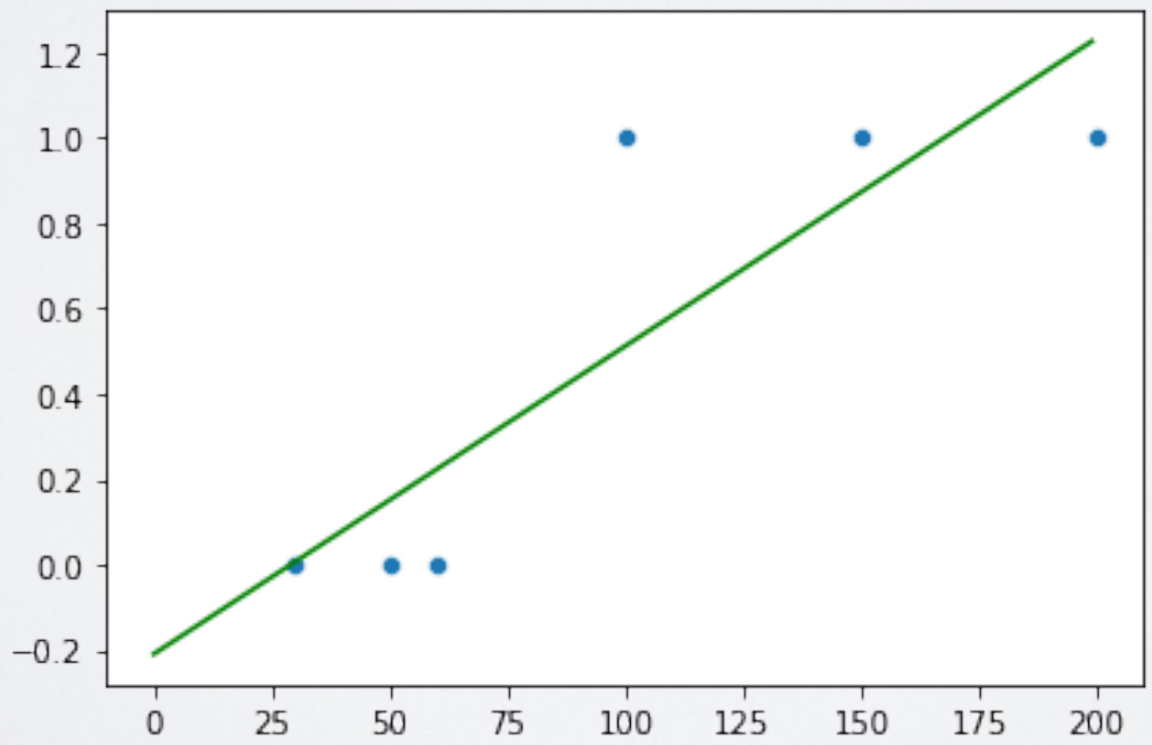
CLASSIFICATION

CLASSIFICATION

- Objective: predict the class of an item
- Methods for regression can be reused with some adaptations
  - Binary Classification is usually simple
  - Multiclass Classification might require more changes
- Evaluation is different

LINEAR CLASSIFICATION

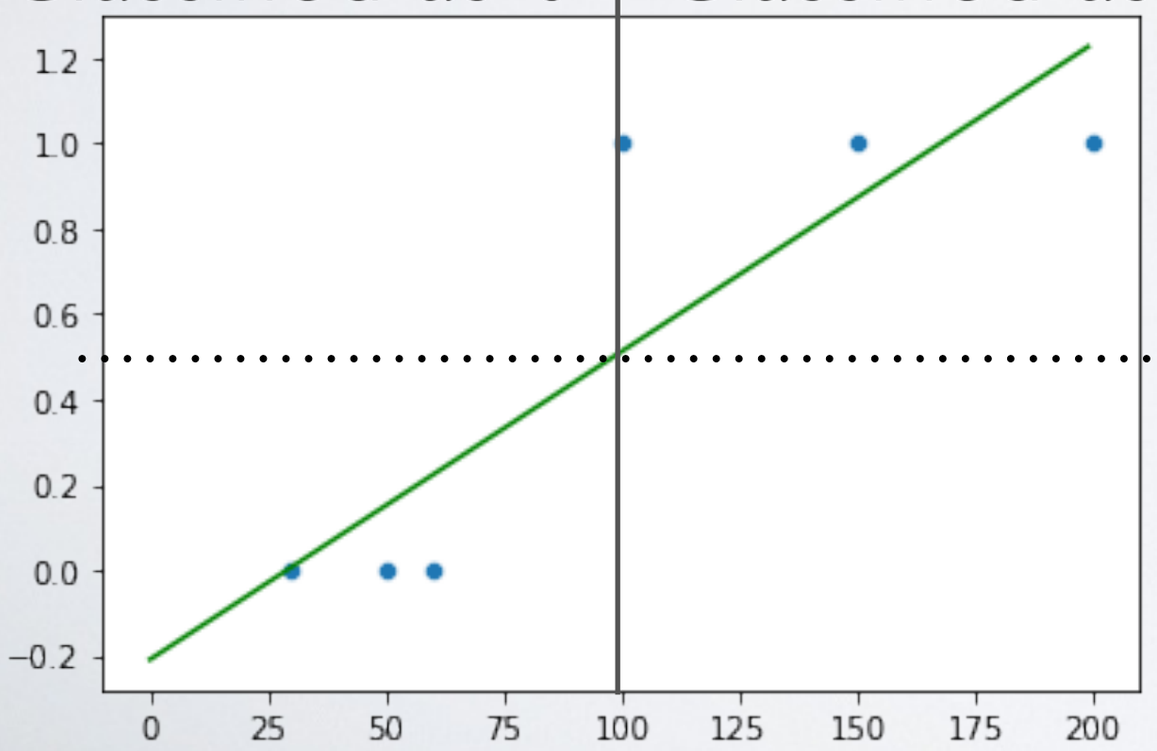
- We can easily adapt linear regression
- Imagine a 1 feature example:
  - We want to classify between apartments and houses
  - Our (unique) feature is dwelling surface



LINEAR CLASSIFICATION

- We can easily adapt linear regression
- Imagine a 1 feature example:
  - We want to classify between apartments and houses
  - Our (unique) feature is dwelling surface

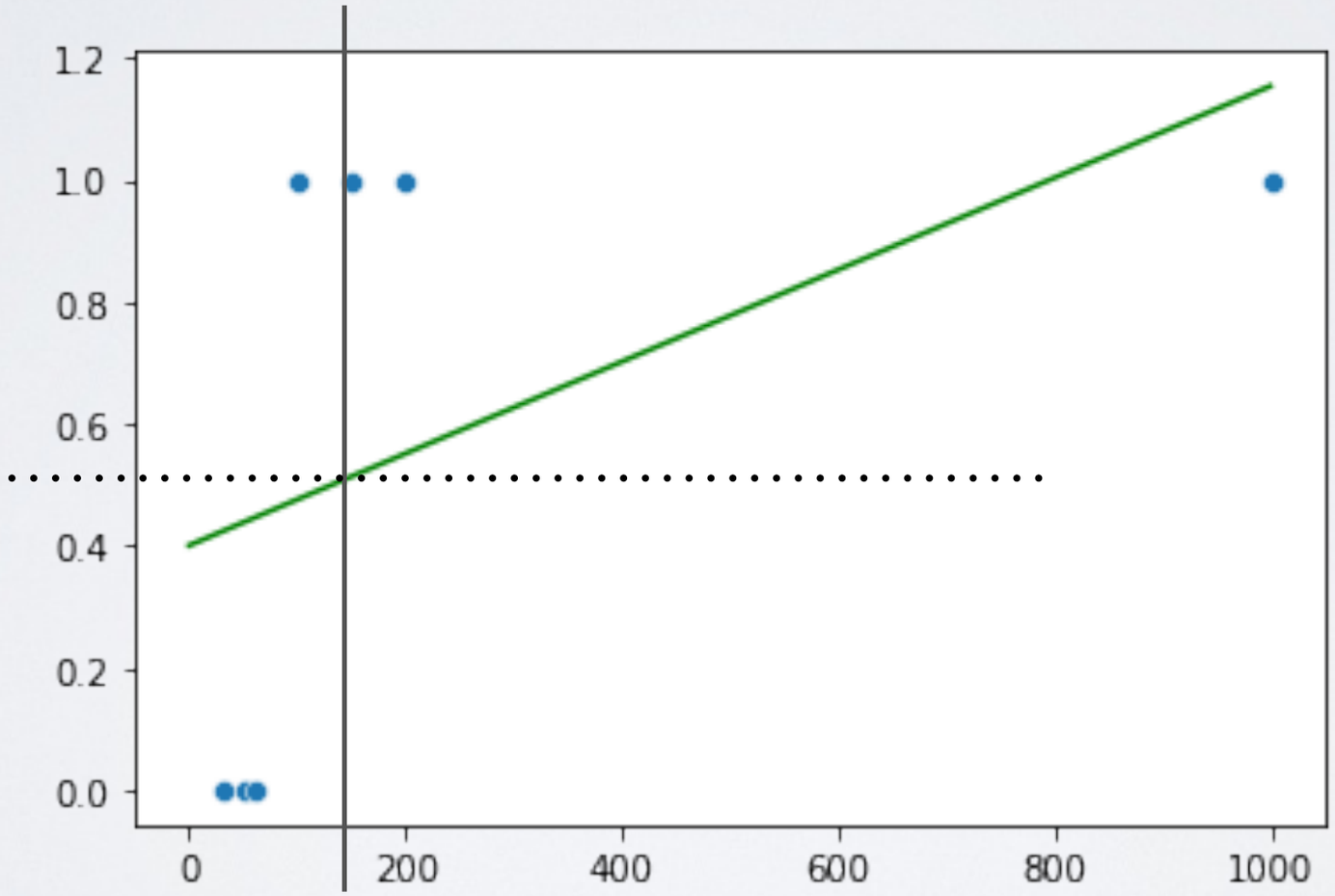
Classified as 0 | Classified as 1




```
MSE 0.0636152055857253 8
RMSE 0.252220549491363 6
MAE 0.205068528575122 92
R2 0.745539177657098 5
```

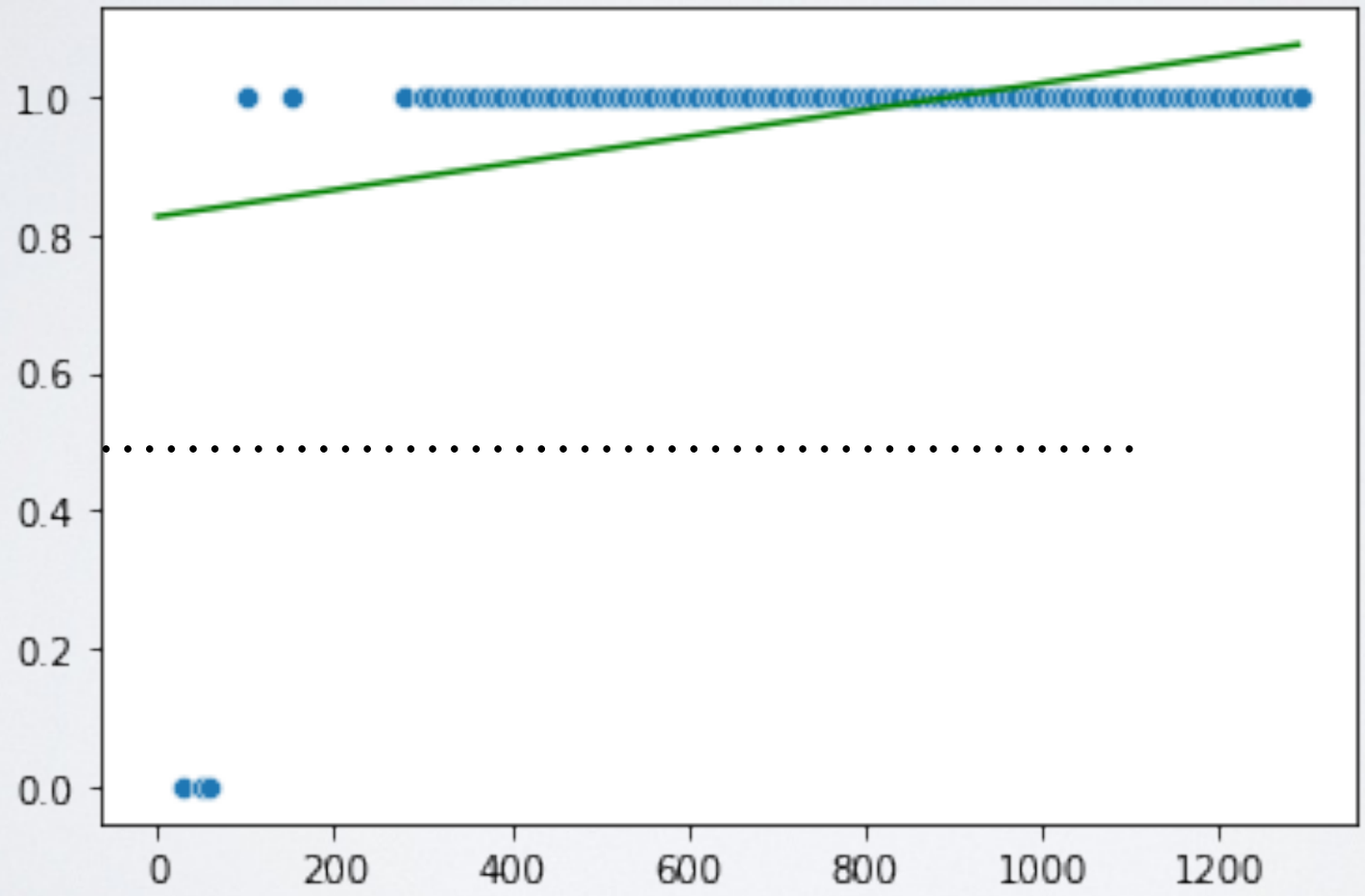
LINEAR CLASSIFICATION

- Weaknesses: Outliers



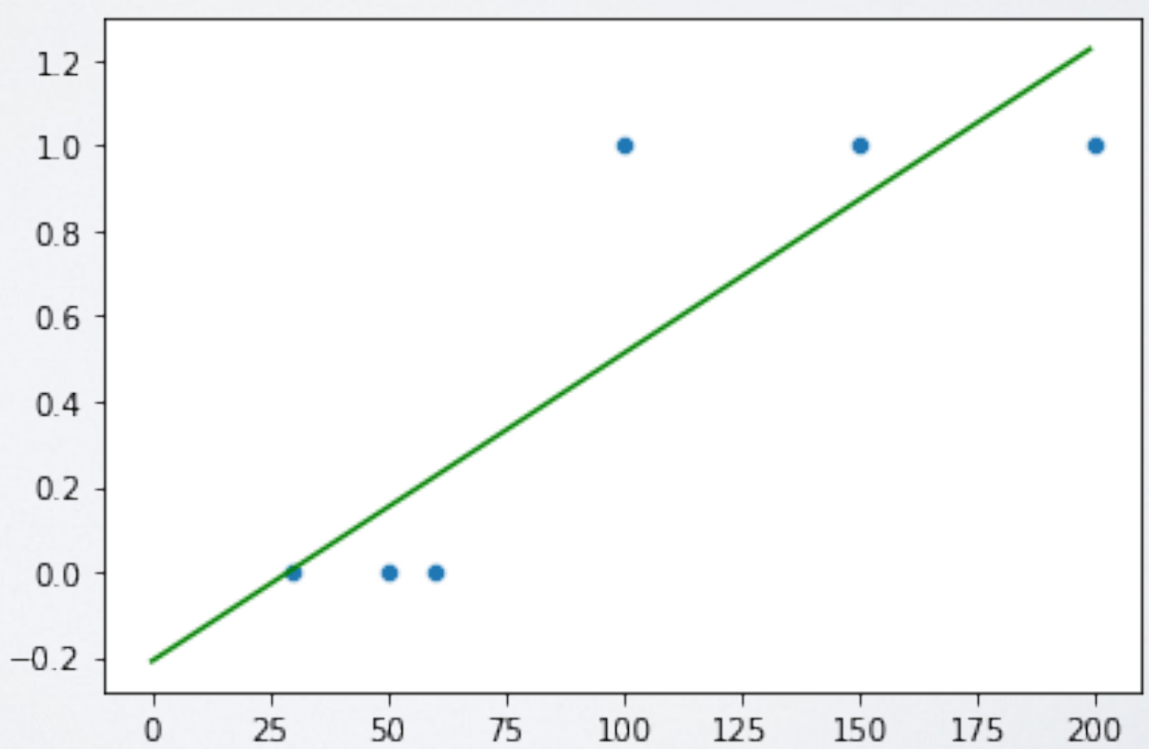
LINEAR CLASSIFICATION

- Weaknesses: Class imbalance

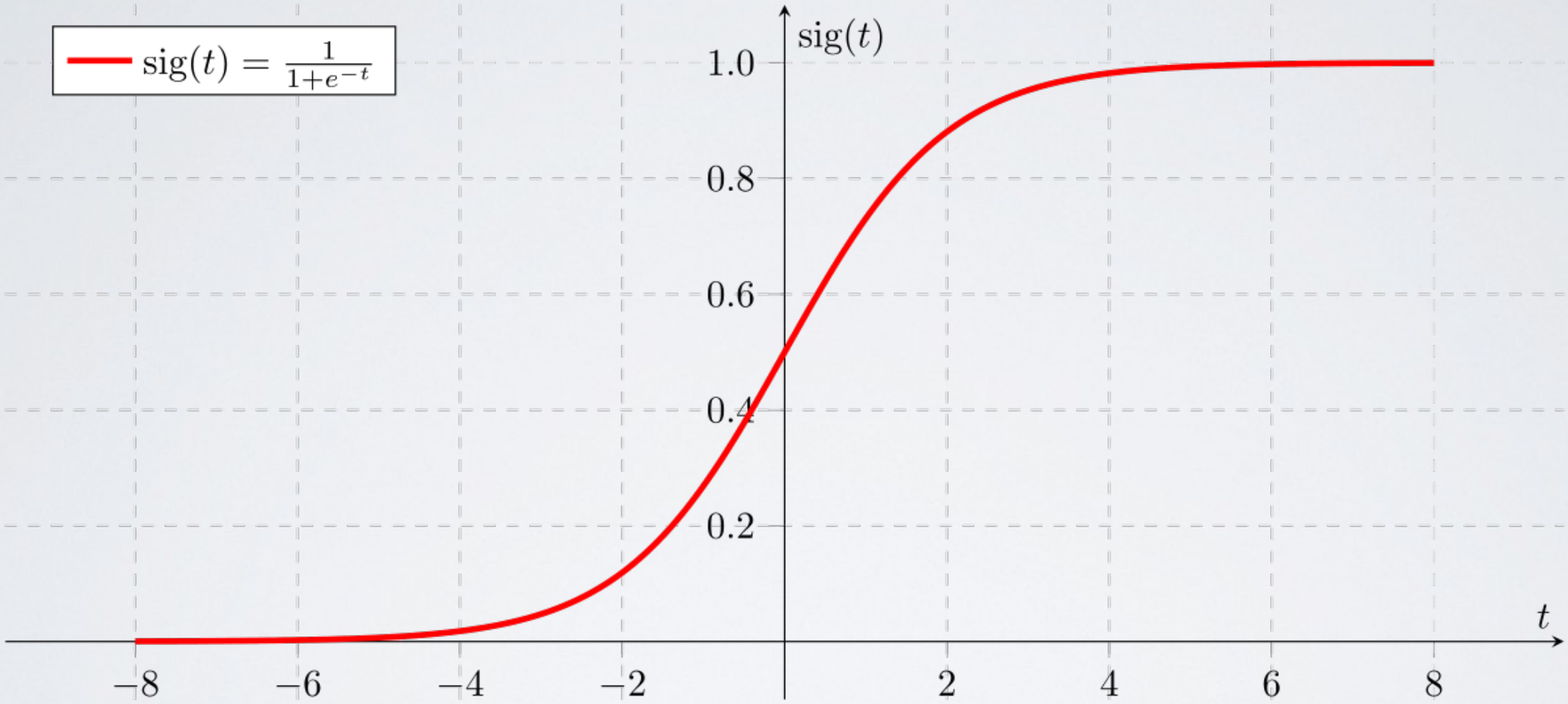


LINEAR CLASSIFICATION

- More generally, inadapted objective:
  - The relation is not linear
  - We minimize a cost function (MSE) which is not meaningful:
    - Some predictions go *beyond* possible values (prediction less than 0 or more than 1 adding error



SIGMOID/LOGISTIC FUNCTION



$$\lim_{t \to -\infty} sig(t) = 0 \qquad \lim_{t \to +\infty} sig(t) = 1 \qquad sig(0) = 0.5$$

LOGISTIC REGRESSION

Logisitic (Sigmoid) function:

$$Sig(x) = \frac{1}{1 + e^{-x}}$$

Linear regression:

$$\hat{y} = \beta_0 + \beta_1 x_i + \beta_2 x_2 + \ldots + \beta_n x_n$$

Logistic Regression:

$$P(y = 1) = Sig(\beta_0 + \beta_1 x_i + \beta_2 x_2 + \ldots + \beta_n x_n)$$

$$P(y = 1) = \frac{1}{1 + e^{-\beta_0 + \beta_1 x_i + \beta_2 x_2 + \ldots + \beta_n x_n}}$$

LOGISTIC REGRESSION

$$P(y=1) = \frac{1}{1 + e^{-\beta_0+\beta_1 x_i+\beta_2 x_2+\ldots+\beta_n x_n}}$$

$$\frac{1}{P(y=1)} = 1 + e^{-\beta_0+\beta_1 x_i+\beta_2 x_2+\ldots+\beta_n x_n}$$

$$\frac{1-P(y=1)}{P(y=1)} = e^{-\beta_0+\beta_1 x_i+\beta_2 x_2+\ldots+\beta_n x_n}$$

$$\frac{P(y=1)}{1-P(y=1)} = e^{\beta_0+\beta_1 x_i+\beta_2 x_2+\ldots+\beta_n x_n}$$

$$ln(\frac{P(y=1)}{1-P(y=1)}) = \beta_0 + \beta_1 x_i + \beta_2 x_2 + \ldots + \beta_n x_n$$

LOGISTIC REGRESSION

$$\frac{P(y=1)}{1-P(y=1)} = e^{\beta_0+\beta_1 x_i+\beta_2 x_2+\ldots+\beta_n x_n}$$

probability to happen / probability not happening =>odds (FR: cote)

Get a 6 in a dice : odds = 1:5=0.2
Get a 5 or 6: odds = 2:4 =0.5
Get everything but a 1: odds = 5:1=5

LOGISTIC REGRESSION

/!\ multiplicative relation between variables

Interpretation as **odd ratios:**

$+1$in x_i =>odds multiplied by e^{β_i}

$$\frac{P(y=1)}{1-P(y=1)} = e^{\beta_0} e^{\beta_1 x_i} e^{\beta_2 x_2} (\dots) e^{\beta_n x_n}$$

https://christophm.github.io/interpretable-ml-book/logistic.html

MULTICLASS LOGISTIC REGRESSION

- In many cases, we have more than 2 classes
  - e.g.: {house, apartment, office, industrial}. {cat,dog,horse,…}
  - Categories are unordered=> conversion to numeric would be catastrophic
- Simple solution: one VS all
  - Train a logistic classifier on one class VS all other classes.
  - Pick the class with the largest confidence
    - e.g.: house: 20%. Apartment: 30%. Office: 70%. Industrial: 80%=>Industrial.
- Alternative approach: softmax regression

SOFTMAX

- Softmax is a generalization of Logistic/Sigmoid to Multiclass
  - Takes several outputs with arbitrary values $\in (-\infty, +\infty)$
  - Convert into a set of (positive) probabilities summing to 1.
- $$\sigma(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$
  - $\mathbf{z}$: vector of real numbers
  - Exponential convert Real into $(0, +\infty)$
  - Division by the sum normalizes (sum of values =1).

CROSS ENTROPY

- The usual loss function associated with softmax is the cross-entropy
  - We have an estimated probability $q(i)$ for each possible outcome i, we compare with the true distribution (one-hot encoding, $p(i) = 1$ for the true label)

- $H(P, Q) = -\sum_i p(i) \log q(i)$

- $H(P, Q) = -\log q(i)$ for i =True label

CLASSIFICATION WITH DECISION TREE

DECISION TREE

- Trees can be easily adapted to the classification task
  - It is even more natural than for regression

- The principle is to divide observations in term of **class homogeneity**
  - We want items in the same branch/leaf to belong to the same class

DECISION TREE

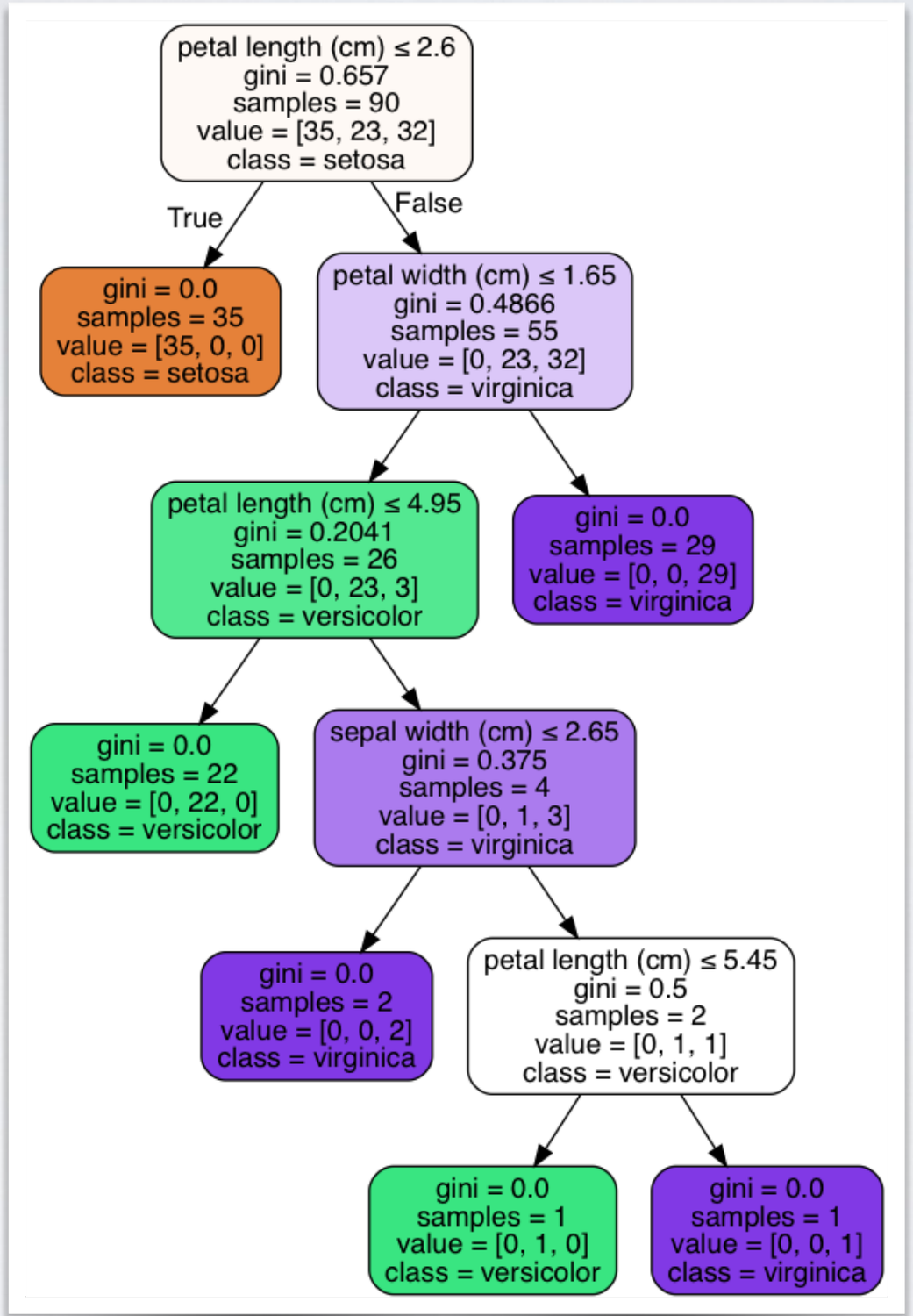
- Most common homogeneity/diversity/inequality/purity scores
  - Gini Coefficient: $1 - \sum_j p_j^2$
    - p_i: fraction of items of class i
    - Min: 0: 1 class only
    - Max: 0.5: (2 classes), 0.66(3classes), 0.75 (4classes), 0.875(8classes)

- Interpretation:
  - If we classify a random item randomly according to class distribution, it is the probability to be wrong.

DECISION TREE

- Most common homogeneity/diversity/inequality/purity scores
  - p_i: fraction of items of class i
  - Entropy: $-\sum_j p_j \cdot log_2 p_j$
    - Min: 0: 1 class only
    - Max: 1 (2 classes), 1.584(3 classes), 2 (4 classes), 3 (8 classes), etc.
  - Interpretation: average # of bits required to encode the information of the class of each item, using optimal coding

DECISION TREE



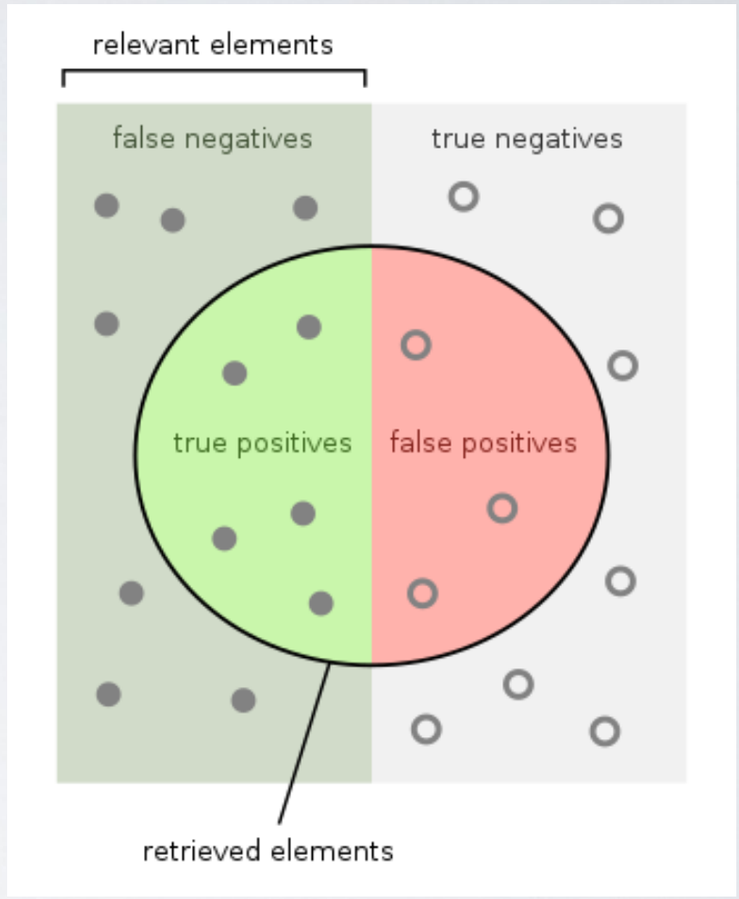
CLASSIFICATION EVALUATION

BINARY CLASSIFICATION

- Many scenarios require binary classification
  - Covid/not covid
  - Give a credit/do not give credit
  - Spam/not-spam
  - Postive sentiment/negative sentiment
  - Face on a photo/no face
  - Normal user/bot
  - Etc.

CLASSIFICATION: EVALUATION

		Actual	
		Positive	Negative
Predicted	Positive	**True Positive**	**False Positive**
	Negative	**False Negative**	**True Negative**



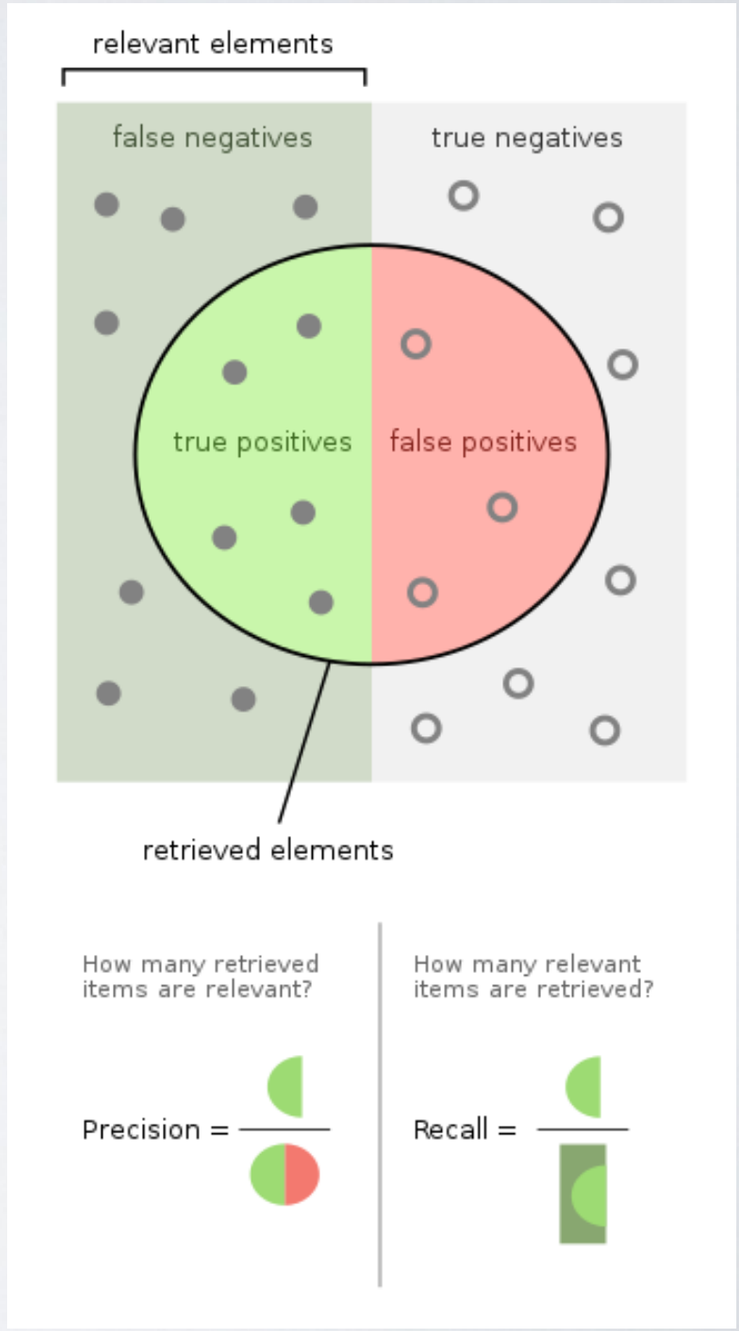
/!\ Positive=1, not 0.
Results change according to which class
Is 1.

CLASSIFICATION: EVALUATION

- Precision=$\frac{TP}{TP+FP}$
  - Among those predicted as True, fraction of really True

- Recall=$\frac{TP}{TP+FN}$
  - Among those really true, what fraction did we identity correctly

- Non-symmetric
  - Precision success != Precision failure.



ACCURACY

- Accuracy: $\frac{TP + TN}{P + N}$

- Fraction of correct prediction, among all predictions
  - Simple to interpret, symmetric

- Main drawback: class imbalance
  - Test whole city, 1 000 people, for Covid
    - 95% don't have covid, i.e., 50 people have covid, 950 don't have it
  - Our test (ML algorithm) is pretty good: TP: 45 - FN: 5 - TN: 900 -FP: 50
    - Accuracy= (45+900)/1 000=0.945
  - Dumb classifier: Always answer: not covid
    - Accuracy: (0+950)/1 000 = 0.95

F1 SCORE

- F1 score: $F_1 = 2\frac{precision * recall}{precision + recall}$
  - Harmonic mean between precision and recall
    - Harmonic mean more adapted for rates.
    - Gives more importance to the lower value
    - Not symmetric

- Scores for the covid predictor:
  - Precision=45/95=0.47
  - Recall = 45/50=0.9
  - F1=0.65

- Score for the naive predictor impossible to compute…
  - You need at least some TP !
  - Assuming 1 "free" TP (Precision=1, Recall=1/50)
    - => F1=0.04

RANKING-BASED EVALUATION SCORES

RANKING-BASED SCORES

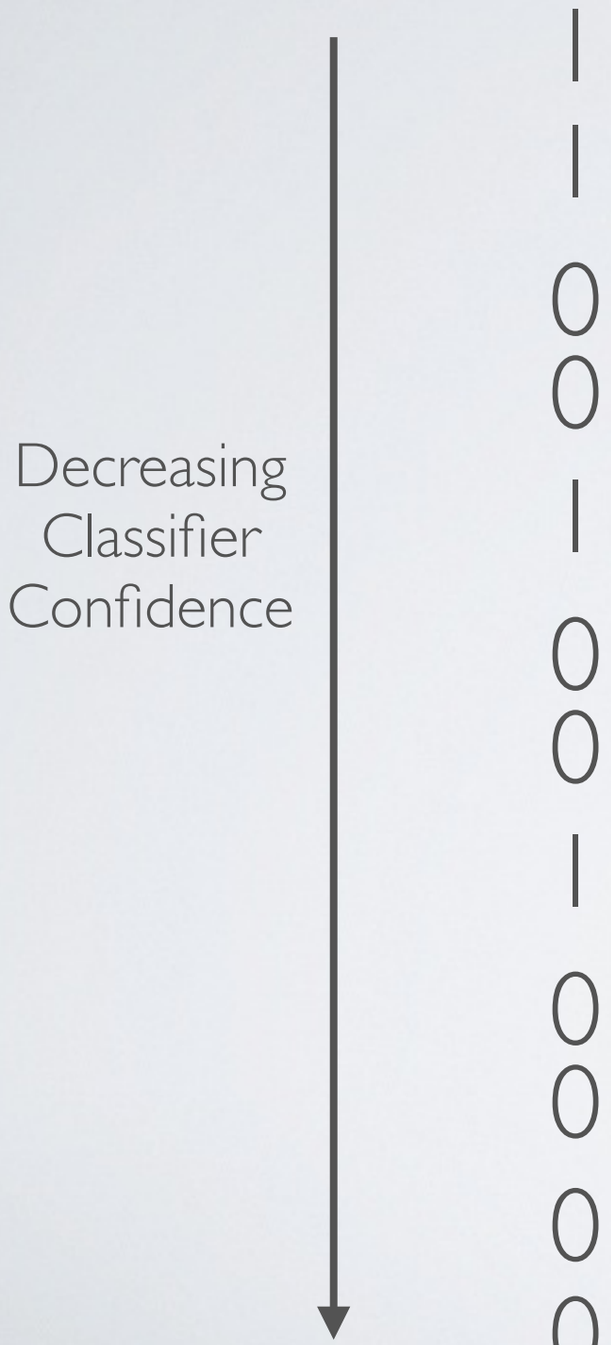
- Most classification methods assign a probability, or score, to their prediction.

- If our objective is not really to answer a yes/no question, we can use ranking-based approaches
  - Typical example: recommendation. Will user X buy product Z?
    - We are not really interested in having a correct classification(impossible problem), but of ranking correctly items.

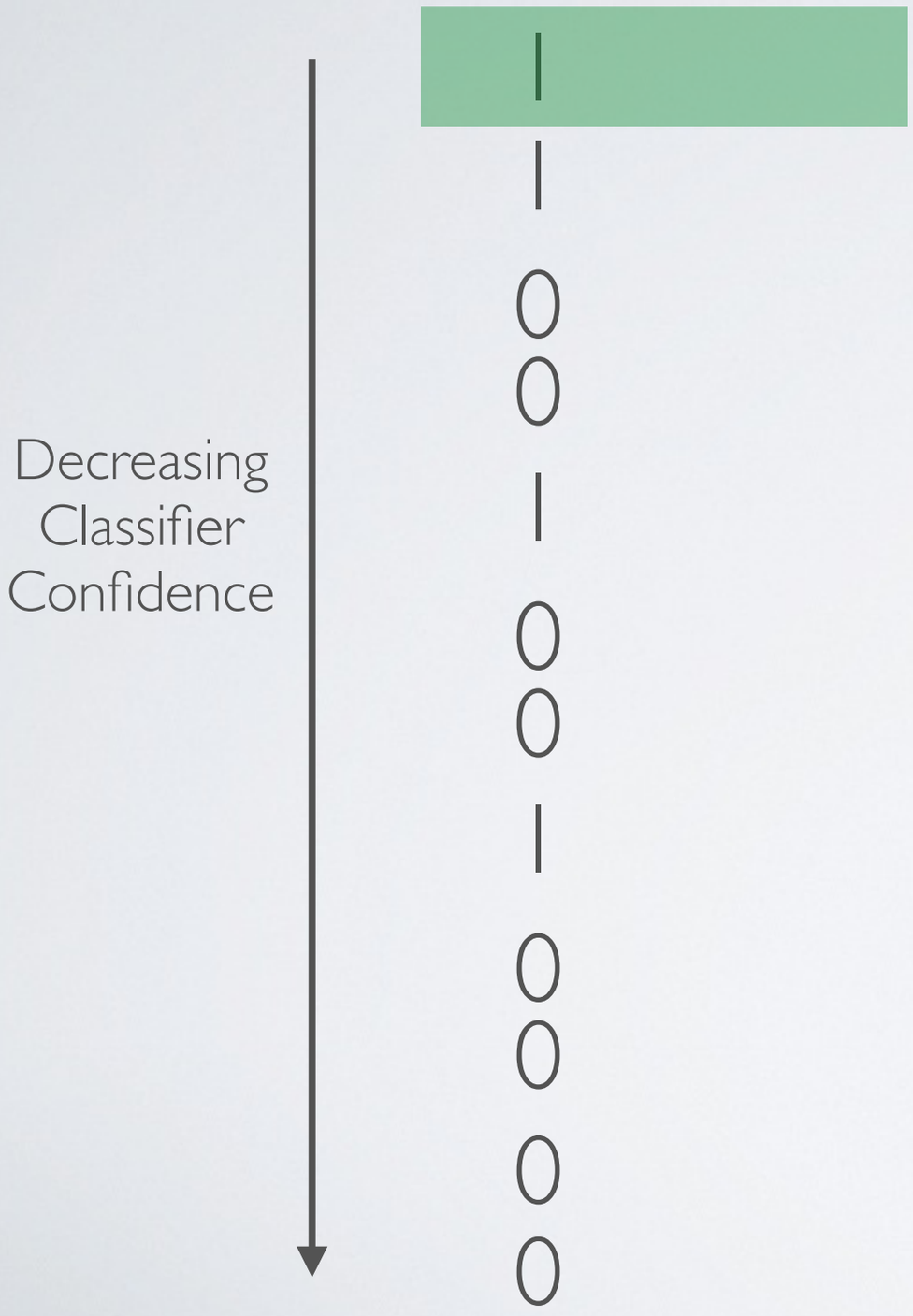
PRECISION@K

- If we know that we will do exactly k recommendations, compute the precision among the k highest scores: Precision@k
  - Typically, search engine-like evaluation
- If we don't know the exact k-value, but we know we care more about the first ones: Average Precision@k
  - Compute the precision for each value of k, weighted by the gain in recall
    - $\sum_{i}^{n} (R_i - R_{i-1}) P_i$
    - It can also be understood as the area under the Precision/Recall Curve

AVERAGE PRECISION



AVERAGE PRECISION



Green is predicted at 1, rest at 0
(Confidence threshold)

TP=1 FP=0

FN=3

$$\text{Precision}=\frac{1}{1},\ \text{Recall}=\frac{1}{1+3}$$

AVERAGE PRECISION

Top2

TP=2 FP=0

FN=2

$$\text{Precision}=\frac{2}{2},\ \text{Recall}=\frac{2}{2+2}$$

AVERAGE PRECISION

Top3

TP=2 FP=1

FN=2

$$\text{Precision}=\frac{2}{2+1},\ \text{Recall}=\frac{2}{2+2}$$

AVERAGE PRECISION

Top5

Decreasing Classifier Confidence

1
1
0
0
1
0
0
1
0
0
0
0

TP=3 FP=2

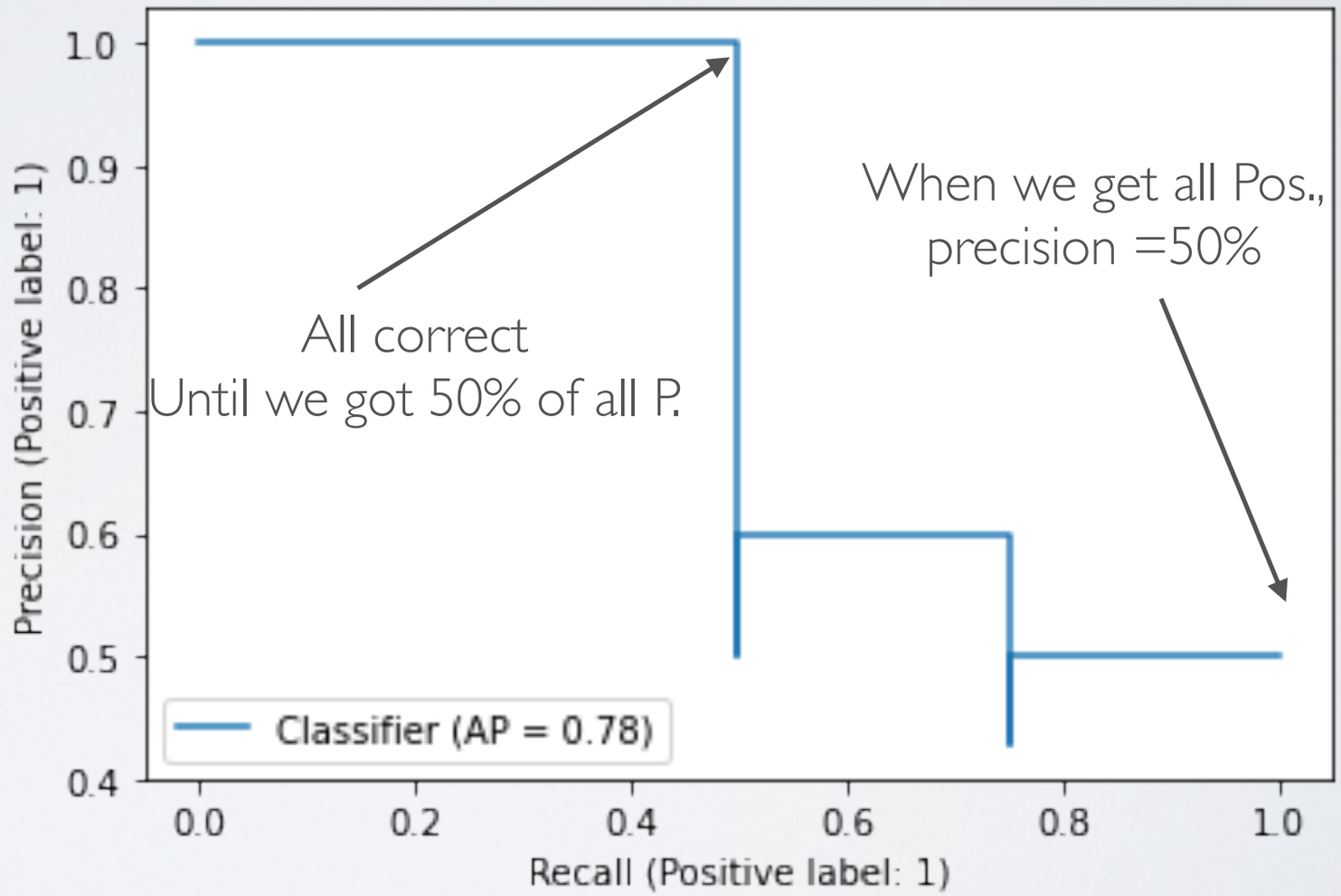
FN=1

$$\text{Precision}=\frac{3}{3+2},\ \text{Recall}=\frac{3}{3+1}$$

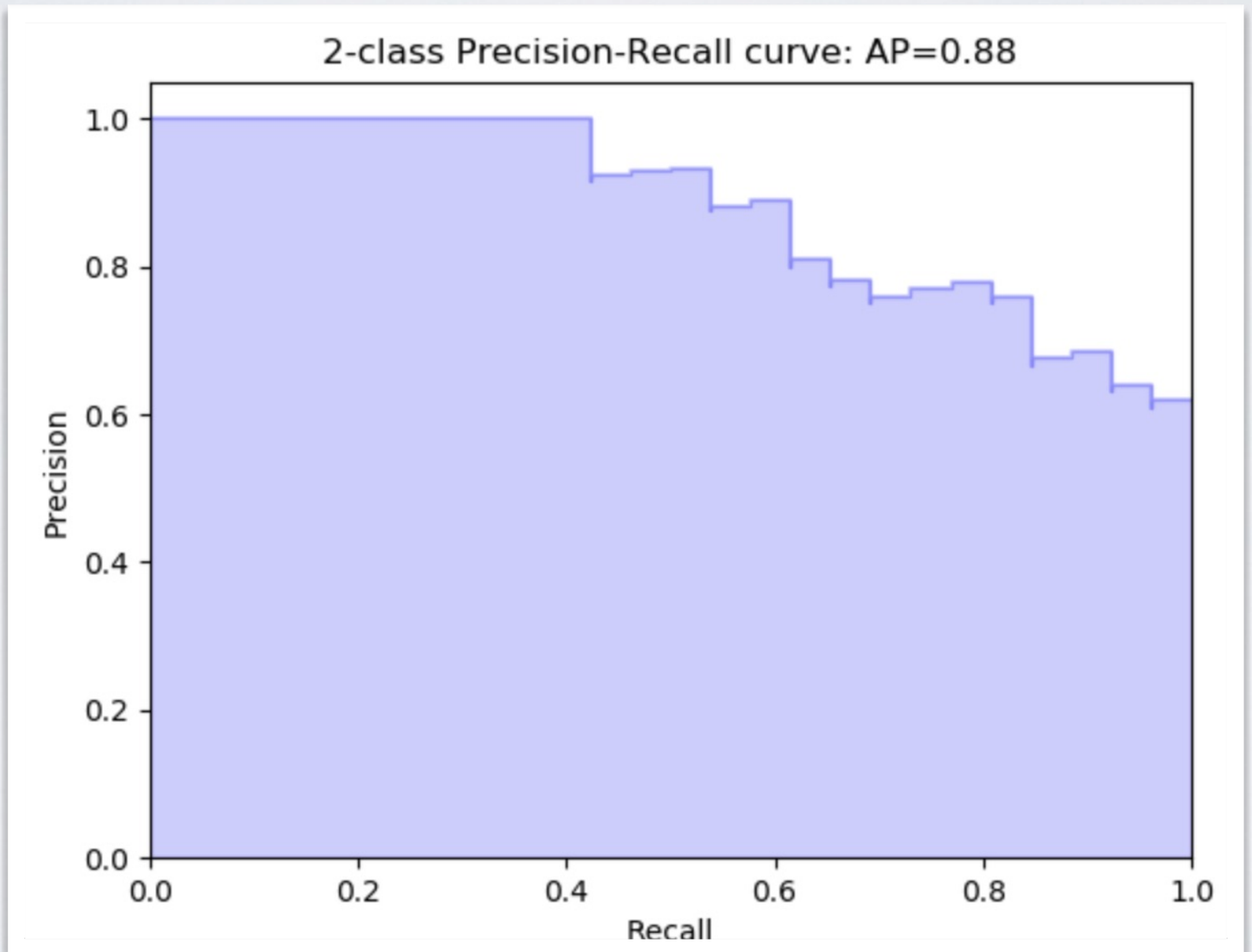
AVERAGE PRECISION

Decreasing Classifier Confidence

0 0 1 0 0 1 0 0 0 0



AVERAGE PRECISION



AVERAGE PRECISION

- Interpretation:
  - 1: all class 1 ranked first

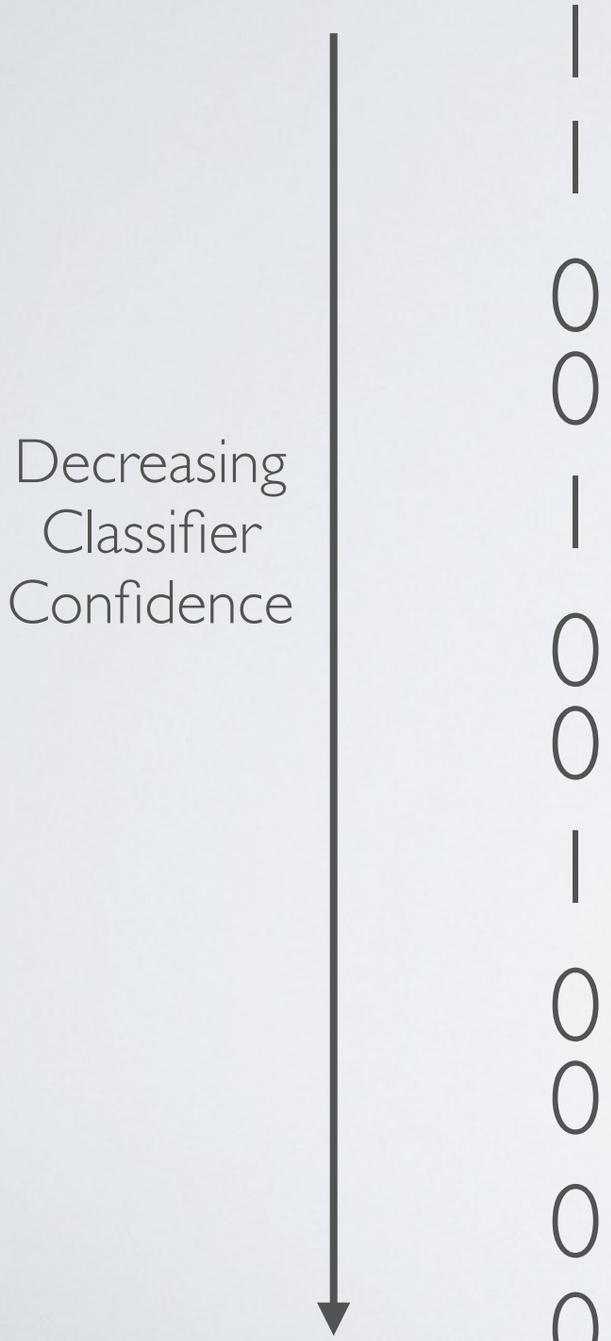
- Pros:
  - No need to arbitrarily decide k

- Cons:
  - Results still depend on the fraction of real positive in the test set:
    - The more positive, the easier it is to have a good score
    - Imagine 90% of class 1 : random order => value of 0.9
    - If 10% of class 1, random order => value of 0.1

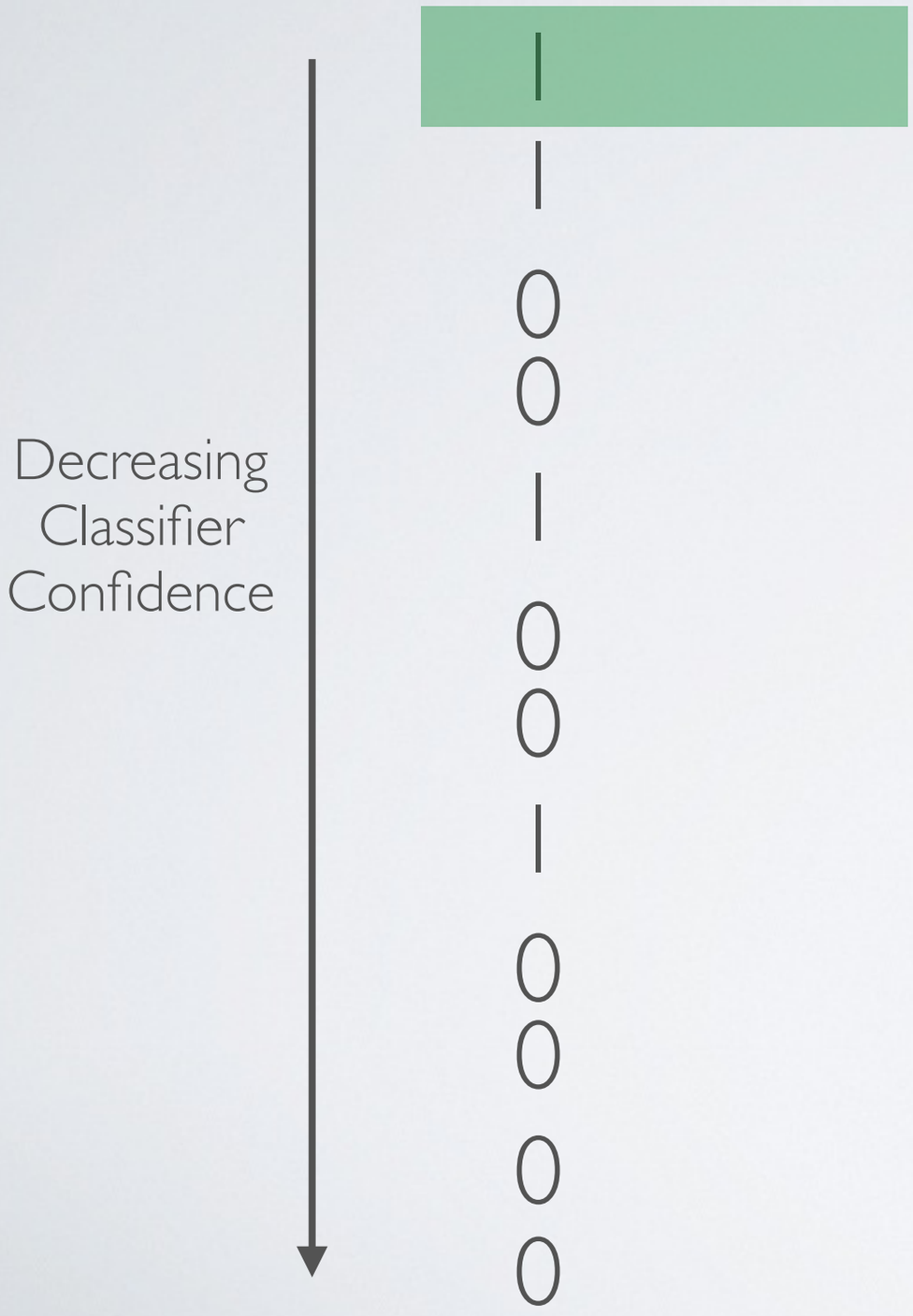
AUC - AUROC

- AUC: Area Under the Curve. Short name for AUROC (Area under the Receiver Operating Characteristic Curve)
- Similar idea than AP, but analyzing the relationship between
  - True positives rate (recall): $TPR = \frac{TP}{TP + FN} = Recall$
    - Among all really positives, those we labelled correctly
  - False positives rate :$FPR = \frac{FP}{FP + TN}$
    - Among all really negatives, fraction we mislabelled.

AUC



AUC



Green is predicted at 1, rest at 0
(Confidence threshold)

TP=1 FP=0

$$TPR=\frac{1}{4}, FPR=\frac{0}{8}$$

AUC

TP=2 FP=0

$$TPR=\frac{2}{4}, FPR=\frac{0}{8}$$

AUC

Top3

TP=2 FP=1

$$TPR=\frac{2}{4}, FPR=\frac{1}{8}$$

AUC

Top5

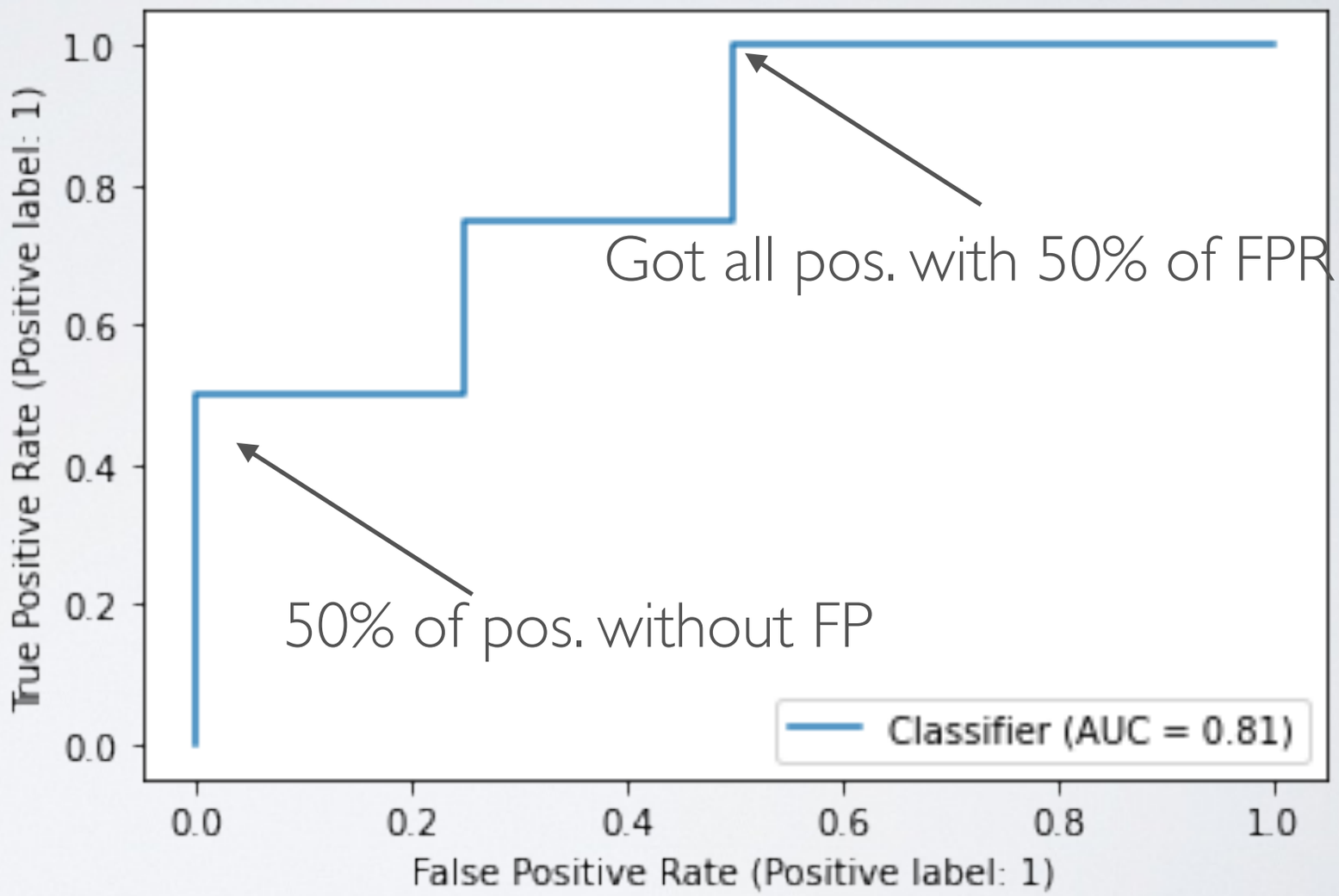
TP=3 FP=2

$$TPR=\frac{3}{4}, FPR=\frac{2}{8}$$

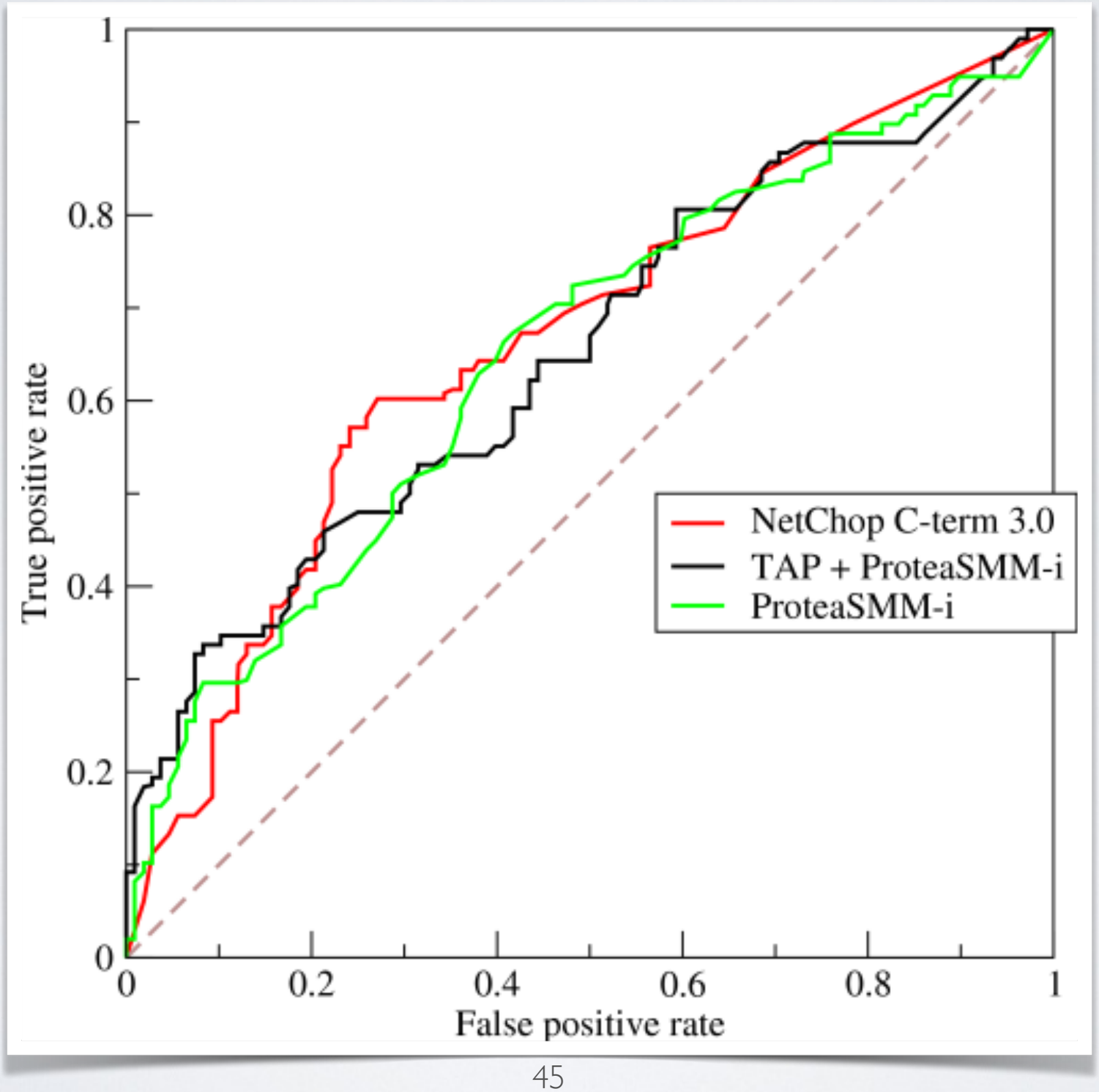
AUC

Decreasing Classifier Confidence

1
1
0
0
1
0
0
1
0
0
0
0



AUC - AUROC


True positive rate
False positive rate
0
0.2
0.4
0.6
0.8
1
NetChop C-term 3.0
TAP + ProteaSMM-i
ProteaSMM-i

AUC - AUROC

- Probabilistic interpretation:
  - If we pick a random positive example and a random negative example, probability that the positive one has a higher score

- Pros:
  - Independent on the fraction of positive examples, i.e., an unbalanced test set can be used
    - If at random we got 30% of all positives, we have also 30% of all negatives

- Cons:
  - Often high values, (>0.95), thus small (relative) improvements
  - Not helpful if you care about the first few elements

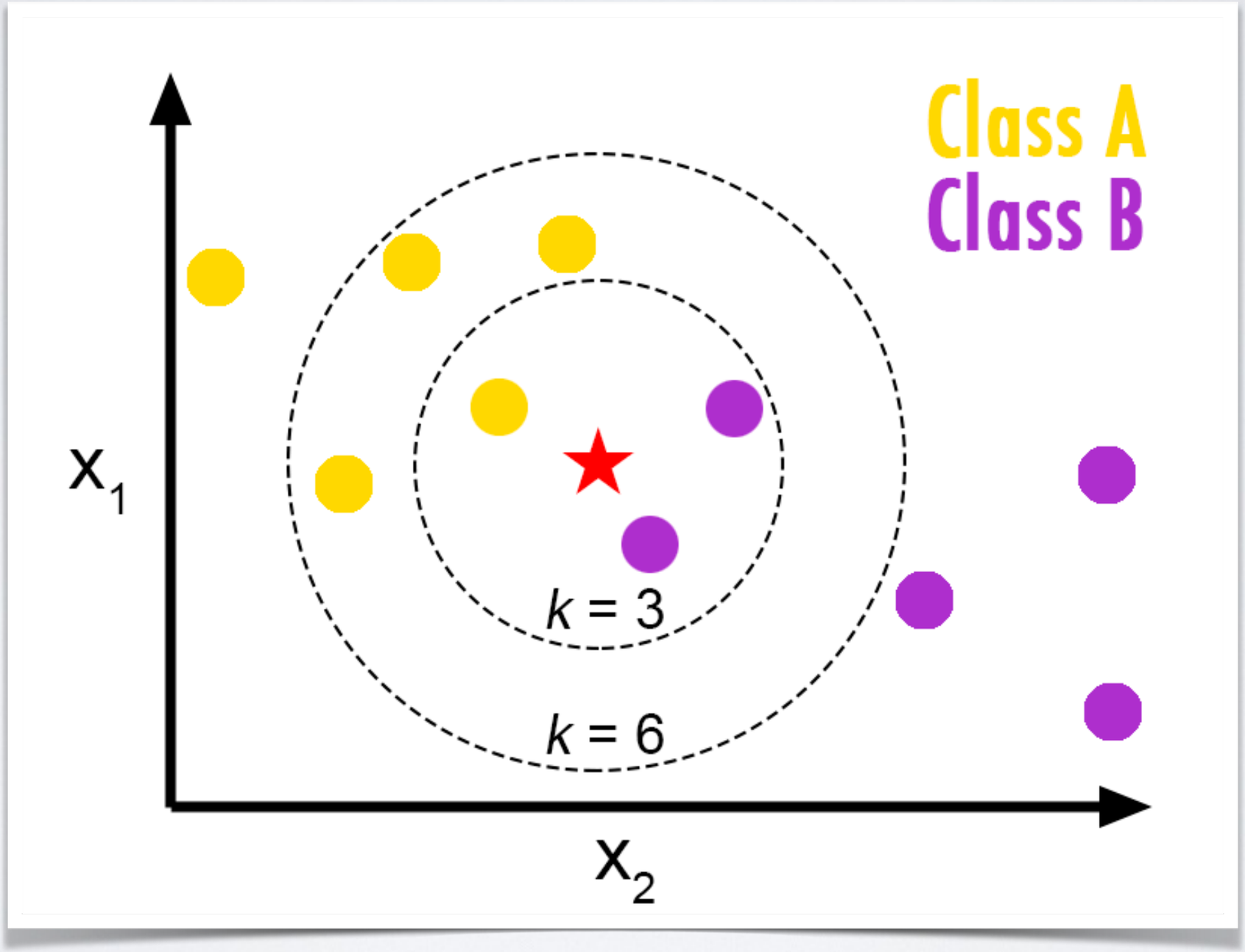
KNN

K nearest neighbors

K-NN

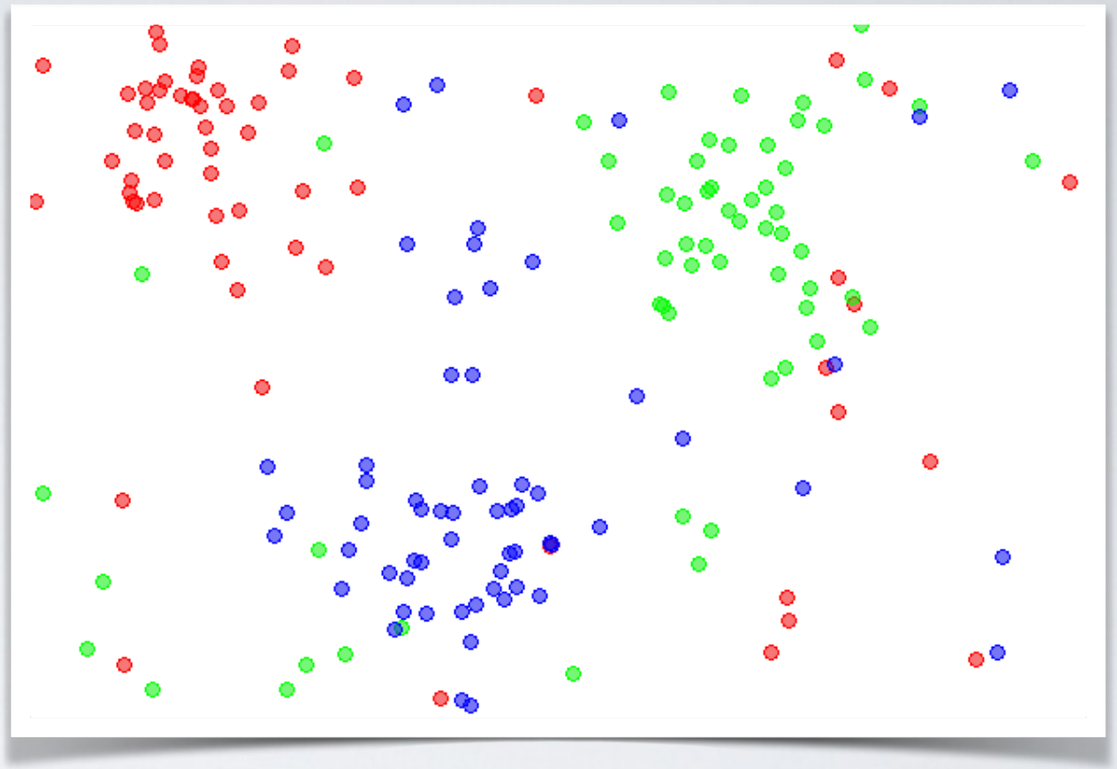
- Extremely simple approach, yet very powerfull in certain cases
- Principle: to classify (or regress) a new observation, we search for the closest one(s) in the training set, and assign the same class/value average.
  - K is obviously a parameter

K-NN

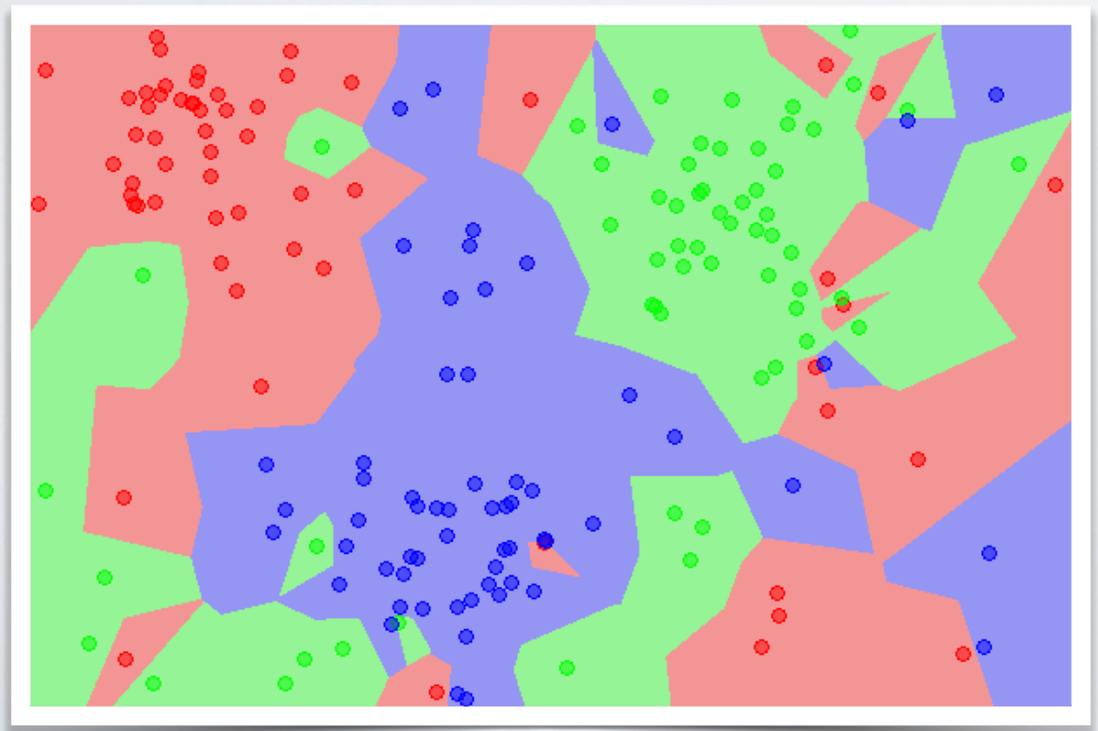


https://helloacm.com/a-short-introduction-to-k-nearest-neighbors-algorithm/

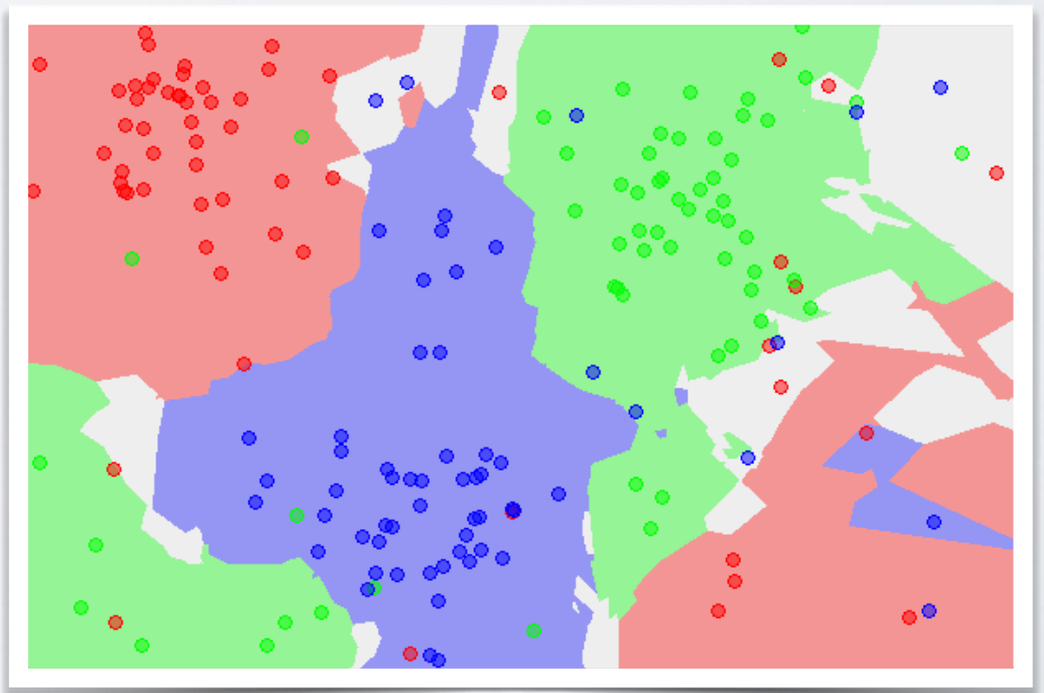
Dataset (2D, 3 classes)



1-NN



5-NN



K-NN

- Strength
  - Extremely efficient with large training set and good covering of the feature space
    - Shown to outperforms more advanced methods in many applications
  - Few parameters, simple to understand
  - No training time (possible precomputation)

- Weaknesses
  - Finding neighbors is done at evaluation time, which can be a problem with large datasets
    - Solutions: K-D tree, Ball tree… but keep dataset in memory. Hashing…
  - Curse of dimensionality=>dimensionality reduction first.
  - Choice of a proper distance

ML ADVANCED

REGULARIZATION

REGULARIZATION

- We have seen that a drawback of ML methods is that they can overfit

- When the ML objective can be clearly expressed, there is a generic way to limit overfitting: regularization
  - Two types of regularization:
    - L1 or Lasso regularization
    - L2 or Ridge regularization

L2 REGULARIZATION

- L2 or Ridge Regularization (for linear regression)
  - $\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - (b + \sum_{j}^{p} (w_j x_{ij})))^2 + \lambda \sum_{j}^{p} w_j^2$
  - $\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - \hat{y}_i)^2 + \lambda \sum_{j}^{p} w_j^2$
  - Notation: $\sum_{j}^{p} w_j^2 = \|w\|_2^2$

L2 REGULARIZATION

- Expressed as a general principle
  - $$\ell(b, w) = \frac{1}{N} \sum_{i}^{N} f(y_i, \hat{y}_i, b, w) + \lambda \sum_{j}^{p} w_j^2$$
    - Some parameters are regularized, and some others might not be (intercept…)

- Intuition: we force coefficients to be small.
  - If λ=0, normal regression
  - If λ->∞, all coefficients tends towards 0
  - /!\ The magnitude of coefficients depends on the magnitude of variables!
    - Important to normalize the variables, else you will constraint more the variables of lower amplitude

L1 REGULARIZATION

- L1 or Lasso Regularization
  - Lasso: Least Absolute Shrinkage and Selection Operator
  - $\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - (b + \sum_{j}^{p} (w_j x_{ij})))^2 + \lambda \sum_{j}^{p} |w_j|$
  - $\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - \hat{y}_i)^2 + \lambda \sum_{j}^{p} |w_j|$
  - Notation: $\sum_{j}^{p} |w_j| = \|w\|_1$

REGULARIZATION

- Similar methods, different results:
  - L1 regularization tends to force some values to be 0
  - L2 regularization tends not to attribute 0

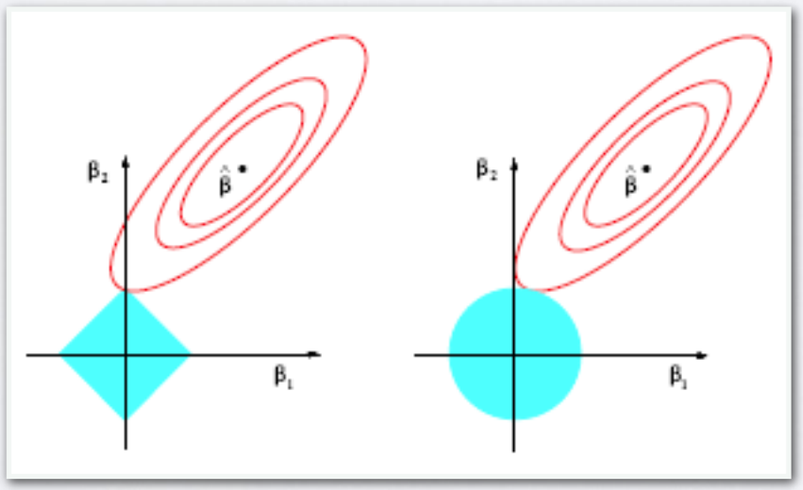
- L1 regularization thus performs **variable selection**
  - Variables for which the coefficient is 0 can be discarded

REGULARIZATION

- Why different behaviors ?
  - We minimize the sum of error+constraints
  - Red lines represent error (every point of a circle have same error)
  - Similarly for blue.
  - Intersection is the optimal solution (for that error, minimize constraint)

- => For a same error, L1 favors some variables to 0

L1



L2

https://online.stat.psu.edu/stat508/book/export/html/749

ELASTIC NET

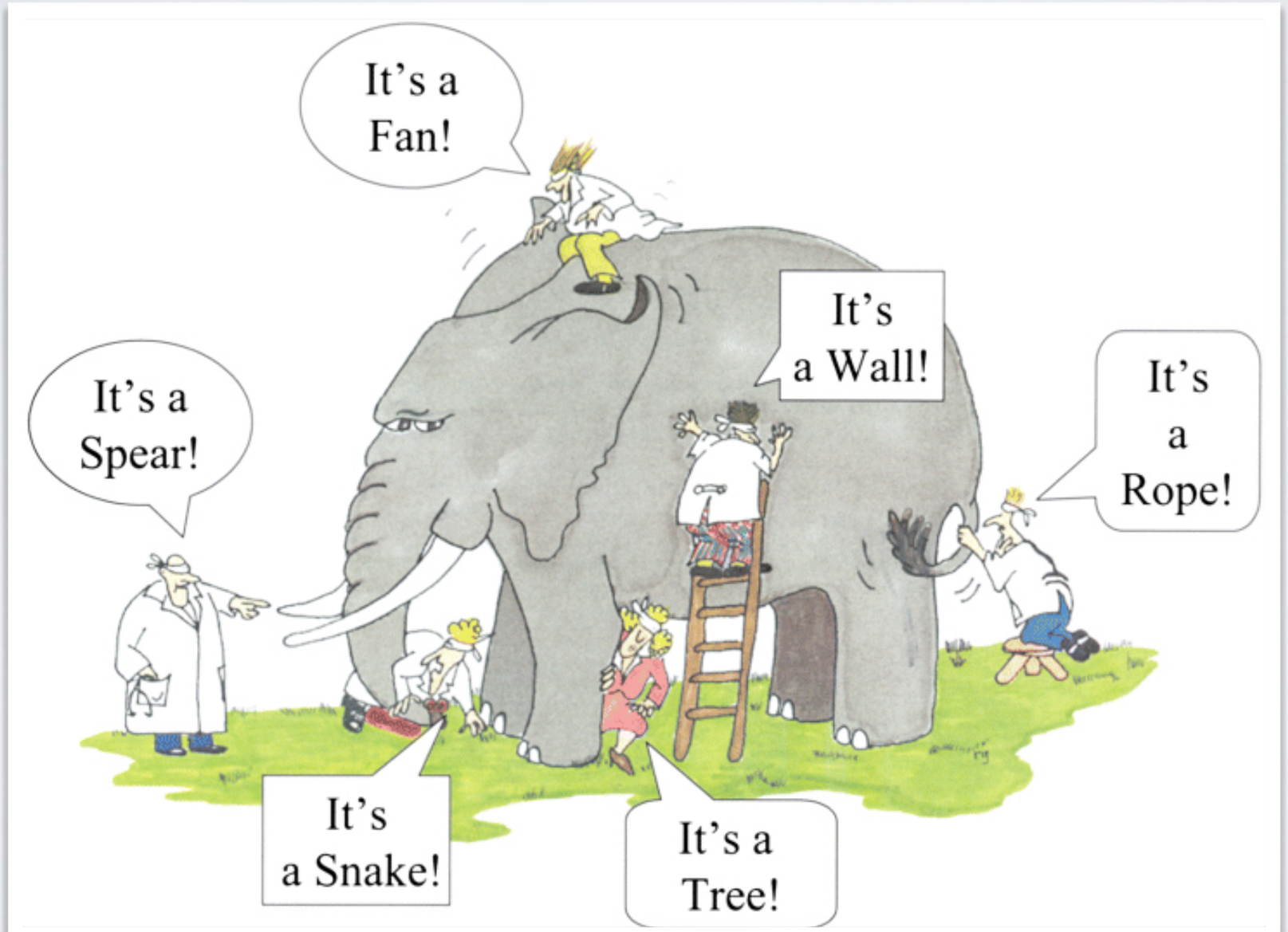
- Best of both worlds :)
- $$\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - \hat{y}_i) + \lambda_1 \sum_{j}^{p} |w_j| + \lambda_2 \sum_{j}^{p} w_j^2$$

ENSEMBLE LEARNING

ENSEMBLE LEARNING

- Ensemble learning is a general principle:
  - All models have strengths and weaknesses
    - e.g., linear models struggle with non-linearities but are good at extrapolation
    - Decision trees are good at capturing non-linearities, but struggle with extrapolation
  - Could we combine the strengths of various models?
    - Direct application: **Stacking**
    - Using multiple times the same model: **Bagging**
    - Training models specifically to solve other weaknesses: **Boosting**

ENSEMBLE LEARNING



STACKING

- In the simplest approach, various models (different approaches, same approach with different parameters) are trained on the same dataset

- Their predictions are then combined:
  - Regression: averaging. Average values of the classifiers (possibly weighted)
  - Classification:
    - Voting: class with the most vote
    - Soft / Averaging: average of probabilities yielded by the classifier

- Weaknesses:
  - What if several models make the same mistake? (Correlation of errors…)
  - What if we merge good models and poor models?

STACKING

- A possible solution to stacking is to use a meta-model:
  - The prediction made by each individual model is considered as a feature for the meta-model
  - The meta-model is trained as any ML model with the original target, but using sub-models outputs as features.
- Any model can be used as meta-model
- Famous for winning the $1M prize of the 2009 Netflix prize.
  - 100+ individual predictors

BAGGING

- Bagging is an ensemble methods, but differ from stacking in two main ways:
  - The various individual predictors are made of the same algorithm
  - Each algorithm is trained on a subset of the original data
    - Different subsets on all variables
    - And/Or trained only on some variables
    - => Various strategies exist.

- Advantages over stacking:
  - All models are comparable, less chances to average "good" and "bad" models
  - Can be understood as "lower the Variance", i.e., prevent overfit.

BAGGING: RANDOM FOREST

- Random forest is the most famous bagging algorithm
  - It is based on decision trees (thus the name *forest*…)
  - A direct application of bagging

- Trees are good candidates for bagging because overfit is their main problem
  - What is similar between trees will stay, and when they disagree, taking the average of all the errors should get close to right answer.
    - Similar to "Wisdom of the crowds"

RANDOM FOREST

- Set
  - Parameters of individual trees (not too simple, not too large…)
  - Averaging function
  - Nb. of trees

- What is specific is the subsamble strategy
  - What is key is to avoid correlation between trees, i.e., train on different data
  - Subsample observations: With replacement. Sample n at random among n items
    - Variants: m among n. Or without replacement: random samples, or "folds" (each observation used in a single tree, but requires lot of data)…
  - Specific to trees: subsample of variables at each node: to chose the best split, restrain to a random fraction of variables.
    - Impose diversity in the trees

BOOSTING

BOOSTING

- Again, a general principle
- We train various models in sequence
  - First, train a normal model
    - Usually, this model will be tuned to be relatively simple, and thus underfit=>Weak learners
  - Then, extract the errors of the model (incorrect classes/residuals).
  - Train a second model, focusing on predicting the errors missed by the first model
  - Update the main model and recompute the errors
  - Repeat until we cannot improve anymore
- Final prediction is the sum of all weak learners (not average: each method *corrects, complements* previous ones)

$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

XGBOOST

XGBOOST

- As of today, certainly the most popular method among those not using neural networks

- Used in winning solution in countless ML challenges
  - And at Google, Amazon, Uber…

- Both :
  - A method described in a scientific paper
  - A library developed and improved by a community
    - Changes in the ML scientific culture…

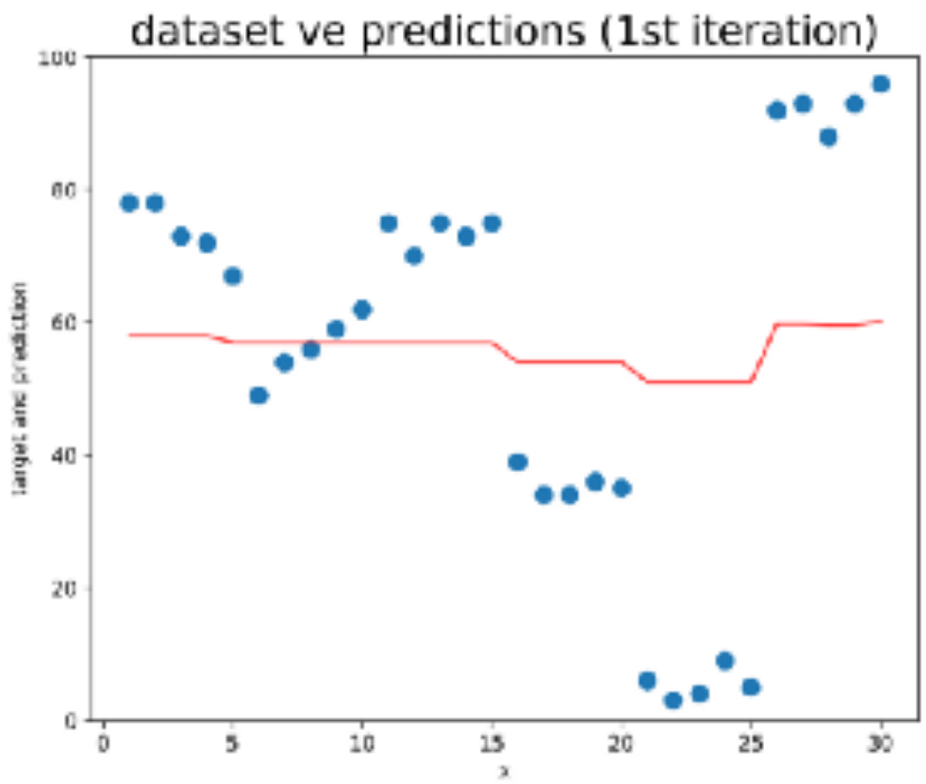
XGBOOST

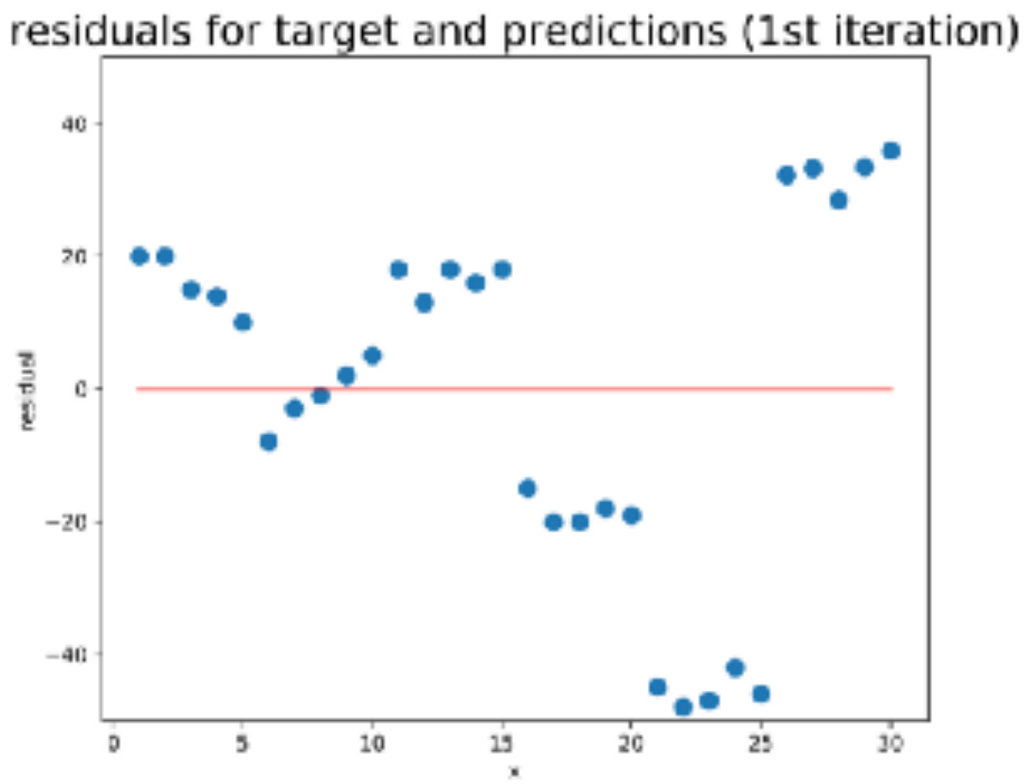
- In a few words:
  - A tree boosting methods
    - Can be used for classification and regression
  - Weak learners
    - Default to 3 or 6 levels max
  - Introduces Regularization
    - Each new leaf adds some regularization cost
  - Gradient Boosting method:
    - Explicitly do a gradient-descent-like approach

GRADIENT BOOSTING

- Gradient boosting is the application of boosting to explicit gradient descent

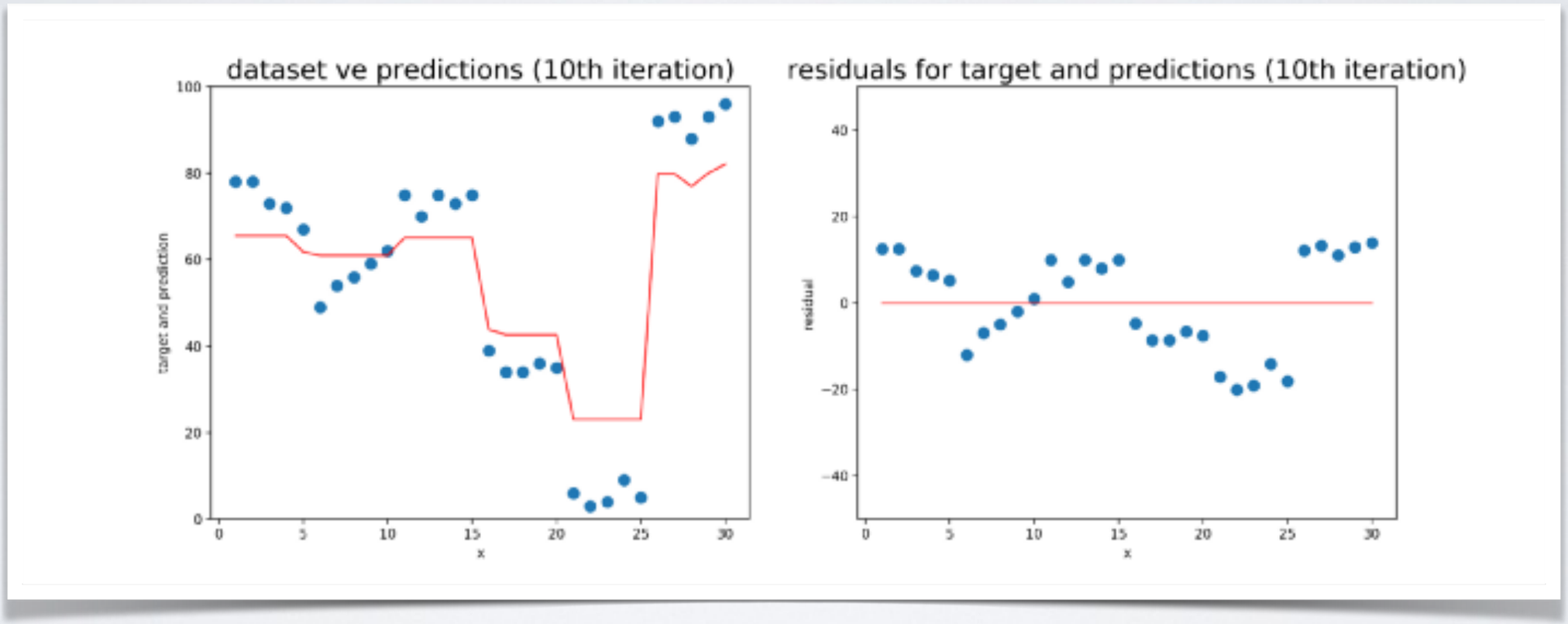
GRADIENT BOOSTING





https://medium.datadriveninvestor.com/how-do-boosting-algorithms-work-5d2c734aca4c

GRADIENT BOOSTING



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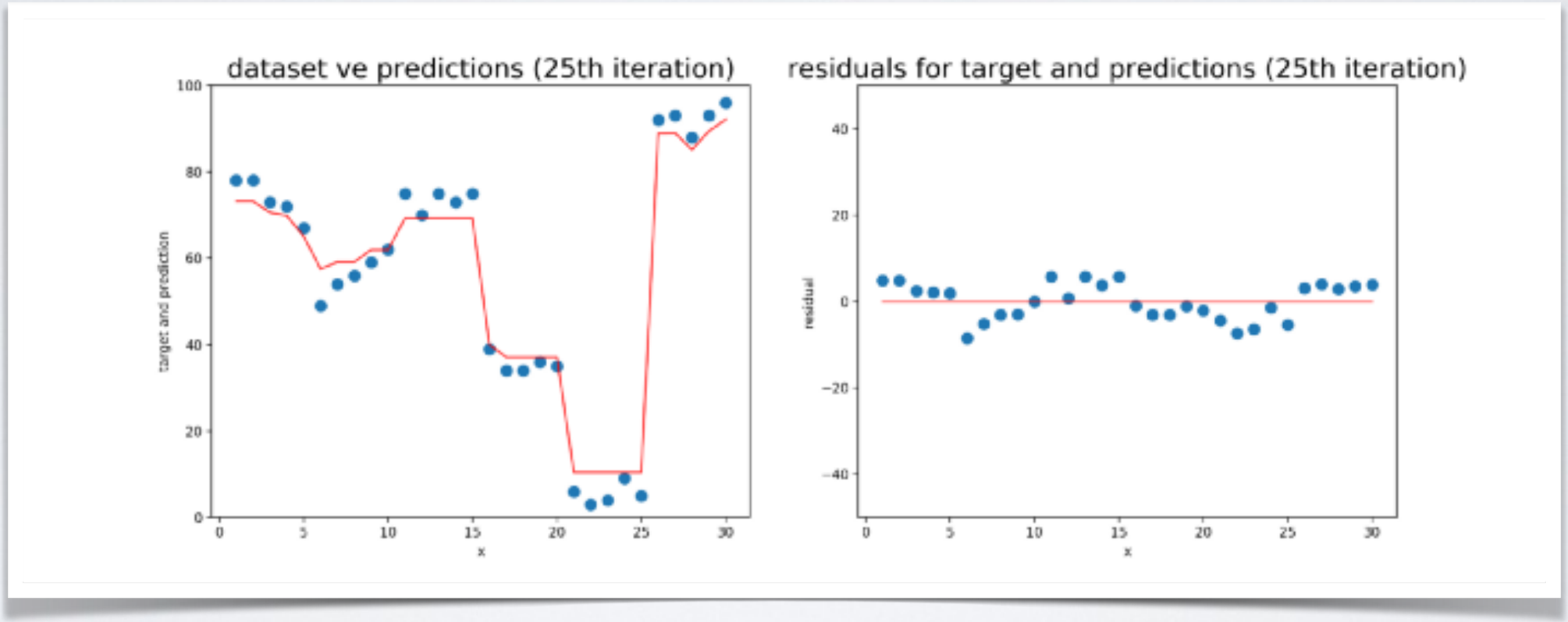
GRADIENT BOOSTING



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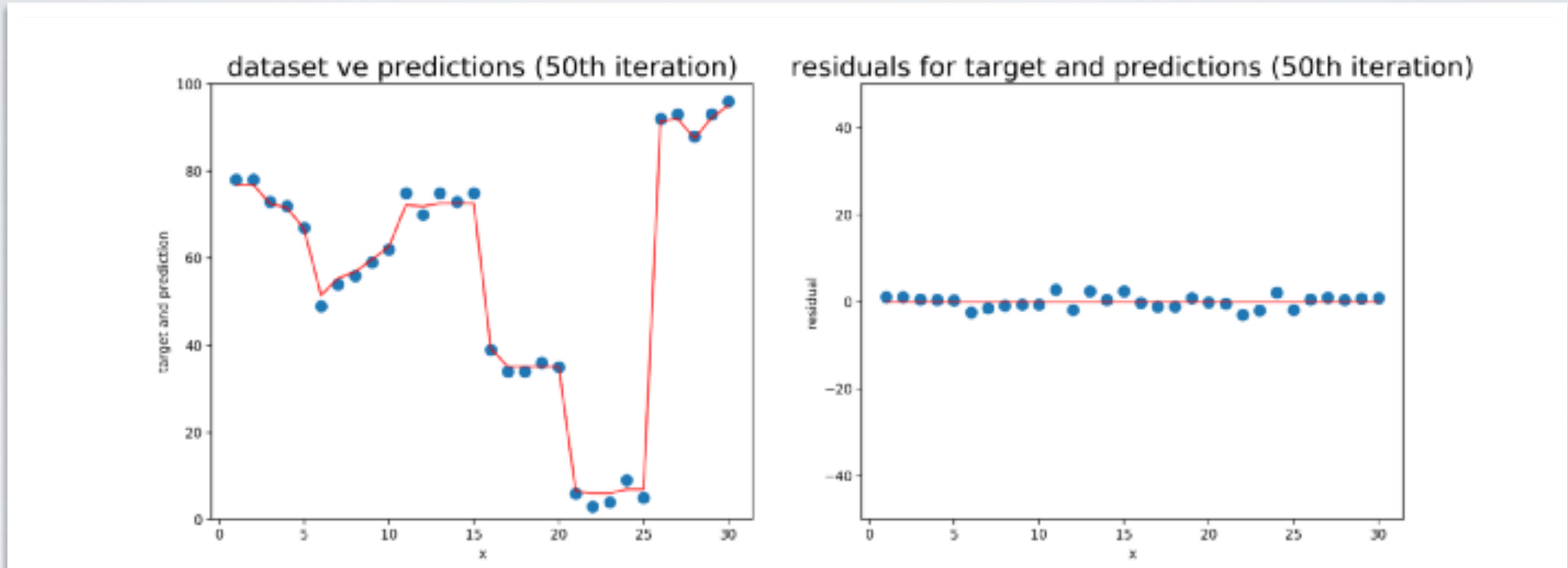
GRADIENT BOOSTING



https://medium.datadriveninvestor.com/how-do-boosting-algorithms-work-5d2c734aca4c

XGBOOST IN A NUTSHELL

$$\text{obj}^{(t)} = \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{t} \omega(f_i)$$

$$= \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \sum_{i=1}^{t} \omega(f_i)$$

- In our loss for the tree, we decompose the prediction $\hat{y}$ as
  - Prediction given by previous tree + prediction of new tree.
  - ω regularization, explained later

XGBOOST IN A NUTSHELL

$$w_j = -\frac{G_j}{H_j + \lambda}$$

- w_j : score of a leaf
- Using RMSE as an objective:
  - G_j: Sum of errors (to residuals)
  - H_j: Number of items in the leaf
  - λ: Regularization parameter

GAIN ON A SPLIT

- $$Gain = \frac{1}{2}\left[\frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda}\right] - \gamma$$

- L, R=> Left and Right children

- Sum of regularized averaged error of the children squared, minus that of parent, minus regularization γ

https://xgboost.readthedocs.io/en/stable/tutorials/model.html

XGBOOST IN A NUTSHELL

- For First tree:
  - For each leaf
    - We compute the gain to find the best possible split,
    - If regularization makes the gain negative, do nothing
    - If we reach the maximal tree depth, do nothing
    - Compute the final score of the leaf : signed error. To add to the final prediction

- Next tree: same process, but compute error relatively to previous tree (residuals)

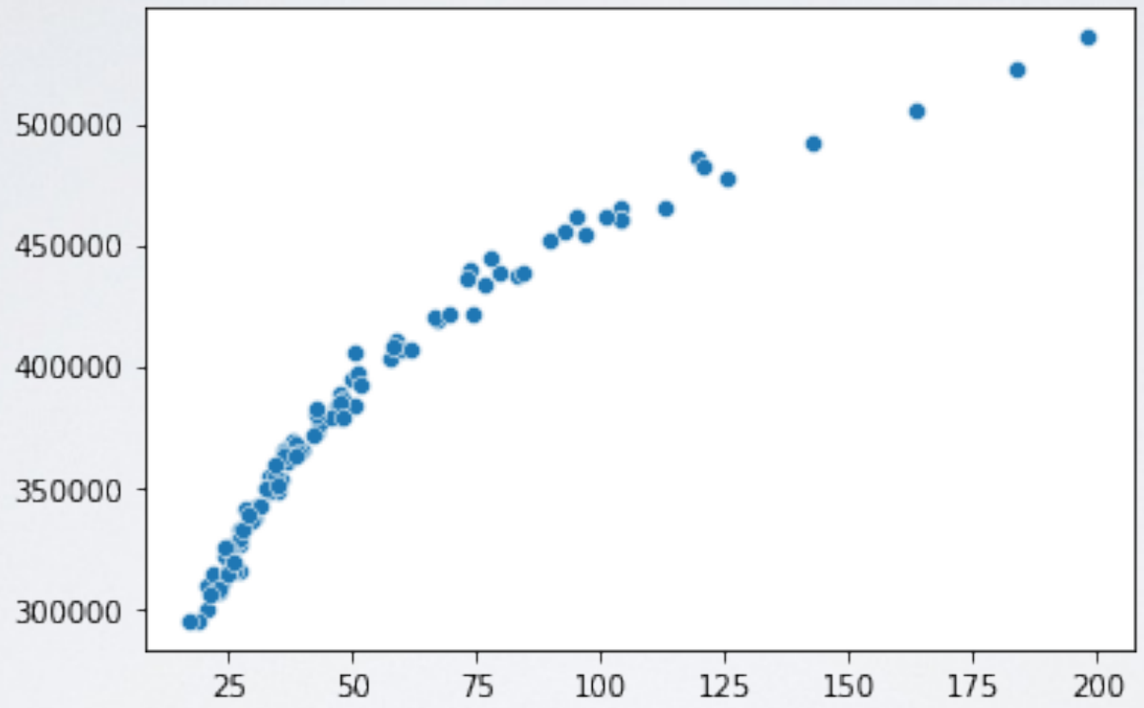
- When finished, for each prediction, sum the (signed) prediction of each tree (weighted by learning rate η)

LEARNING RATE

- As in most gradient descent methods, there is a learning rate η (eta) parameter, allowing to tune how fast we converge
  - To avoid the "ping-pong" effect around global minimum
  - In practice, the prediction of the previous tree is shrinked by η

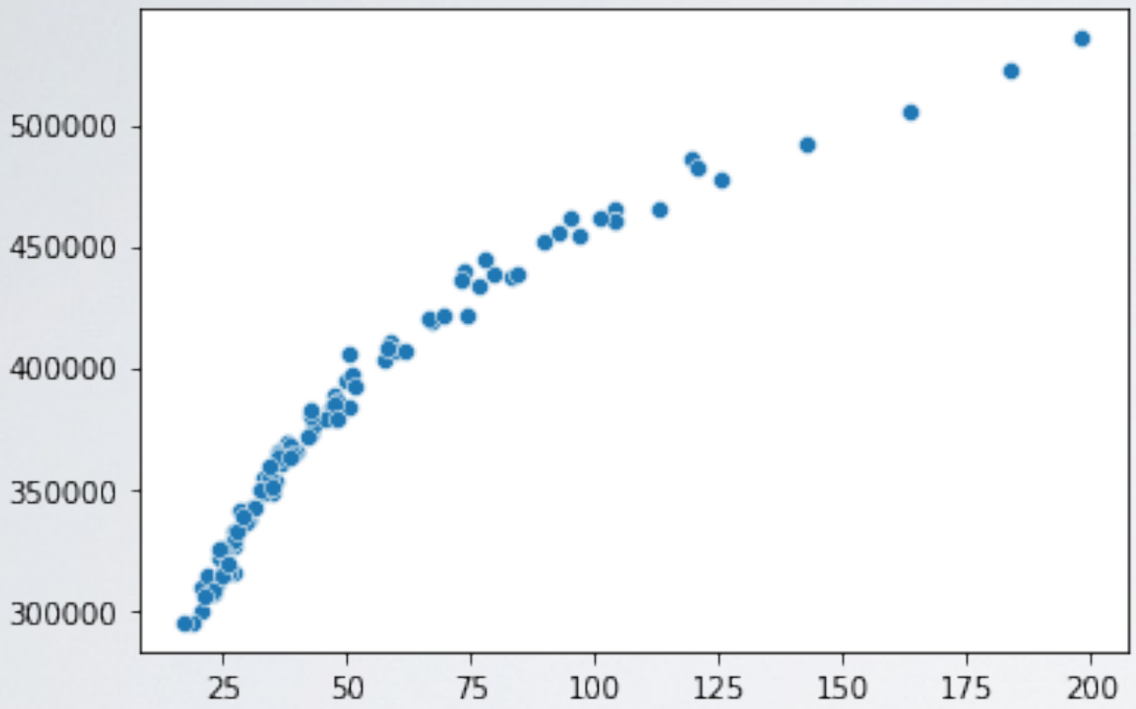
- $\hat{y} = \eta \hat{y}_i^{(t-1)} + f_t(x_i)$

XGBOOST: EXAMPLE

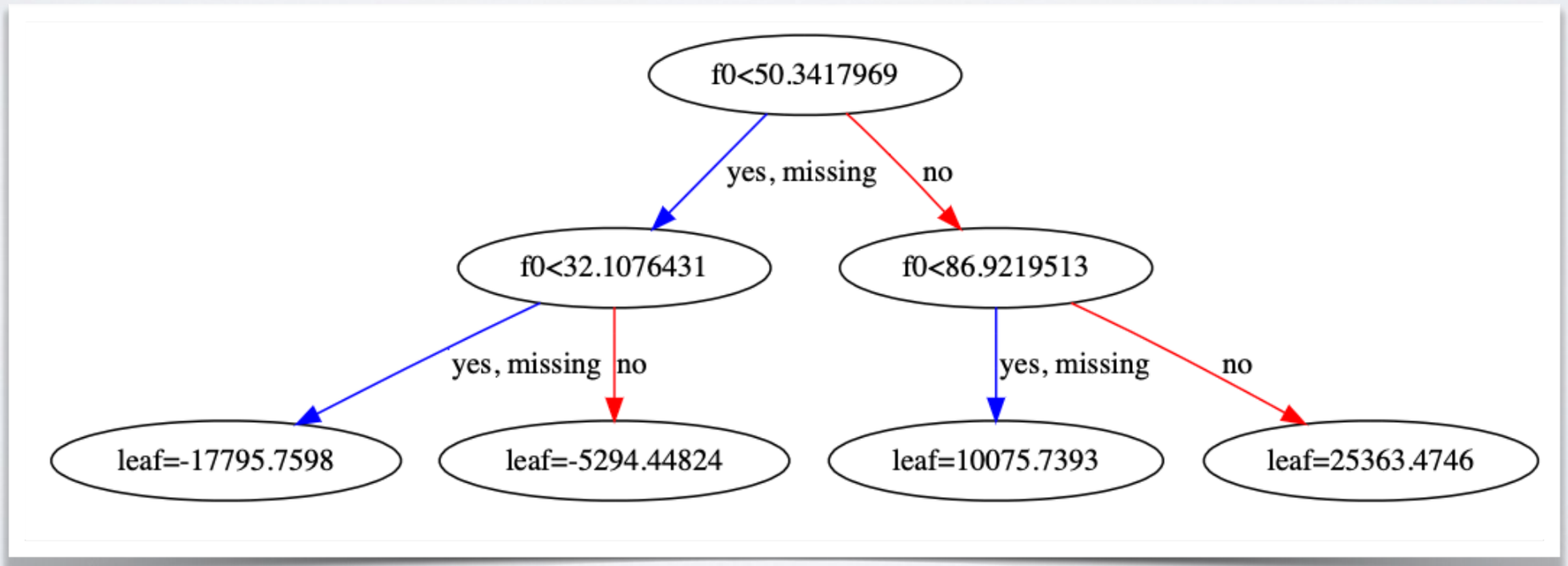


objective="reg:squarederror",
learning_rate=0.3,
base_score=np.mean(Ytrain),
max_depth=2

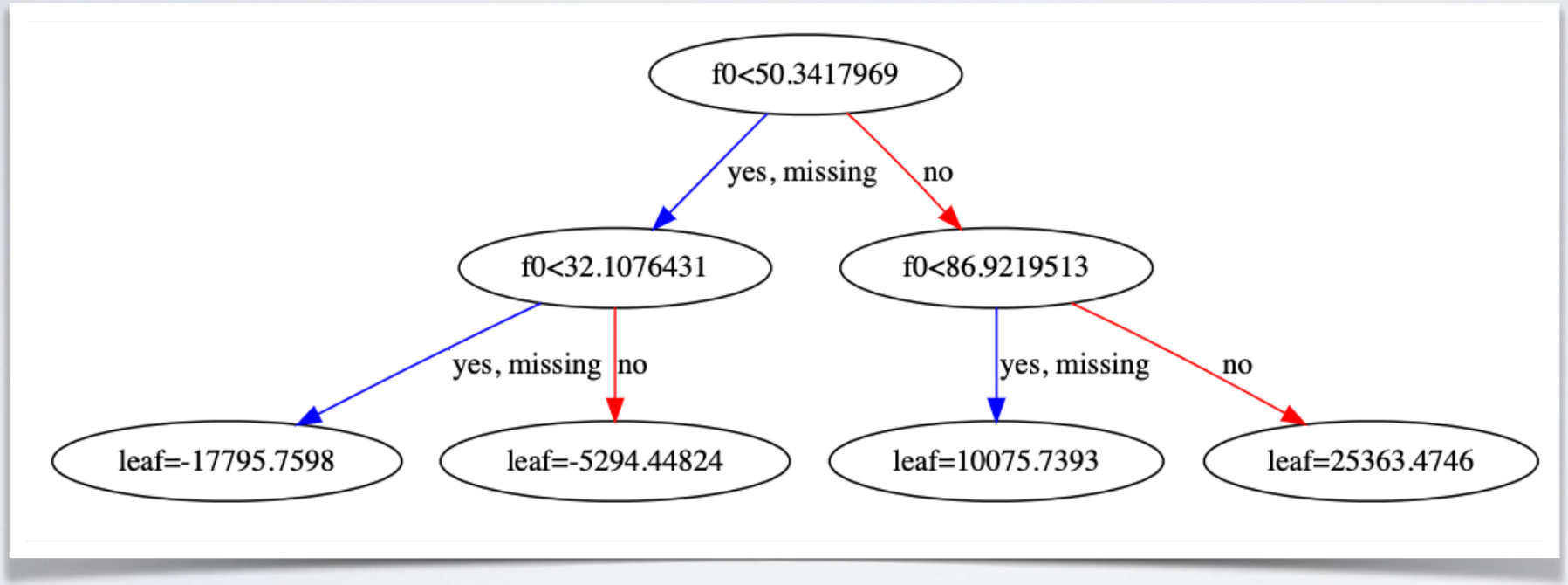
XGBOOST: EXAMPLE

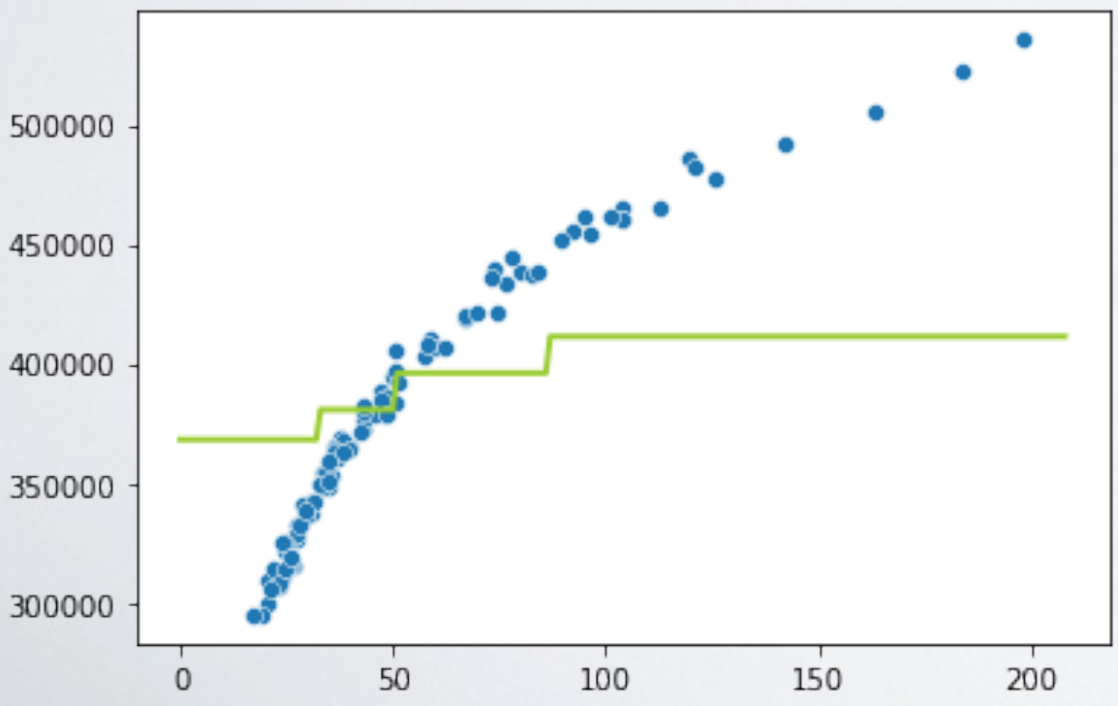


First tree



XGBOOST: EXAMPLE

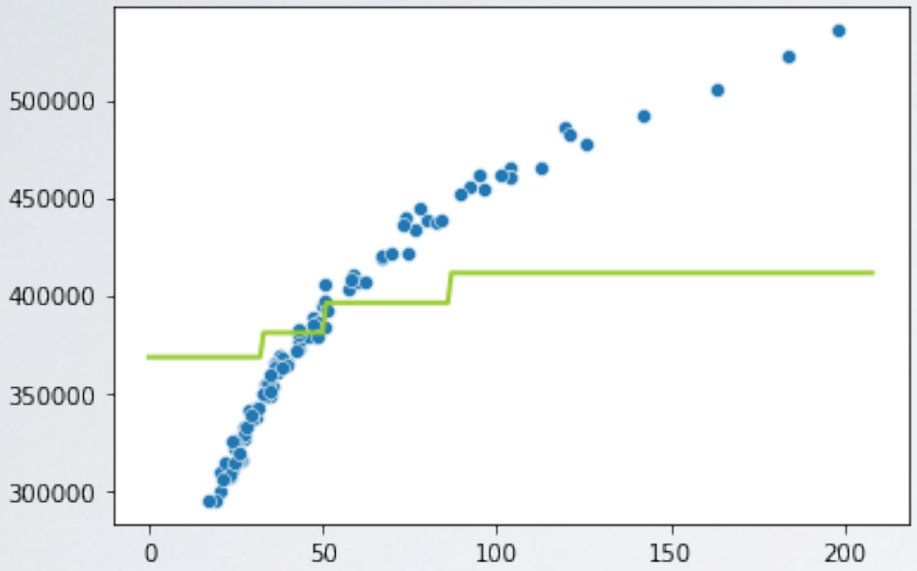




1 single tree for prediction:
Learning rate effect…

XGBOOST: EXAMPLE

1



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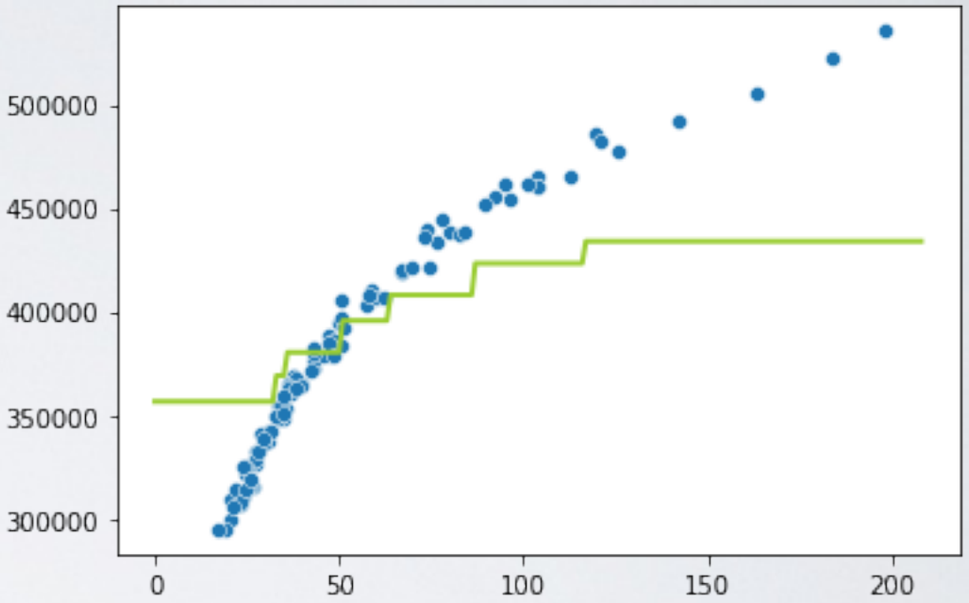

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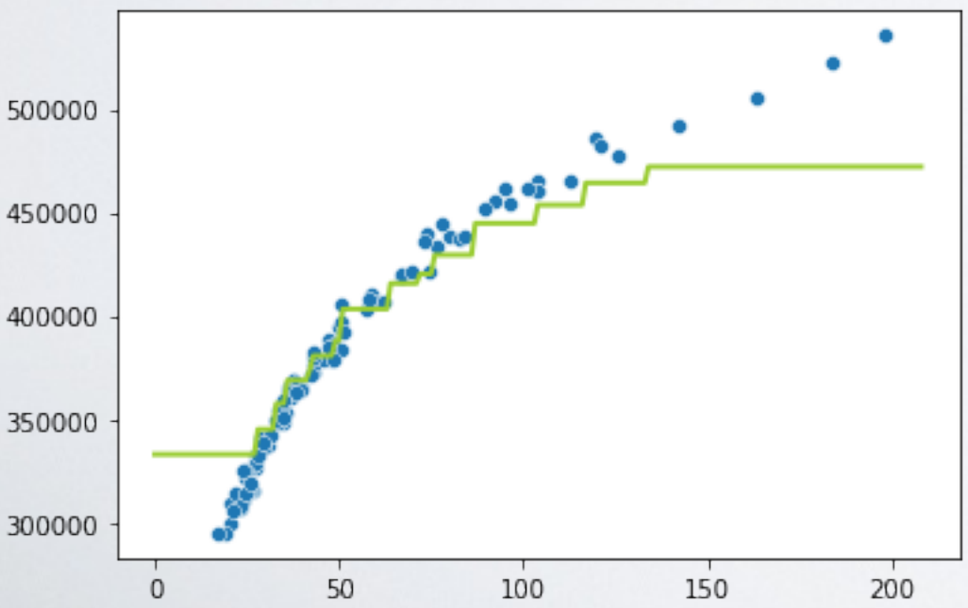

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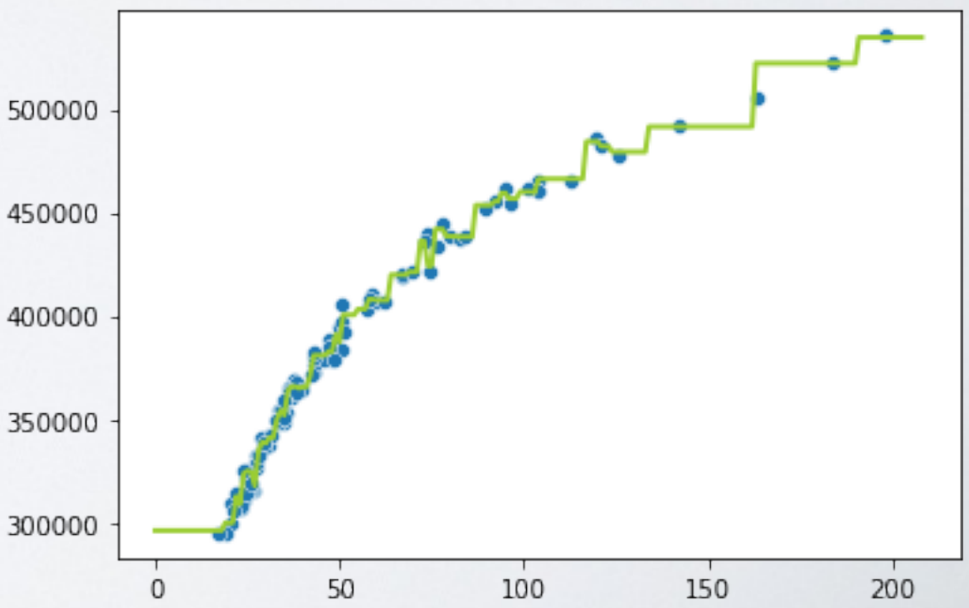

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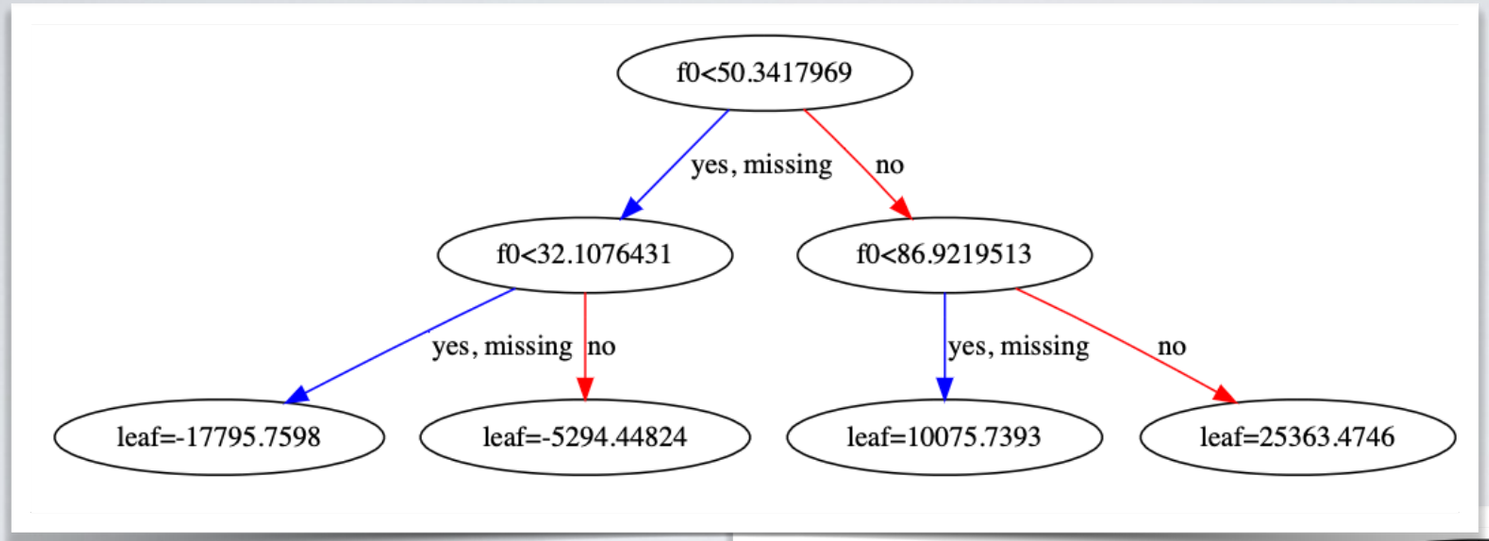
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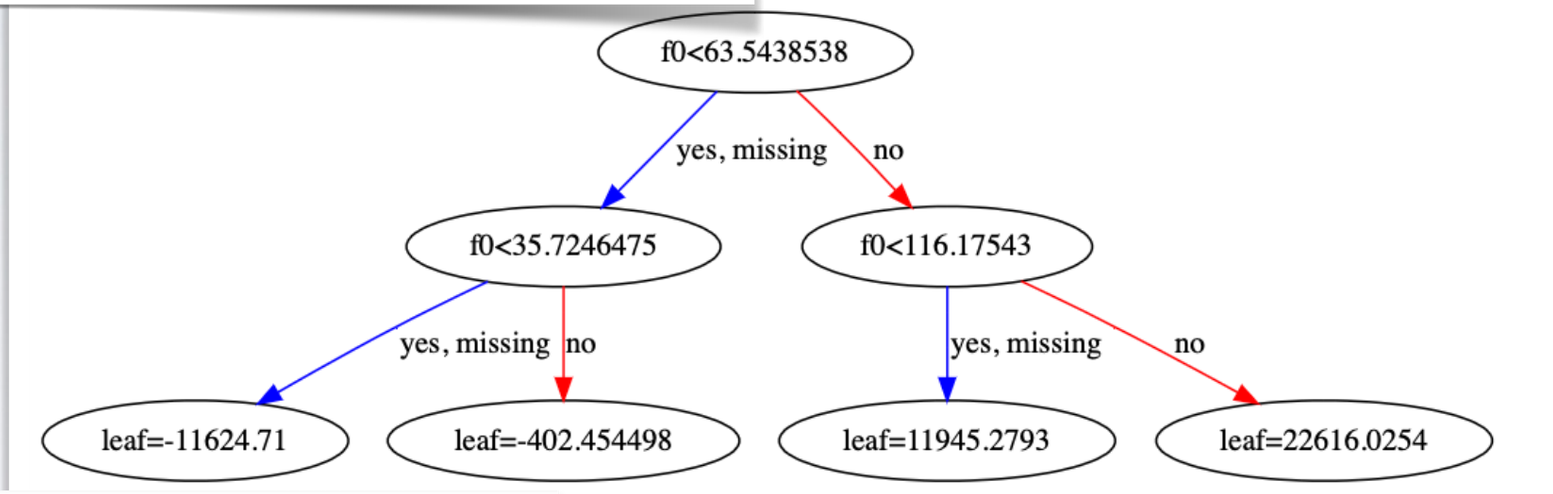
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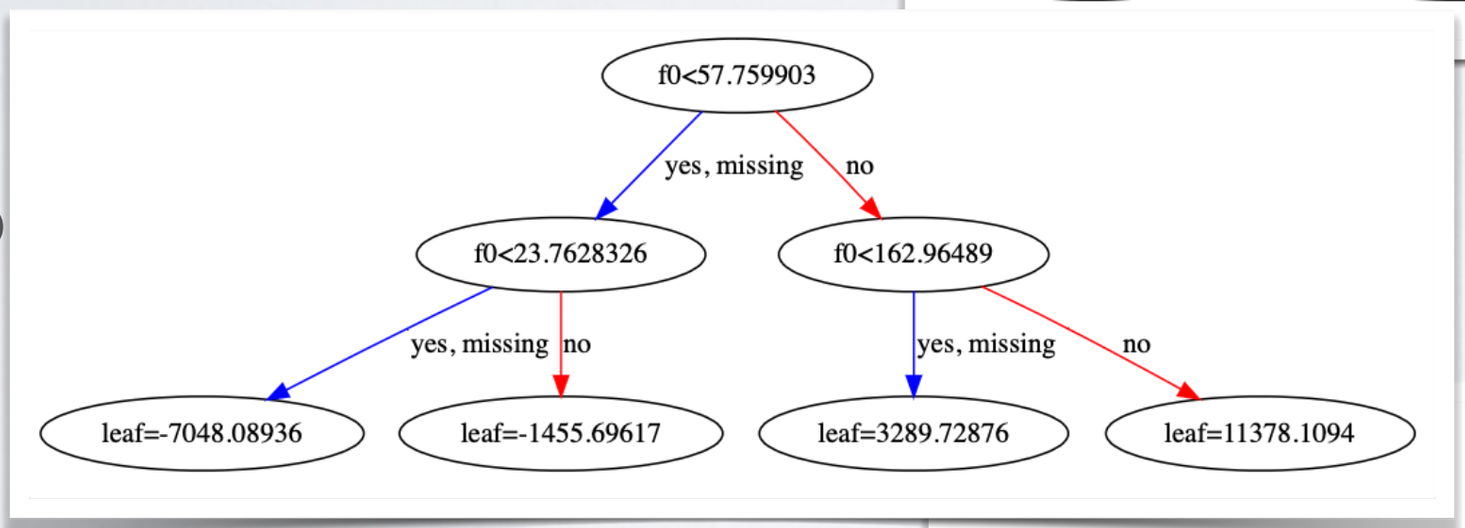
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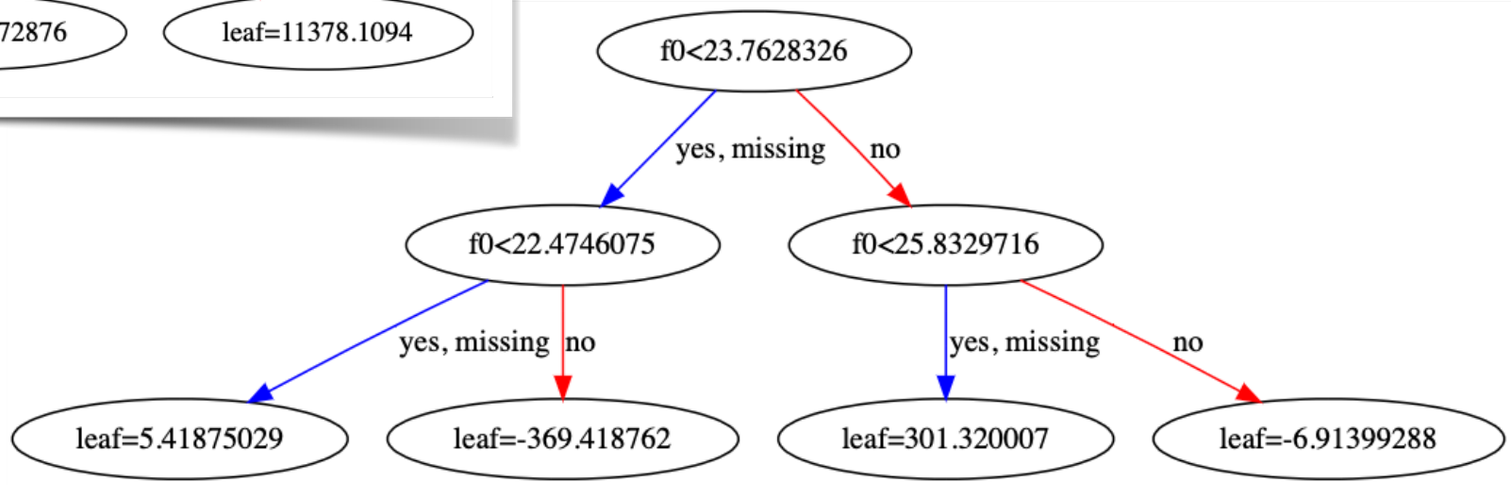
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CLASSIC ML VS DNN

- Until now, I have presented "classic" methods.
- In the news, we hear often about Neural networks methods when talking about IA. Are classic obsolete?
  - DNN are mostly "chained" classic methods. Nothing different in the theory
  - DNN are good for problems with
    - Huge quantity of data
    - Huge quantity of attributes
    - Attributes being semantically related to each other, but of the same nature (adjacent pixels, following words…)
    - =>Structured data
  - If limited data, set of unrelated, loosely known features: XGboost & Co. are the most used and usually most efficient methods