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
 - Evaluate the risks of recidivism of a convict (don't do that!)
 - What else ?

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.

SUPERVISED ML: DNN

- Many recent successes thanks to Deep Neural Networks
- This class: only "classic" methods
- DNN are just an *evolution* of methods presented in this class, all principles stay the same.

FICTIONAL EXAMPLE

- 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.

EVALUATION/OBJECTIVE

- Before applying any method, set up an objective/a quality score/an error measure
- We want to be able to compare several prediction methods to see which one is the most efficient. But how to compare them ?
- Typical scores:
 - MAE: Mean Absolute Error
 - MSE, RMSE: (Root) Mean Square Error

• R^2

MEAN ABSOLUTE ERROR

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

- Similarity with the MAD (Mean Absolute Deviation), comparing values with predictions instead of simple mean.
- Simple to interpret
 - lower the value, lower the error, better the prediction
 - 0: perfect prediction

MEAN SQUARED ERROR

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

- Similarity with the Variance
- Using squared errors give stronger importance to large errors
- RMSE = \sqrt{MSE} , can be easier to interpret

 R^2 (R-SQUARED)

$$R^{2} = 1 - \frac{\sum_{i} e_{i}^{2}}{\sum_{i} y_{i} - \bar{y}} = 1 - \frac{MSE}{Var(y)}$$

- Quantifies the fraction of the variance that is explained by the prediction
 - Sometimes called coefficient of determination for linear regression
- I=>Perfect prediction.
 - Negative if the prediction is worst than taking the average (=Variance)

R^2 (R-SQUARED)



EVALUATION/OBJECTIVE

- Which one should you use?
 - Different literature have their favorite one. RMSE is probably the most popular.
 - If your ML algorithm use the RMSE as objective (loss function), then you should probably use RMSE
- 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".

BASELINE

- Let's define our baseline, our reference to improve on
- Let's assume we only know the target variable values
- Using statistics, we know that the best "prediction" we can do for the price of a future apartment will be
 - The average (for MSE) =>Variance
 - The median (for MAE) => MAD



(Some imaginary values)

BASELINE



Using Mean=51676

MSE 1105345073.7155044 RMSE 33246.73027104326 MAE 22740.967725747014 R2 0.0

25

20

RMSE lower

Using Median=43086

MSE 1179133659.4166086 RMSE 34338.51568452848 MAE 21658.66828240126 R2 -0.06675615376207489

MAE lower

- 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



- 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: $\hat{y} = \beta_0 + \beta_1 x$

• We solve this problem, and obtain:

- ▶ β₀=987
- β₁=779



MSE 20668278.463901177 RMSE 4546.237836266508 MAE 3512.3861644882704 R2 0.9813015148342528

• We solve this problem, and obtain:

- ▶ β₀=987
- β₁=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 -0.06675615376207489

Using Linear Regression

MSE 20668278.463901177 RMSE 4546.237836266508 MAE 3512.3861644882704 R2 0.9813015148342528

- Note: To generate the data, I used indeed a linear model, with parameters
 - β₀=987 0
 - β₁=779 1000

Using Linear Regression

MSE <u>20668278.463901177</u> RMSE <u>4546.237836266508</u> MAE 3512.3861644882704 R2 <u>0.9813015148342528</u>

Using "Real" generative model

MSE 20863741.73315057 RMSE 4567.68450455486 MAE <u>3506.783422078361</u> R2 0.9811246802204318

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



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 RMSE 19702.800445600322 MAE 16757.480694933285 R2 0.7329146952183824

MSE 785600976.607142 RMSE 28028.57428780747 MAE 22165.777484397917 R2 0.34222807880552575 MSE 22157971.6387145 RMSE 4707.225471412486 MAE 3617.346073048316 R2 0.9847551176123155

Generative Parameters Found Parameters

• $\beta_0 = 0 \ \beta_1 = 1 \ 000, \beta_2 = 10 \ 000$ • $\beta_0 = 579 \ \beta_1 = 994, \beta_2 = 9 \ 821$

- Linear regression works :)
- But what happens if relations are not linear?

• Assume that Price $\approx \log(\text{surface})^* | 00 000 ?$



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 0.9922842323758786

- 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 ?

- OLS (Ordinary Least Square Linear regression) is simple to understand and flexible:
 - If I know that a relation is log-linear, or other, I can transform my variables beforehand to fall back on a linear problem (but...)
- Linear regression is interpretable:
 - The meaning of each coefficient β can be interpreted (positive/negative, strength, significance), and thus the relative strength of the corresponding features
 - /!\True only if strict conditions are respected:
 - No multicollinearity (correlations between variables)
 - No endogeneity (correlation between variables and errors (ϵ))
 - No heteroskedasticity (inhomogeneous distribution of errors)
 - Etc.

(OLS?)

- Common question: Is OLS machine learning or stat/ econometrics?
- In my opinion:
 - Not a very meaningful question. Is tomato a vegetable or a fruit?
 - If we focus mainly on the coefficients, and not on the prediction => not classic machine learning
 - If we focus mainly on the prediction and compare with other models => Yes, a ML method like any other

- 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, later during the class

- Another strength of OLS is that it is equivalent to MLE
- MLE (Maximum Likelihood Estimation) is a model-based approach
 - IF we make the assumption that our data has been generated by a random model of the form: $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_n x_n + \epsilon$

- And that variables are normally distributed and independent

- Then MLE finds the parameters of this model that generate the observed data with the highest probability (likelihood).
- It's a less 'intuitive'', more 'scientifically grounded' way to arrive at the same method

- Intuitive reason to use MSE instead of MAE
 - Single, "intuitive" solution (blue)
 - MSE: all the green line fits equally (a | +a2, b | +b2, c | +c2=constant)



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
 - I Level of splitting





MSE 1106922922.7787206 RMSE 33270.45119589935 MAE 27836.40899704275 R2 0.6351425995939648

DECISIONTREE

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





MSE 299670892.805488 RMSE 17311.00496232059 MAE 13262.652619929546 R2 0.9012242490634346

DECISION TREE

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





MSE 90552465.56733872 RMSE 9515.905924678886 MAE 7434.910779663157 R2 0.9701526307682573

DECISION TREE

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





MSE 0.0 RMSE 0.0 MAE 0.0 R2 1.0 MACHINE LEARNING: SOLVED

OR IS IT ? OVERFITTING...
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 method with as many parameters as you want on the training set.
- Only when all your models are trained, you can evaluate it on the test set
 - You can never, ever reuse that (exactly same) test set.

AVOIDING OVERFIT

Decision Tree, **levels=10**

Scores on	MSE 0.0 RMSE 0.0
Train Set	MAE 0.0

Decision Tree, levels=5

MSE 9675372.95170697 RMSE 3110.5261535159884 MAE 2364.5552169188454 R2 0.9968108606746918

Scores on Test Set

MSE 60522590.58807978 RMSE 7779.626635519199 MAE 6427.594619486819 R2 0.9689849224913336

MSE 47482936.48734139 RMSE 6890.786347532579 MAE 5748.307144423111 R2 0.9756671526915104

TRAIN/EVALUATION/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 an evaluation set for intermediary steps (hidden like test set, but not for final evaluation)
 - You can do whatever you want with your evaluation set, it's part of your training process
- Keep a test set, that you will <u>use only once at the end</u>

TRAIN/TEST SPLIT

• What size should your test set have?

No good answer. 66% Train, 33% Test is often a default choice

• Rule of thumb:

- You need <u>enough</u> 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
 - e.g.: predict weight of a Tomato based on its species...
- Problem is if data is scarce
 - =>Cross validation

- Golden rule: One test set must be used only once
- But from a single dataset, you can create multiple test sets
 If you just want to restart you training differently, make a new 66/33 split
- If you have too few data to put 33% aside for training:
 - 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











Iteration N/N

dataaspirant.com

- Do you need Cross validation and which one?
- In my opinion:
 - If your data is very scarce, you need it from the beginning
 - If you are at a point in which every fraction of a % of accuracy count.
- A simple train/test is enough for most cases.

FIGHTING OVERFIT BACKTOTHE METHOD

FIGHTING OVERFIT

• Implicit limit to overfit:

- Because a method has a limited power of expression, it cannot overfit "too much".
 - <u>Trivial solution</u>: 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
- Not necessarily a clear boundary between the 2

FIGHTING OVERFIT





Train

MSE 474131230.6072998 RMSE 21774.554659218633 MAE 16958.426496791166 R2 0.8437196622358905

MSE 9675372.95170697 RMSE 3110.5261535159884 MAE 2364.5552169188454 R2 0.9968108606746918

Test

MSE 297361867.9984524 RMSE 17244.18359907051 MAE 14666.202886910516 R2 0.8476155548782759 MSE 47482936.48734139 RMSE 6890.786347532579 MAE 5748.307144423111 R2 0.9756671526915104

FIGHTING OVERFIT

- Avoiding overfit in decision trees: Pruning strategies
 - One way to see: Artificially limit the expressivity of the model
 - I)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.
 - What the weather be like in 5 years ? Extrapolation from current condition...

OVERFIT/UNDERFIT, HIGH BIAS HIGH VARIANCE



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 methods change
- Imbalanced datasets might become a problem

- 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



- 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



MSE 0.06361520558572538 RMSE 0.2522205494913636 MAE 0.20506852857512292 R2 0.7455391776570985

• Weaknesses: Outliers



• Weaknesses: Class imbalance



- 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 FUNCTION



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

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



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

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

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

LOGISTIC REGRESSION

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

Problem to solve similar to a linear regression. We minimize the error between true $y \in \{0,1\}$ and estimated probability of being 1

LOGISTIC REGRESSION

/!\ log transform of the target variable => multiplicative relation between variables Interpretation as **odd ratios:** +1in x_i =>prediction 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 <u>catastrophic</u>
- Simple solution (often used): one VS all
 - Train a logistic classifier on one class VS all other classes.
 - Attribute the class with the largest confidence
 - e.g.: house: 20%. Apartment: 30%. Office: 70%. Industrial: 80%=>Industrial.
 - Rather a heuristic than principled method.
- Alternative approach: softmax regression
 - Later in class

- 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

- Most common homogeneity/diversity/inequality/purity scores
 - p_i : fraction of items of class i

Gini Coefficient:
$$1 - \sum p_j^2$$

Entropy:
$$-\sum_{j} p_{j} \cdot log_{2}p_{j}$$

- Most common homogeneity/diversity/inequality/purity scores
 - p_i : fraction of items of class i

Gini Coefficient:
$$1 - \sum p_j^2$$

- Min: 0: 1 class only
- Max: 0.5: (2 classes), 0.66(3classes), 0.75 (4classes), 0.875(8classes)
- Interpretation:

- If we classify by taking an element at random, probability to be wrong.

- 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: I (2 classes), I.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


CLASSIFICATION: EVALUATION

		Actual	
		Positive	Negative
cted	Positive	True Positive	False Positive
Predi	Negative	False Negative	True Negative



CLASSIFICATION: EVALUATION

• Precision= $\frac{TP}{TP+FP}$

 Among those predicted as True, fraction of really True

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

Among those really true, what fraction did we identity correctly



ACCURACY

• Accuracy:
$$\frac{TP + TN}{P + N}$$

- Fraction of correct prediction, among all predictions
 - Simple to interpret
- Main drawback: class imbalance
 - Test whole city, I 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)/1000 = 0.95

FI SCORE

- . FI 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
- Scores for the covid predictor:
 - <u>Precision</u>=45/95=0.47
 - $\underline{\text{Recall}} = 45/50 = 0.9$
 - ► FI=0.65
- Score for the naive predictor impossible to compute...
 - You need at least some TP !
 - Assuming I "free" TP (Precision=I, Recall=1/50)
 - => FI=0.04

AUC

- Method adapted for strong class imbalance
 - Typical example: recommendation. Will user X buy product Z?
 - We are not really interested in having a correct classification, but of ranking correctly items
 - Top k strategy: Accuracy among the top-k items with higher score/probability?
- Will see in link prediction class