# SUPERVISED ML

# SUPERVISED ML

- Certainly the most successful branch of ML currently
- Training a computer program (algorithm) to learn through examples
- Tasks:
  - Predict the weather, the climate
  - Recognize objects/people in pictures
  - Etc.

# SUPERVISED ML

- Two main objectives, with similar solutions
- Regression: predict a numerical value
  - Temperature, cost, grade, etc.
- Classification: predict a class/label/category
  - Success/Failure, Blue/Red/Yellow, which animal among 1000 possibles, etc.

# PREDICTING VS EXPLAINING

- Final goal is prediction:
  - Supervised ML is obviously what you need
    - No need of interpretability, you just care about accuracy

- Final goal is understanding your data
  - "Is product X causing cancer ?"
  - => If your model is the best at predicting if people will get cancer or not, it is likely the best at capturing the effect of X on cancer.
    - But of course, problem of explainability … XAI ?

# PROGRAM

- ML process
- Simple methods
  - Linear Regression
  - Decision trees
- Objectives for regression
- Overfit
- Cross-validation

# SUPERVISED ML - PROCESS

- Let's say we want to predict the price of apartments. We have a collection of examples, for now in comparable settings (same neighborhood of the same city…)
- We have access to some characteristics of apartments:
  - Surface Area, # of rooms, # of windows, Elevator…
- This is typically a Regression problem.

# SUPERVISED ML - PROCESS

- STEP 1: Define the objective
  - Objective function / Score
  - =>Measurement of average errors made by the model
    - RMSE, etc.

# STEP 1: THE OBJECTIVE

- **Before applying any method**, set up an objective/a quality score/an error measure

- We want to decide on the best method among candidates

- Typical scores for regression:
  - MSE, RMSE: (Root) Mean Square Error
  - MAE: Mean Absolute Error
  - $R^2$

# MEAN SQUARED ERROR

- $\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2 = \frac{1}{n}\sum_{i=1}^{n} e_i^2$

- Similarity with the **Variance**

- Using *squared* errors give stronger importance to large errors
  - Strenght and weakness (outliers)

- $\mathrm{RMSE} = \sqrt{\mathrm{MSE}}$, can be easier to interpret

- Simple to interpret
  - The lower the value, lower the error, better the prediction

# MEAN ABSOLUTE ERROR

- $$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \hat{y}_i\right| = \frac{1}{n}\sum_{i=1}^{n}\left|e_i\right|$$

- Similarity with the MAD (Mean Absolute Deviation), comparing values with predictions instead of simple mean.
- Intuitive interpretation (not a root of a square)
- =>Better with heavy tailed distribution in the target

# $R^2$ (R-SQUARED)

- $R^2 = 1 - \frac{\sum_i e_i^2}{\sum_i y_i - \bar{y}} = 1 - \frac{MSE}{Var(y)}$

- Normalized MSE
  - Quantifies the fraction of the variance that is explained by the prediction
  - Sometimes called the *coefficient of determination* for linear regression

- 1=>Perfect prediction.
  - Negative if the prediction is worse than using the average for prediction (=Variance)

# EVALUATION/OBJECTIVE

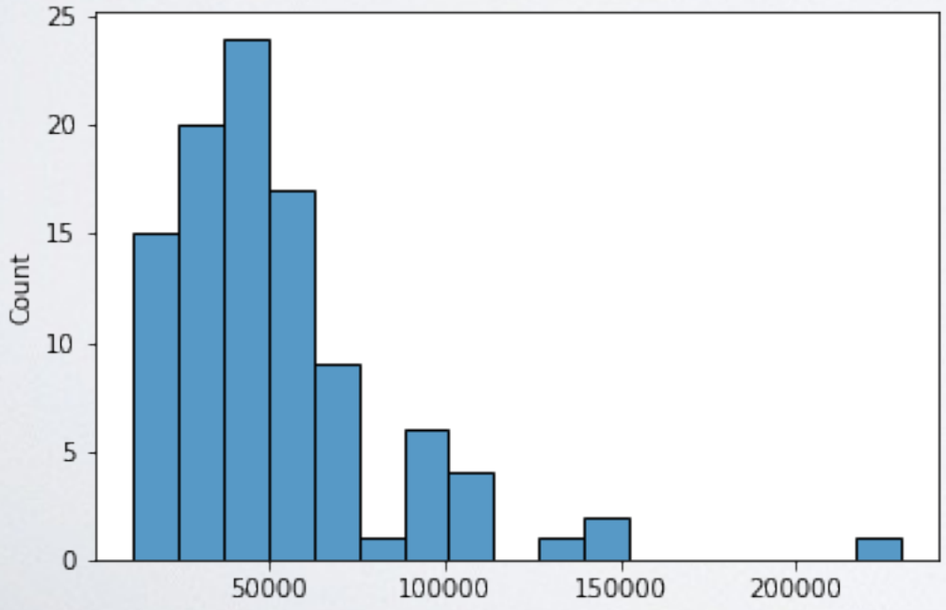
- Which one should you use?
  - Different literature have their favorite one. RMSE is probably the most popular currently
- If you're not writing a paper or playing a competition, use all of them
  - More information can allow you to judge better. There is no "truth".

# SUPERVISED ML - PROCESS

- STEP 2: Define baselines
  - How good is the prediction with a naive model?
  - Can our model improve over those models?
    - How much?

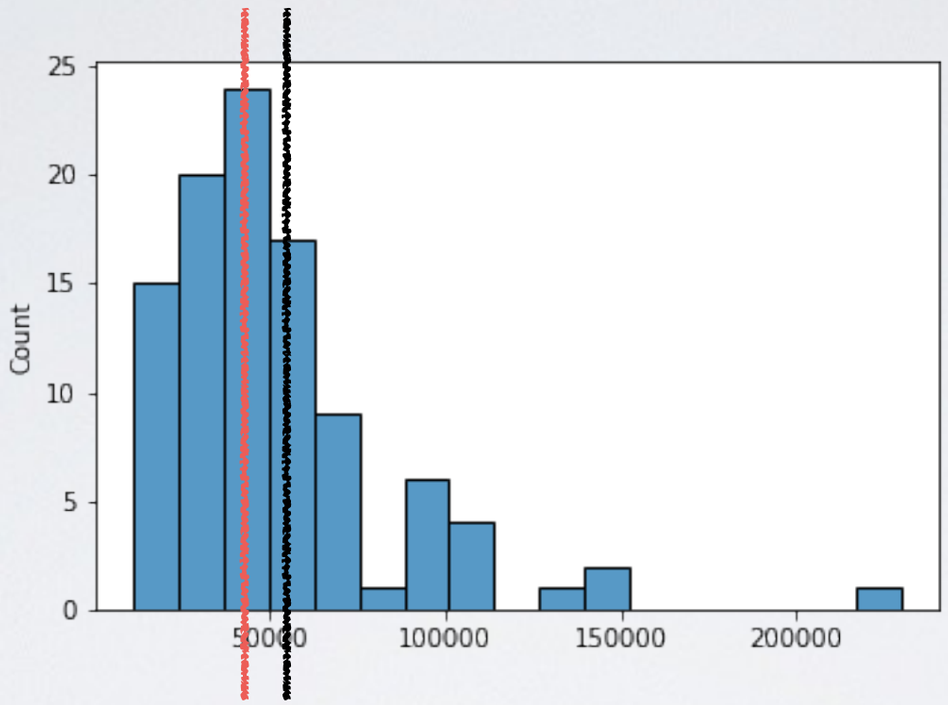
# BASELINE

- Let's define our baseline, our reference to improve on
- Let's assume we **only know** the **target** variable
- Using statistics, we know that the best "prediction" we can do for the price of a future apartment, with no additional information (features) will be
  - The average (for MSE)
  - The median (for MAE)




(Some imaginary values)

# BASELINE




Using **Mean**=51676

```
MSE 1105345073.7155044
RMSE 33246.73027104326
MAE 22740.967725747014
R2 0.0
```

RMSE lower

Using Median=43086

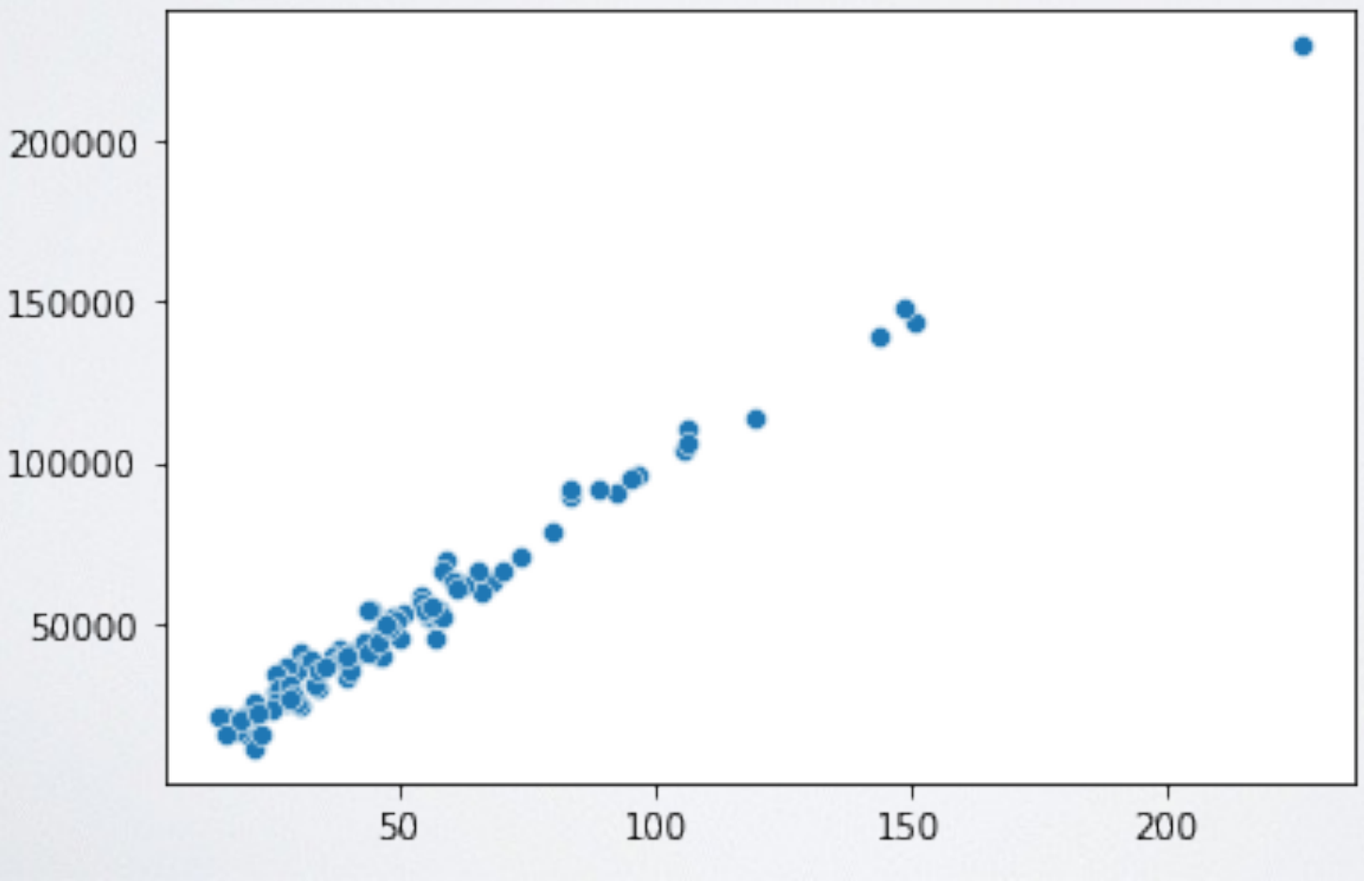
```
MSE 1179133659.4166086
RMSE 34338.51568452848
MAE 21658.66828240126
R2 -0.0667561537620748 9
```

MAE lower

# LINEAR REGRESSION

- Let's assume that we know one apartment attribute: Surface area. We can plot the relation between Surface and Price

- There seems to be a linear relationship



# LINEAR REGRESSION

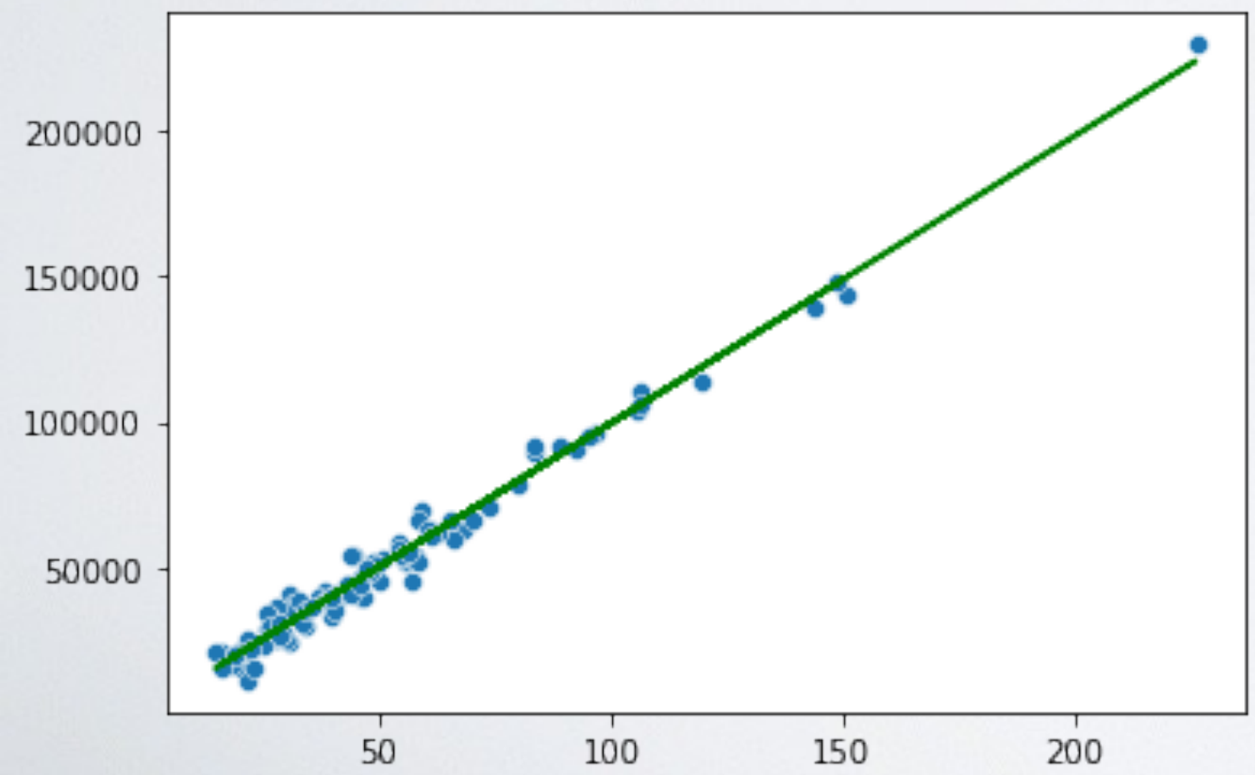
- We will use **linear regression** method, and more specifically **Ordinary Least Square**. First, with a single variable:

- We assume that: $y_i = \beta_0 + \beta_1 x_i + \epsilon$
  - Target value=constant+(constant*feature)+normally distributed (random) errors
  - i=>ith example in our dataset

- The objective of linear regression is to find parameters $\Theta = \{\beta_0, \beta_1\}$
  - Such as to minimize the **MSE**,
  - Considering that the prediction is: $\hat{y}_i = \beta_0 + \beta_1 x_i$
    - Equivalently: $\hat{y} = \beta_0 + \beta_1 x$

# LINEAR REGRESSION

- We solve this problem, and obtain:
  - $\beta_0$=987
  - $\beta_1$=779




```
MSE 20668278.463901177
RMSE 4546.237836266508
MAE 3512.3861644882704
R2 0.981301514834252 8
```

# LINEAR REGRESSION

- We solve this problem, and obtain:
  - $\beta_0$=987
  - $\beta_1$=779

## Using Mean

```
MSE 1105345073.7155044
RMSE 33246.73027104326
MAE 22740.967725747014
R2 0.0
```

## Using Median

```
MSE 1179133659.4166086
RMSE 34338.51568452848
MAE 21658.66828240126
R2 -0.0667561537620748 9
```

## Using Linear Regression

```
MSE 20668278.463901177
RMSE 4546.237836266508
MAE 3512.3861644882704
R2 0.9813015148342528
```

# LINEAR REGRESSION

- Note: To generate the data, I used indeed a linear model, with parameters
  - $\beta_0$=~~987~~ 0
  - $\beta_1$=~~779~~ 1000
-

Using
Linear Regression

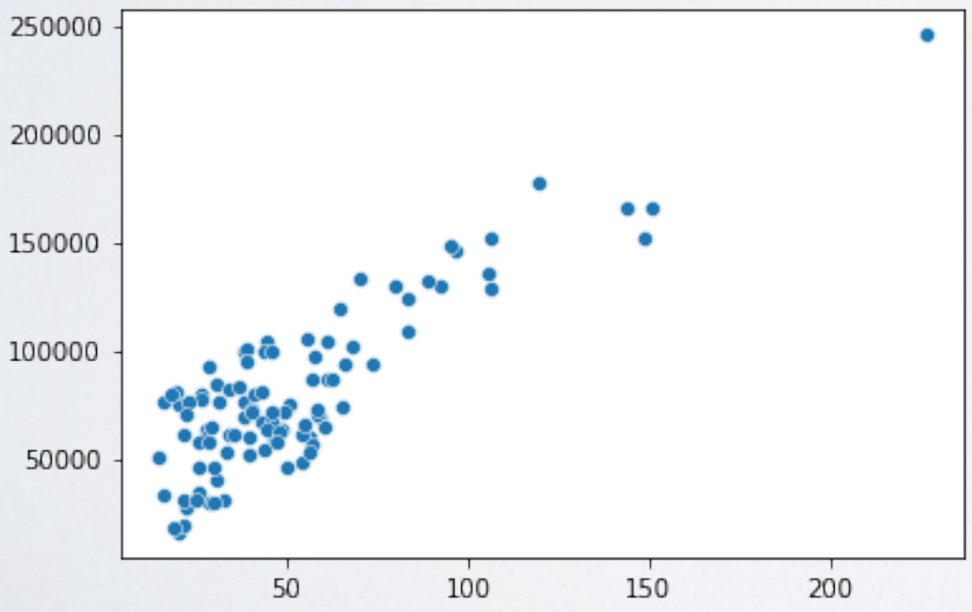
```
MSE 20668278.463901177
RMSE 4546.237836266508
MAE 3512.3861644882704
R2 0.981301514834252 8
```

Using
"Real" generative model

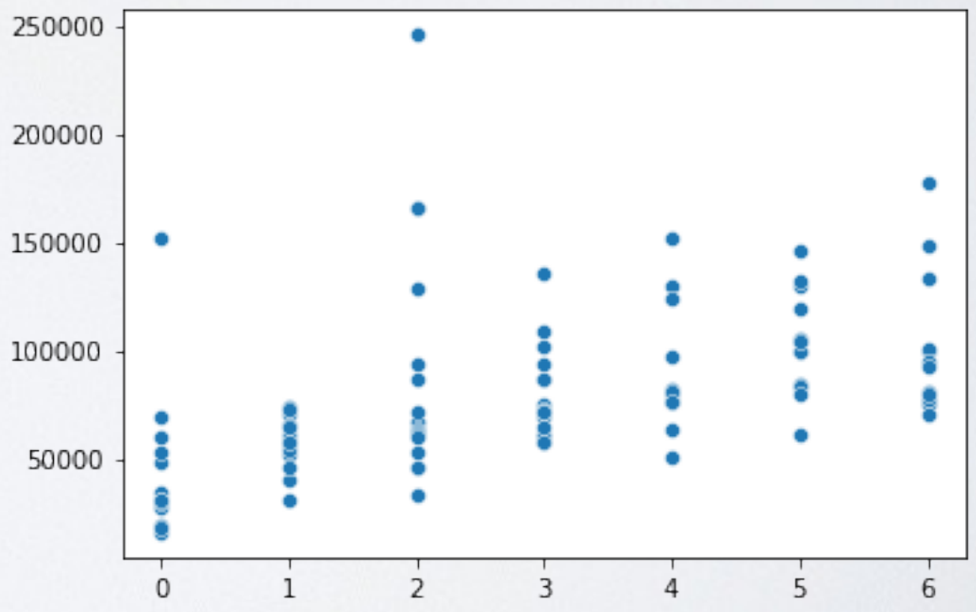
```
MSE 20863741.73315057
RMSE 4567.68450455486
MAE 3506.783422078361
R2 0.9811246802204318
```

# LINEAR REGRESSION

- In real life, we usually have more than 1 parameter
  - New dataset, prices depends on surface AND floor




Surface




Floor

# LINEAR REGRESSION

- General formulation with any number of attribute
  - $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n + \epsilon$
  - Searching for the different coefficients

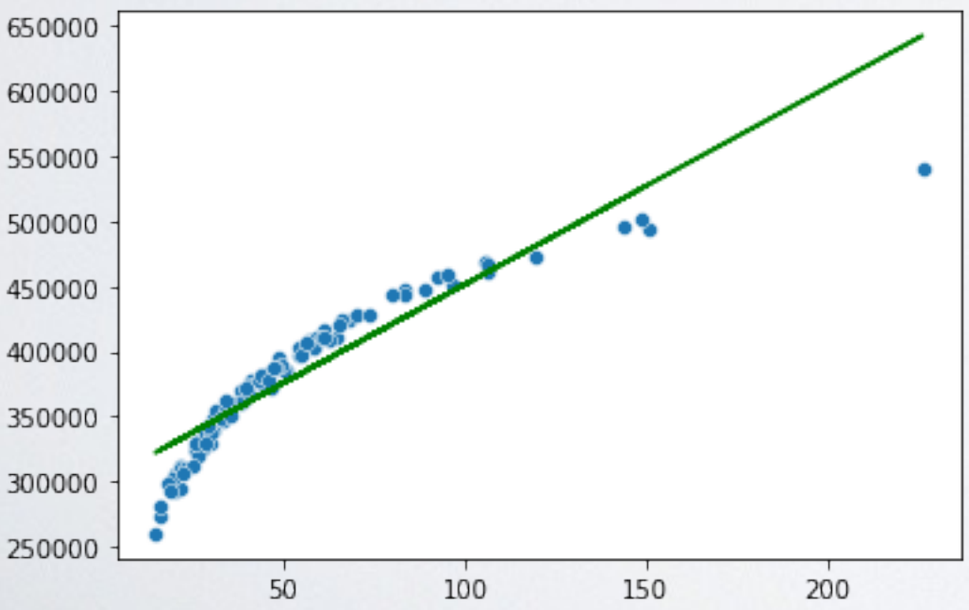
| Surfaces only | Floor only | All features |
|---|---|---|
| MSE 388200345.3991482<br>RMSE 19702.800445600322<br>MAE 16757.480694933285<br>R2 0.7329146952183824 | MSE 785600976.607142<br>RMSE 28028.57428780747<br>MAE 22165.777484397917<br>R2 0.3422280788055257 5 | MSE 22157971.6387145<br>RMSE 4707.225471412486<br>MAE 3617.346073048316<br>R2 0.984755117612315 5 |

Generative Parameters
- $\beta_0 = 0\ \beta_1 = 1\,000, \beta_2 = 10\,000$

Found Parameters
- $\beta_0 = 579\ \beta_1 = 994, \beta_2 = 9\,821$

# LINEAR REGRESSION

- Linear regression works :)
- But what happens if relations are not linear?
  - Assume that Price ≈ log(surface)*100 000 ?




## Linear regression

```
MSE 474131230.6072998
RMSE 21774.554659218633
MAE 16958.426496791166
R2 0.8437196622358905
```

## Real model

```
MSE 23408487.920127597
RMSE 4838.231900201518
MAE 4057.809620606243
R2 0.992842323758786
```

# LINEAR REGRESSION

- Linear regression works if there are indeed linear relations
  - But there is no particular reason for relations to be linear

- In many scientific domains (e.g., epidemiology, biology, econometrics, etc.), linear regression is still widely used.
  - Why?
    - Force of habits
    - Explainability
    - Good enough with scarce data

# OLS STRENGTH

- Analytical solution: $\hat{\beta} = (X^T X)^{-1} X^T y$
  - With X the feature matrix

- An analytical solution guarantees to find the optimal solution

- Possible to do before the generalization of computers

- If there are
  - Many variables, matrix inversion becomes a bottleneck $\mathcal{O}(v^3)$
  - Many observations, matrix multiplication goes $\mathcal{O}(nv)$
  - Solution=>Gradient descent (Reach global optimum for OLS)

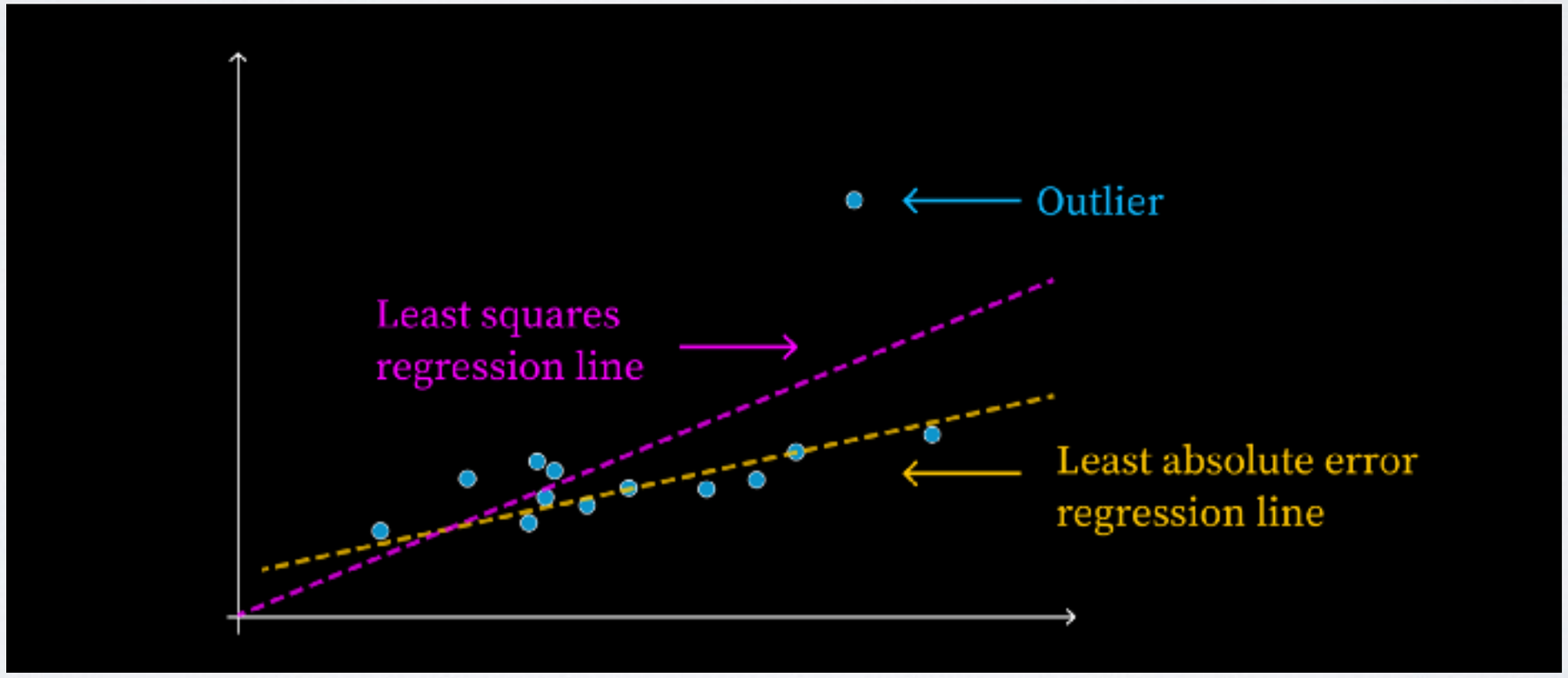
# OLS OPTIMALITY

- If some conditions are respected, OLS is **optimal** to solve the problem. No other method can outperform it.
  - The problem is that these conditions are not realistic for many real problems

- OLS conditions for optimality
  - Relations between features and targets are <u>really</u> linear
  - All necessary features are present, and all present features are necessary

# OLS KNOWN WEAKNESS

- MSE is known to be sensitive to outliers



# NON-LINEAR REGRESSION:

# DECISION TREE REGRESSION

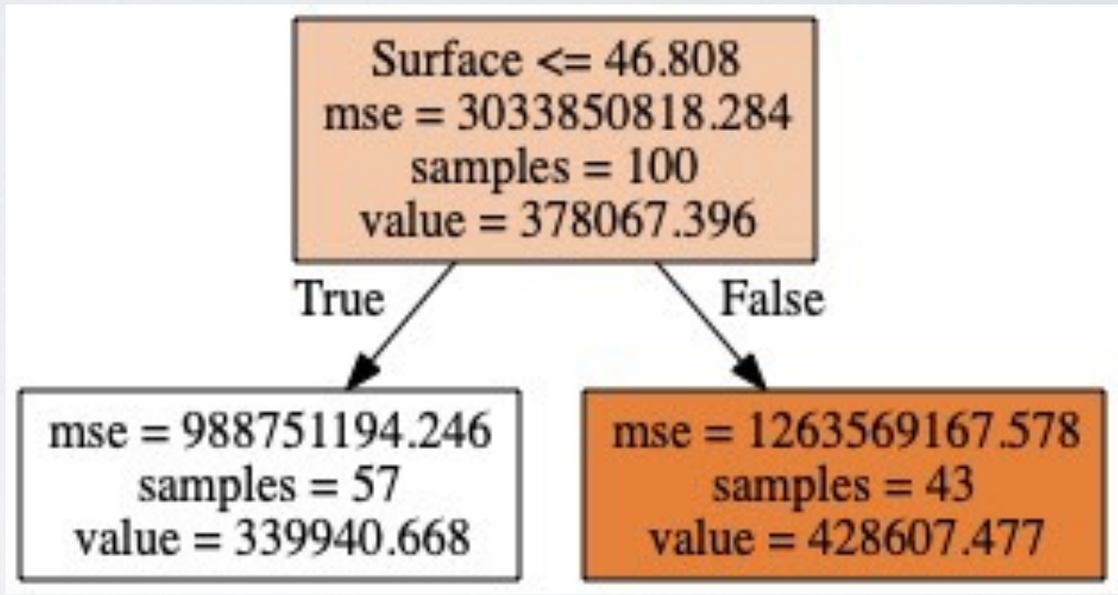
# DECISION TREE

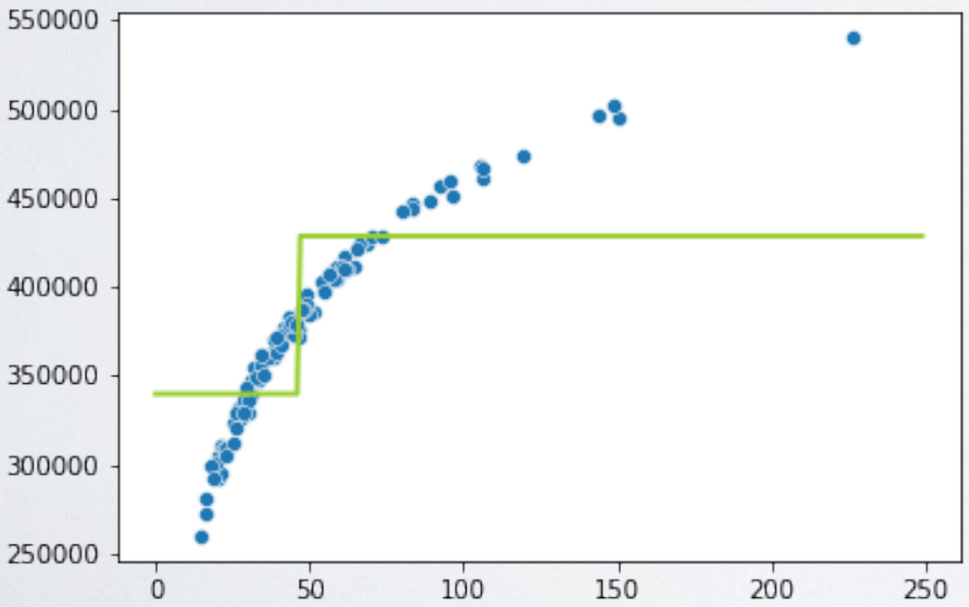
- Decision tree is a simple yet powerful way to do machine learning.

- Meta-algorithm:
  - Recursively split the data in 2 groups of items, based on a chosen attribute, so that elements in the same group have as close target values as possible
  - Predict that the value of a new item is the same as those of the group it belongs to.

# DECISION TREE

- Ex: Using
  - MSE as split criteria
  - 1 Level of splitting

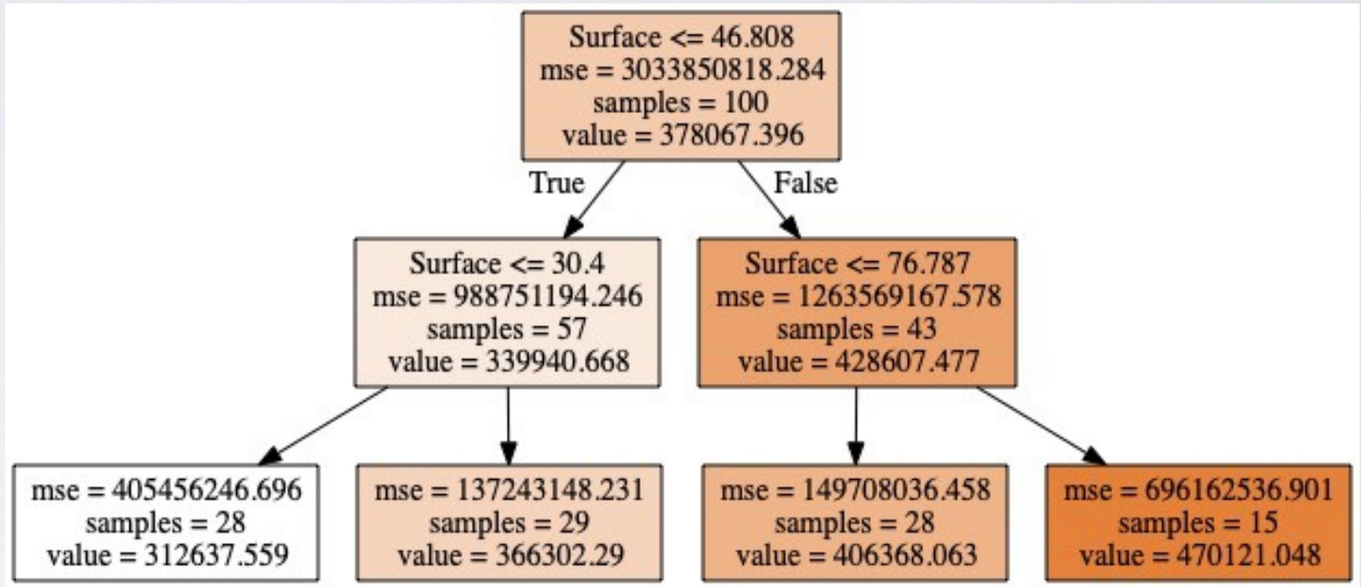


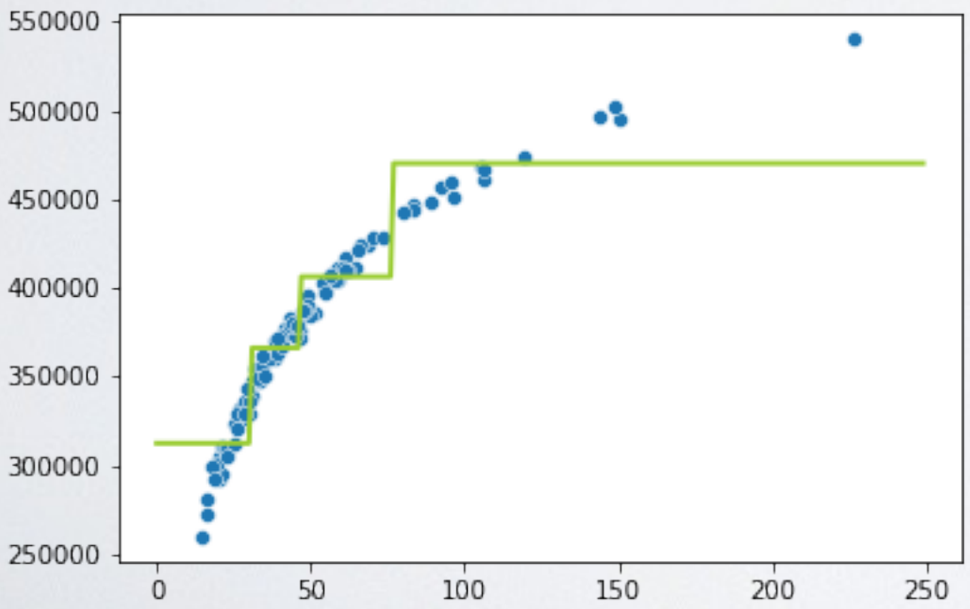




```
MSE 1106922922.7787206
RMSE 33270.45119589935
MAE 27836.40899704275
R2 0.6351425995939648
```

# DECISION TREE

- Ex: Using
  - MSE as split criteria
  - 2 Level of splitting

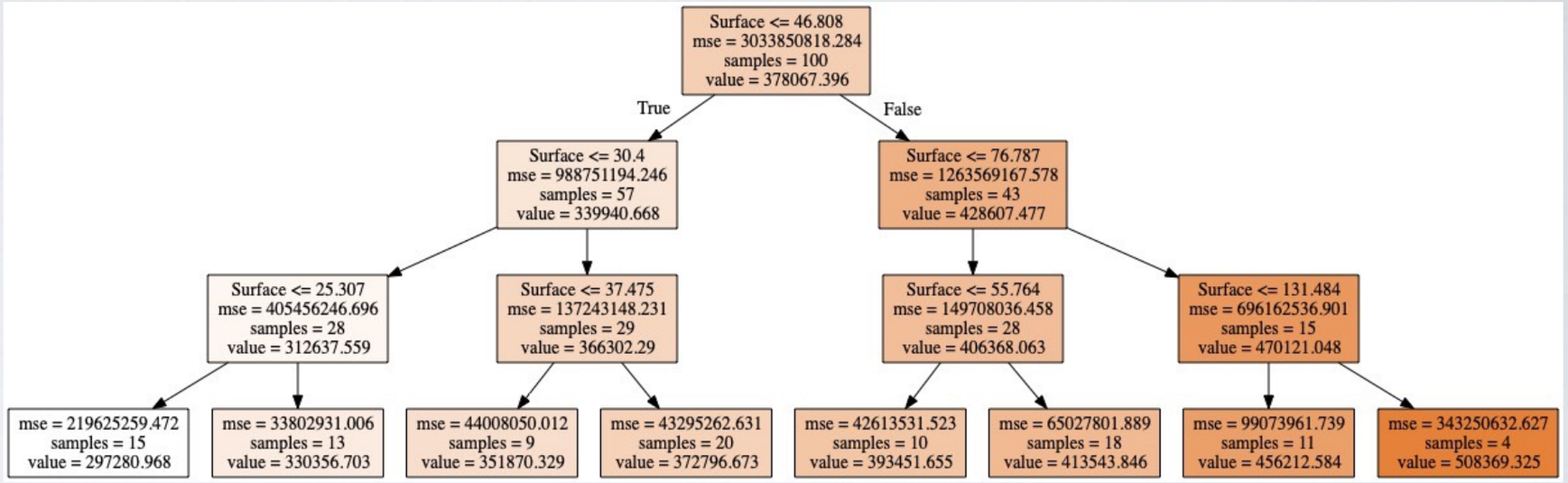


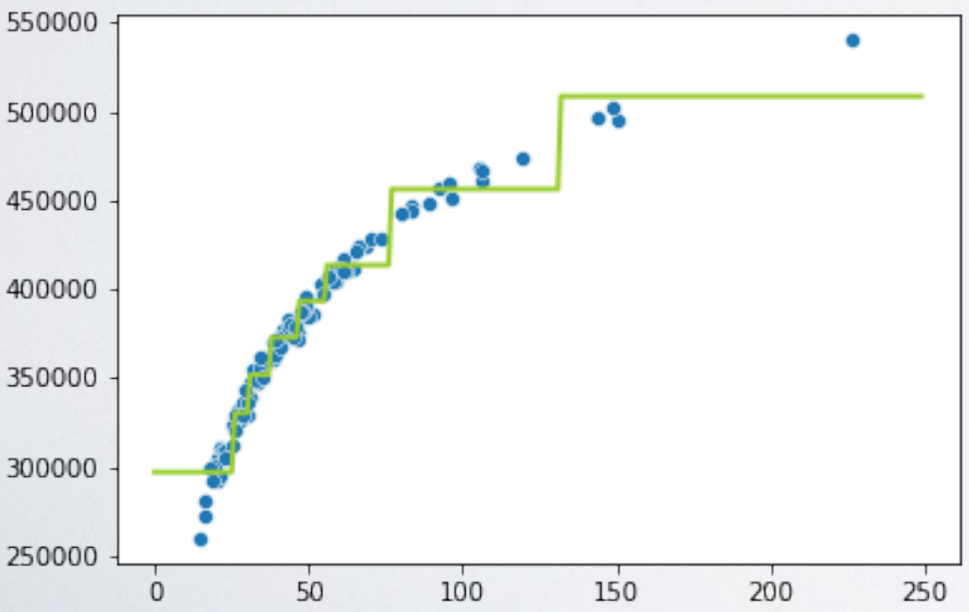




```
MSE 299670892.805488
RMSE 17311.00496232059
MAE 13262.652619929546
R2 0.901224490634346
```

# DECISION TREE

- Ex: Using
  - MSE as split criteria
  - 3 Level of splitting

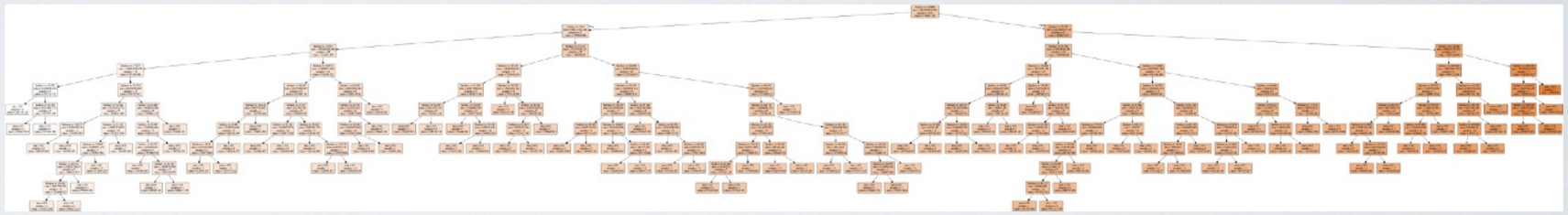


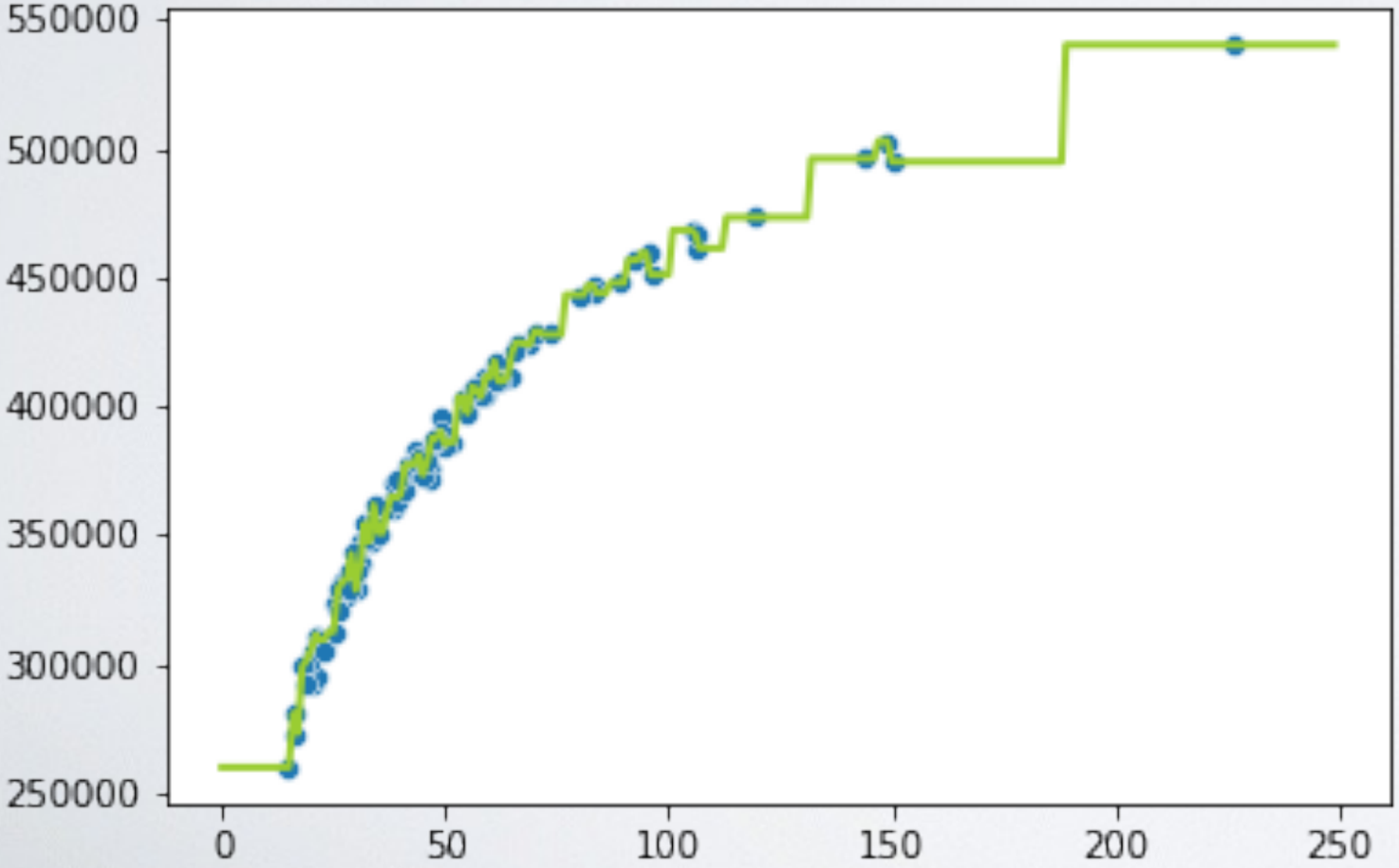




MSE 90552465.56733872
RMSE 9515.905924678886
MAE 7434.910779663157
R2 0.970152630768257 3

# DECISION TREE

- Ex: Using
  - MSE as split criteria
  - 10 Level of splitting





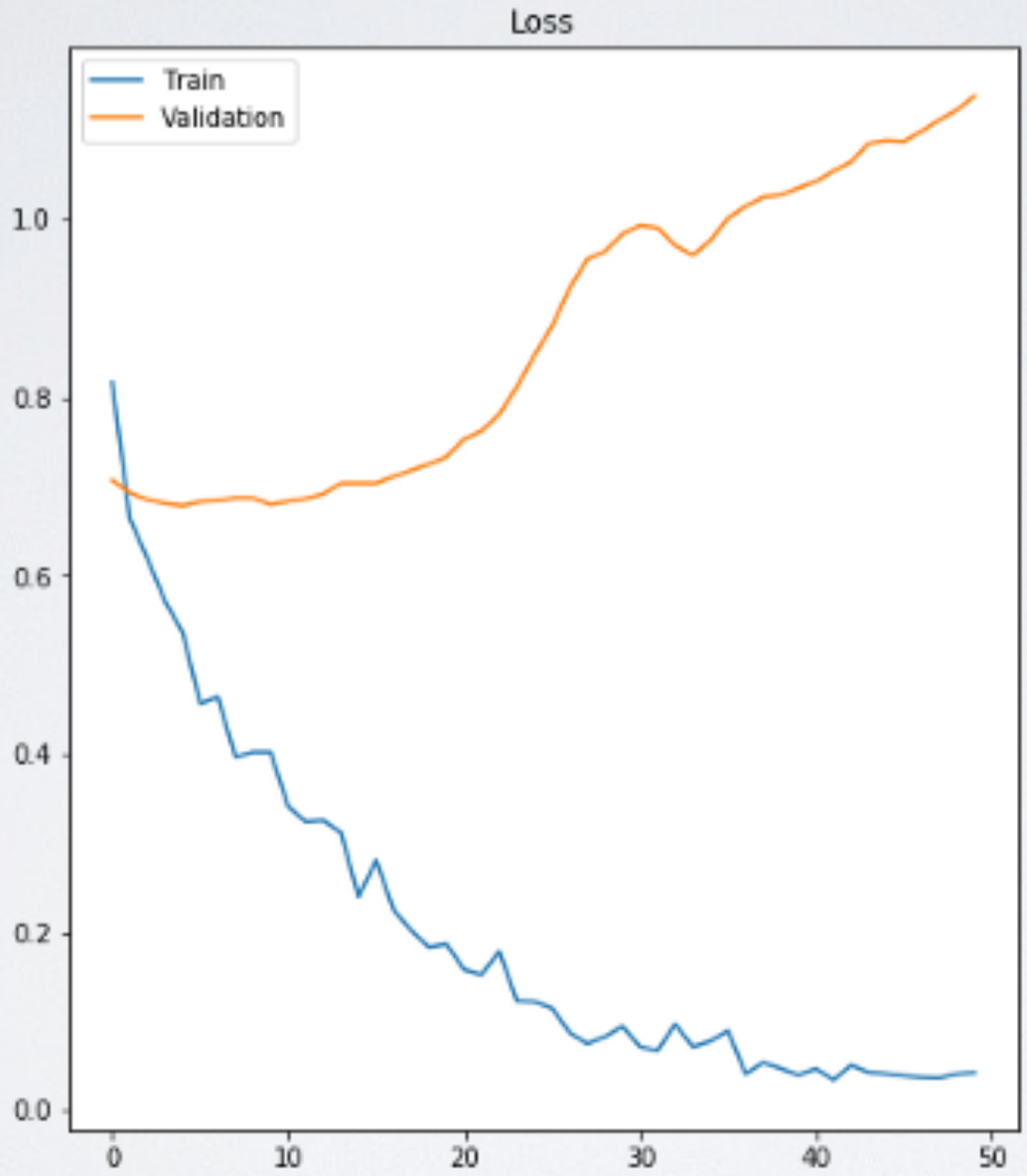

```
MSE 0.0
RMSE 0.0
MAE 0.0
R2 1.0
```

# MACHINE LEARNING: SOLVED

# OR IS IT ?

# OVERFITTING…

# OVERFIT SIGN: EMPIRICAL




Training steps/model complexity

# AVOIDING OVERFIT

- The most important rule of machine learning
  - And essential part of the scientific process

- Predicting what you already know is cheating
  - Even if you genuinely try not to cheat, you can cheat unintentionally
  - Experimental scientific experiments are done in **double blind:**
    - Neither the tested subject **nor the experimenter** know the placebo from real pill

- You must hide a **test set**, that you will **never** use when learning, and that you will **only use once**, for evaluating.

# AVOIDING OVERFIT

- When your data is ready, before any learning, split your data into:
  - A **training** set
  - A **test** set

- You can train as many methods with as many parameters as you want on the training set.

- Only when all your models are trained, you can evaluate them on the test set
  - You can never, ever reuse that (exactly same) test set.

# AVOIDING OVERFIT

| | Decision Tree, **levels=10** | Decision Tree, **levels=5** |
|---|---|---|
| Scores on Train Set | MSE 0.0<br>RMSE 0.0<br>MAE 0.0<br>R2 1.0 | MSE 9675372.95170697<br>RMSE 3110.5261535159884<br>MAE 2364.5552169188454<br>R2 0.996810860674691 8 |
| Scores on Test Set | MSE 60522590.58807978<br>RMSE 7779.626635519199<br>MAE 6427.594619486819<br>R2 0.968984922491333 6 | MSE 47482936.48734139<br>RMSE 6890.786347532579<br>MAE 5748.307144423111<br>R2 0.975667152691510 4 |

# TRAIN/**VALIDATION**/TEST

- In some cases, you need to see the results on the test set to know how to improve your prediction
  - Ex: how many levels in my decision tree? The right level is the one with the best results on the test set.
  - More generally: *hyperparameter tuning*.
    - If my learning method has parameters, how to fix those parameters? (Coefficient of learning, number of layers in deep NN, etc.)

- => Solution:
  - Use a **validation set** for intermediary steps (hidden like test set, but not for final evaluation)
    - You can do whatever you want with your validation set, it's part of your training process
  - Keep a test set, that you will use only once at the end

# TRAIN/TEST SPLIT

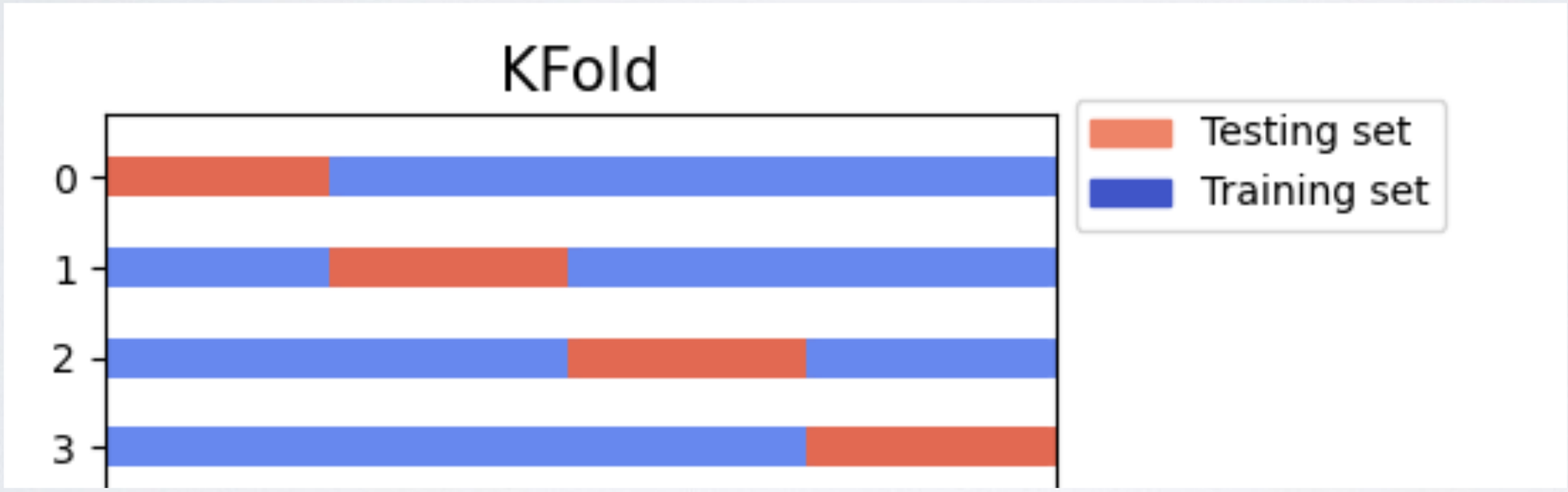
- What size should your test set have?
  - No good answer. 80% Train, 20% Test is often a default choice

- Rule of thumb:
  - You need enough data for training. If your problem is simple (few features…) and you have many examples, then a random sample of 5% of it can be enough

- Problem is if data is scarce
  - =>Cross validation

# CROSS VALIDATION

- General idea: From your data, create 10 datasets, each using 90% of the data as train and 10% as test/validation



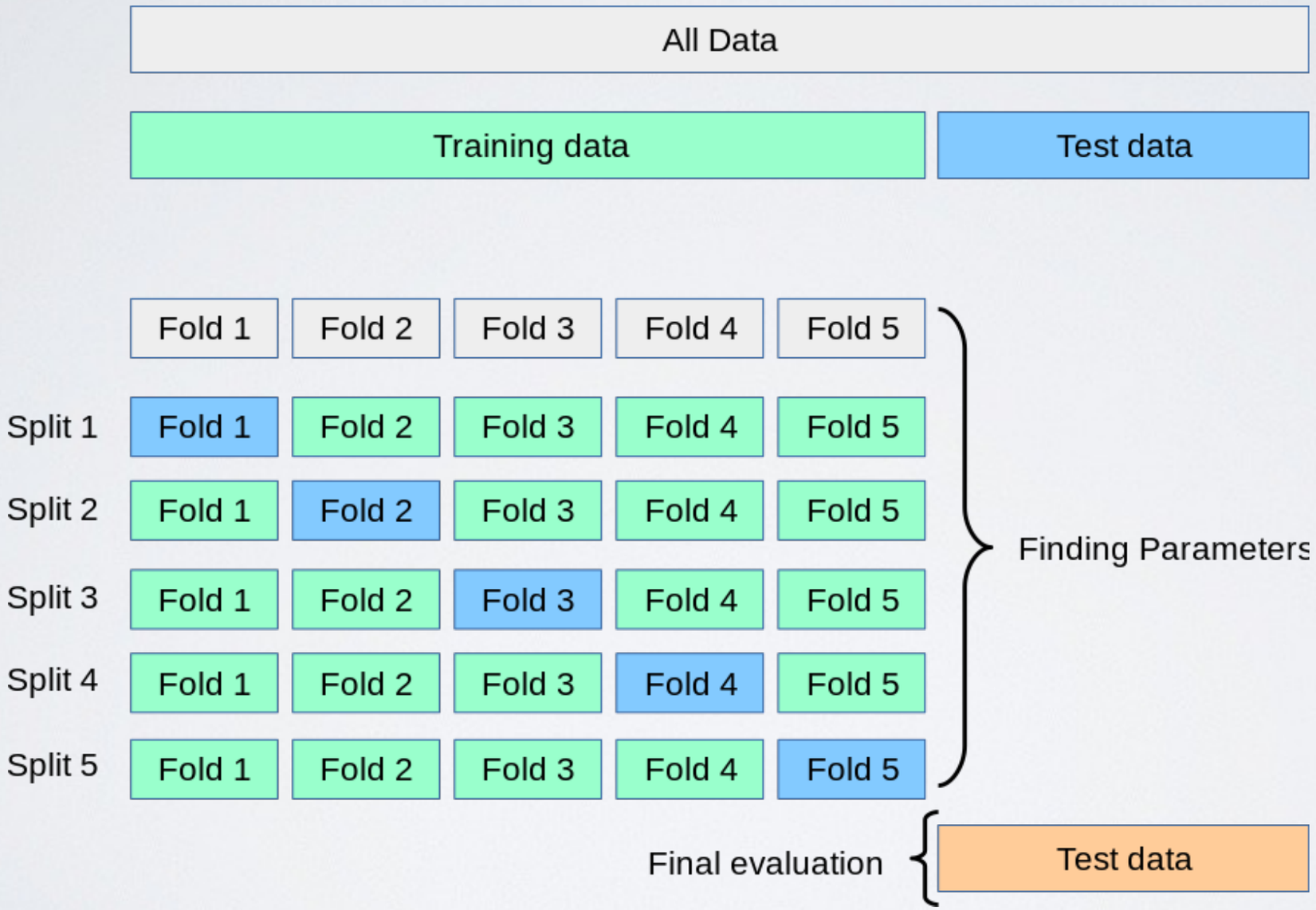
# CROSS VALIDATION

- Usage 1: small dataset
  - If you have too few data to put 33% aside for a test set:
    - Use only, e.g., 10% for the test set
    - But creates 10 train/test sets, each with different test sets
    - Then, compute the average scores over the 10 sets

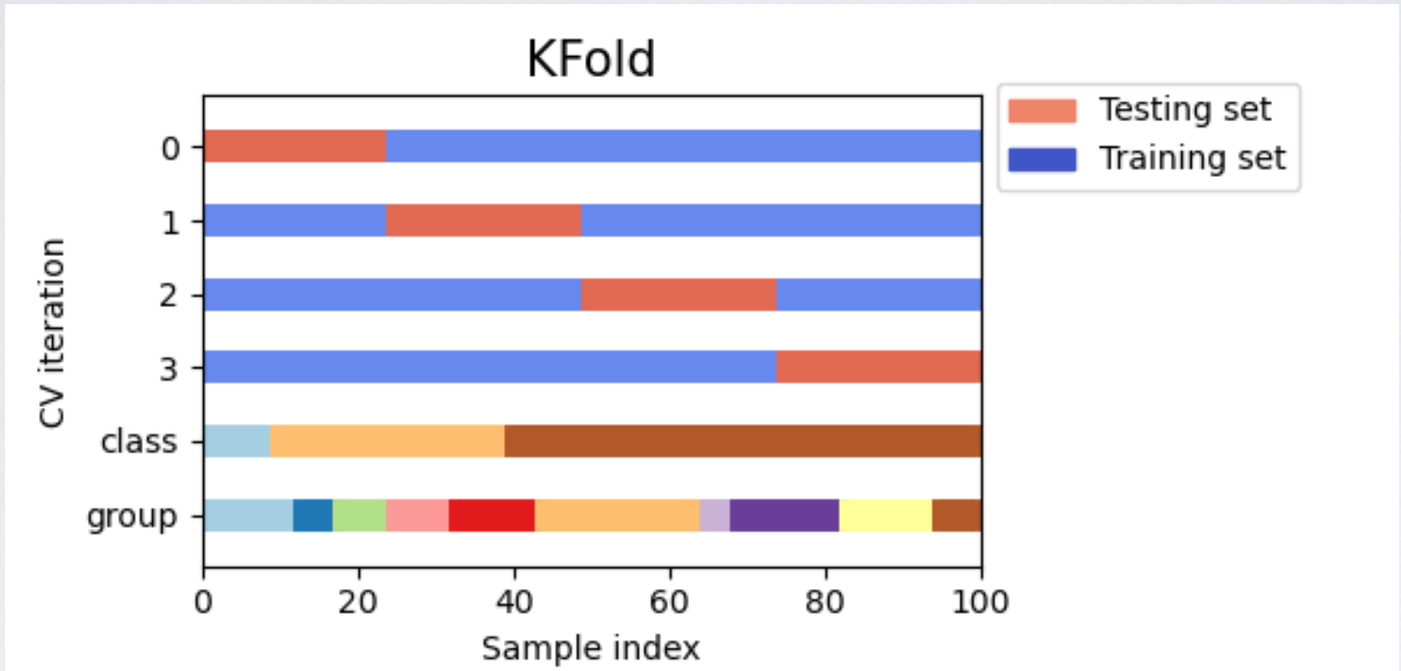
- Usage 2: Robustness and variability
  - By running several times the test, you can check that you were not just "lucky" with your test set
  - You can report the variance of the score

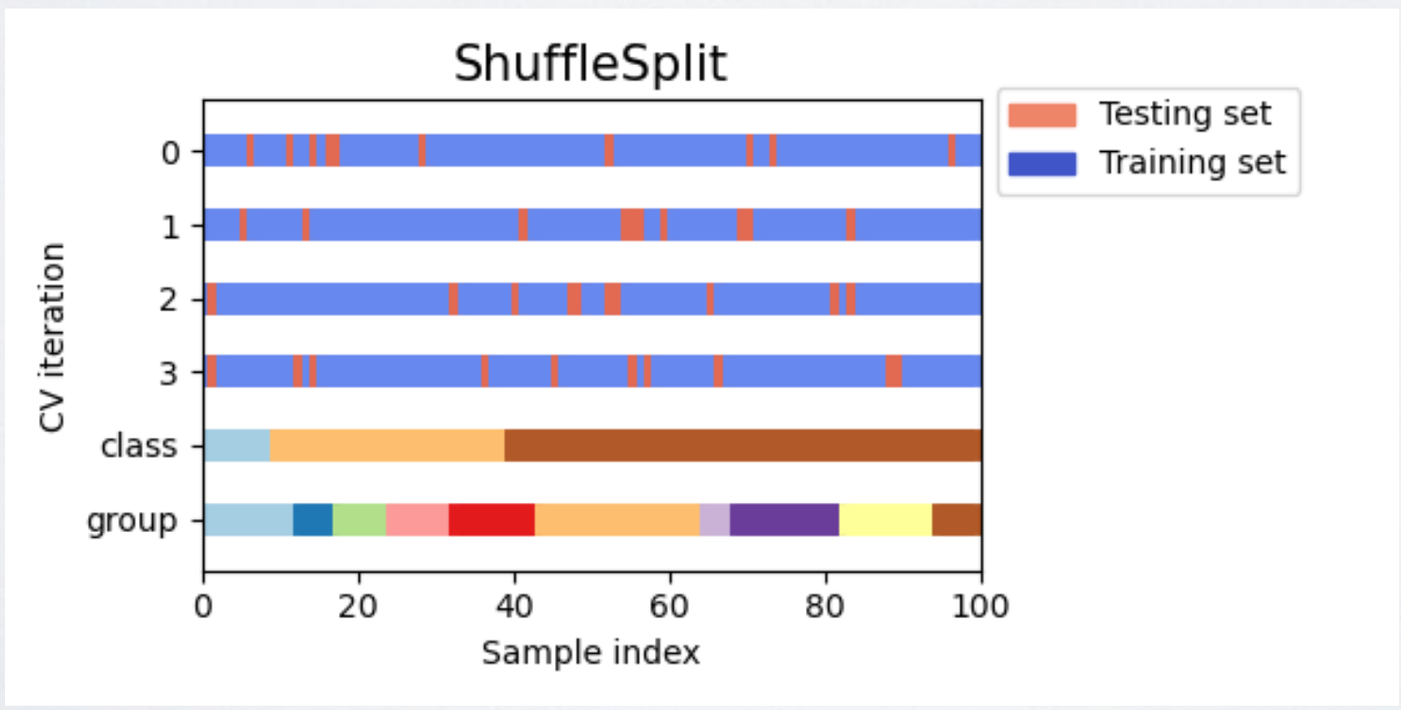
- Usage 3: as validation set

# CROSS VALIDATION

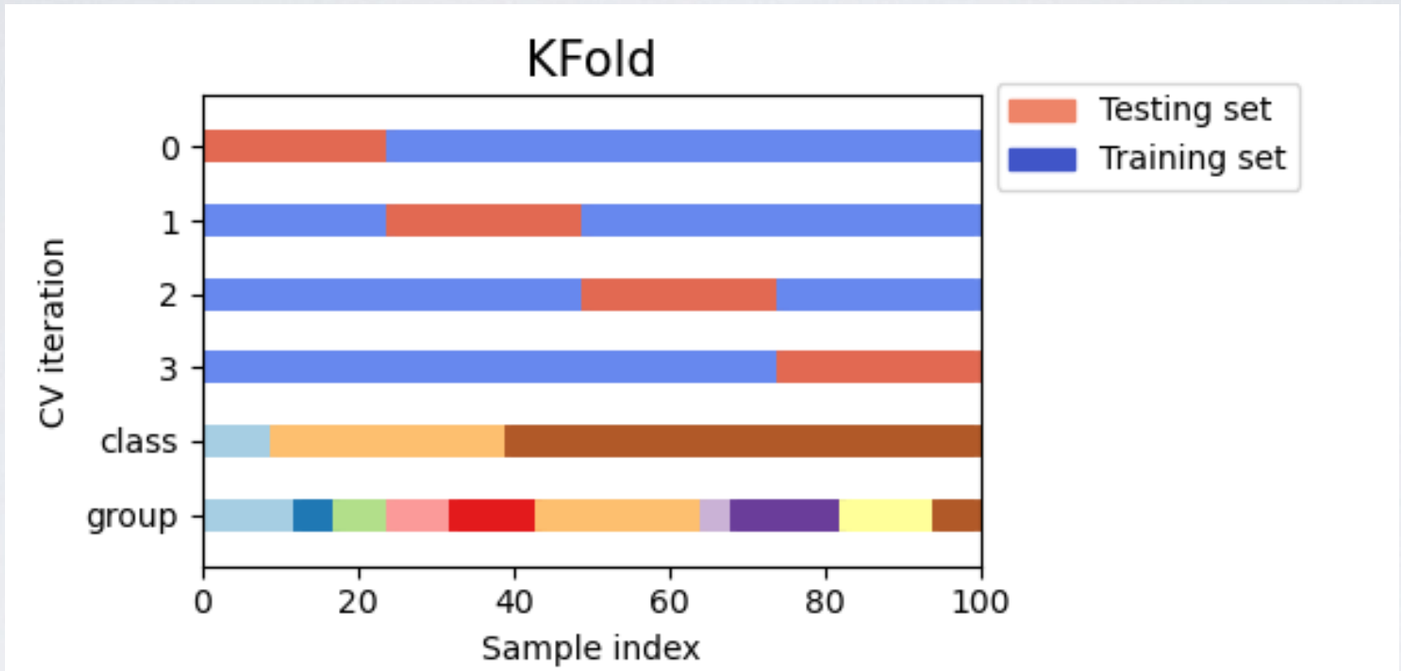


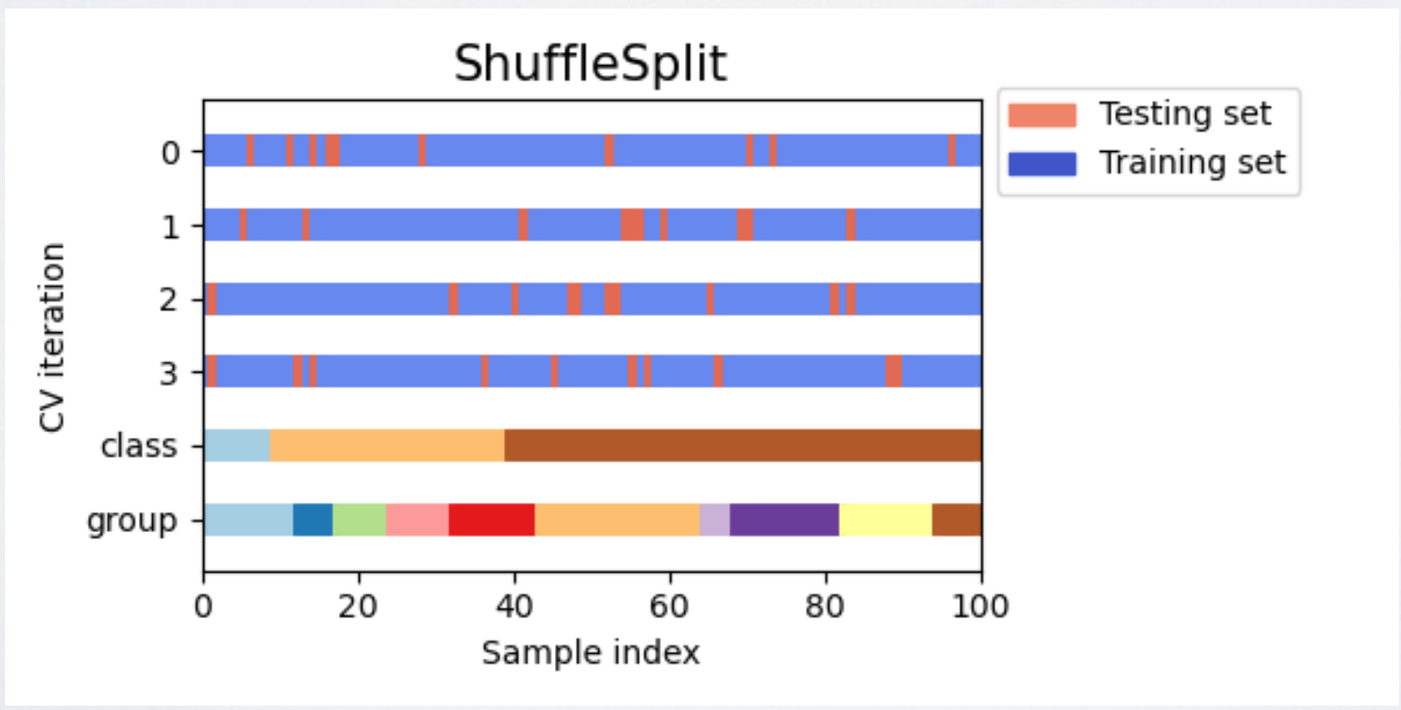
# CROSS VALIDATION



# CROSS VALIDATION

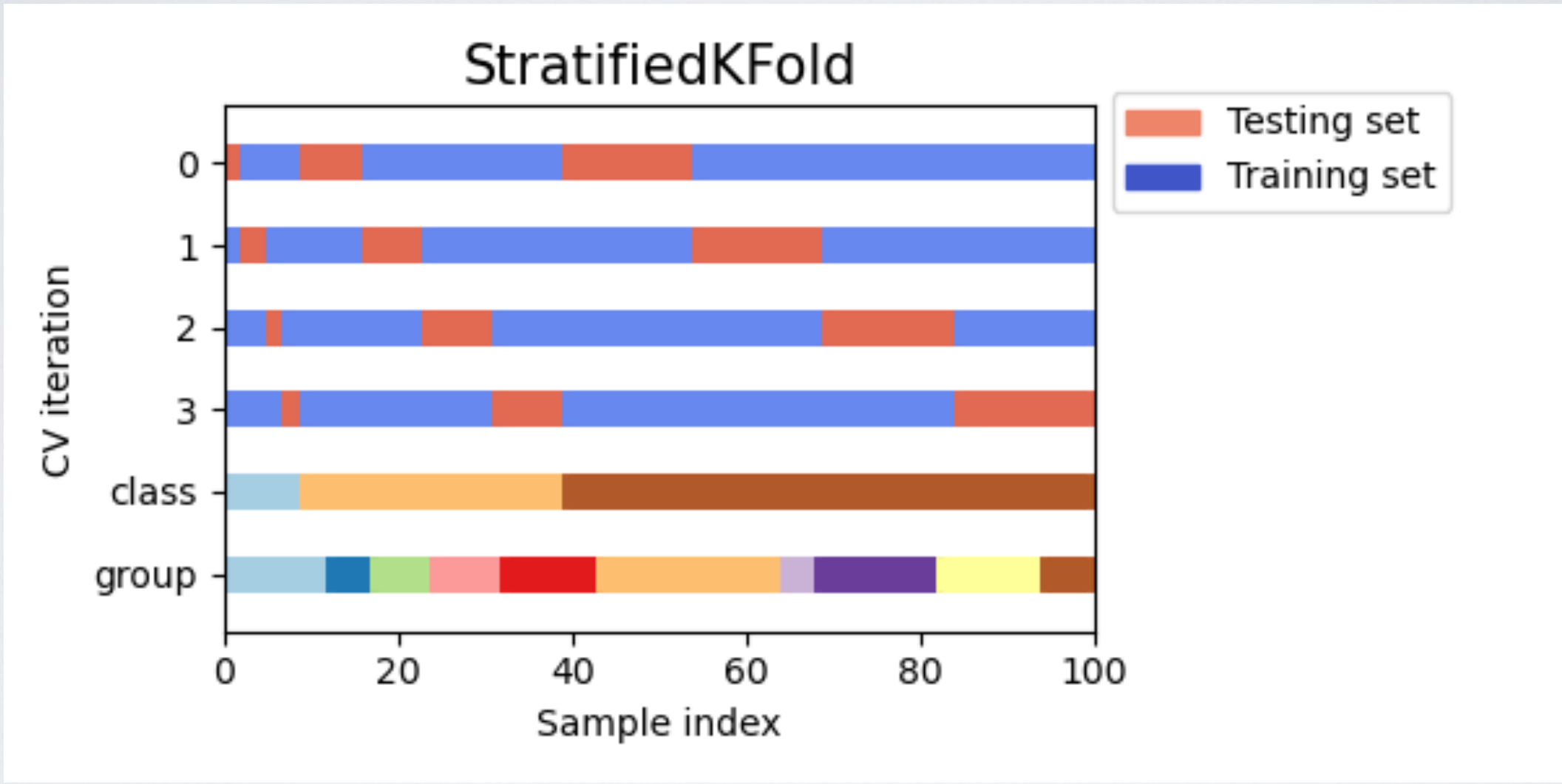


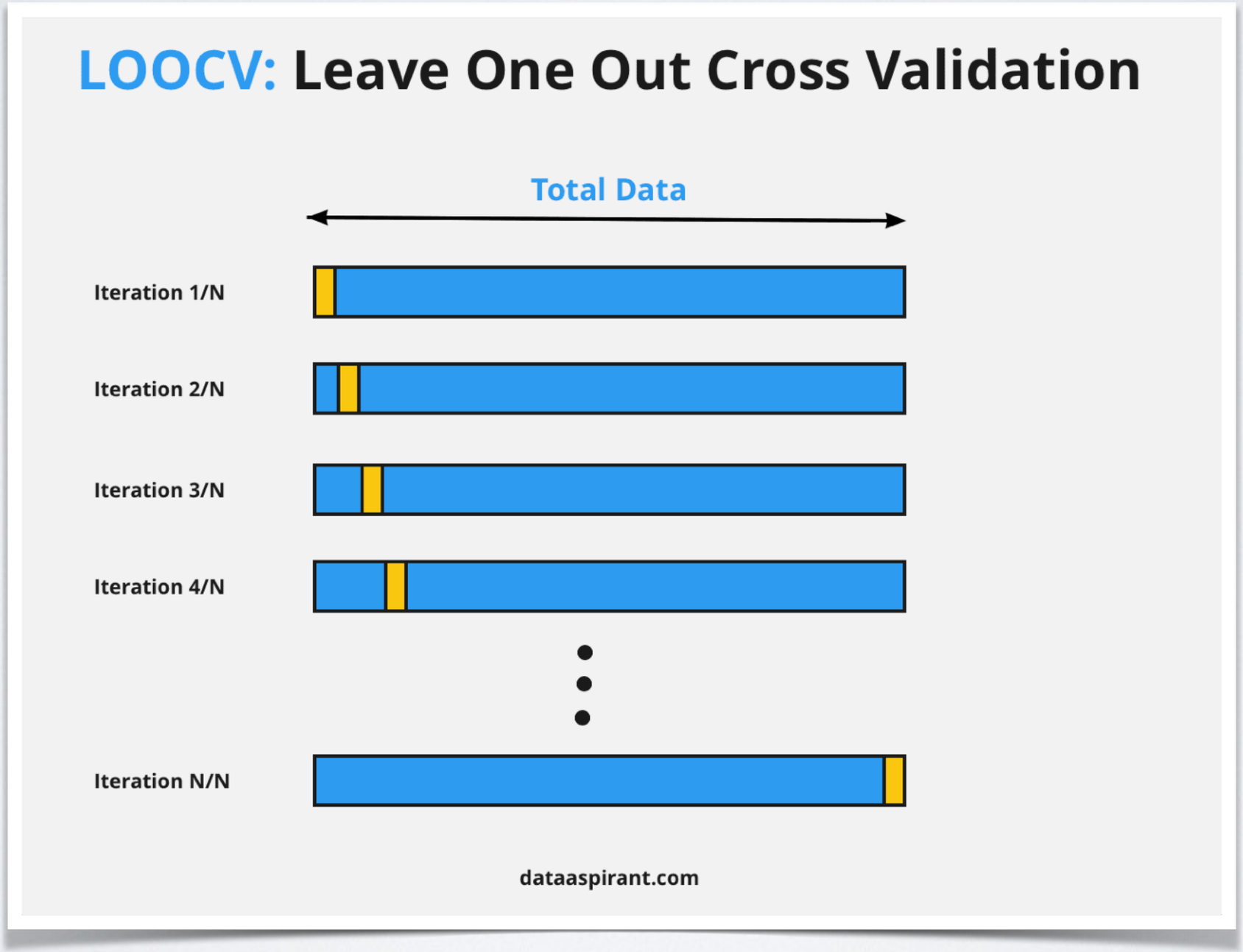
# STRATIFIED K-FOLD

- Variant in which you take into account the target classes
  - In a classification problem, your test set might have more elements of one class, just by chance
    - In particular if strong class imbalance
    - Think of a rare class, that might not be present in a random test set

# CROSS VALIDATION



# CROSS VALIDATION



# FIGHTING OVERFIT

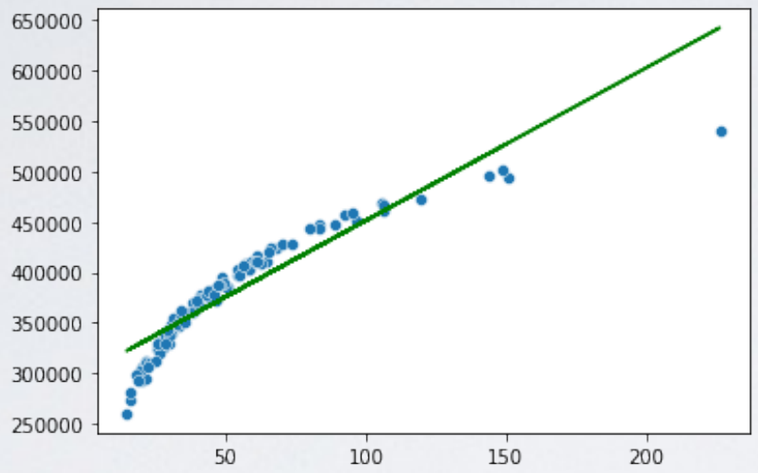
# BACK TO THE METHOD

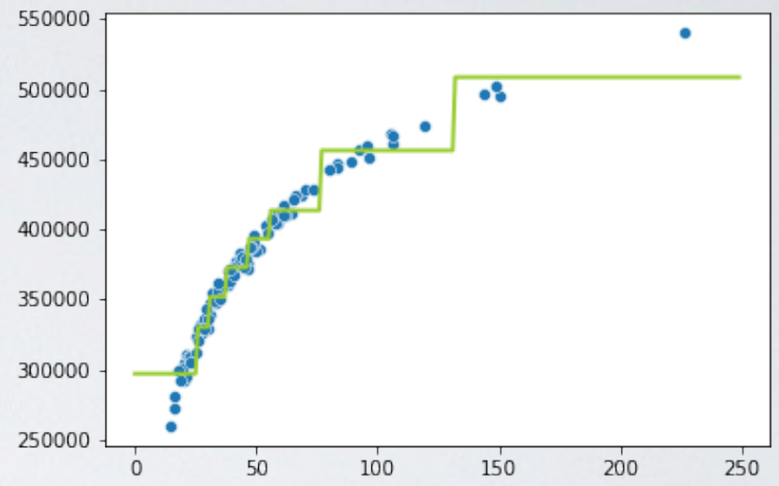
# FIGHTING OVERFIT

- Implicit limit to overfit:
  - Because a method has a limited power of expression, it cannot overfit "too much".
    - Trivial solution: each point has its own prediction. No **generalization**
  - =>A linear regression method cannot overfit to the trivial solution, unlike decision tree
    - Unless there are enough variables…

- Explicit limit to overfit:
  - The method is not limited in its power of expression, but contains a safeguard against overfit (Regularization)

# FIGHTING OVERFIT



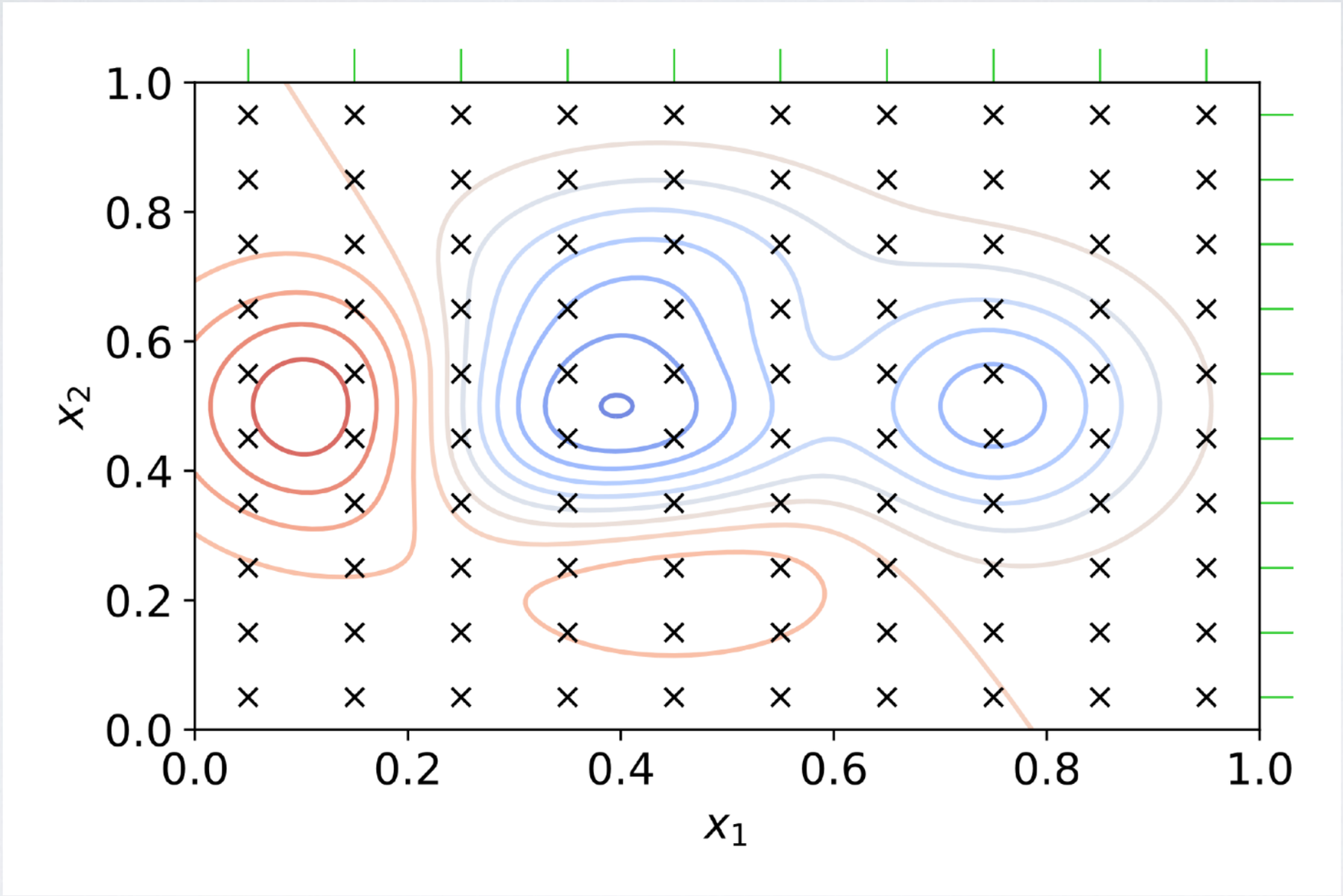

| | | |
|---|---|---|
| Train | MSE 474131230.6072998<br>RMSE 21774.554659218633<br>MAE 16958.426496791166<br>R2 0.843719662235890**5** | MSE 9675372.95170697<br>RMSE 3110.5261535159884<br>MAE 2364.5552169188454<br>R2 0.996810860674691**8** |
| Test | MSE 297361867.9984524<br>RMSE 17244.18359907051<br>MAE 14666.202886910516<br>R2 0.847615554878275**9** | MSE 47482936.48734139<br>RMSE 6890.786347532579<br>MAE 5748.307144423111<br>R2 0.975667152691510**4** |

# FIGHTING OVERFIT

- Avoiding overfit in decision trees: Pruning strategies
  - One way to see: Artificially limit the expressivity of the model
  - 1)Limit the number of levels (Simple but naive)
  - 2) Limit the number of leaves
    - =>Split nodes in priority where it improves the most
  - 3) Limit the size of leaves
    - => Explicitly forbids the naive solution

- Hyperparameter tuning/optimization
  - Typical approach: Grid search.
  - Fix a set of possible parameters. Test all possibilities on a validation test

# GRID SEARCH




More clever methods exist: Bayesian optimization, etc.

# NOTE: GENERALIZATION

- A very important notion in machine learning is Generalization
  - Can we extract generic principles underlying our data?
  - Can we generalize our observations to unseen cases?

- Linear regression can predict an unseen value, while decision tree cannot.
  - Alcohol in wine example:
    - we know how alcohol degree in wines correlates with summer temperatures today
    - Can we make predictions for the next 50 years, when we will encounter never seen summer temperatures ? (Linear regression: yes. Decision tree: no)