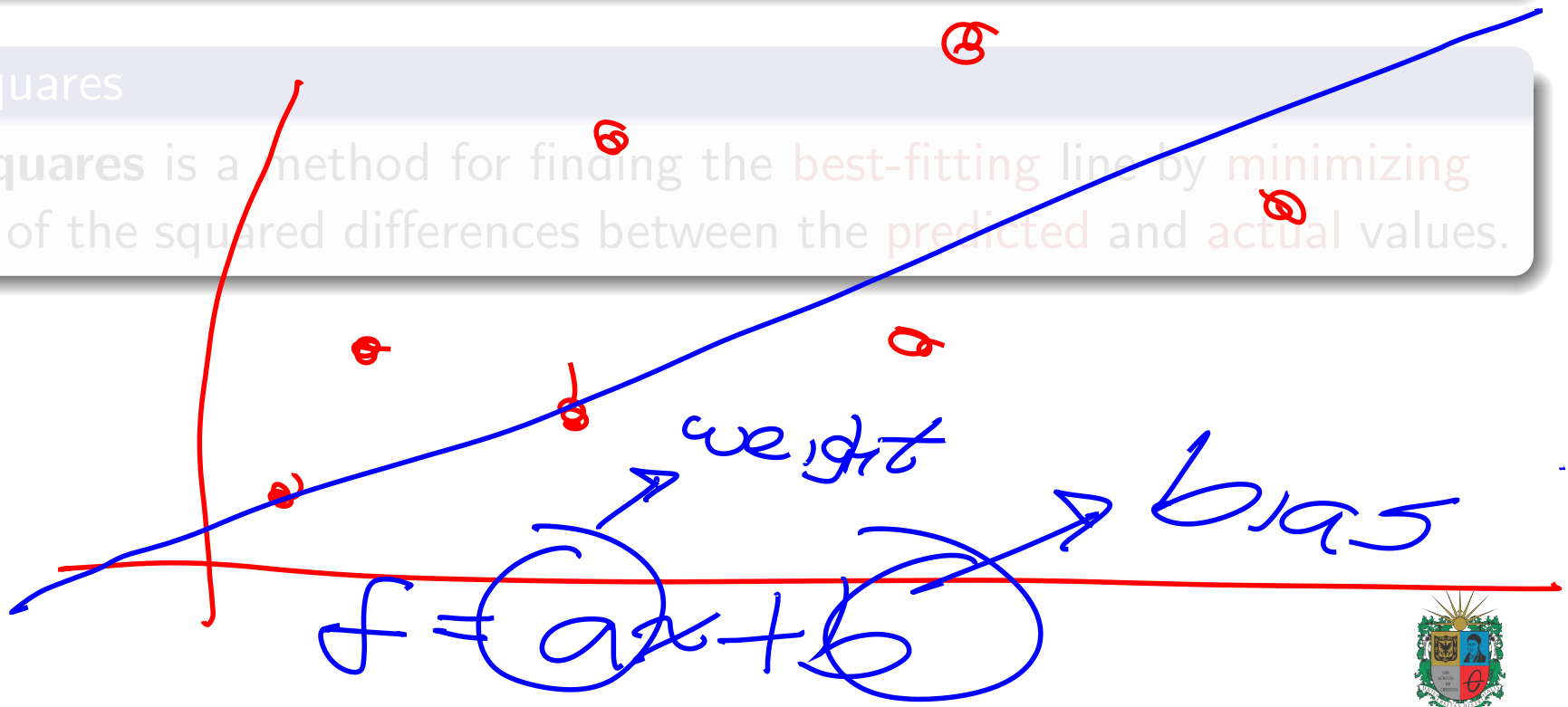
Linear Regression with Least Squares

Linear Regression

- **Linear regression** is a type of regression analysis used for predicting the value of a continuous dependent variable.
- It works by finding the line that best fits the data.

Least Squares

Least squares is a method for finding the best-fitting line by minimizing the sum of the squared differences between the predicted and actual values.



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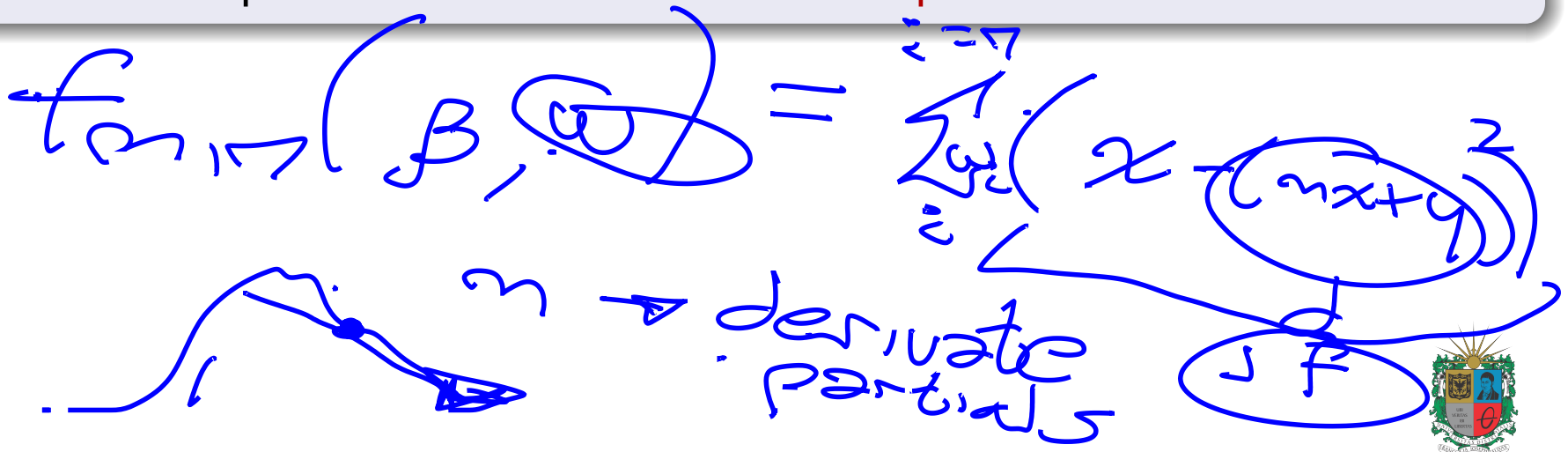

Ridge & Lasso

Ridge Regression

Ridge regression is a type of linear regression that includes a penalty term to prevent overfitting. It works by adding a regularization term to the least squares objective function.

Lasso Regression

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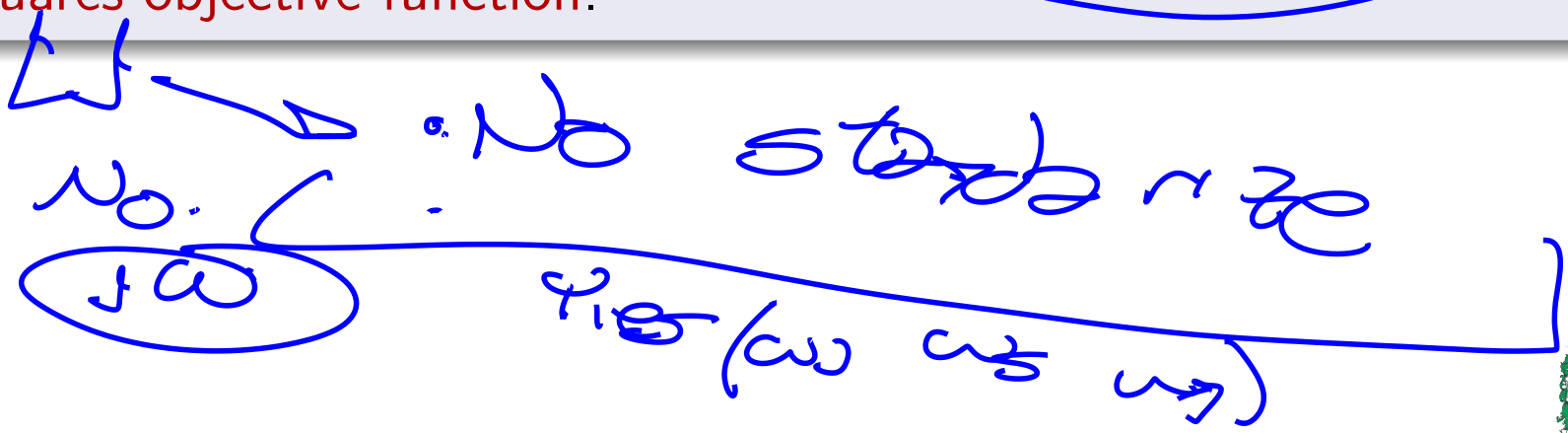
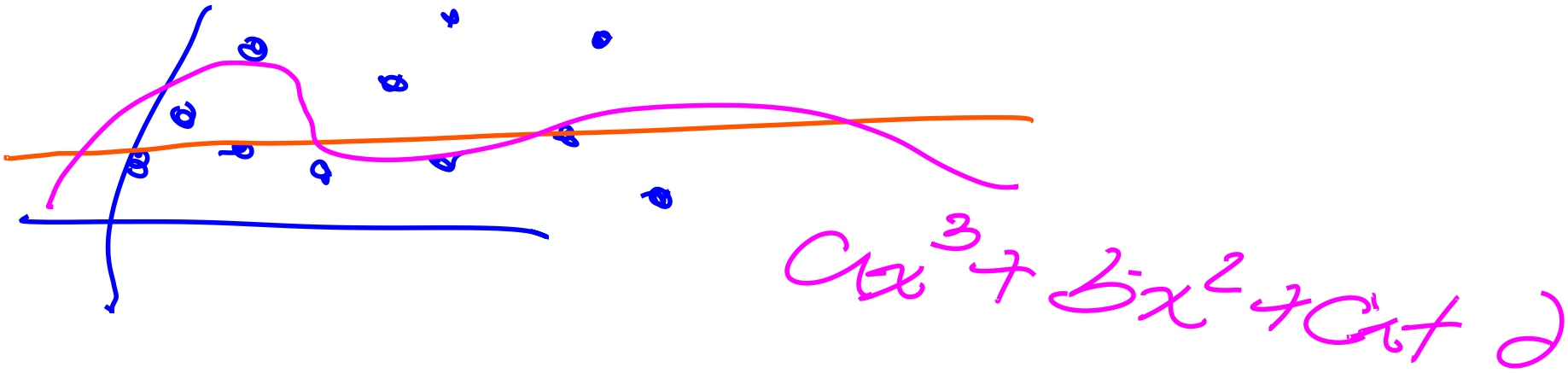


Polynomial Regression

Polynomial Regression

- **Polynomial regression** is a type of regression analysis that models the relationship between the independent and dependent variables as an nth-degree polynomial.
- It can capture non-linear relationships between the variables.



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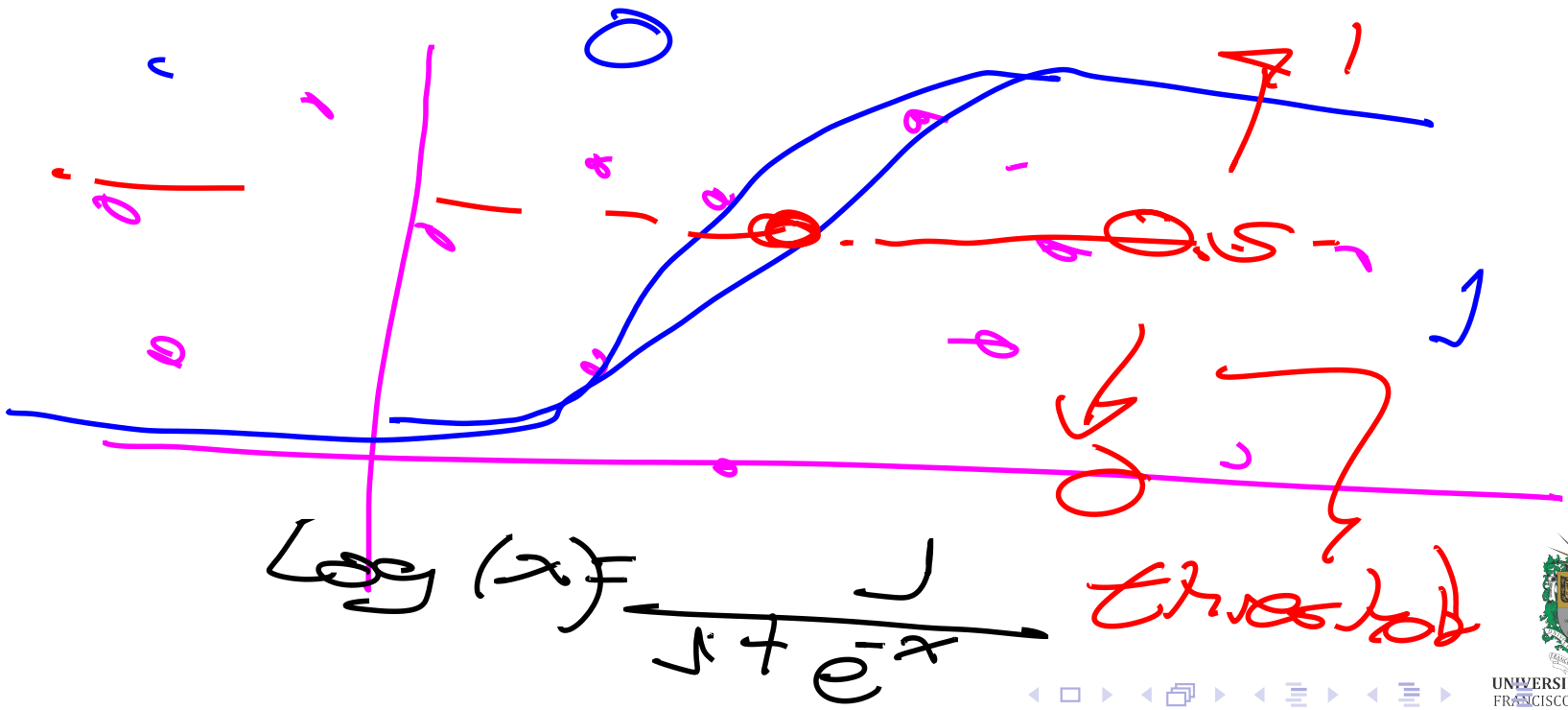
Logistic Regression

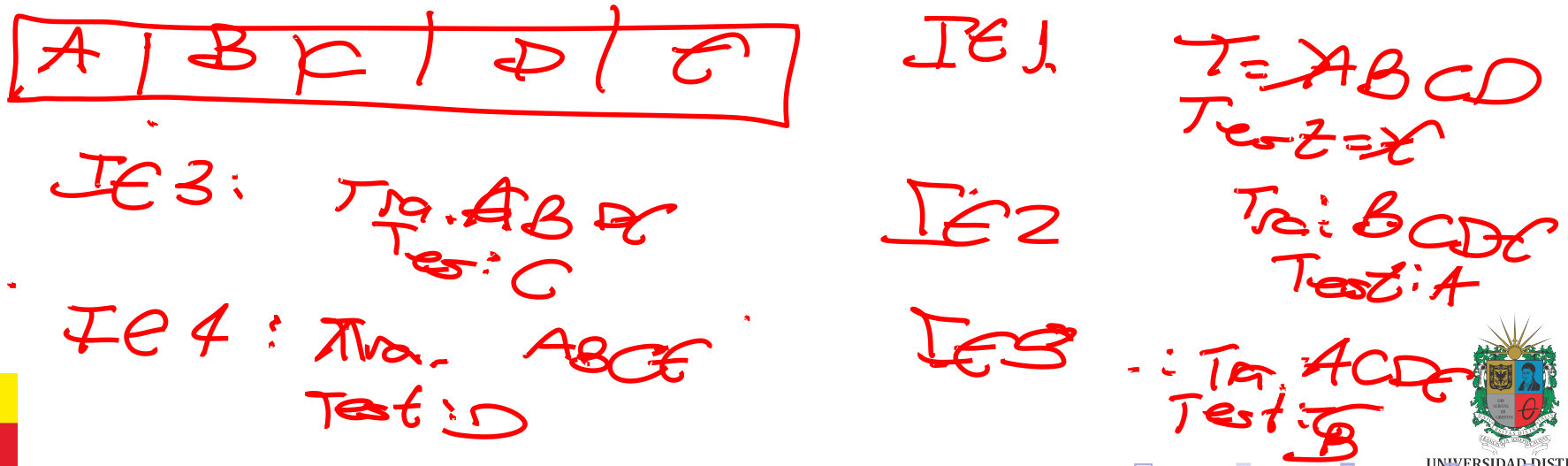
Logistic Regression

- **Logistic regression** is a type of regression analysis used for predicting the outcome of a categorical dependent variable.
- It is used for binary classification tasks, where the output is a probability between 0 and 1.



Cross-Validation

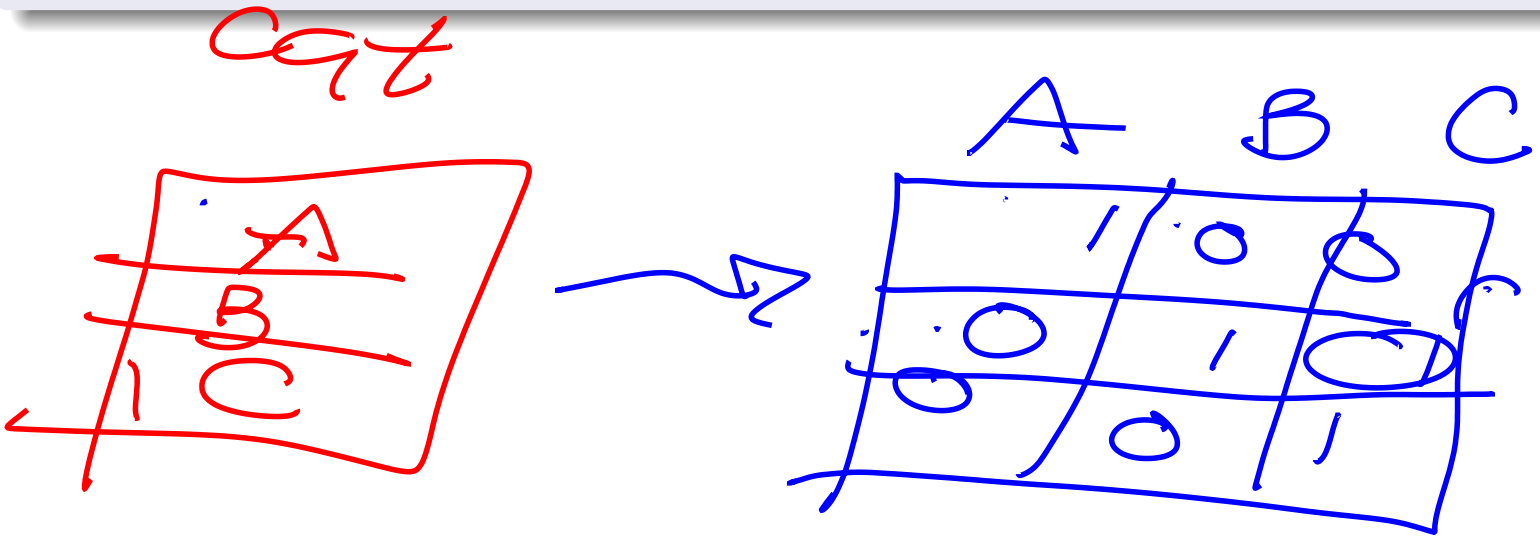
- **Cross-validation** is a technique for assessing the performance of a model.
- It involves splitting the data into multiple subsets, training the model on some subsets, and evaluating it on others.
- Common cross-validation **techniques** include k-fold cross-validation and leave-one-out cross-validation.
- Cross-validation helps to reduce overfitting and provides a more accurate estimate of the model's performance.



One-Hot Encoding

One-Hot Encoding

- **One-hot encoding** is a technique for converting categorical variables into numerical variables.
- It creates a binary vector for each `category`, with a 1 for the *category* and 0s for all other categories.



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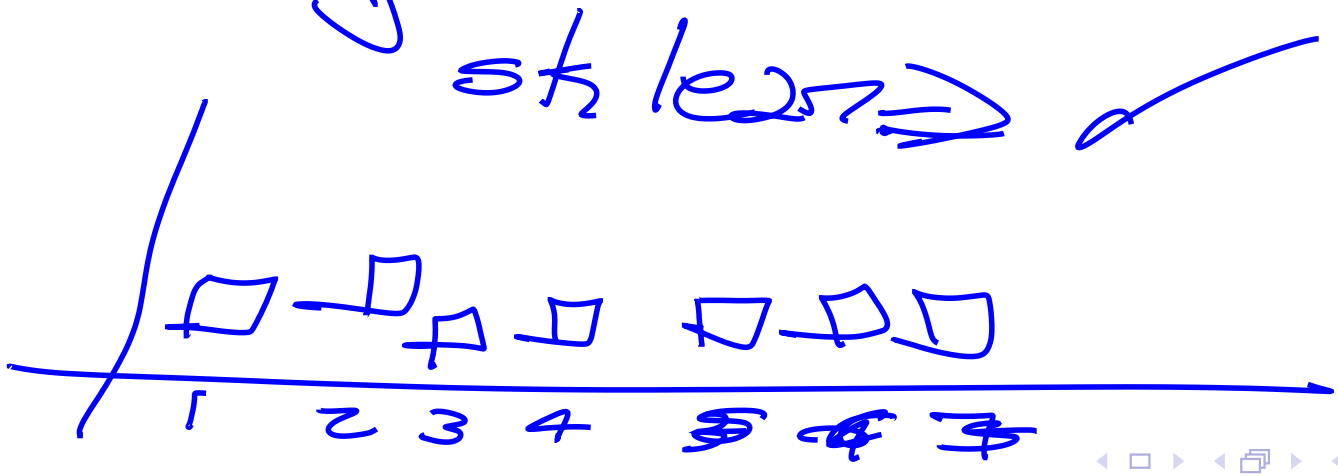
Data Leakage

- **Data leakage** occurs when information from the test set is inadvertently used to train the model.
- It can lead to overfitting and inflated performance metrics.
- Common sources of **data leakage** include target leakage, train-test contamination, and information leakage.
- To prevent **data leakage**, it is important to carefully separate the training and test data and avoid using information from the test set during training.



Outline

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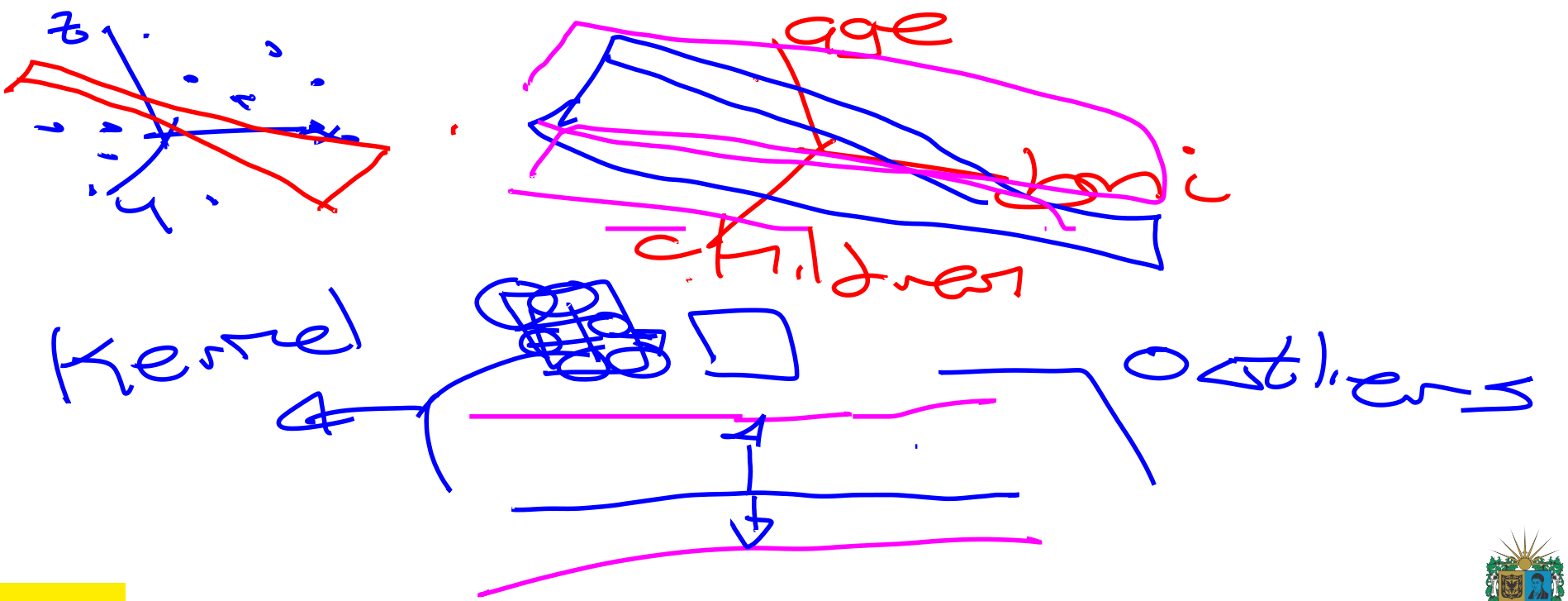
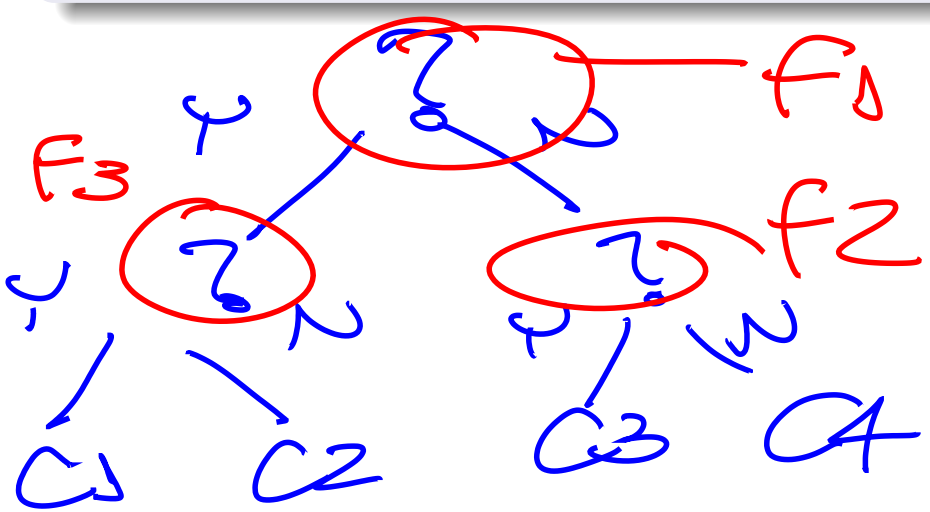
Support Vector Machines

- **Support vector machines** are a type of machine learning model that can be used for both classification and regression tasks.
- They work by finding the hyperplane that best separates the data into different classes.



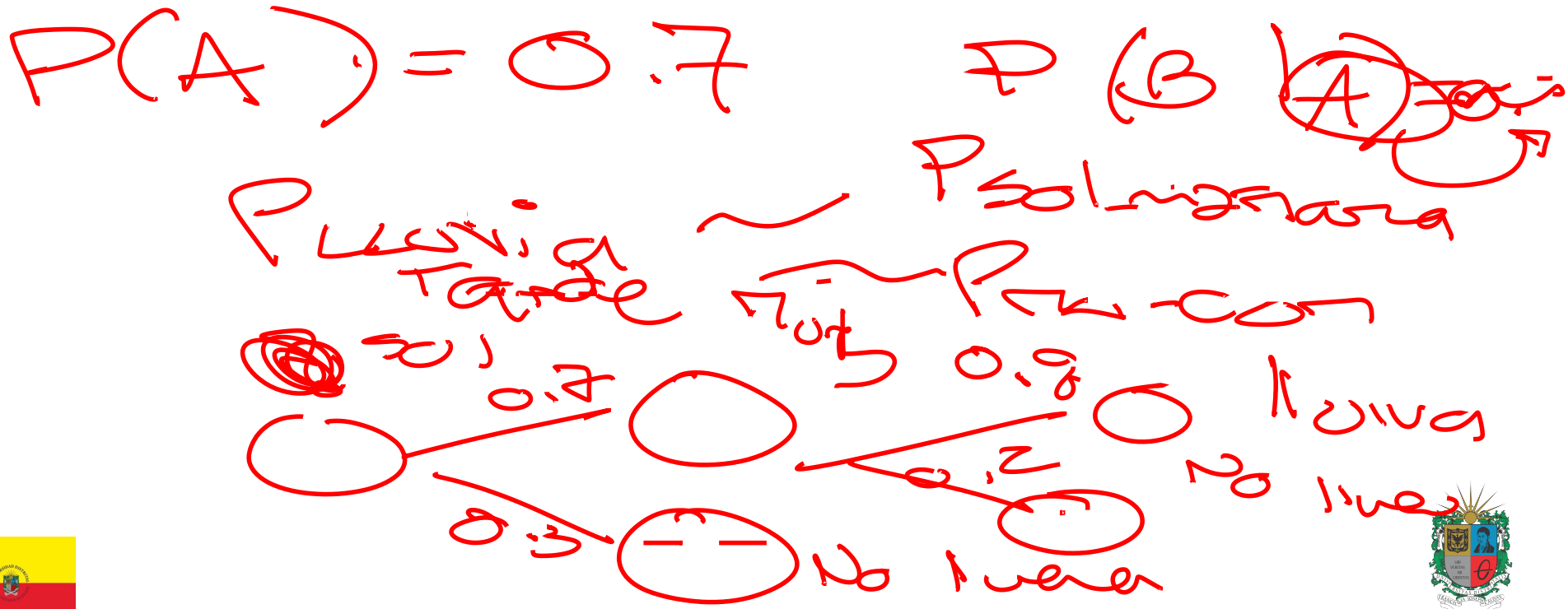
Decision Trees

- **Decision trees** are a type of machine learning model that can be used for both classification and regression tasks.
- They work by recursively partitioning the data into subsets based on the values of the features.



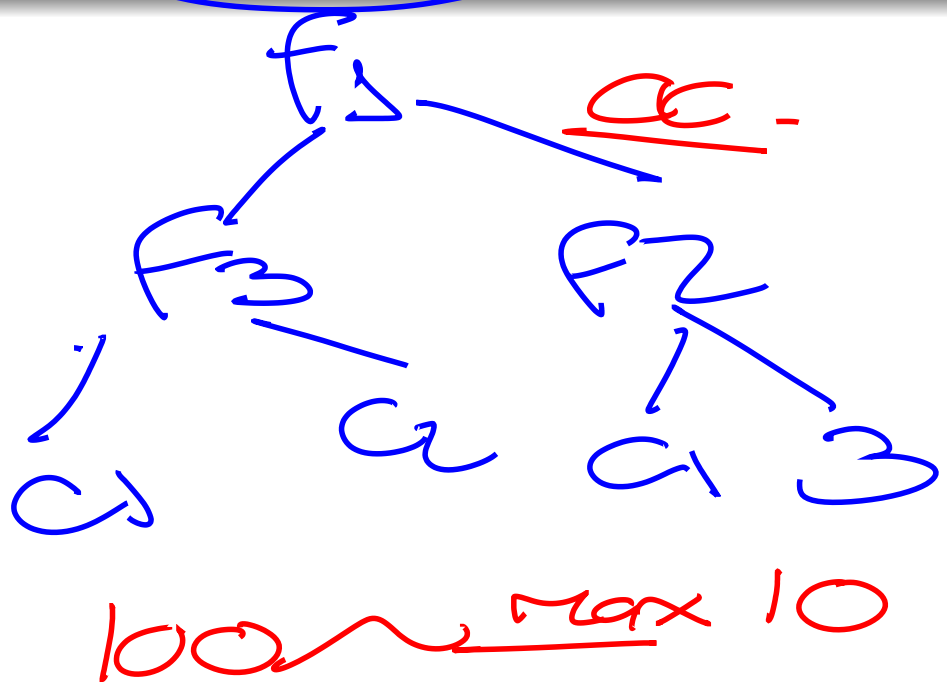
Naive Bayes Classifier

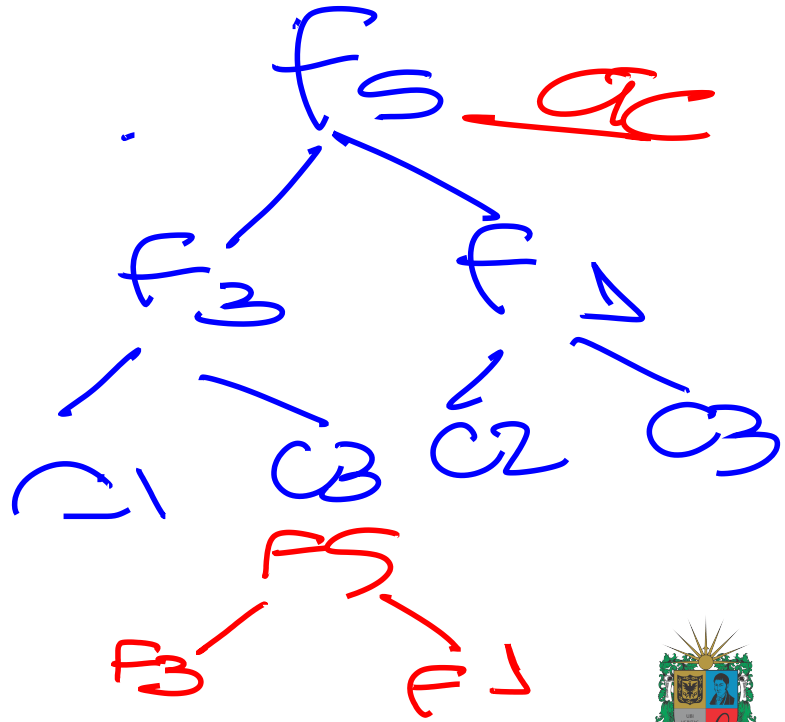
- The **naive Bayes classifier** is a simple probabilistic classifier based on Bayes' theorem.
- It assumes that the features are conditionally independent given the class label.



Random Forest

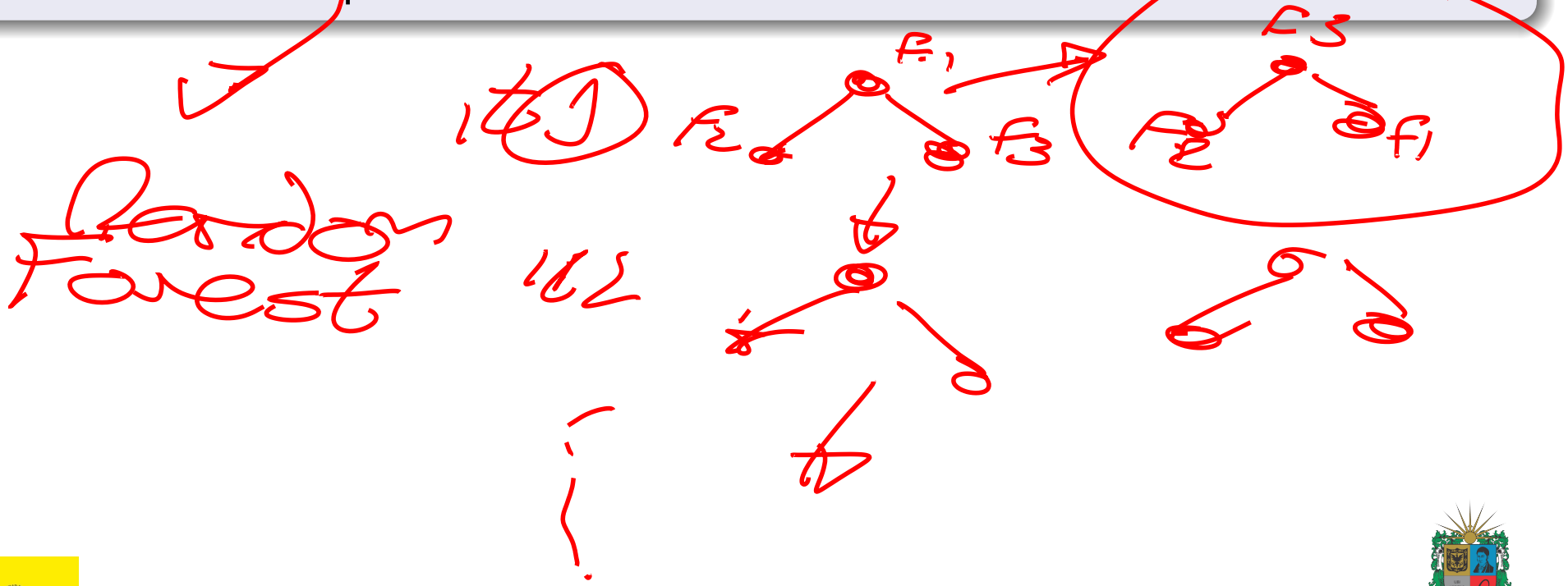
- **Random forest** is an ensemble learning method that combines multiple decision trees to create a `strong predictive model`.
- It works by building multiple trees and averaging their predictions to reduce overfitting.





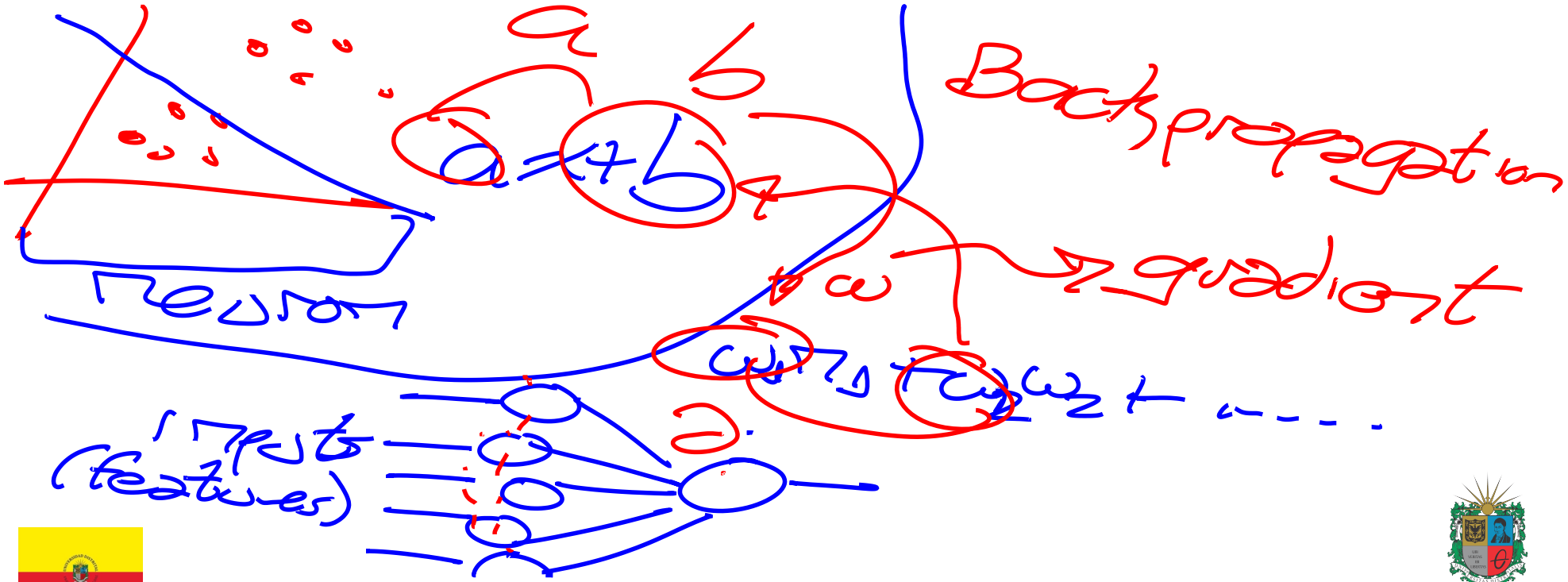
Gradient Boosted Decision Trees

- **Gradient boosted decision trees** are an ensemble learning method that combines multiple decision trees and gradient descedent optimization to create a strong predictive model.
- They work by building trees sequentially, with each tree correcting the errors of the previous trees.

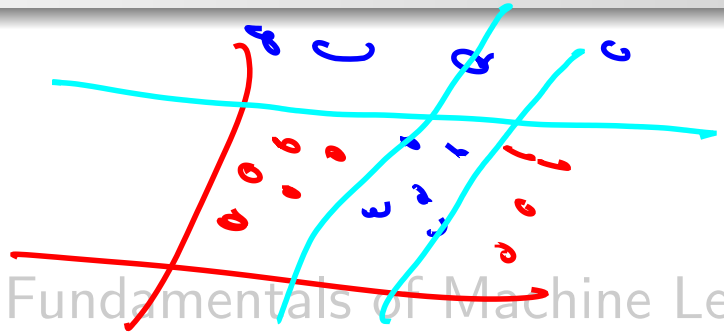


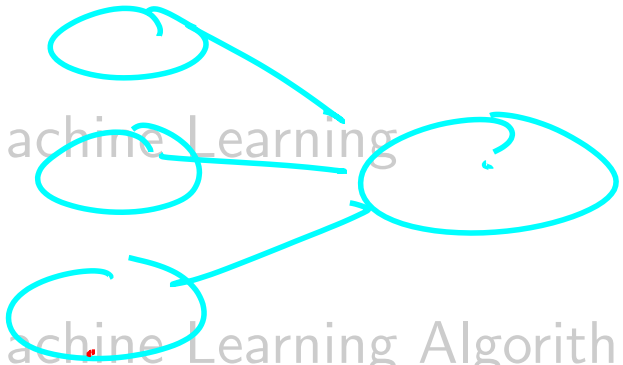
Neural Networks

- **Neural networks** are a type of machine learning model inspired by the human brain.
- They consist of layers of interconnected nodes that process input data and produce output data.



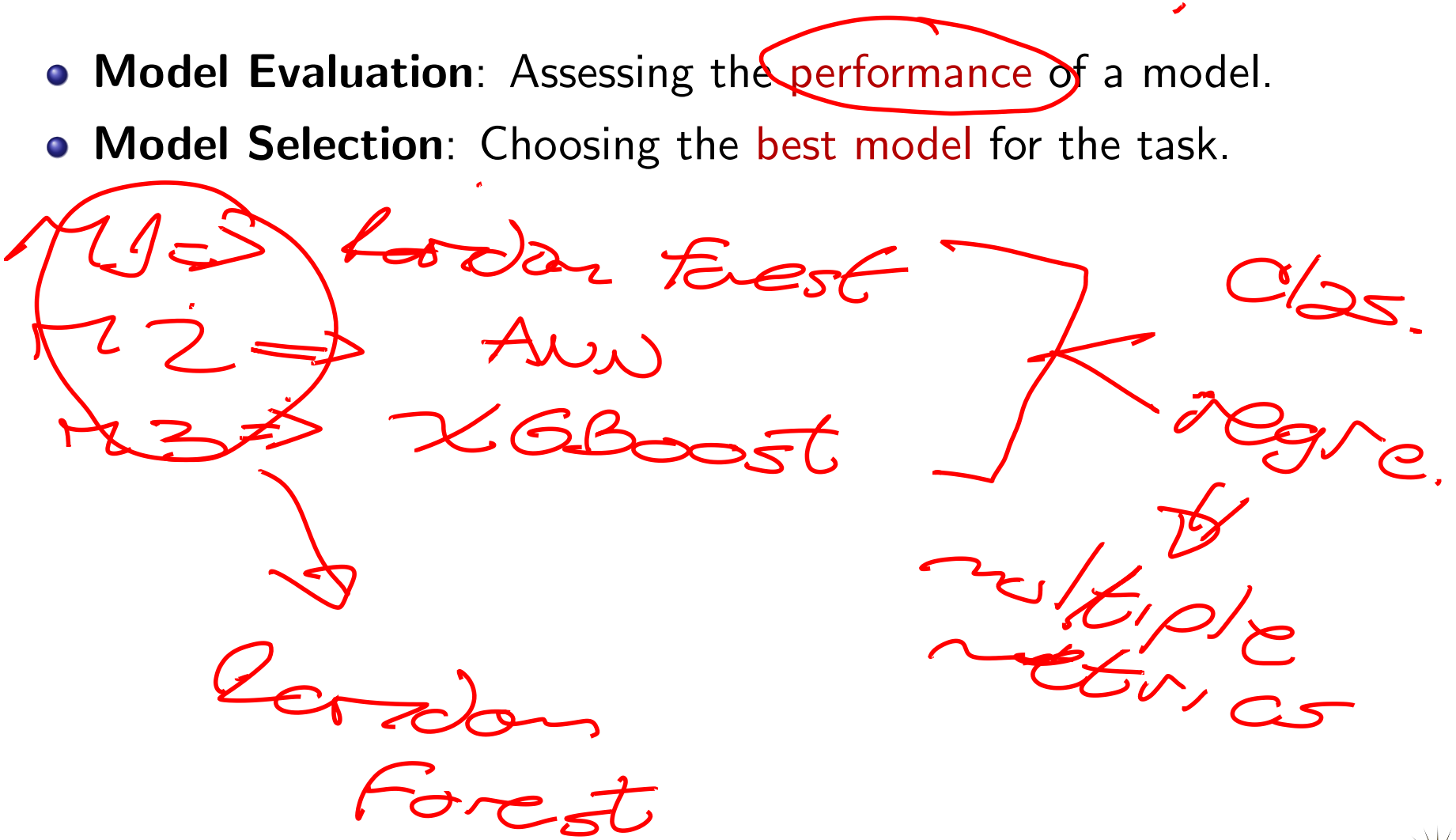
Outline





Model Evaluation & Selection

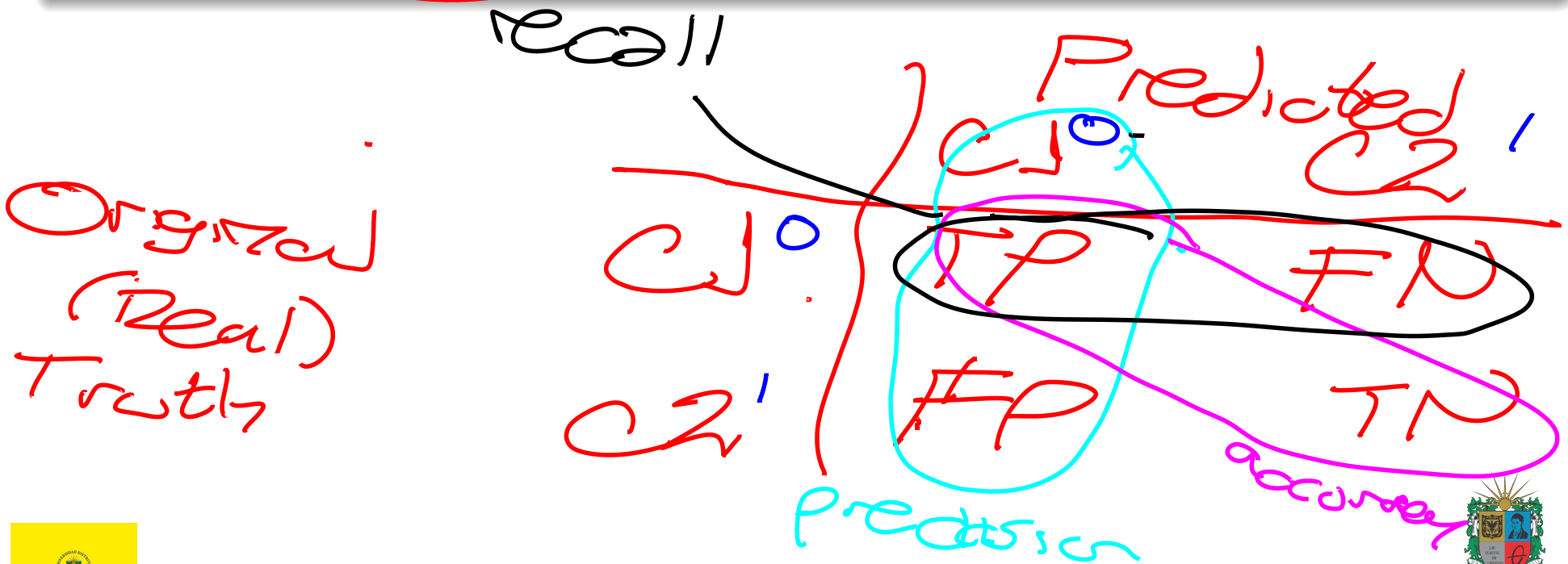
- **Model Evaluation**: Assessing the performance of a model.
- **Model Selection**: Choosing the best model for the task.



Confusion Matrices

Definition

- A **confusion matrix** is a table that summarizes the performance of a classification model.
- It shows the number of true positives, true negatives, false positives, and false negatives.



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Basic Evaluation Metrics

Classification

- **Accuracy**: The proportion of correct predictions.
- **Precision**: The proportion of true positives among all positive predictions.
- **Recall**: The proportion of true positives among all actual positives.
- **F1 Score**: The harmonic mean of precision and recall.

$$Ac = \frac{TP + TN}{TP + FP + FN + TN}$$

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

$\approx 1 \Rightarrow$ Predicted True is True

$\approx 0 \Rightarrow$ Predicted True is Falsepositive

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

1 => Expected True is Predicted True

0 => Expected True is False

Basic Evaluation Metrics

- **Accuracy**: The proportion of correct predictions.
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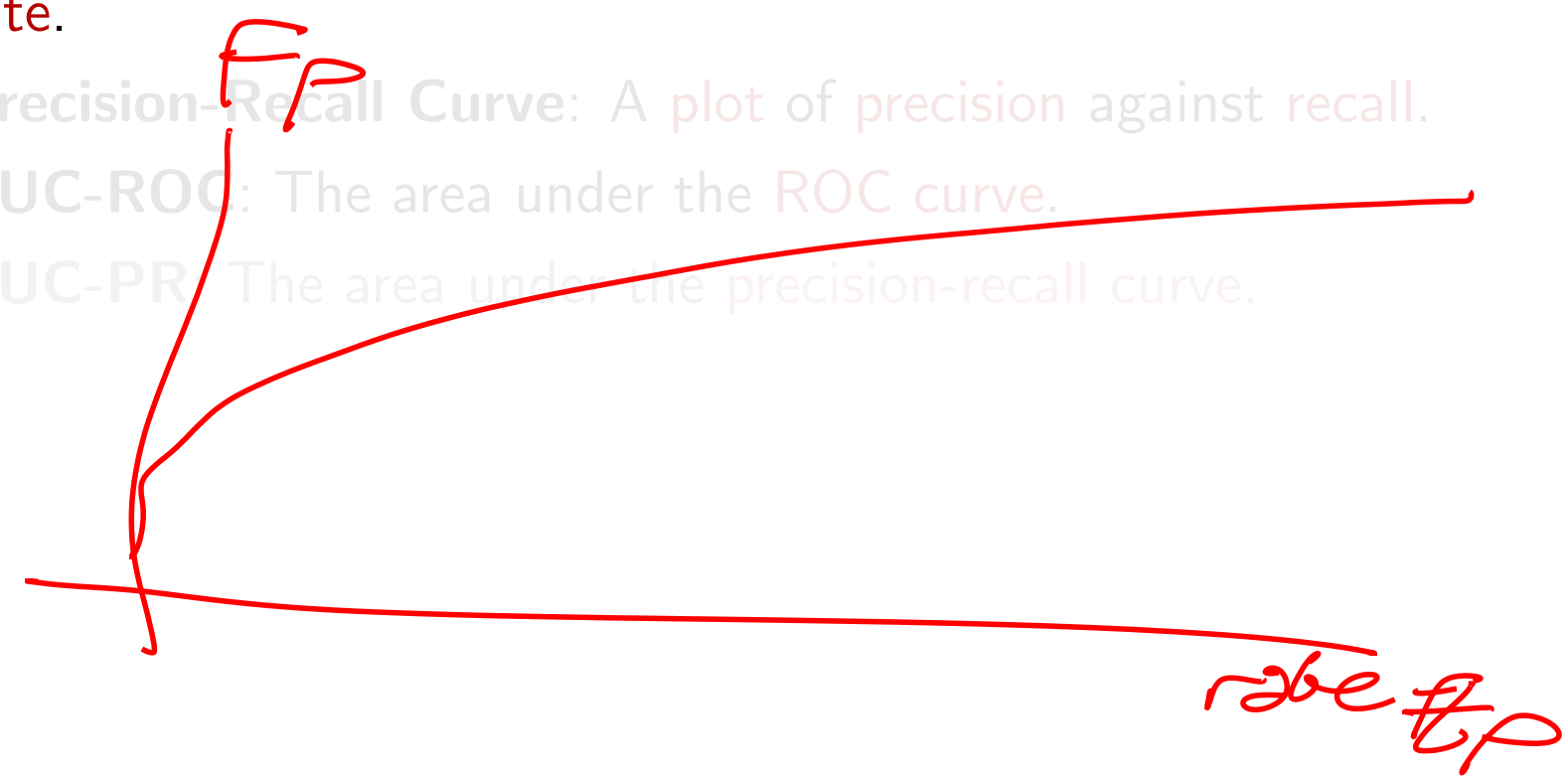
- **Recall**: The proportion of true positives among all actual positives.
- **F1 Score**: The harmonic mean of precision and recall.

$$F1 = 2\,\frac{precision * recall}{precision + recall}$$

$$precision = recall = 1 \Rightarrow 2 * \frac{1}{2} = 1$$

Classifier Decision Metrics

- **ROC Curve**: A plot of the true positive rate against the false positive rate.
- **Precision-Recall Curve**: A plot of precision against recall.
- **AUC-ROC**: The area under the ROC curve.
- **AUC-PR**: The area under the precision-recall curve.



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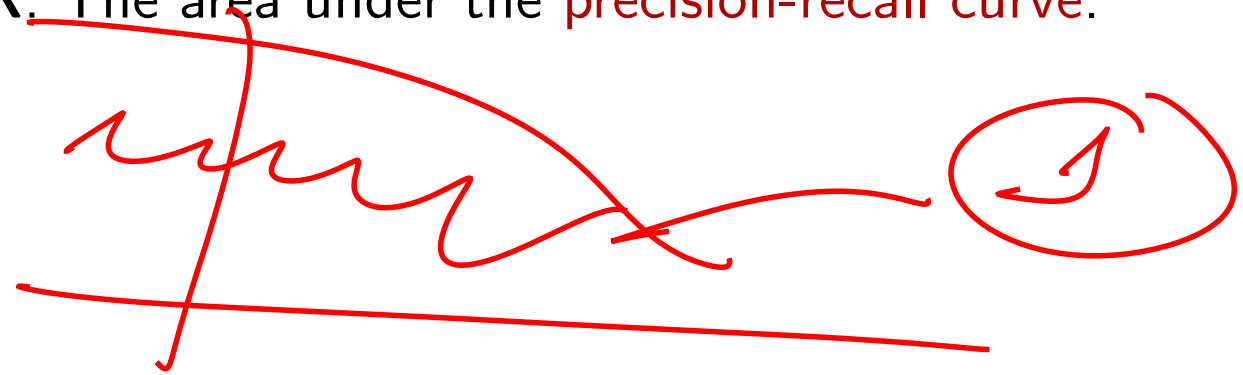
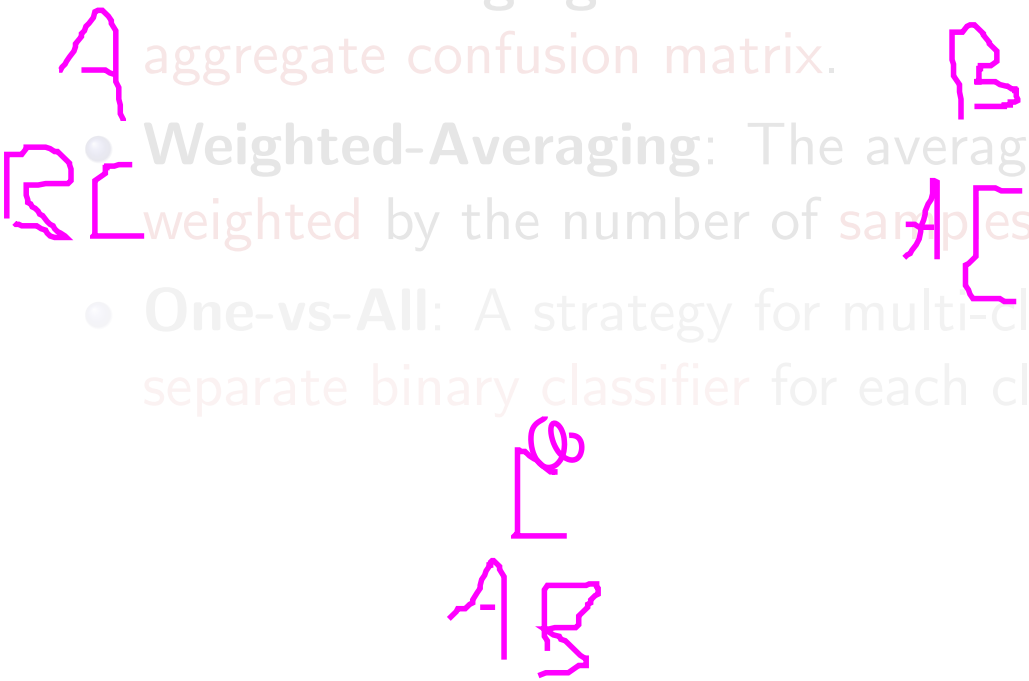


Multi-Class Evaluation

- **Macro-Averaging**: The average of the evaluation metrics for each class.
- **Micro-Averaging**: The evaluation metrics calculated on the aggregate confusion matrix.
- **Weighted-Averaging**: The average of the evaluation metrics weighted by the number of samples in each class.
- **One-vs-All**: A strategy for multi-class classification that trains a separate binary classifier for each class.



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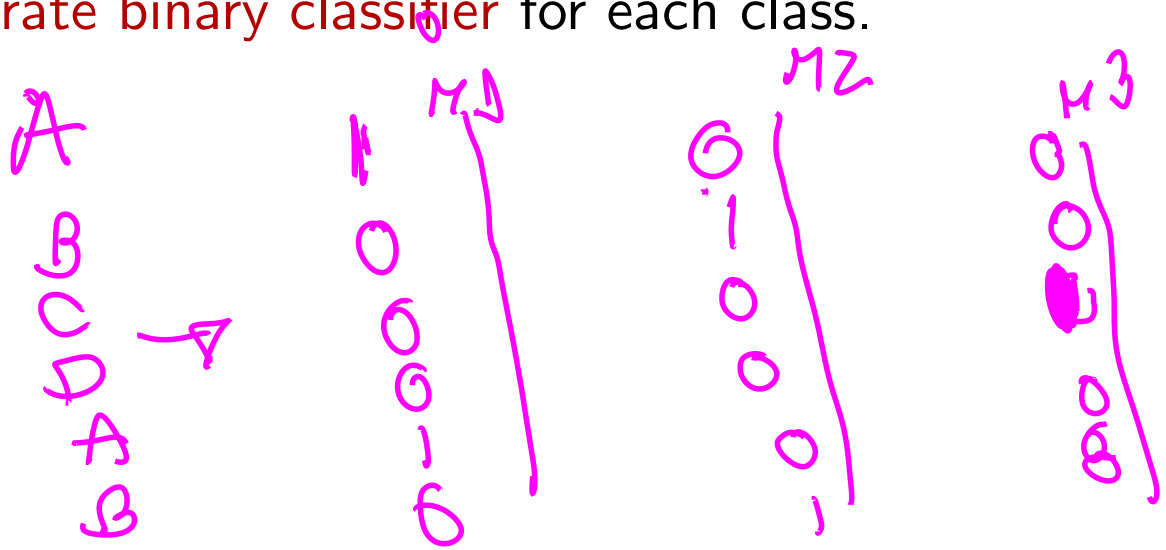
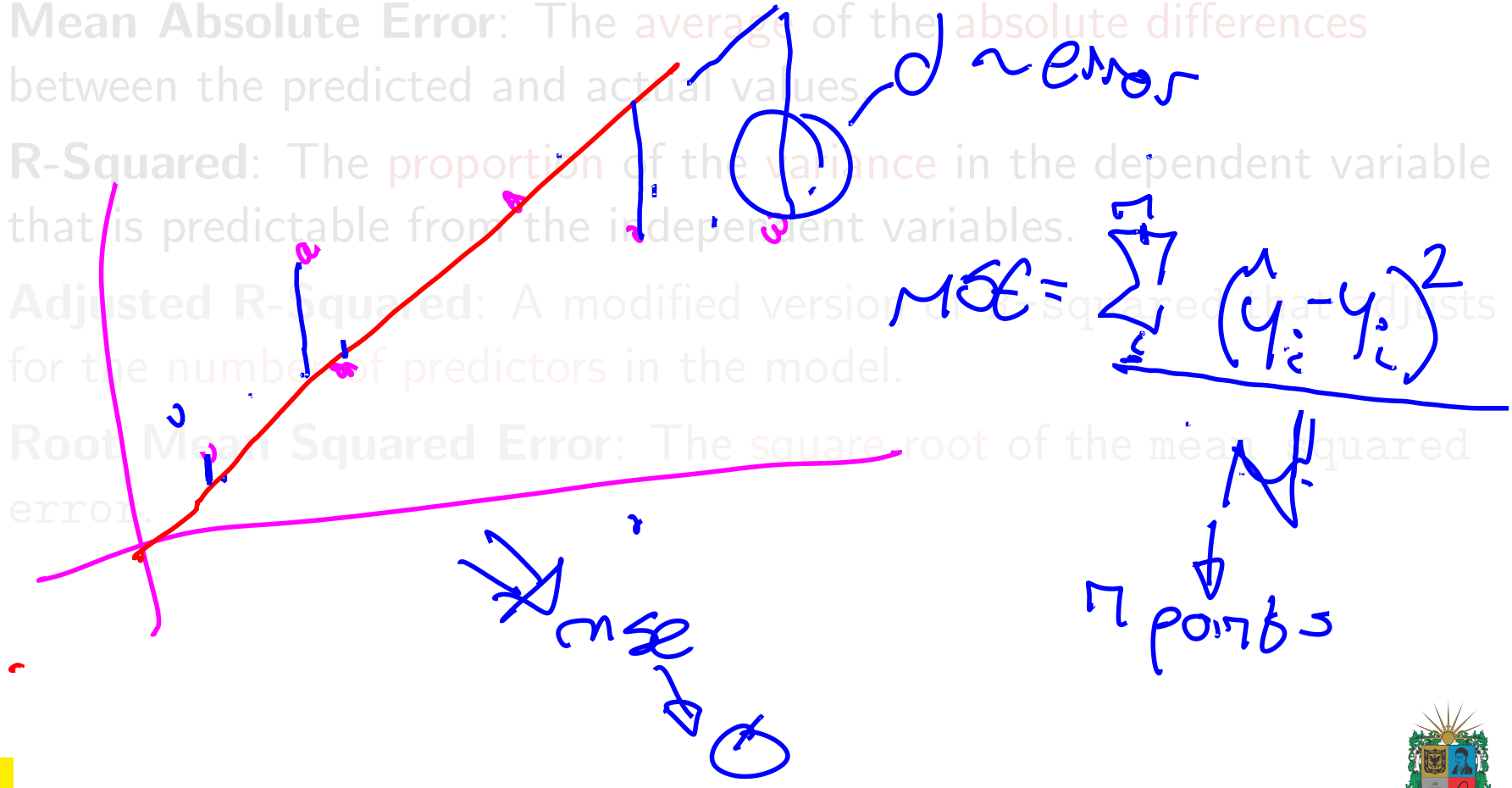


Regression Evaluation

- **Mean Squared Error**: The average of the squared differences between the predicted and actual values.
- **Mean Absolute Error**: The average of the absolute differences between the predicted and actual values.
- **R-Squared**: The proportion of the variance in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared**: A modified version of R-Squared that adjusts for the number of predictors in the model.
- **Root Mean Squared Error**: The square root of the mean squared error.



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$$MAE = \frac{\sum_{i=1}^{n} |\hat{y}_i - y_i|}{N}$$

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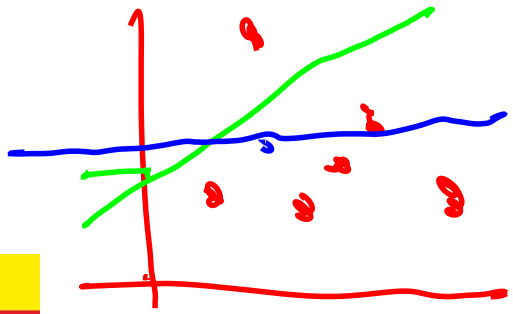
$$R^2 = 1 - \frac{\sum_{i=1}^{M} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{M} (\bar{y} - y_i)^2}$$

M => total points

$\bar{y}$ => average



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$$\sqrt{MSE} = \sqrt{\sum_{i=1} (y_i - \hat{y}_i)^2}$$

Model Calibration

- **Model calibration** is the process of adjusting the output of a model to match the true probability distribution.
- It is important for models that *output probabilities*, such as logistic regression and support vector machines.

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Outline

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Thanks!

Questions?

Repo: *https://github.com/EngAndres/ud-public/tree/main/courses/data-science-introduction*

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