



# Ensemble Methods

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Room HC3

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# Part 1: Summary

## Ensemble Methods

- Bagging (Random Forest)
- Boosting (Gradient Boosting)

## Model Parameters

- **Number of estimators:** 15, 50, 100, 150, 250 (**bagging** and **boosting**)
- **Maximum depth:** None, 3, 5, 10 (**bagging** and **boosting**)
- **Learning rate:** 0.05, 0.1, 0.5 (**boosting**)

## Pipeline

- Standard scaling
- Noise (0%, 30%, 60%, 90%)
- Train (80%) and test (20%) splitting
- Stratified fold splitting (3 folds)

## Analysis

- **F1 Score** (cross-validation, train and test)

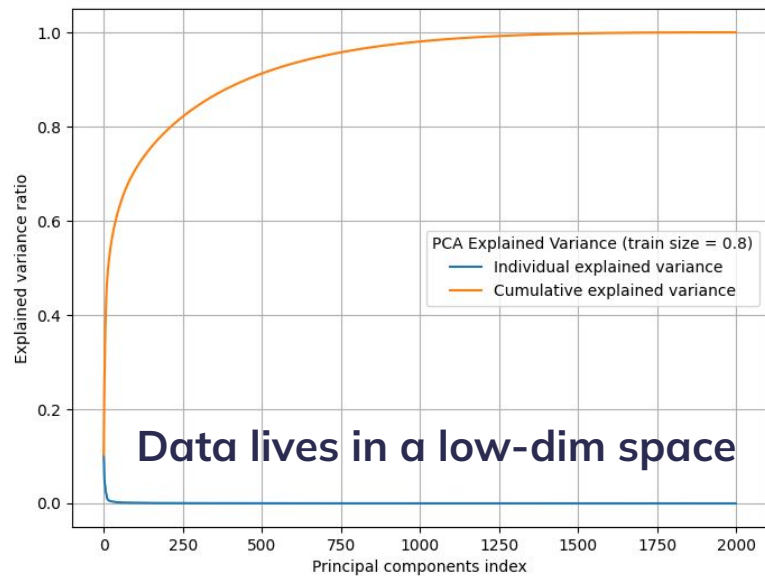
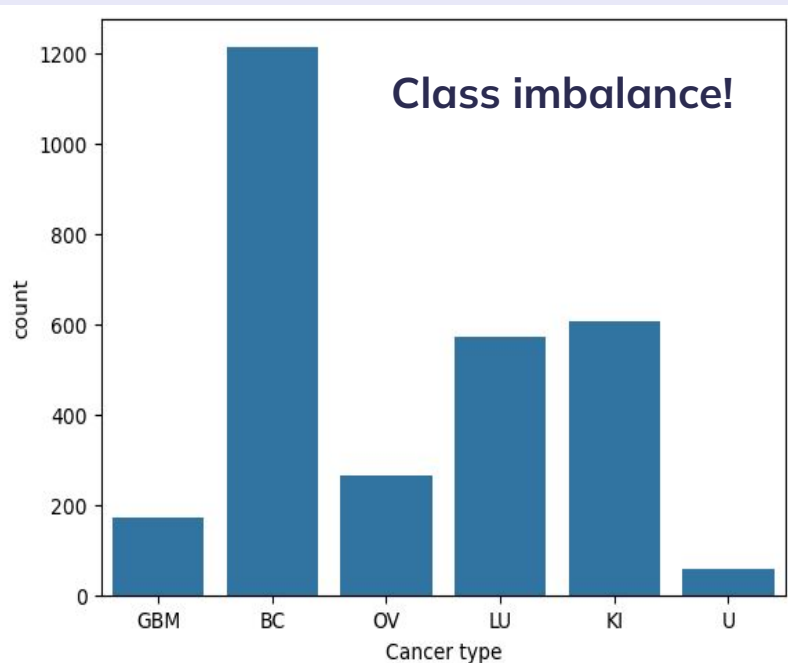


# Cancer Dataset

# Cancer dataset exploration

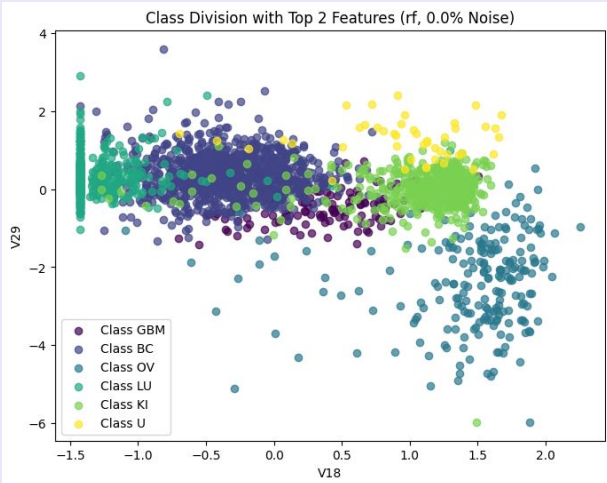


Meaningless features



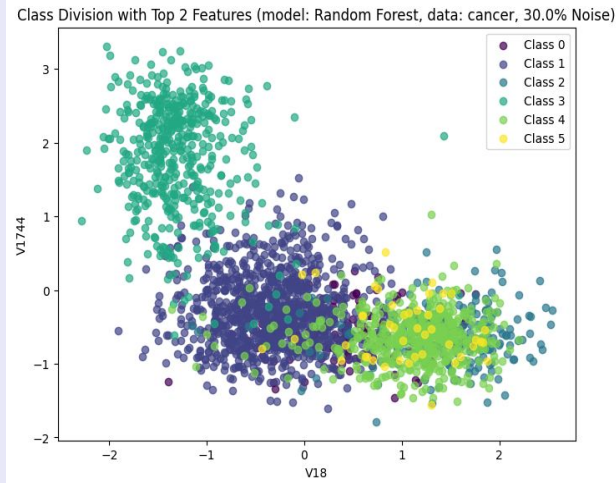
# Random Forest: Top 2 Features

0% Noise



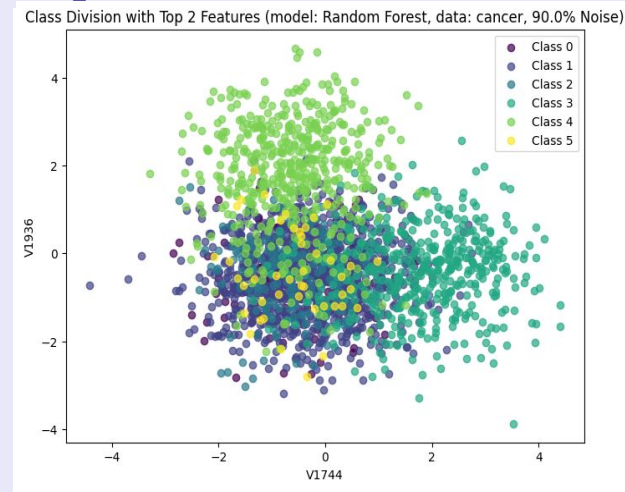
2 features allow to see  
class **separation**

30% Noise



Three classes are **still**  
**separable**

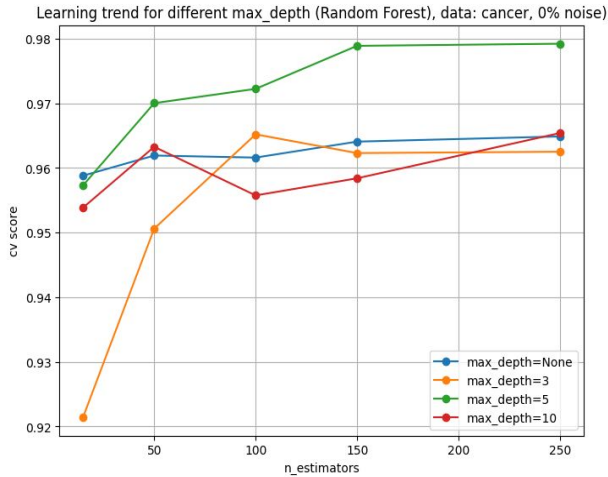
90% Noise



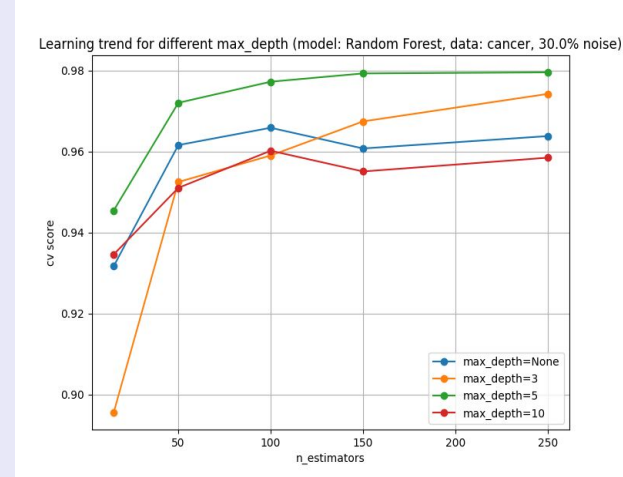
Classes **intertwined**  
with only 2 features

# RF: Nr. of Trees and Maximum Depth

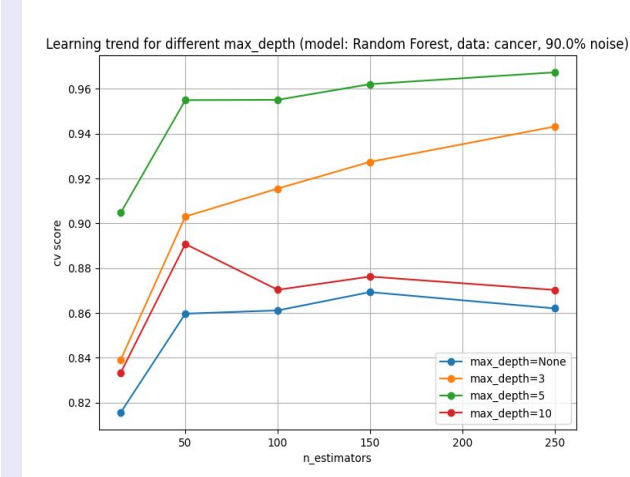
0% Noise



30% Noise



90% Noise



A small number of **deep trees** is sufficient

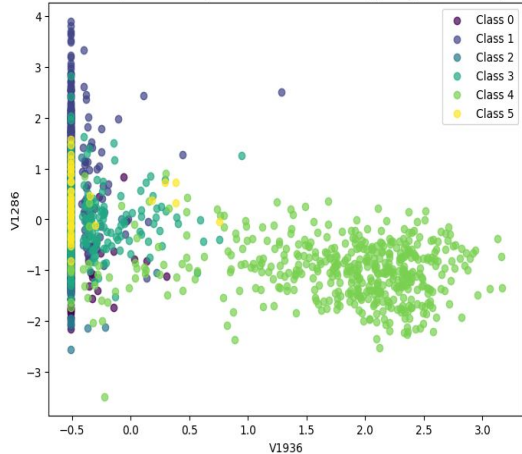
Good results especially for **enough estimators**

No benefits from a **depth** larger than 5 levels

# Gradient Boosting: Top 2 Features

0% Noise

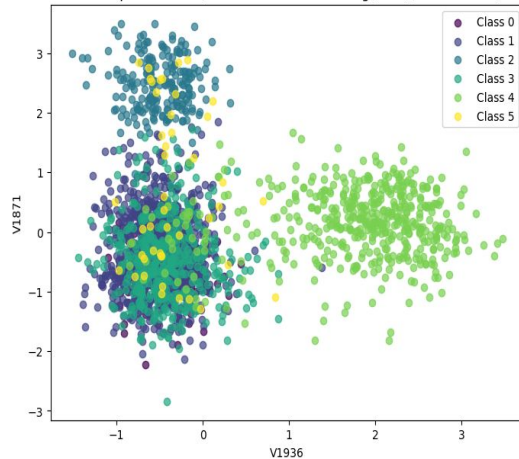
Class Division with Top 2 Features (model: Gradient Boosting (XGB), data: cancer, 0.0% Noise)



Gene **V1936** allows to  
separate **class 4**

30% Noise

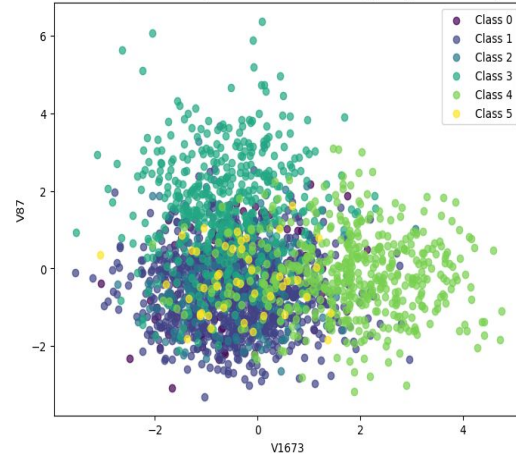
Class Division with Top 2 Features (model: Gradient Boosting (XGB), data: cancer, 30.0% Noise)



With only 2 genes some  
classes are **separable**

90% Noise

Class Division with Top 2 Features (model: Gradient Boosting (XGB), data: cancer, 90.0% Noise)

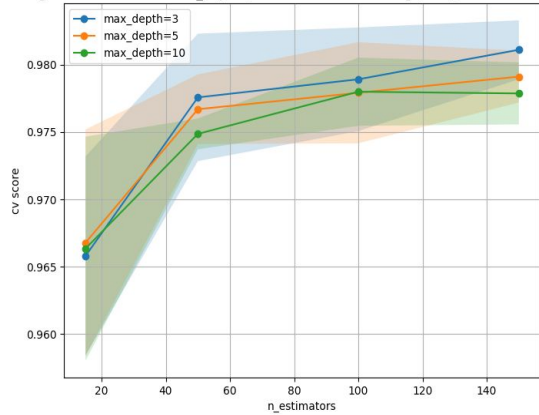


No clear **separation**  
with only two features

# GB: Nr. of Trees and Maximum Depth

0% Noise

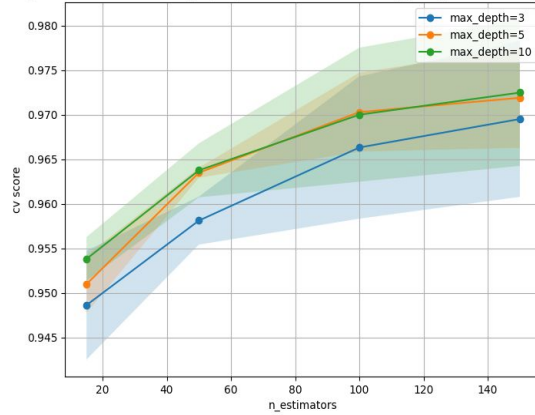
Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cancer, 0% noise)



Maximum depth **does not change** F1 score

30% Noise

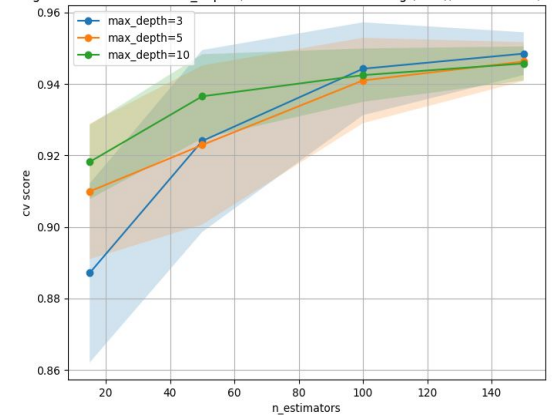
Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cancer, 30.0% noise)



Results **worsen** but still **good**

90% Noise

Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cancer, 90.0% noise)



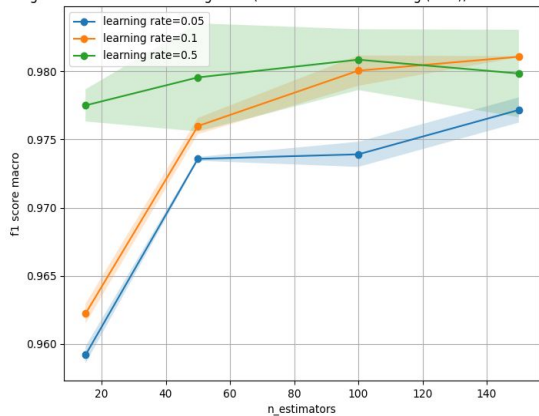
**Similar** scores with **enough** estimators



# GB: Nr. of Trees and Learning Rate

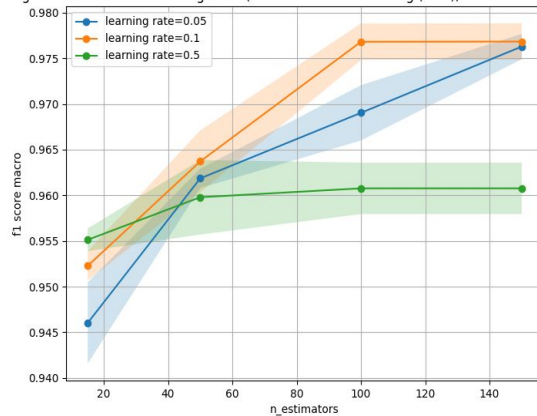
0% Noise

Learning trend for different learning rates (model: Gradient Boosting (XGB), data: cancer, 0% noise)



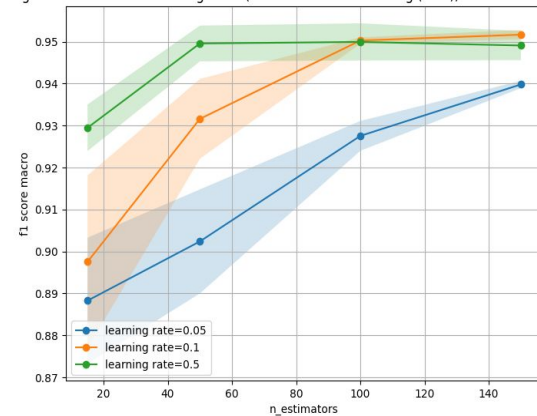
30% Noise

Learning trend for different learning rates (model: Gradient Boosting (XGB), data: cancer, 30.0% noise)



90% Noise

Learning trend for different learning rates (model: Gradient Boosting (XGB), data: cancer, 90.0% noise)

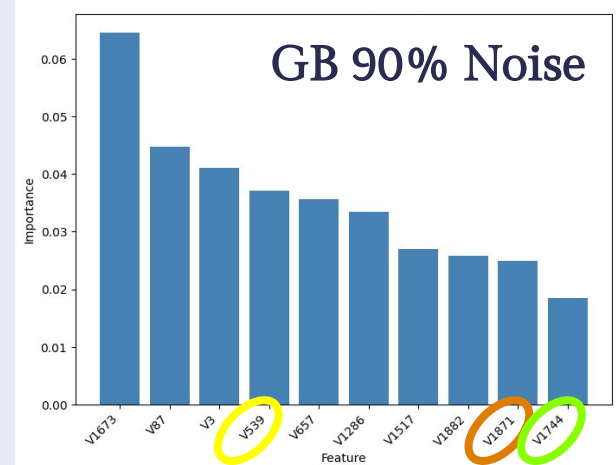
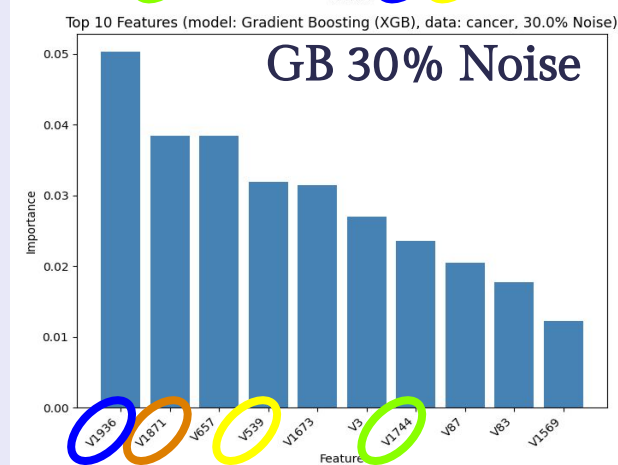
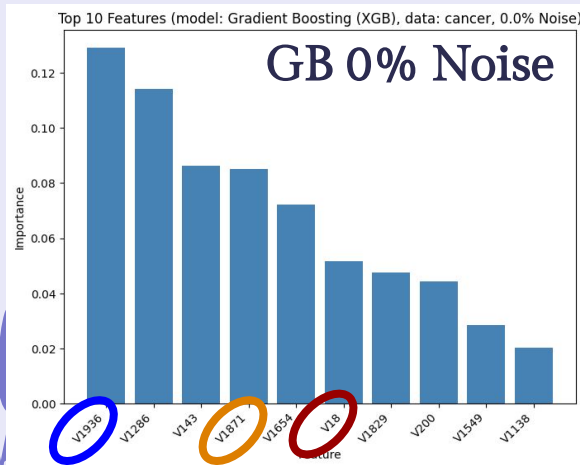
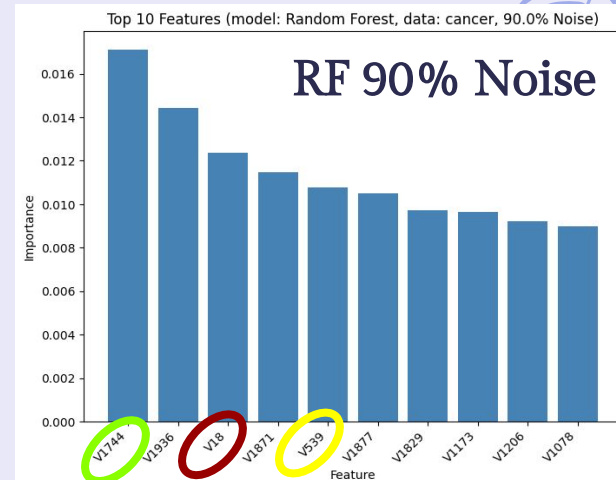
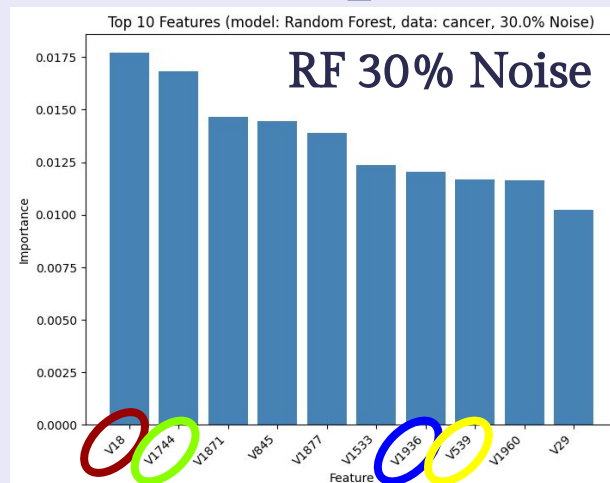
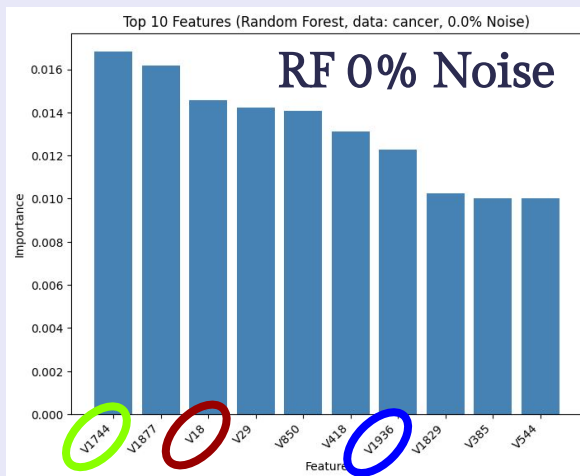


50 trees are enough  
for **large** learning rates

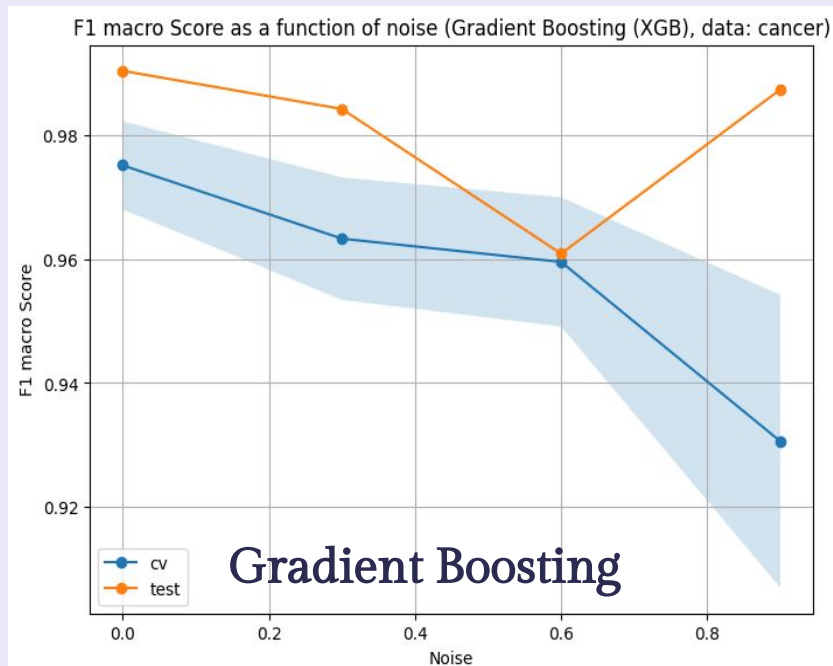
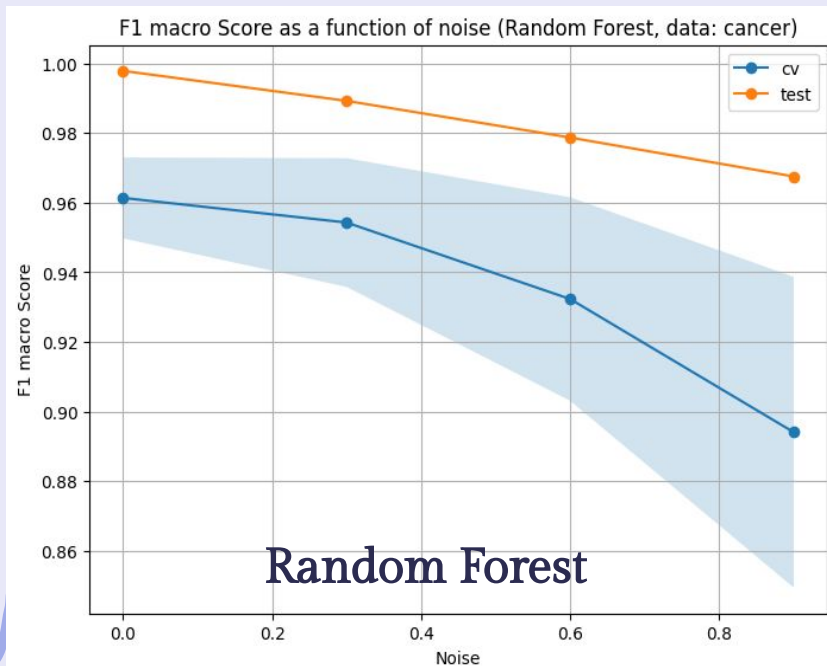
Best results for a **small**  
learning rate

**Early stopping** effect  
for small learning rates

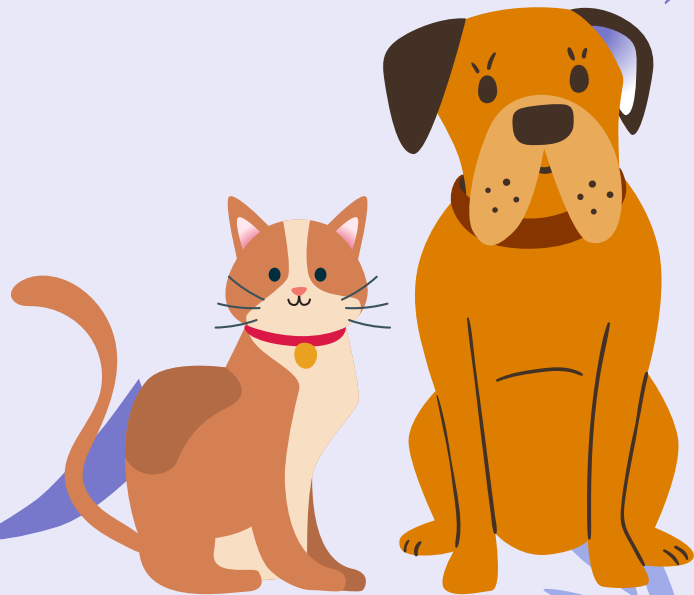
# RF vs GB: Top 10 Features



# RF vs GB: Performance Comparison



# Cats and Dogs Dataset



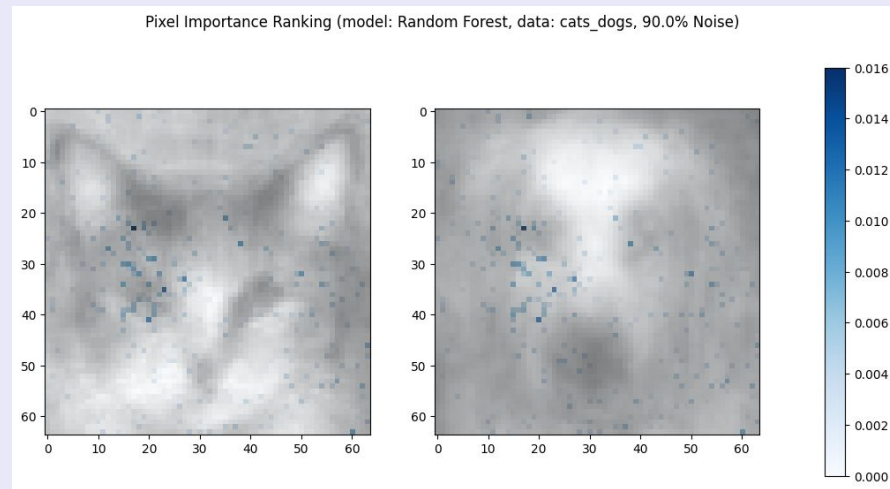
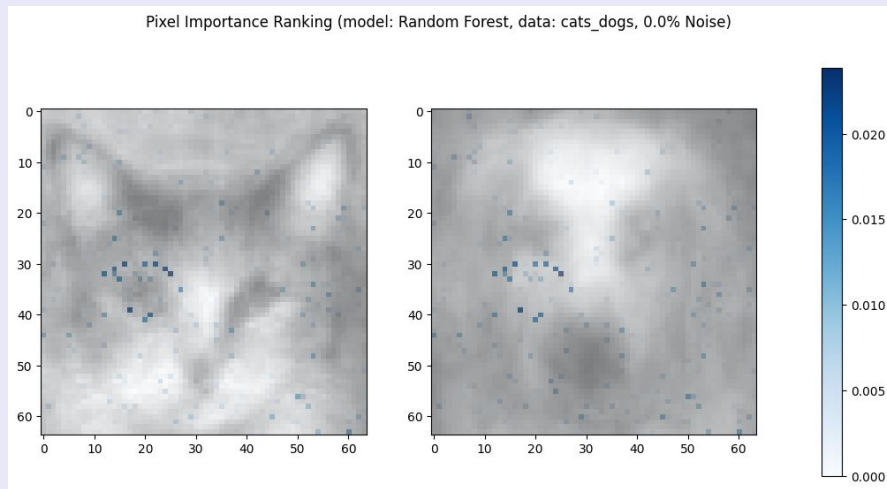
# Random Forest: Top Pixels



0% Noise



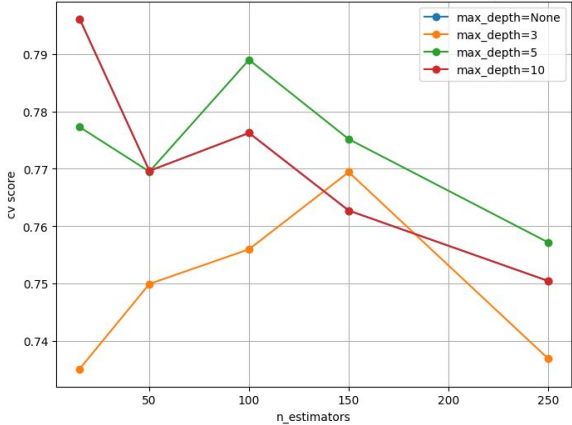
90% Noise



# RF: Nr. of Trees and Maximum Depth

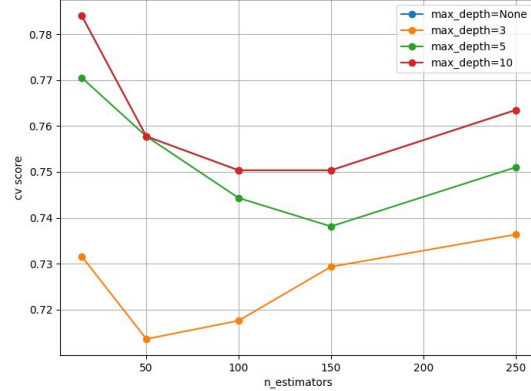
0% Noise

Learning trend for different max\_depth (Random Forest), data: cats\_dogs, 0% noise)



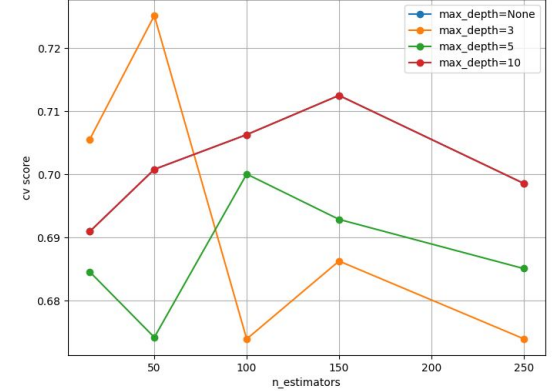
30% Noise

Learning trend for different max\_depth (model: Random Forest, data: cats\_dogs, 30.0% noise)



90% Noise

Learning trend for different max\_depth (model: Random Forest, data: cats\_dogs, 90.0% noise)



Depths **larger than 3**  
allow good training

Maximum depth of 10  
**outperforms**

Performance **worsens**,  
even with more trees

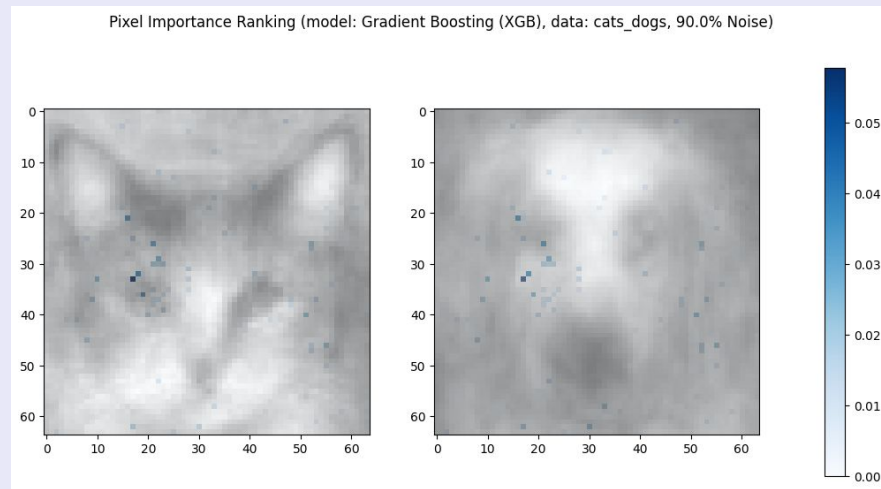
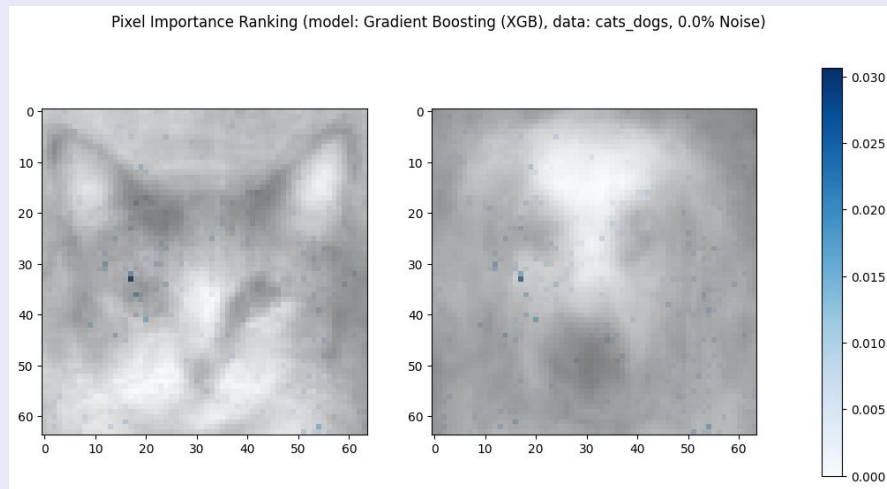
# Gradient Boosting: Top Pixels



0% Noise



90% Noise



Same area of focus as with RF: around the **cat's eye** and the **dog's cheek**

With noise, **maximum** value of importance **increased**

# GB: Nr. of Trees and Maximum Depth

0% Noise

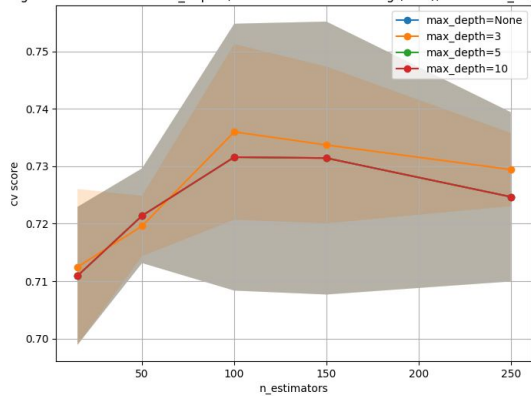


30% Noise

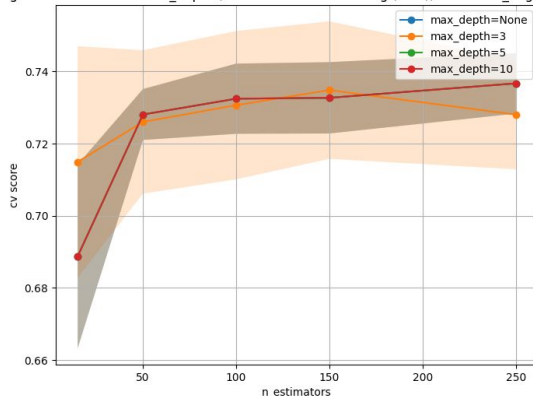


90% Noise

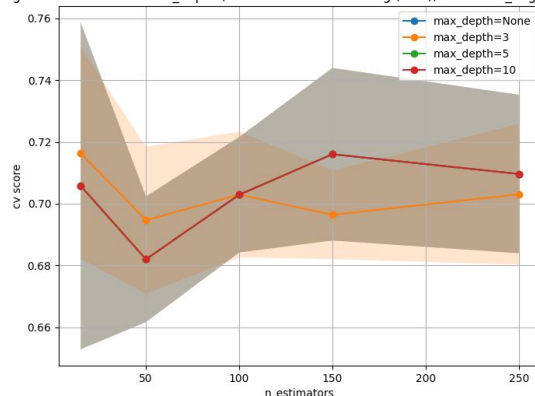
Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cats\_dogs, 0% noise)



Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cats\_dogs, 30.0% noise)



Learning trend for different max\_depth (model: Gradient Boosting (XGB), data: cats\_dogs, 90.0% noise)



F1 score always  
below 0.74

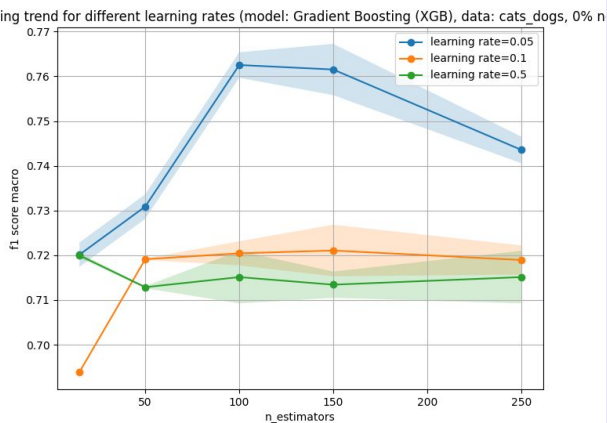
Minimal changes for  
different learning rates

Unstable F1 scores  
for all estimators

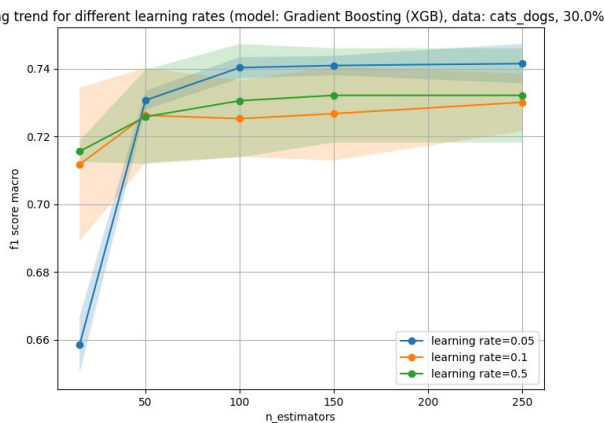


# GB: Nr. of Trees and Learning Rate

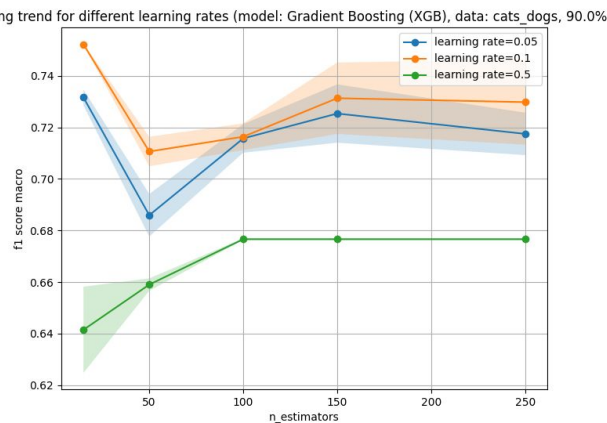
0% Noise



30% Noise



90% Noise

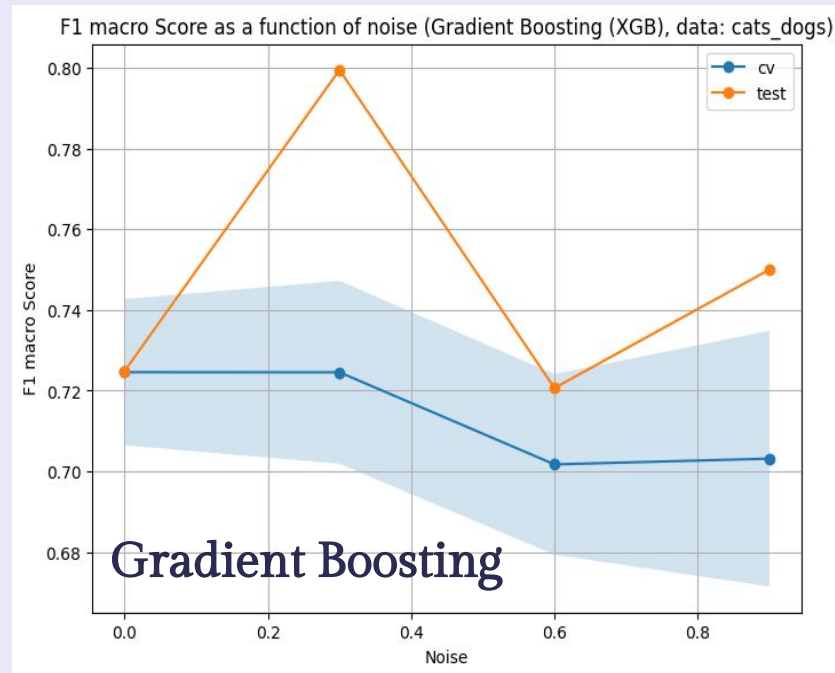
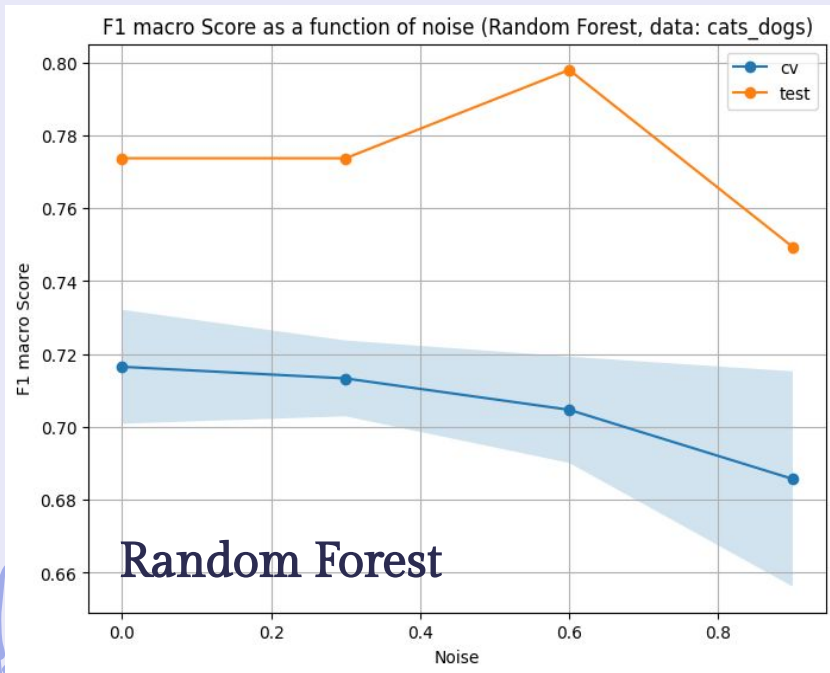


A low learning rate outperforms

More than 50 trees **don't improve** F1 score clearly

No improvements for forests with more trees

# RF vs GB: Performance Comparison





# Simulated data

## Gradient Boosting

# Part 2: Summary

## Simulated dataset

- 400 samples for 400 features:
- 100 informative features
- 3 classes with weights 20%, 30%, 50%
- 70% of class separation

## Model Parameters

- **Number of estimators:** 100 (default)
- **Maximum depth:** 1, None (default)
- **Learning rate:** 0.1 (default), 10

## Ensemble Method

- Boosting (Gradient Boosting)

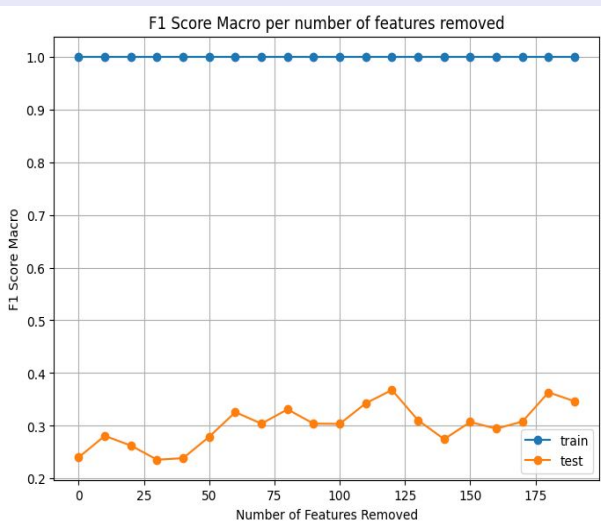
## Procedure

- Recursively eliminate features

## Analysis

- **F1 Score**

# GB: Maximum Depth and Nr. of Trees

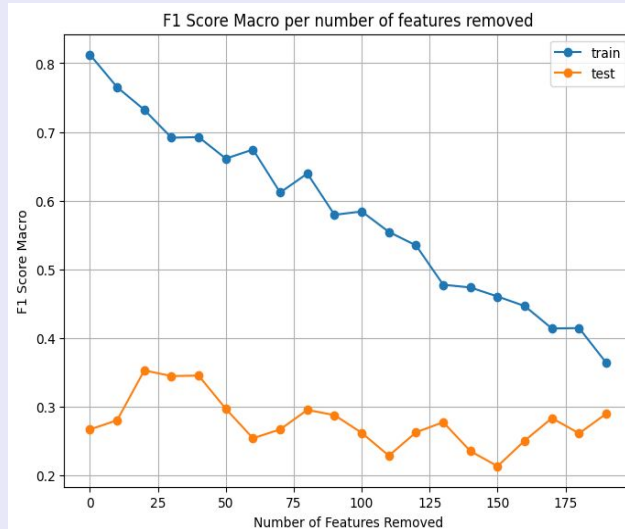


**Immediate overfitting**

Default parameters

Maximum Depth = None

Learning rate = 0.1

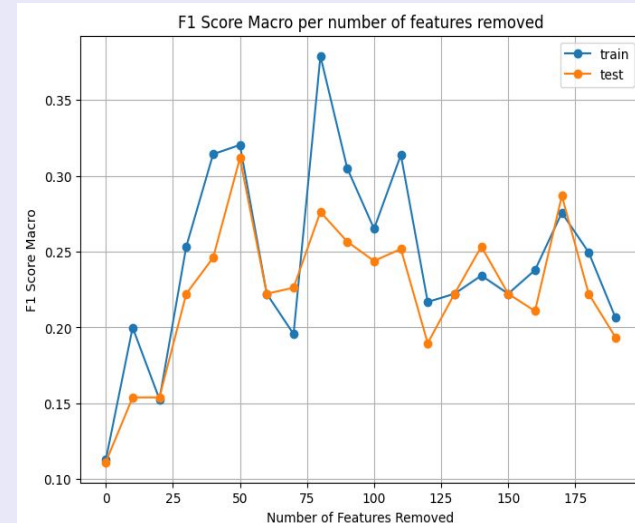


**Train scores worsen**

Shallow decision trees

Maximum Depth = 1

Learning rate = 0.1



**Low F1 scores**

High learning rate

Maximum depth = None

Learning rate = 10

# Thanks

Does anyone have any questions?

Elínborg Ásbergisdóttir  
İpek Korkmaz  
Luca Modica  
Patrícia Marques

