MACHINE LEARNING BASIC CONCEPTS

SUPERVISED MACHINE LEARNING CLASSIFICATION TASK.

future data

Years	Amount	Salary	Own house?	Overdue accounts?	Repay loan
10	50000	3000	Yes	0	??

T = training set

Attributes, **features**, predictors, Input variables, Independent variables, explanatory variables

Label, **class**, output variable, dependent variable, **response**, predictand, target

Instances, examples, data points

Years	Amount	Salary	Own house?	Overdue accounts?	Repaid loan
15	60000	1900	Yes	2	No
2	30000	3500	Yes	0	Yes
9	9000	1700	Yes	1	No
15	18000	3000	No	0	Yes
10	24000	2100	No	0	No
	…	…	…	…	…

Algorithm

Model

IF OA >0 **THEN** NO

IF OA==0 **AND** S>2500 **THEN** Yes

Repaid loan = yes

DEFINITIONS: ATTRIBUTES AND RESPONSE

- **Attributes / features / input variables**
  - A feature is an individual measurable property of an instance
  - Types:
    - Numeric: (real numbers or integers):
      - 0, 1, 2
      - 1.3, 7.9, 10.798, …
    - Categorical: yes / no ; red / green / yellow
      - Many ML algorithms cannot deal with them: they must be encoded into numbers (one-hot-encoding, …)
    - Ordinal: cold, lukewarm, hot
      - Most ML cannot deal with them, they are encoded as integer numbers

Categorical need to be encoded: one-hot encoding

there is no sense of order

Encoding might add or reduce information

In ordinal variables, the encoding is obvious

- **Response / output variable**
  - If categorical (e.g. cancer / no cancer) => classification problem
    - If it has two values: binary classification, otherwise, multi-class problem
  - If real / integer number => regression problem

better results expected for binary classification

DEFINITIONS: FEATURE SPACE (INSTANCE SPACE)

Instances = Rows

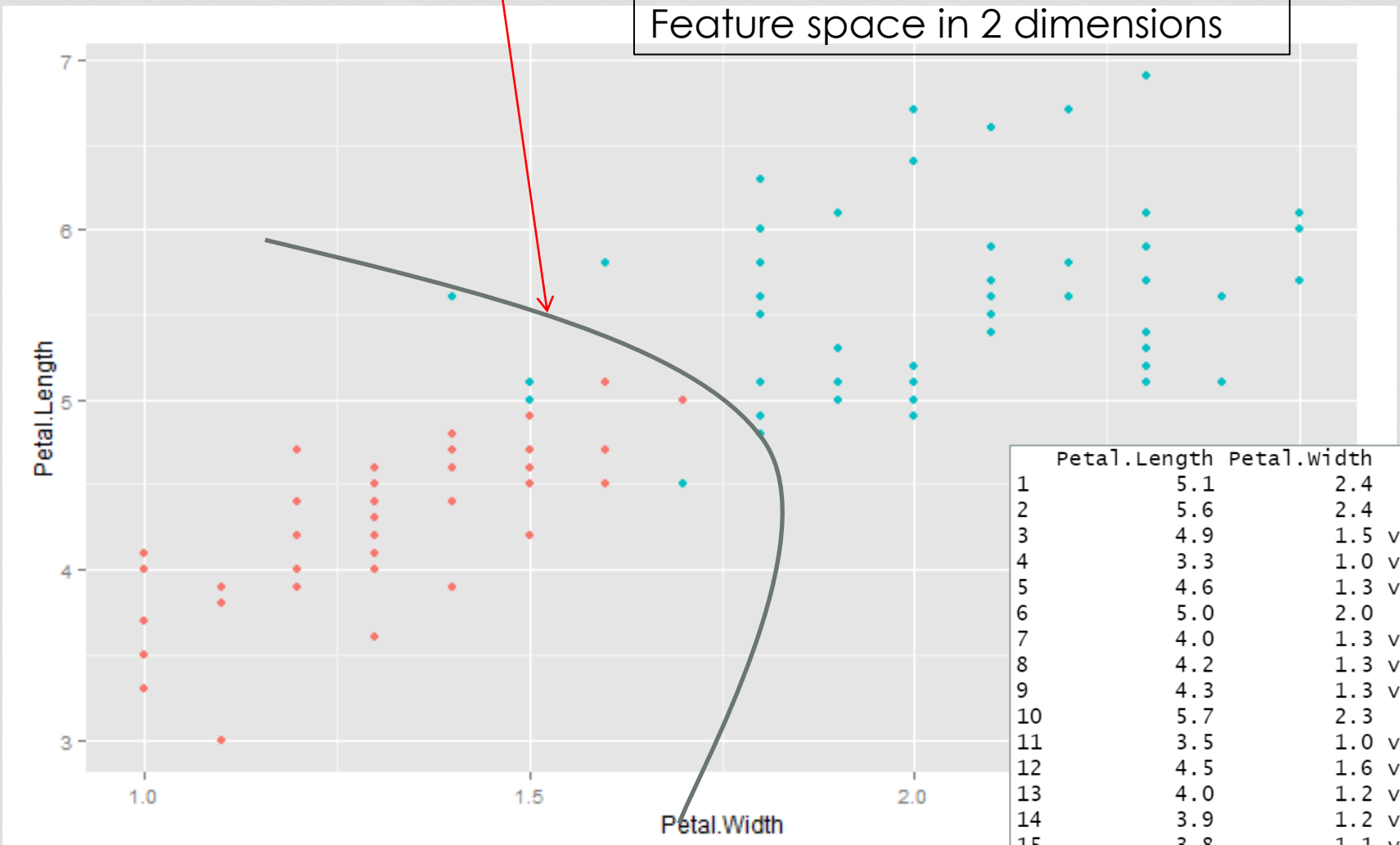
- Instances, examples = tuples
  - In general, they inhabit a d-dimensional space (instance space)
  - (input, output) = $(\mathbf{x}_i, y) = (x_{i1}, x_{i2}, \ldots, x_{id}, y) \in (\mathbf{R}^d, Y)$
    - *Note:* ***boldface*** *means vector*
    - This instance has 5 inputs and 1 output. It inhabits a 5-dimensional space

Years	Amount	Salary	Own house?	Overdue accounts?	Repaid loan
15	60000	1900	Yes	2	No

    - In 2-dimensions (2 attributes), each instance is a point in instance space

- Example: classify plants into two classes ("versicolor“ / red vs. "virginica“ / blue)
- 2 attributtes = (Petal.Width, Petal.Length) = 2 dimensions
- Classification = finding a boundary between the classes

the other approach is to see a model as transformation between inputs into output



	Petal.Length	Petal.Width	Species
1	5.1	2.4	virginica
2	5.6	2.4	virginica
3	4.9	1.5	versicolor
4	3.3	1.0	versicolor
5	4.6	1.3	versicolor
6	5.0	2.0	virginica
7	4.0	1.3	versicolor
8	4.2	1.3	versicolor
9	4.3	1.3	versicolor
10	5.7	2.3	virginica
11	3.5	1.0	versicolor
12	4.5	1.6	versicolor
13	4.0	1.2	versicolor
14	3.9	1.2	versicolor
15	3.8	1.1	versicolor

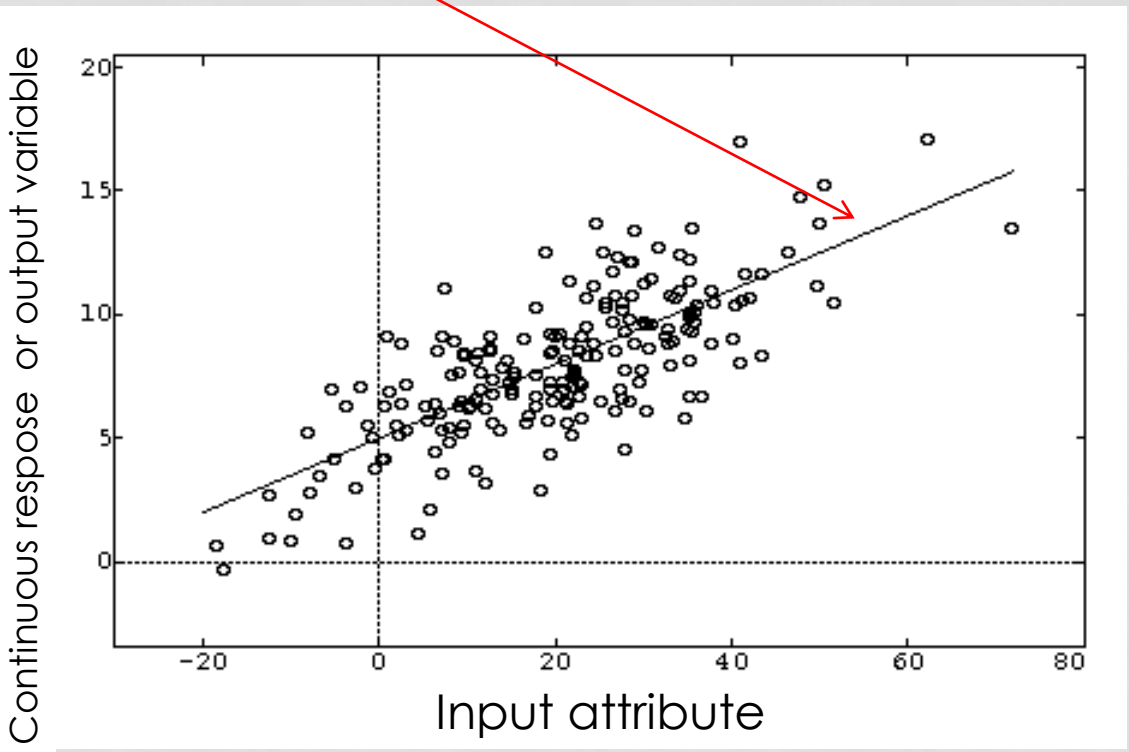
FEATURE SPACE IN REGRESSION

- In the following case, there is one input variable and the output variable / response (continuous "label")
- Regression = finding a function that transforms the inputs into the output

There is an extra axis for the output as we cannot assign a colour to the output

input output

rooms	HousingPrice
6.575	24.0
6.421	21.6
7.185	34.7
6.998	33.4
7.147	36.2
6.430	28.7
6.012	22.9
6.172	27.1



SUPERVISED MACHINE LEARNING CLASSIFICATION TASK. AN EXAMPLE:

future data

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Algorithm

Model

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Repay loan = yes

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Algorithm

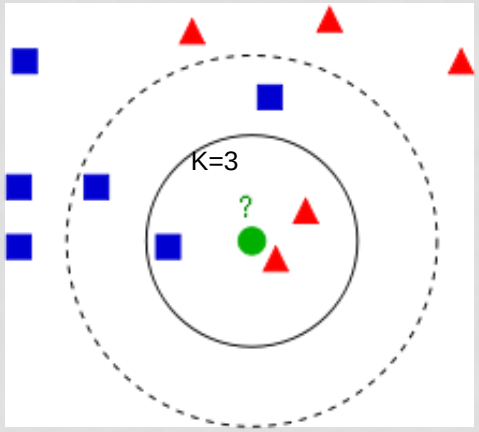
Model

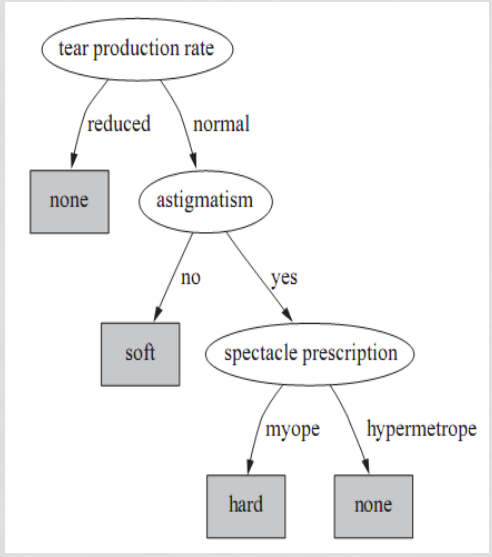
- K-Nearest neighbors (KNN)
- Trees, rules
- Ensembles (bagging, boosting, stacking, …)
- Functions: neural networks, support vector machines, deep learning. …

Repay loan = yes

SYLLABUS

1. Introduction to Machine Learning: tasks, algorithms & models
2. Basic methods for training classification and regression models:
   - **K Nearest Neighbours (KNN)**
   - Classification / regression trees & rules
3. Methodology
4. Methods for preprocessing
5. Advanced training methods based on ensembles of models
6. Large Scale Machine Learning. Big Data
7. Advanced topics
8. Software tools





KNN: K-NEAREST NEIGHBOURS

KNN is a lazy method, because the "model" is the training data

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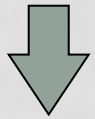

?

El modelo son los propios datos de entrenamiento de los que se aprende y generaliza

Training data

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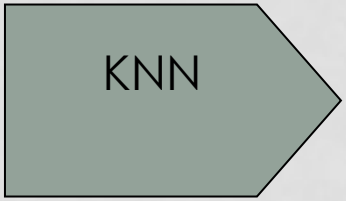

Model

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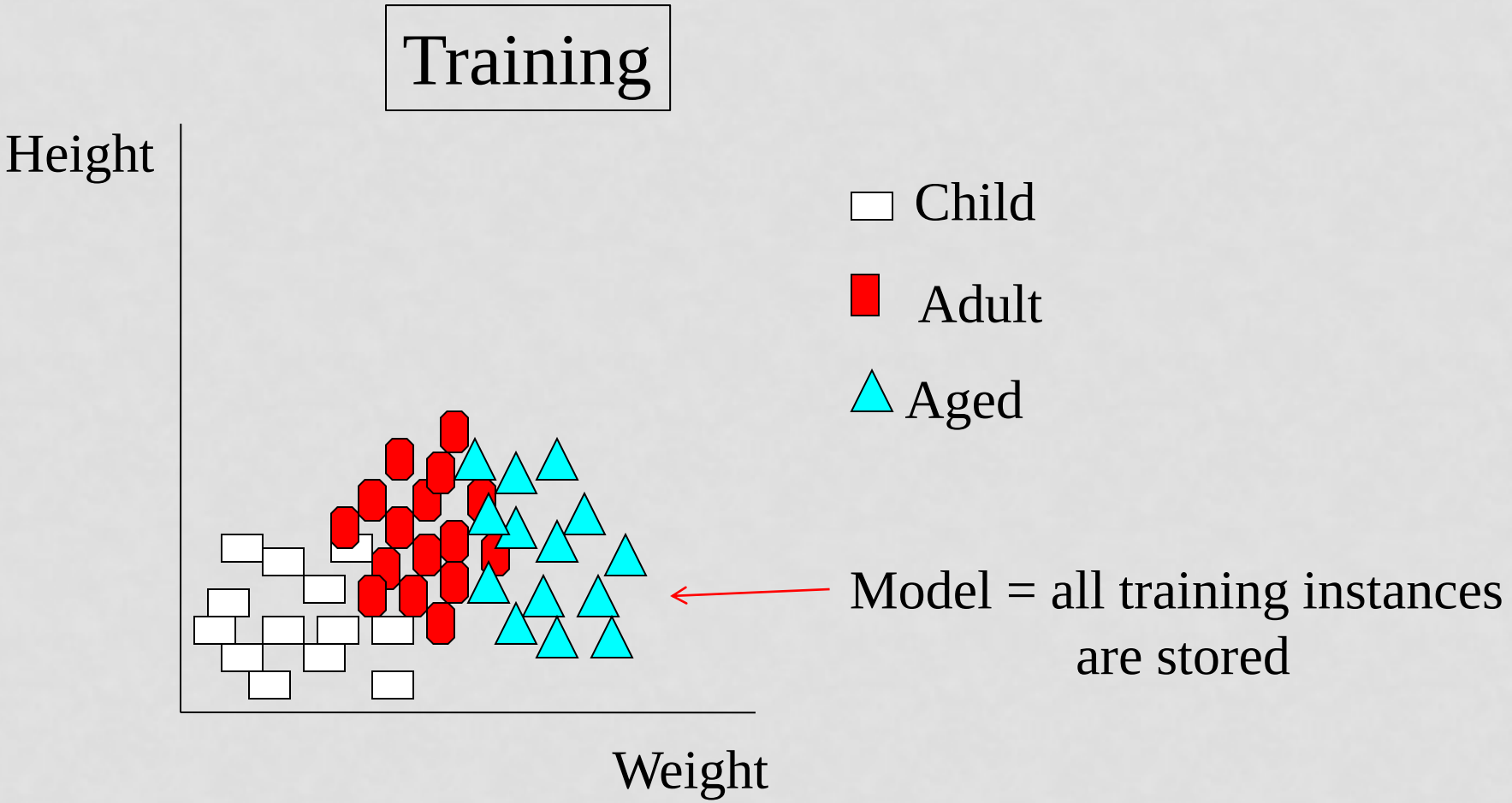
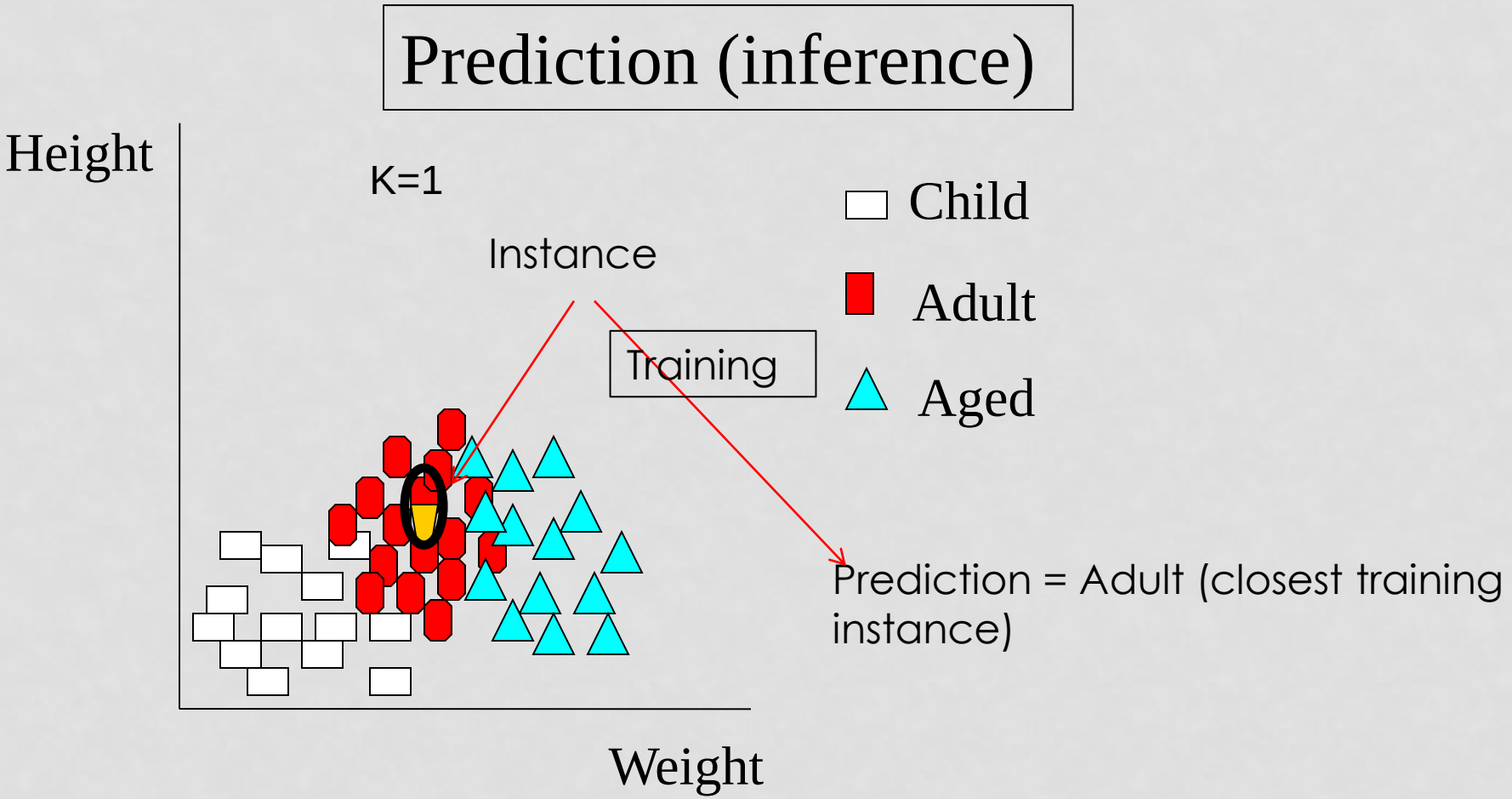
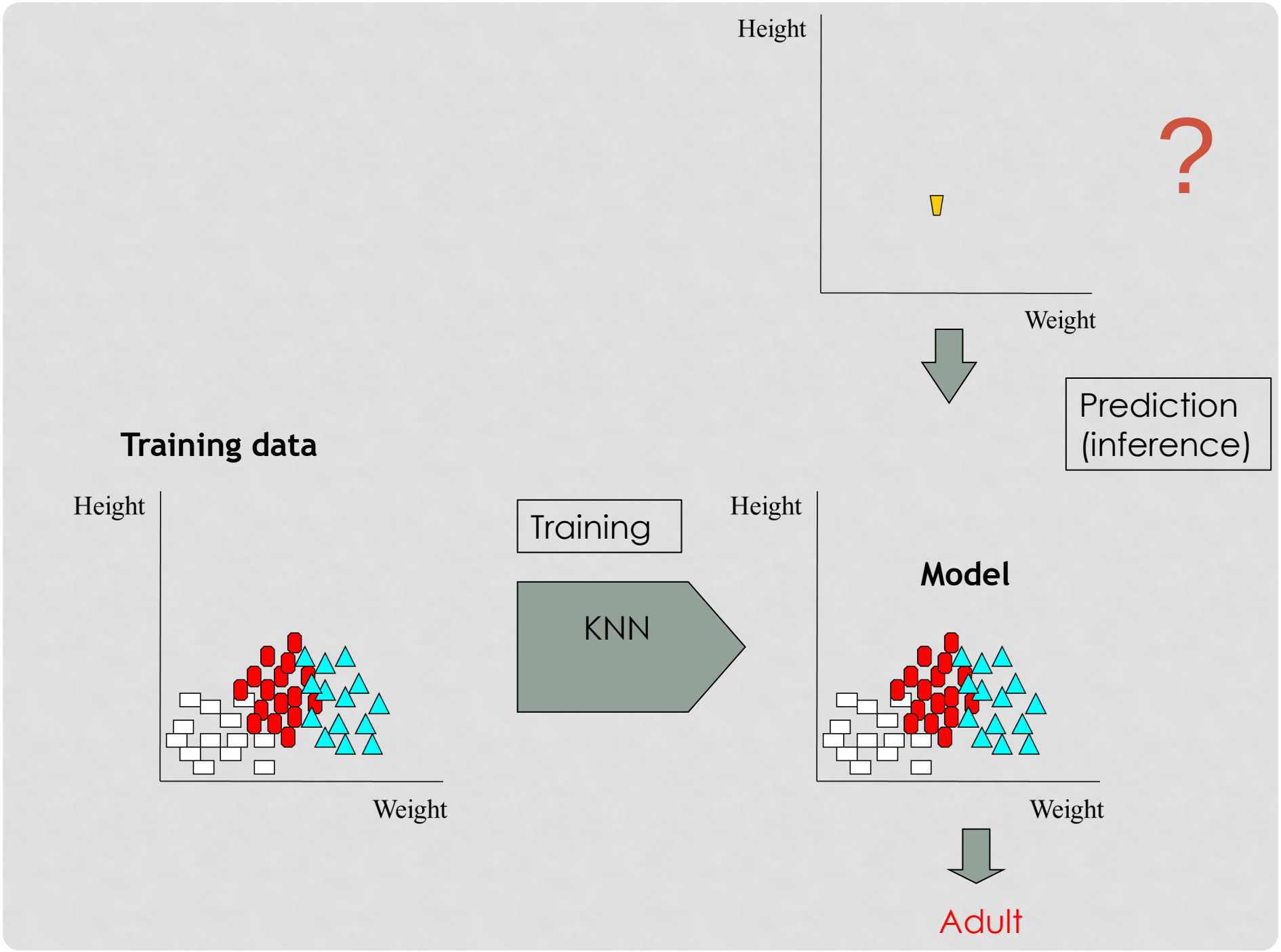
Yes

K-NEAREST NEIGHBORS (KNN): training



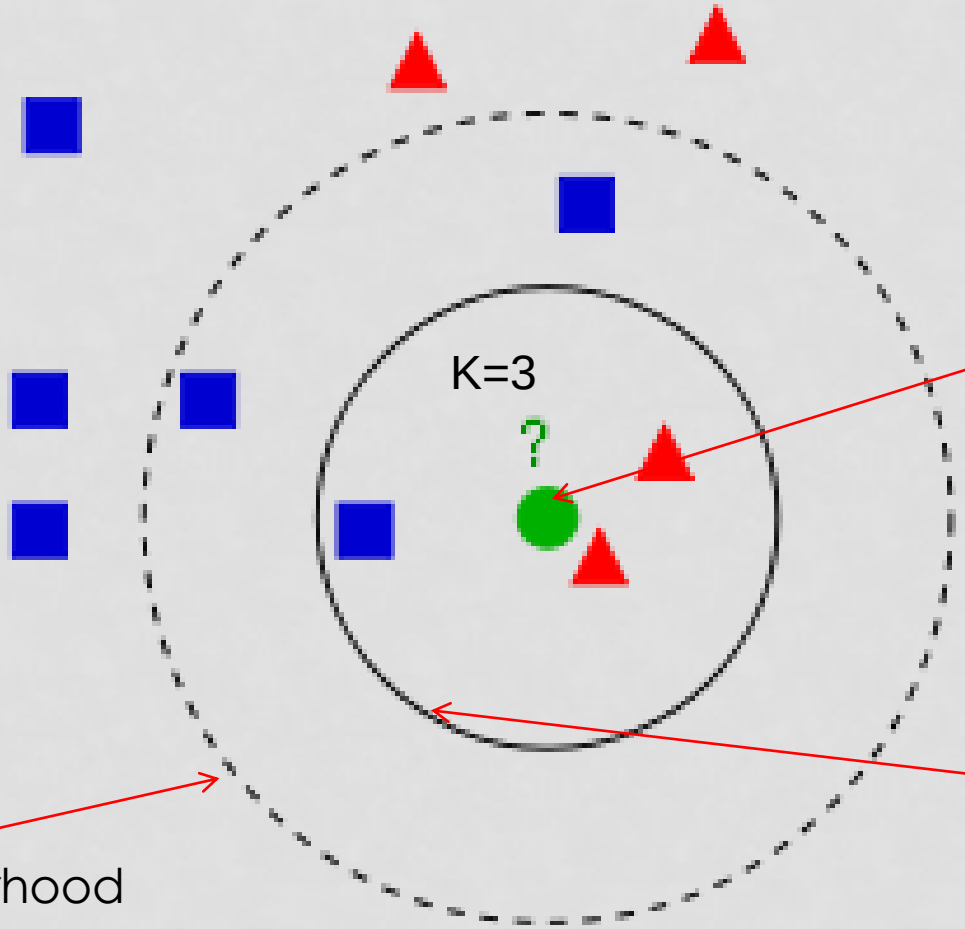
K-NEAREST NEIGHBORS (KNN): prediction




Height
?
Weight
Prediction
(inference)
Training data
Height
Weight
Training
KNN
Height
Model
Weight
Adult

K-NEAREST NEIGHBORS (KNN)

K> 2 => classify new instances as the majority class of the k-nearest neighbours



Prediction instance

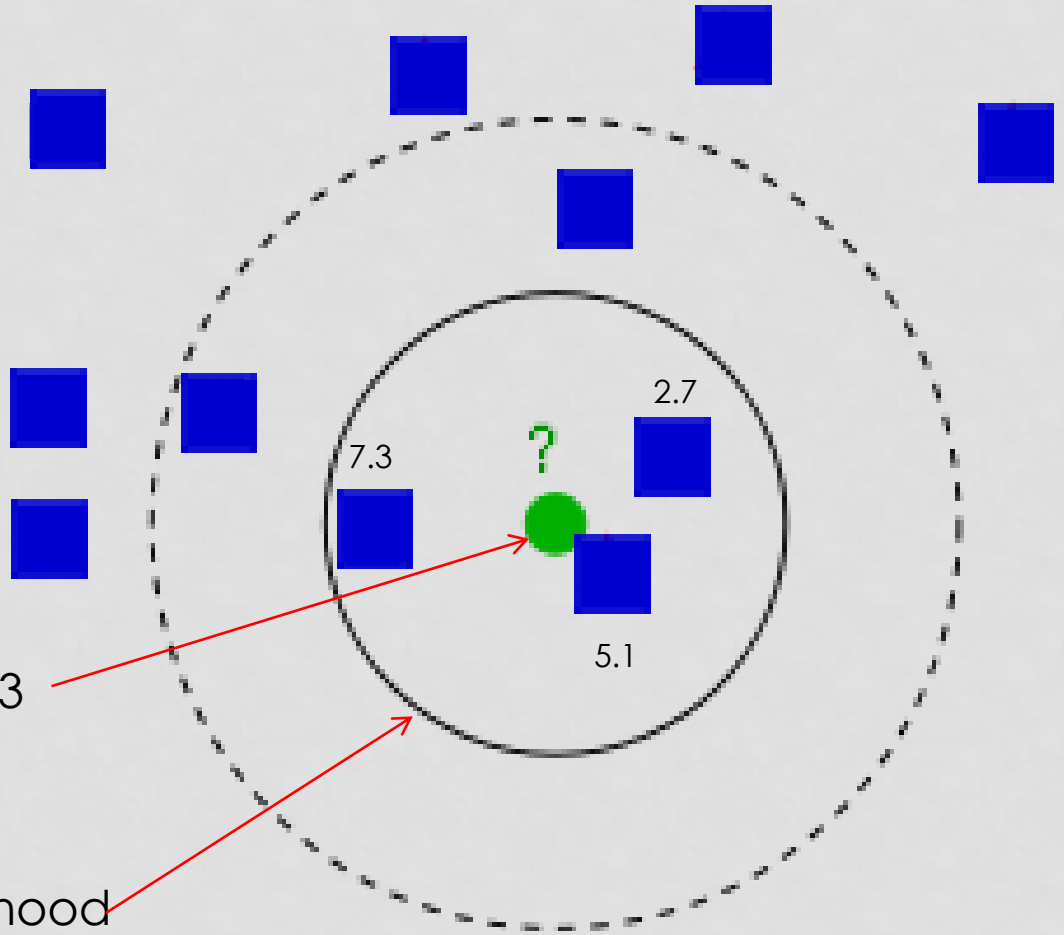
Triangles = 2
Squares = 1
Prediction (majority class in the neighbourhood) = **Triangle**

Neighbourhood with k=3

Neighbourhood with k=5

KNN FOR REGRESSION

It can be easily extended for **regression** by computing the average of the k-nearest neighbours

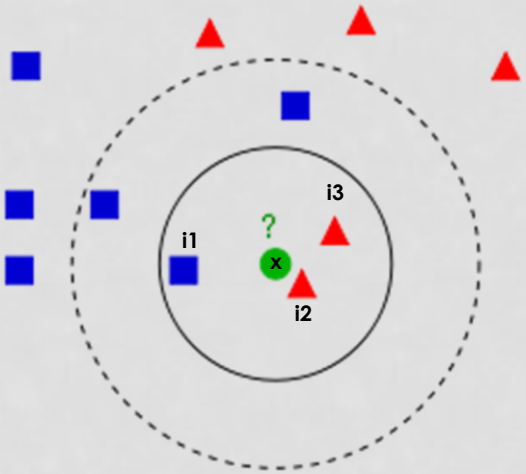


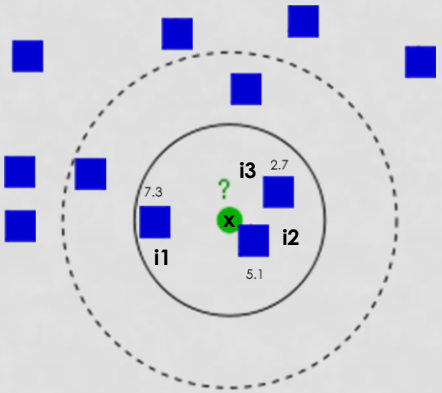
Prediction = (7.3+2.7+5.1)/3

Neighbourhood with k=3

INVERSE EUCLIDEAN DISTANCE WEIGHTING

- In some cases, it may be better to weight the neighbors so that nearer neighbors contribute more to the classification or regression
- The inverse of the distance is typically used
- "uniform" (euclidean distance) vs. "distance" (inverse euclidean distance)





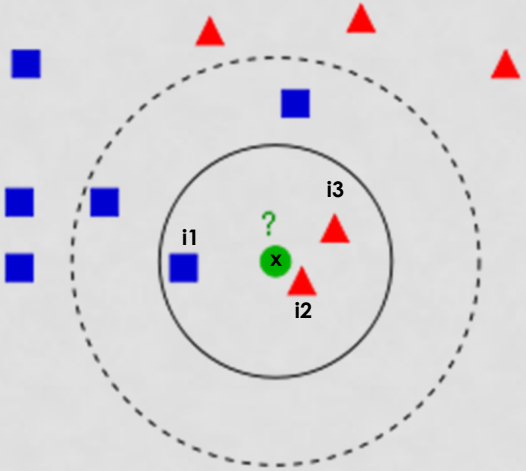
- Blue square: $\frac{1}{d1}$
- Red triangle: $\frac{1}{d2} + \frac{1}{d3}$

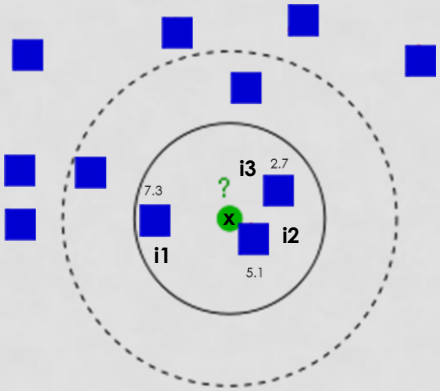
The weight would be the inverse of the distance

$$\frac{\frac{7.3}{d1} + \frac{5.1}{d2} + \frac{2.7}{d3}}{\frac{1}{d1} + \frac{1}{d2} + \frac{1}{d3}}$$

INVERSE EUCLIDEAN DISTANCE WEIGHTING

- In some cases, it may be better to weight the neighbors so that nearer neighbors contribute more to the classification or regression
- The inverse of the distance is typically used





weights : *{'uniform', 'distance'}, callable or None, default='uniform'*

In scikit-learn

Weight function used in prediction. Possible values:

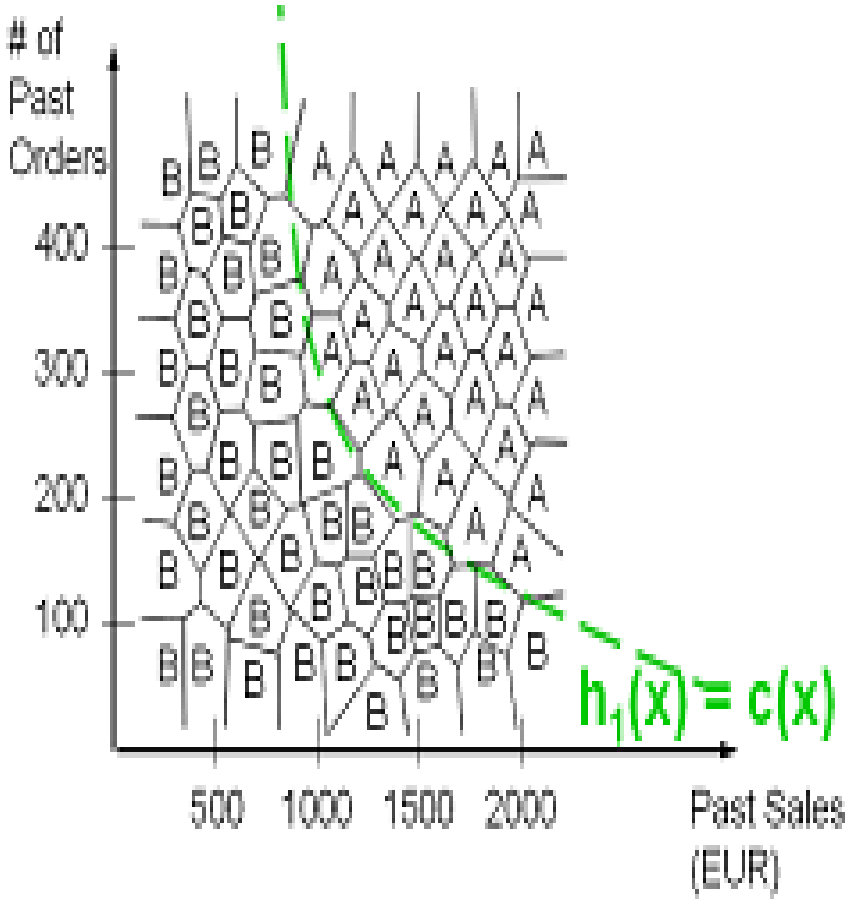
- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.

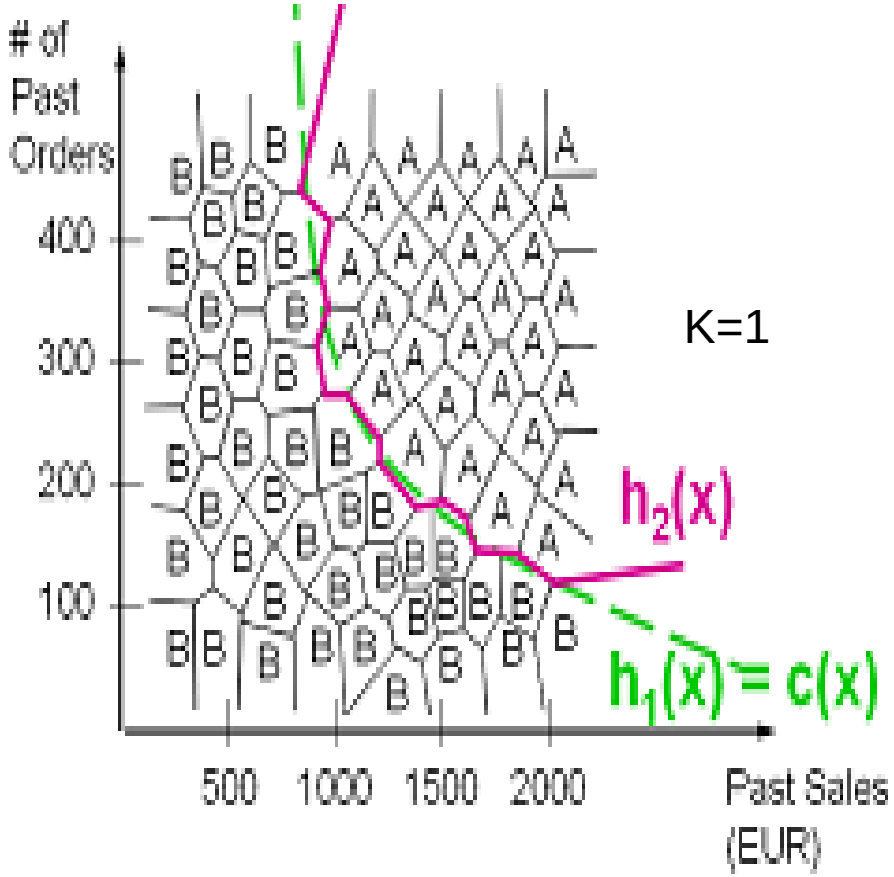
WHY USE K>1? → avoid noissy data

KNN doesnt use voronoi, its just for explanation

VORONOI TESSELLATION in Instance space

The true boundary should separate perfectly the two classes





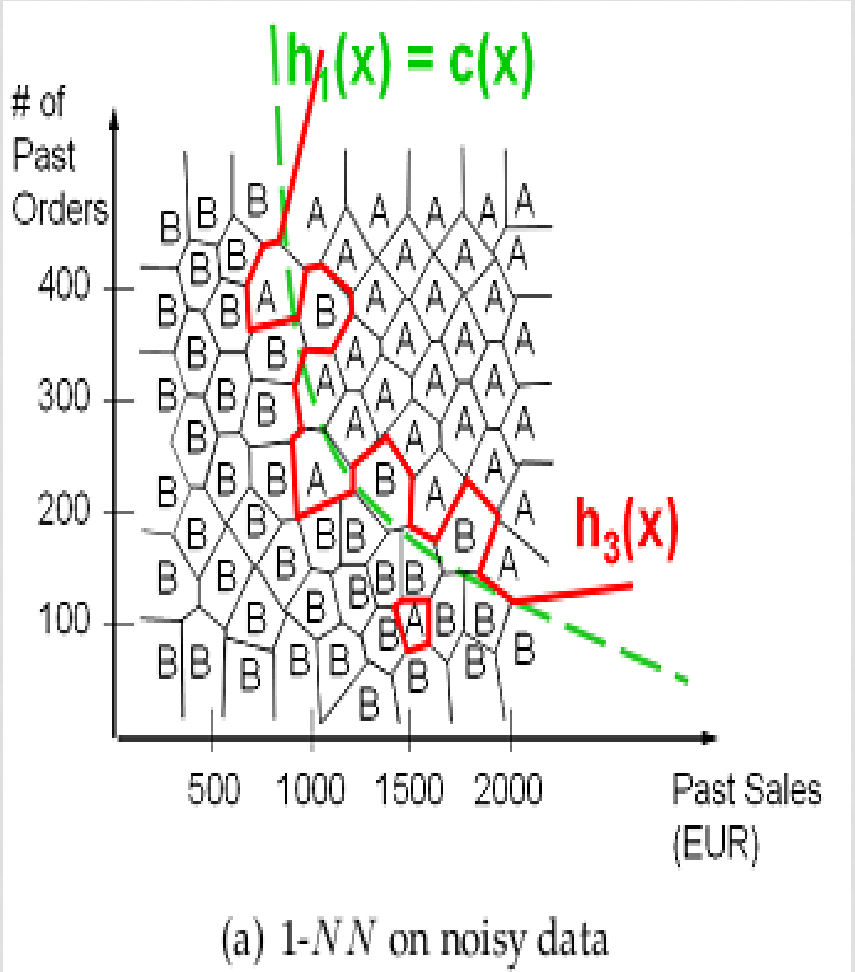
Too Complex: Overfitting
Too Simple: Underfitting

Complexity of the model = Hyperparameters tunning. Length from the tree = 10 is more complex than length =5

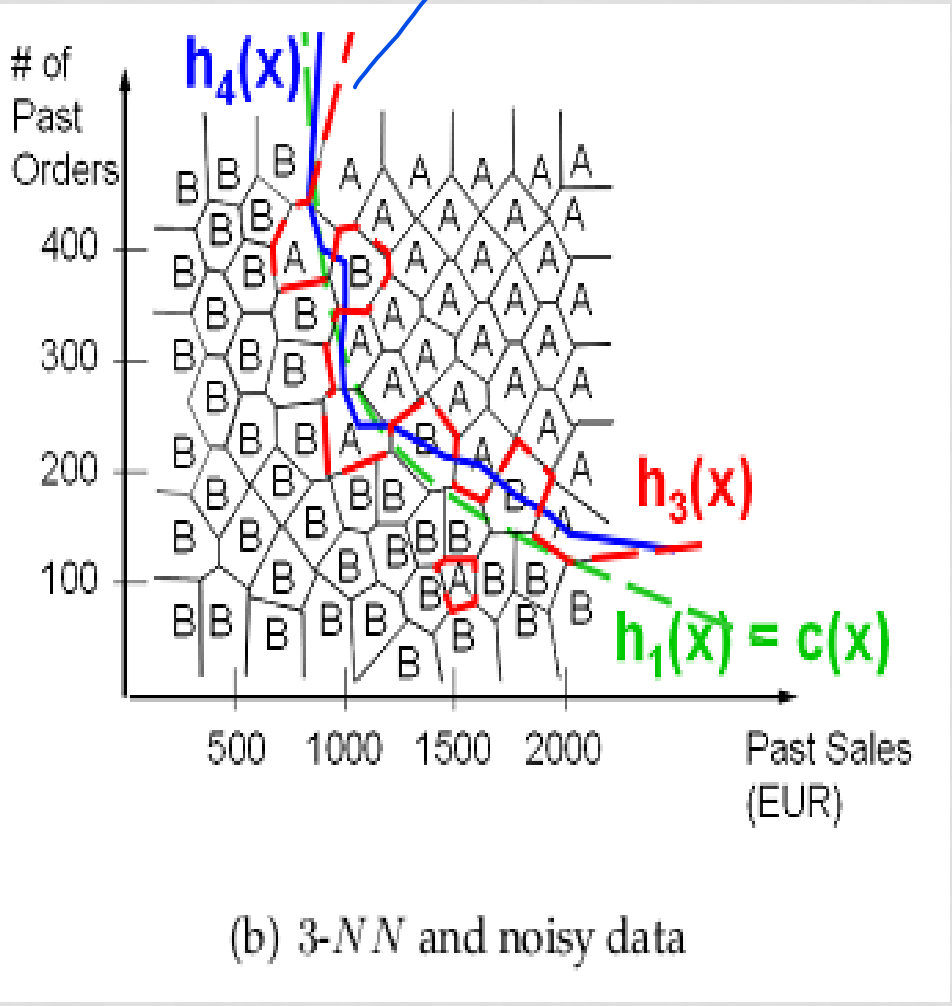
WHY USE K>1?

In KNN, K=1 is more complex than K=5 (k=1, adjust more to training data)

complexity of the model = complexity of the boundary

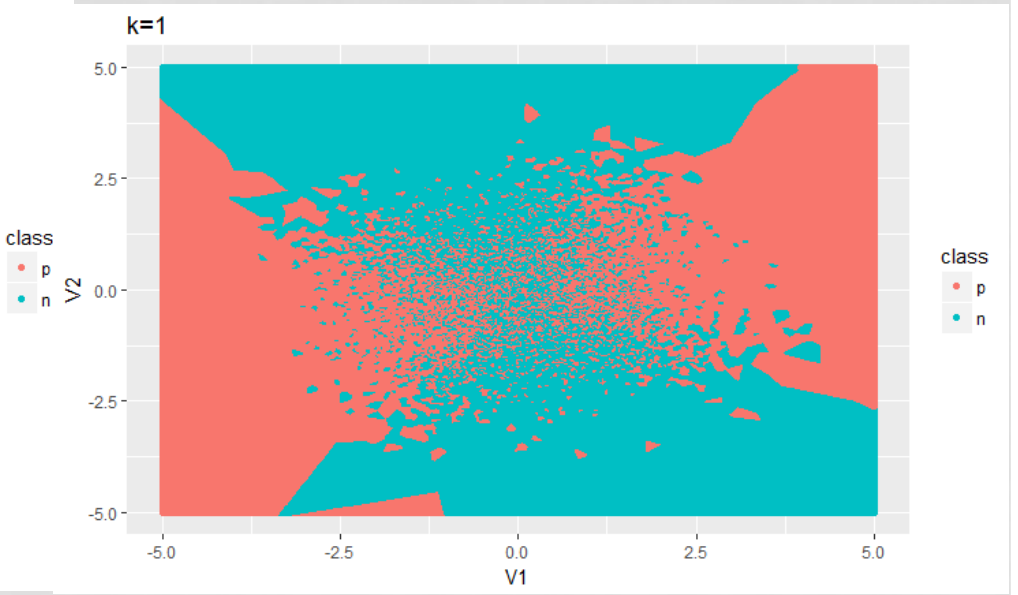


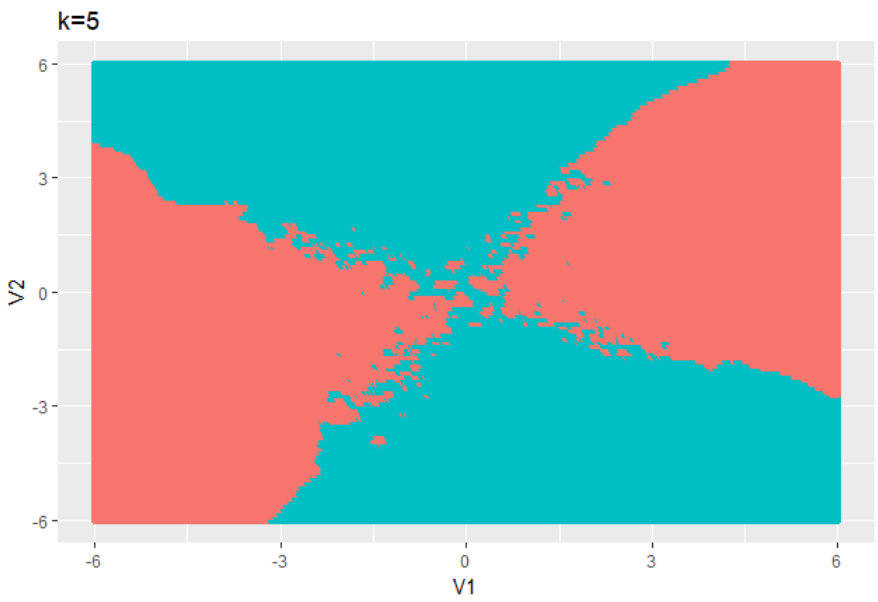
(a) 1-NN on noisy data

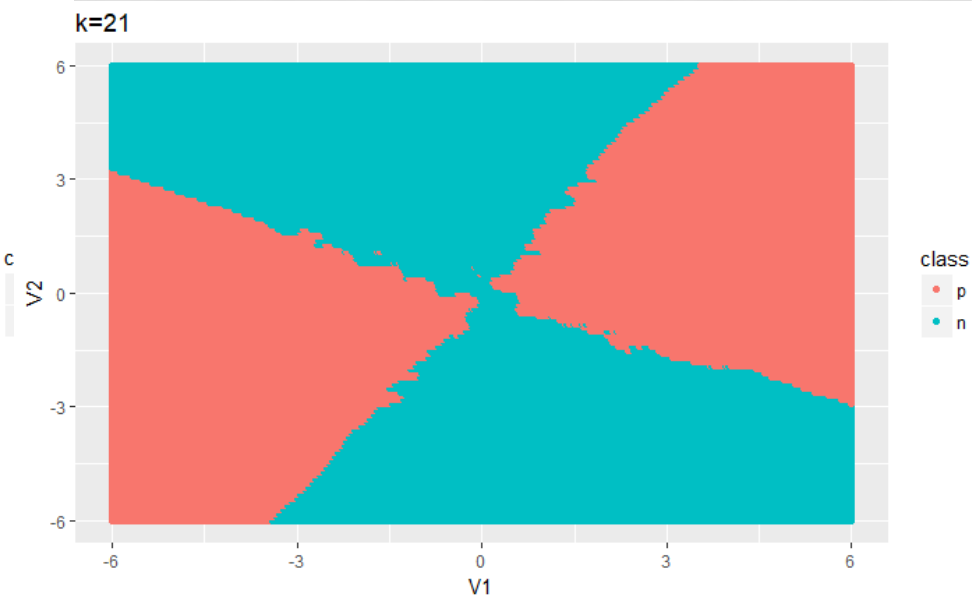


(b) 3-NN and noisy data


4
0
-4
V2
-6
-3
0
3
6
V1


k=1
5.0
2.5
0.0
-2.5
-5.0
V2
-5.0
-2.5
0.0
2.5
5.0
V1
class
p
n


k=5
6
3
0
-3
-6
V2
-6
-3
0
3
6
V1


k=21
6
3
0
-3
-6
V2
-6
-3
0
3
6
V1
class
p
n

Setting	Effect when k = n
Classification	Always predicts the majority class
Regression	Always predicts the mean of the target variable
Variance	Very low (model doesn't vary across point
Bias	Extremely high (model ignores local structur

WHY USE K>1?

- With k=1, noisy instances (i.e. class overlap) have a large influence
- With k>1, more neighbors are considered and noisy instances have less influence (it is like averaging)
- But if k is very large, locality is lost
  - What is KNN if k=number of instances?

Important

- If the number of classes is two, use odd k in order to avoid draws
- K is the main **hyper-parameter** of KNN and has to be tuned properly. Hyperparameter tuning is part of the ML workflow, and we will talk about it in future lectures

SUMMARY OF KNN

- KNN classifies test instances as the majority class in the neighbourhood of the training set
- KNN is a lazy ML algorithm
  - During training, no model is constructed, but all training instances are stored (model = training instances)
- It is based on the idea that the best model of data is the data itself
- It can be easily extended for **regression** by computing the average of the k-nearest neighbours

ISSUES WITH THE USE OF THE EUCLIDEAN DISTANCE IN KNN

- instance #i: $\mathbf{x_i}$ = ($weight_i$, $height_i$) = (w_i, h_i)
- instance #k: $\mathbf{x_k}$ = ($weight_k$, $height_k$) = (w_k, h_k)
- For numerical attributes, the Euclidean distance is typically used:
  - 2D: $d(\mathbf{x_i},\mathbf{x_k})^2 = (w_i-w_k)^2 + (h_i-h_k)^2$
    - $d(\mathbf{x_i},\mathbf{x_k}) = sqrt[\ (w_i-w_k)^2 + (h_i-h_k)^2\ ]$
  - dD: $d(\mathbf{x_i},\mathbf{x_k})^2 = (x_{i1}-x_{k1})^2 + (x_{i2}-x_{k2})^2 + \ldots + (x_{id}-x_{kd})^2$
- Consequences/issues of using the Euclidean distance in KNN:
  1. What to do with categorical variables?
  2. Different features may have different value ranges
  3. Sensitivity to irrelevant features
  4. What if the Euclidean distance is not the most appropriate?

Euclidean distance = focuse too much on variables with large range and ignores features with a low range

Ex: 1 relevant feature and 99 irrelevant features: the classification is going to be based on the irrelevant features

ISSUE #1. WHAT TO DO WITH CATEGORICAL VARIABLES

TREES ARE NOT AFFECTED BY MULTICOLINEALITY AND IS BETTER TO USE ALL THE VARIABLES

- instance #i: $\mathbf{x_i} = (weight_i, height_i) = (w_i, h_i)$
- instance #k: $\mathbf{x_k} = (weight_k, height_k) = (w_k, h_k)$
- For numerical attributes, the Euclidean distance is typically used:
  - $d(\mathbf{x_i},\mathbf{x_k})^2 = (x_{i1}-x_{k1})^2 + (x_{i2}-x_{k2})^2 + \ldots + (x_{id}-x_{kd})^2$

It is the same as doing one-hot encoding

- For categorical attributes: Hamming distance:
  - If attribute *e* is nominal (categorical), instead of $(x_{ie}-x_{ke})^2$, the following is used: $\delta(x_{ie}, x_{ke})$: 0 if $x_{ie}=x_{ke}$ and 1 otherwise
    - e.g. δ("high", "high")= 0; δ("high", "low")= 1
- or transform the categorical attribute to one-hot encoding)

Redundancy = Multicolineality

Ex One-hot encoding: Colour = {Green, Yellow, Red}

Green	Red	Yellow
0	1	0
1	0	0
0	0	1

There is redundancy because if you know 2 columns (0,0) you know the third one (1)

Eliminate redundancy = Dummy Variables

ISSUES WITH THE USE OF THE EUCLIDEAN DISTANCE IN KNN

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- instance #k: $\mathbf{x_k} = (weight_k, height_k) = (w_k, h_k)$
  - $d(\mathbf{x_i},\mathbf{x_k})^2 = (w_i-w_k)^2 + (h_i-h_k)^2$

Important: Distnace depends on the range of the variable not if the variable is relevant or not

Arbitrary reason: considering more relevant weight because its measured in grams compared to height in meters

- Consequences of using the Euclidean distance in KNN:
  1. What to do with categorical variables?
  2. **Different features may have different value ranges**
  3. Sensitivity to irrelevant features
  4. What if the Euclidean distance is not the most appropriate?

ISSUE #2. SCALING (NORMALIZATION)

- It is important to scale (normalize) attributes, because ranges can be different (e.g. human body temperature ranges from 35º to 45º celsius, body weight ranges from 0 to 100kg, body height ranges from 0 to 2m, age ranges from 0 to 100 years, etc.)
- Otherwise, attributes with a large range have more weight on the distance
- Scaling attribute x_1:
  - MinMax (to 0-1 range): $x'_{1j} = \frac{x_{1j} - \min(x_1)}{\max(x_1) - \min(x_1)}$ — convert into a 0-1 range
  - Standarization: $x'_{1j} = \frac{x_{1j} - \bar{x}_1}{\sigma_1}$
  - Robust scaler: $x'_{1j} = \frac{x_{1j} - median(x_1)}{\mathrm{IQR}(x_1)}$ — when the variable has outliers
    - Scale features using statistics that are robust to outliers
    - The IQR (interquartile range) is the range between the 1st quartile (25th quantile) and the 3rd quartile (75th quantile)
    - The number of instances between the 1st quartile and the 3rd quartile is 50%

How to choose the best model: Compute the 3 methods and evaluate it in your model

Sky	Temperature	Humidity	Wind	Tennis
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Overcast	83	86	No	Yes
Rainy	70	96	No	So
Rainy	68	80	No	Yes
Overcast	64	65	Yes	Yes
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Rainy	75	80	No	Yes
Sunny	75	70	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes
Rainy	71	91	Yes	No

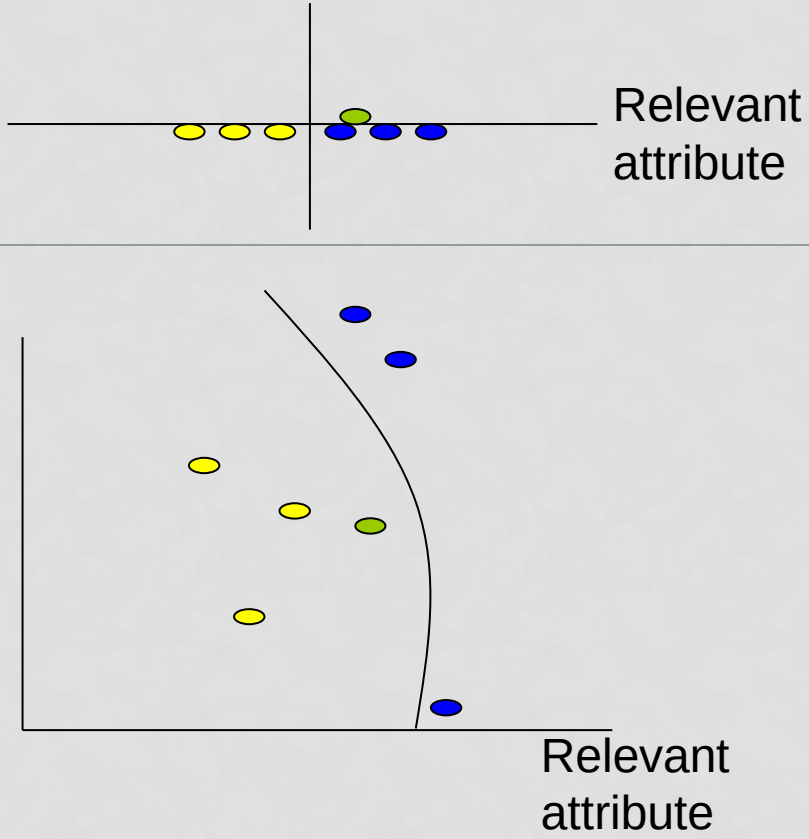
min(T) min(H)
max(T) max(H)

ISSUES WITH THE USE OF THE EUCLIDEAN DISTANCE IN KNN

- $d(\mathbf{x_i},\mathbf{x_k})^2 = (x_{i1}-x_{k1})^2 + (x_{i2}-x_{k2})^2 + \ldots + (x_{id}-x_{kd})^2$

- Consequences of using the Euclidean distance in KNN:
  1. What to do with categorical variables?
  2. Different features may have different value ranges
  3. **Sensitivity to irrelevant features**
  4. What if the Euclidean distance is not the most appropriate?

ISSUE #3. SENSITIVITY TO IRRELEVANT ATTRIBUTES

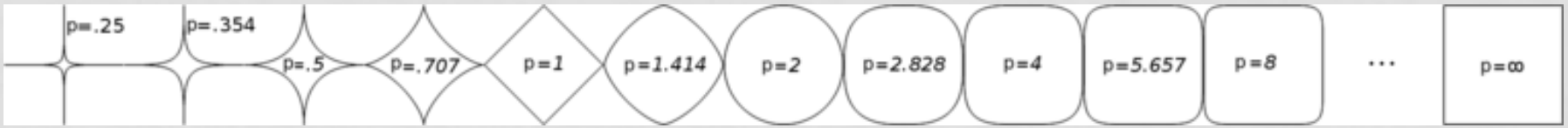


ISSUES WITH THE USE OF THE EUCLIDEAN DISTANCE IN KNN

- instance #i: $\mathbf{x_i} = (weight_i, height_i) = (w_i, h_i)$
- instance #k: $\mathbf{x_k} = (weight_k, height_k) = (w_k, h_k)$
  - $d(\mathbf{x_i},\mathbf{x_k})^2 = (x_{i1}-x_{k1})^2 + (x_{i2}-x_{k2})^2 + \ldots + (x_{id}-x_{kd})^2$
- Consequences of using the Euclidean distance in KNN:
  1. What to do with categorical variables?
  2. Different features may have different value ranges
  3. Sensitivity to irrelevant features
  4. **What if the Euclidean distance is not the most appropriate for a particular problem?**

OTHER DISTANCES: MINKOWSKY

$$\left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p}.$$



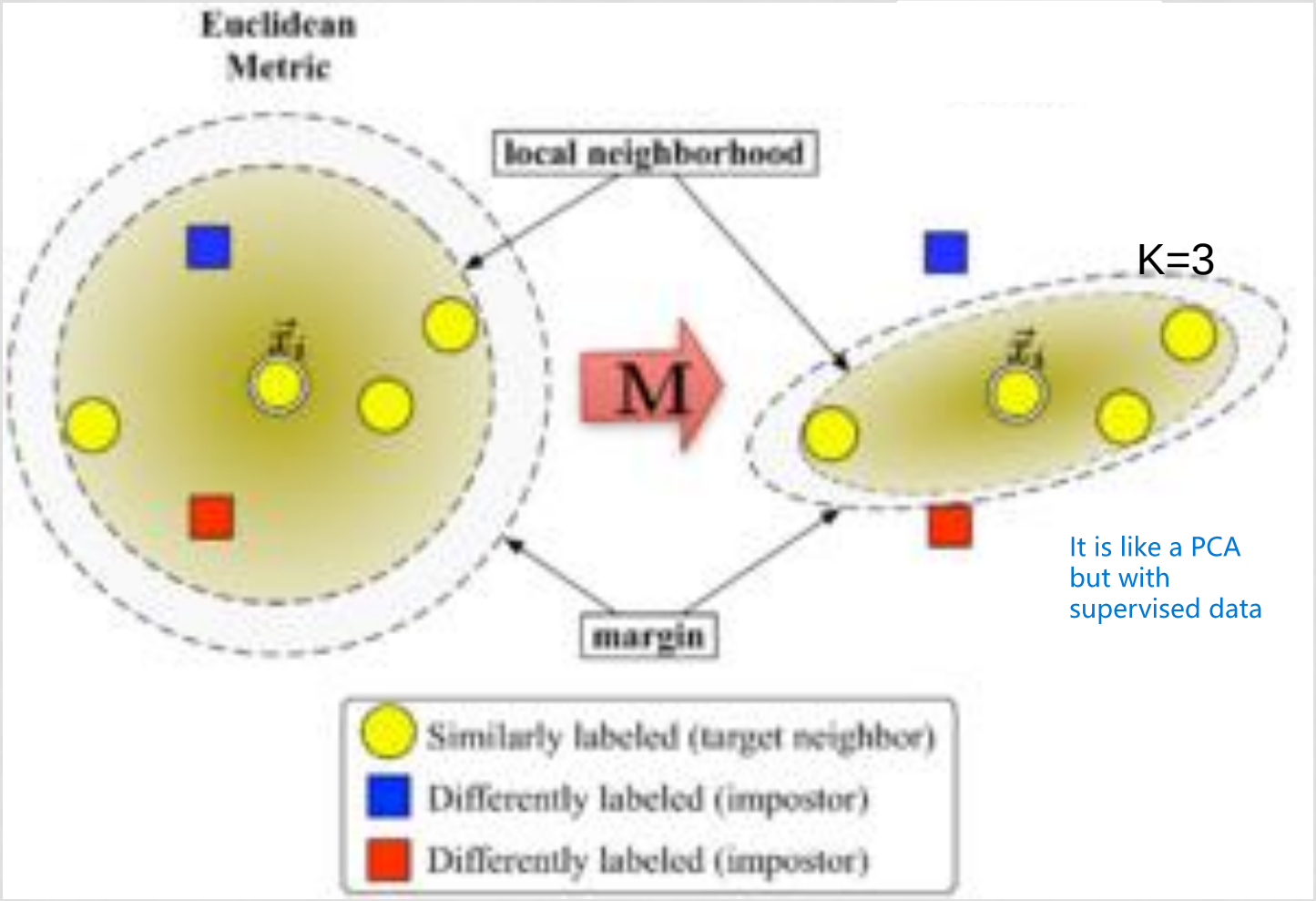
p is another hyper-parameter in scikit-learn

p : *int, default=2*

Power parameter for the Minkowski metric. When p = 1, this is equivalent to using manhattan_distance (l1), and euclidean_distance (l2) for p = 2. For arbitrary p, minkowski_distance (l_p) is used.

OTHER DISTANCES: METRIC LEARNING

The risk of overfitting is reduced by hyperparameter tunning



It is like a PCA but with supervised data

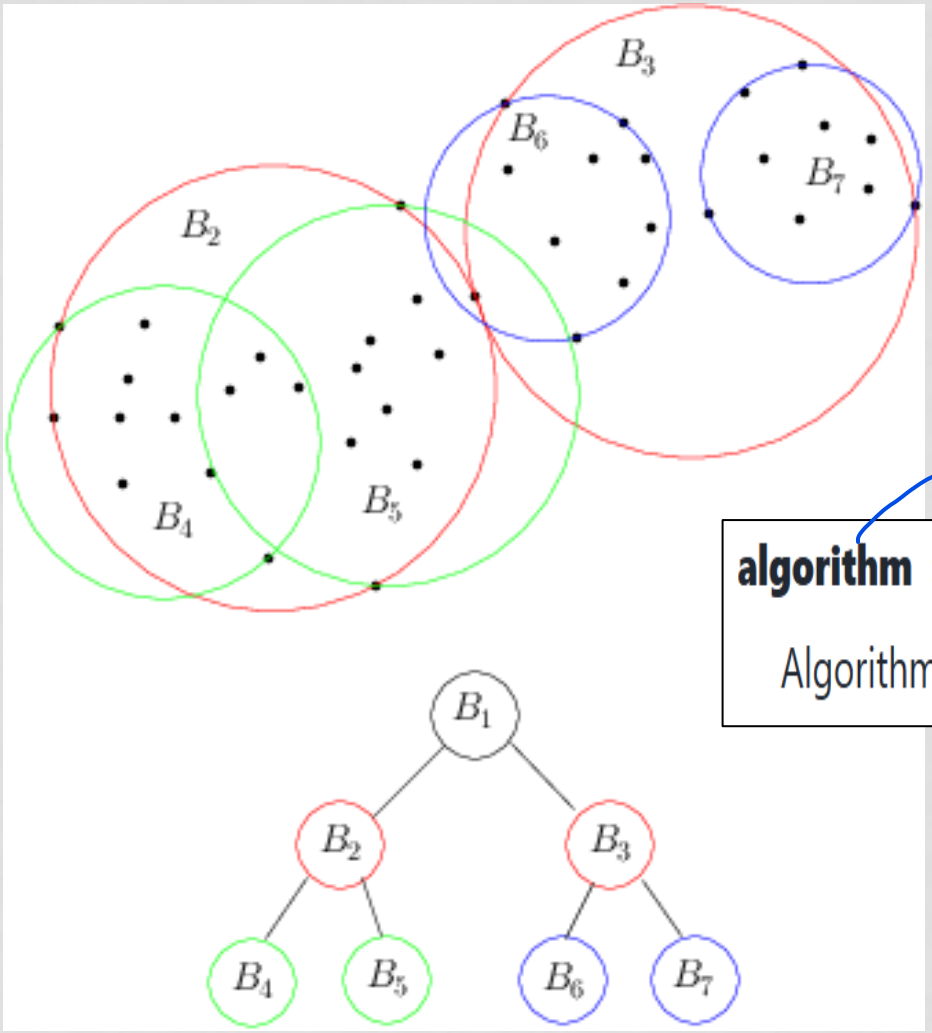
http://contrib.scikit-learn.org/metric-learn/

LIMITATIONS OF KNN

- Slow (when making predictions): all distances to each training instance must be computed. Solution: ball-trees Improves efficiency
- Large storage requirements (all training data must be stored). Possible solution: pre-processing with "condensation"
  The most important instances are the ones defining the border between groups
- Very sensitive to noise. Solutions:
  - Large K's
  - Pre-processing with Wilson editing
- Very sensitive to irrelevant attributes and the curse of dimensionality. Solutions: pre-processing with feature selection / feature extraction
- Depends on the metric (euclidean by default): Solution:
  - Minkowsky Distance
  - Metric learning

BALL-TREES

implemented by scikit-lea



Data is organised in ball-trees (clusters). If a new instance arrives, we will clasiffy it depending on its ball_tree

It is not a hyperparameter because it doesnt change the behaviour of the model, it just makes it more efficient.

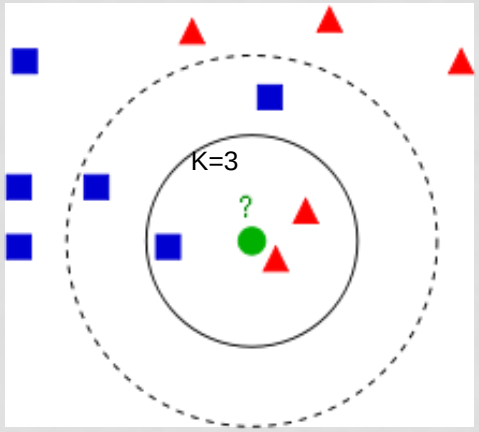
In scikit-learn

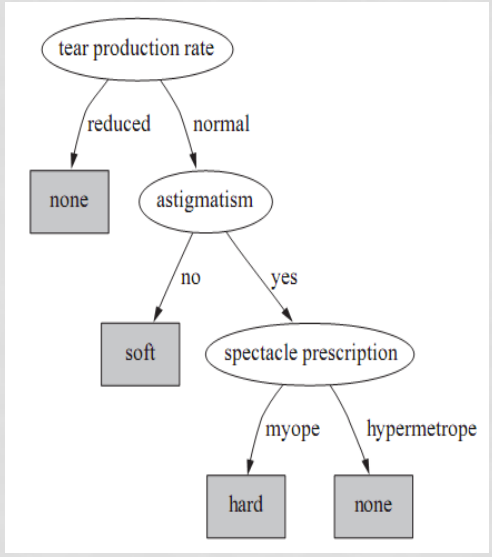
algorithm : *{'auto', 'ball_tree', 'kd_tree', 'brute'}, default='auto'*

Algorithm used to compute the nearest neighbors:

SYLLABUS

1. Introduction to Machine Learning: tasks, algorithms & models
2. Basic methods for training classification and regression models:
   - K Nearest Neighbours (KNN)
   - **Classification / regression trees & rules**
3. Methodology
4. Methods for preprocessing
5. Advanced training methods based on ensembles of models
6. Large Scale Machine Learning. Big Data
7. Advanced topics
8. Software tools





MODELS: TREES (AND RULES) FOR CLASSIFICATION AND REGRESSION

MODELS: DECISION TREES

Attributes, features, Input variables, Independent variables

Label, class, output variable, dependent variable

Sky	Temperature	Humidity	Wind	Tennis
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Over cast	83	86	No	Yes
Rainy	70	96	No	Yes
Rainy	68	80	No	Yes
Over cast	64	65	Yes	Yes
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Rainy	75	80	No	Yes
Sunny	75	70	Yes	Yes
Over cast	72	90	Yes	Yes
Over cast	81	75	No	Yes
Rainy	71	91	Yes	No

Instances, examples

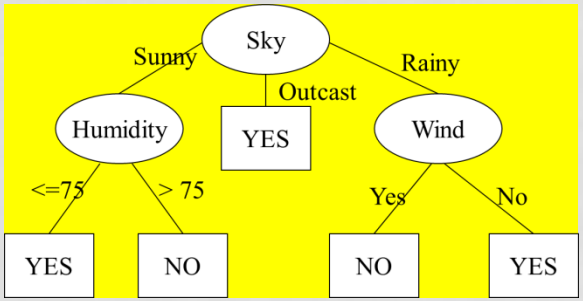
Training Data

Future data

Sky	Temperature	Humidity	Wind	Tennis
Sunny	60	65	No	?????

ML Algorithm

DECISION TREE



Model (Classifier)

Class = Yes

Prediction

MODELS (CLASSIFICATION): RULES

Attributes, features, Input variables, Independent variables

Label, class, output variable, dependent variable

Sky	Temperature	Humidity	Wind	Tennis
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Overcast	83	86	No	Yes
Rainy	70	96	No	Yes
Rainy	68	80	No	Yes
Overcast	64	65	Yes	Yes
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Rainy	75	80	No	Yes
Sunny	75	70	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes
Rainy	71	91	Yes	No

Instances, examples

Training Data

Future data

Sky	Temperature	Humidity	Wind	Tennis
Sunny	60	65	No	?????

ML Algorithm

RULES

IF Sky = Sunny **AND** Humidity <= 75

THEN Tennis = Yes ...

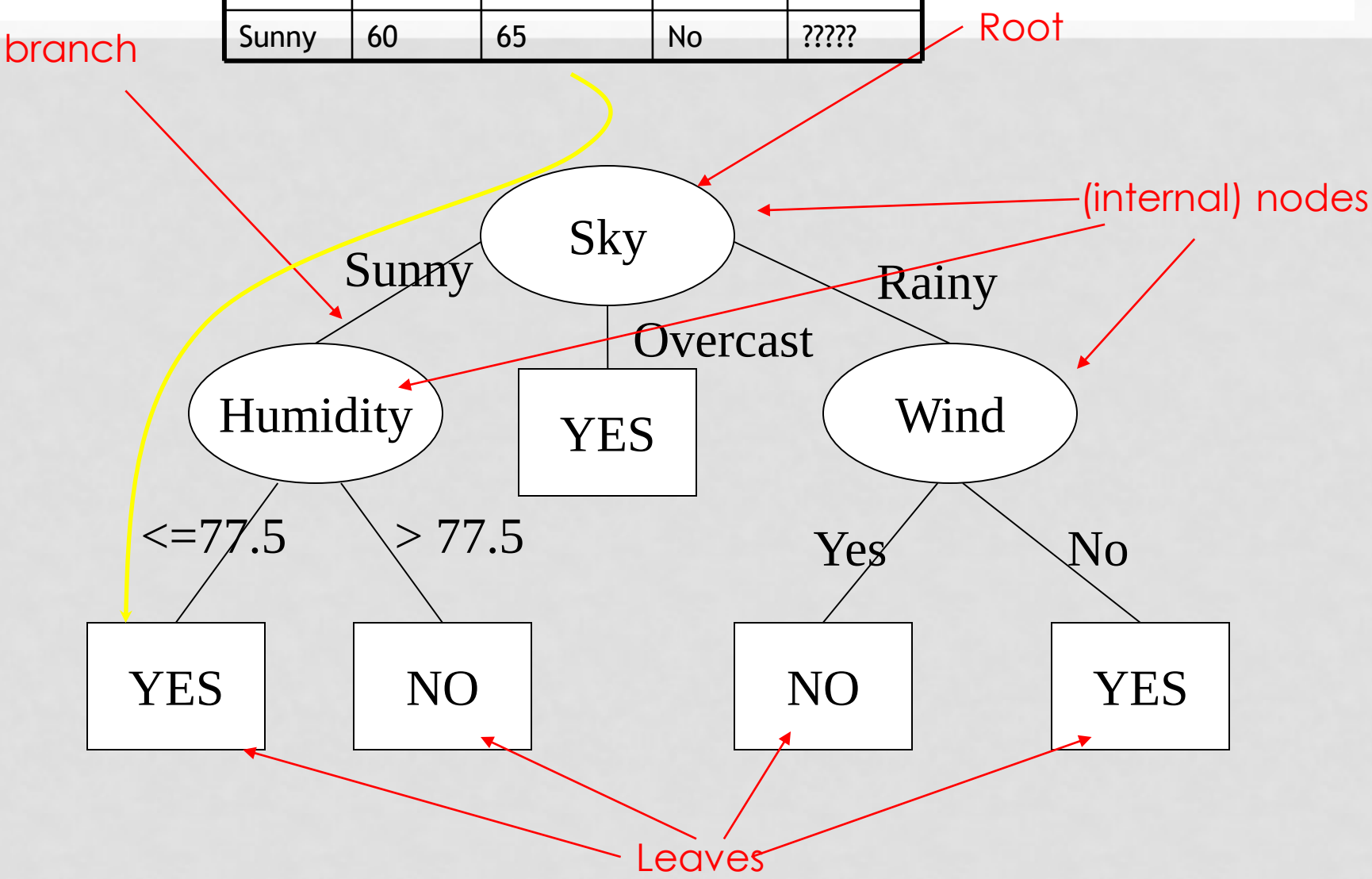
Model (Classifier)

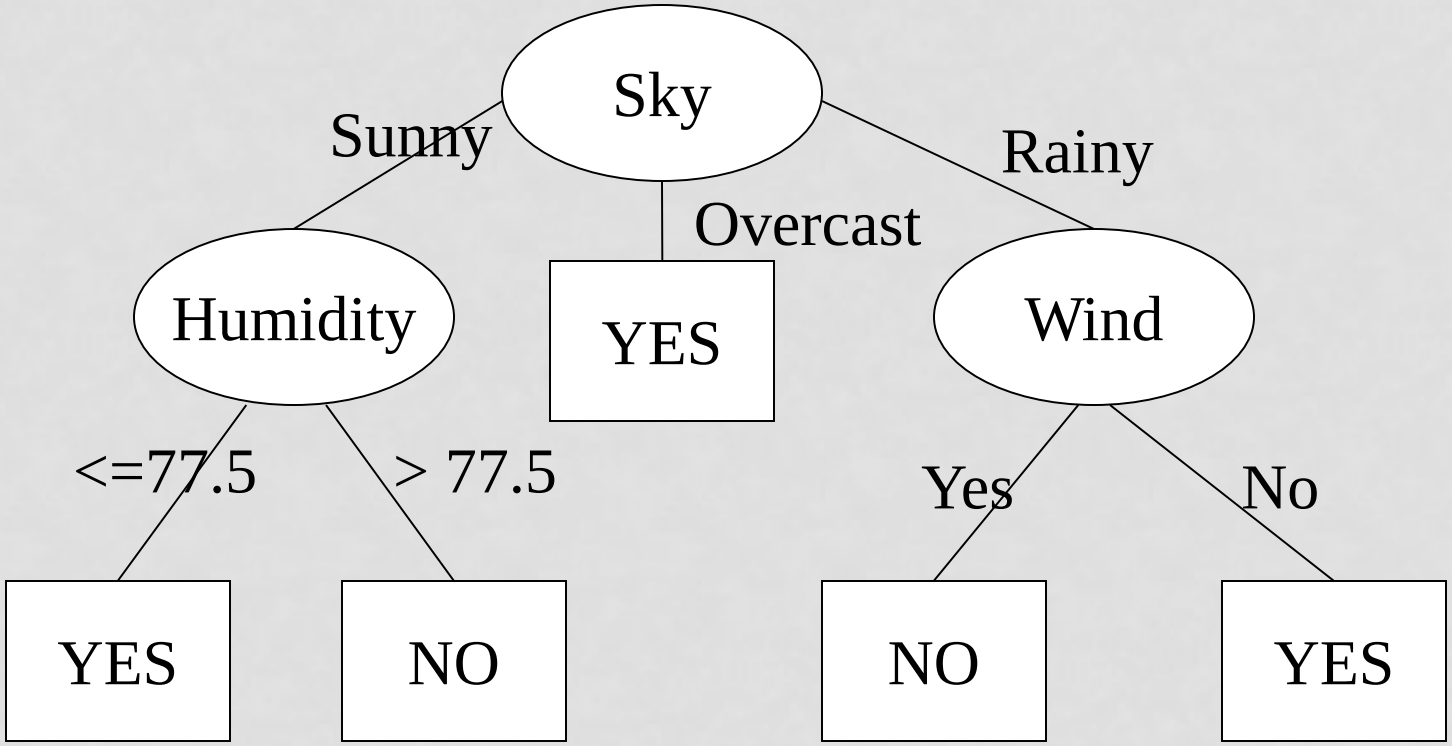
Class = Yes

Prediction

Decision trees

Sky	Tempe rature	Humidity	Wind	Tennis
Sunny	60	65	No	?????





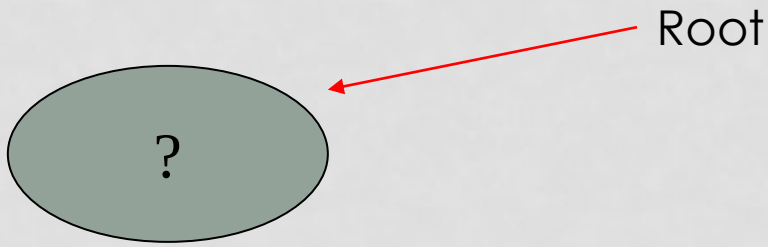
Decision trees

DECISION TREE ALGORITHM

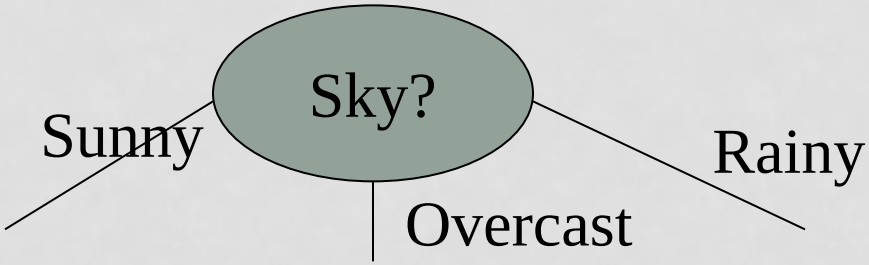
- There are many algorithms for training trees: ID3, C4.5 (J48), C5.0, CART, …
- Here, the basic ideas for all of them will be explained:
  - Trees are constructed iteratively (iterative improvement), starting from the empty tree
  - The main step in the algorithm (repeated many times) is selecting the best feature for each tree node, using some criterion (such as entropy minimization).
  - Growing the tree stops when it is not possible to continue splitting the data or hyper-parameters force to stop the growth process.

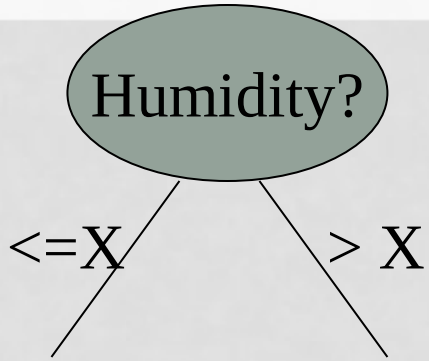
repeated step ->

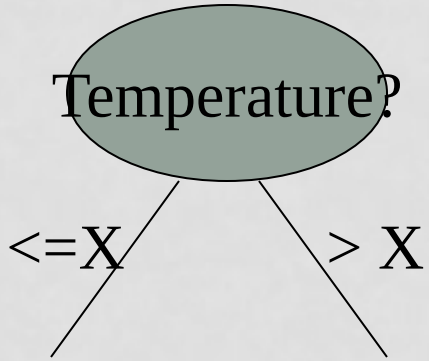
THE CONSTRUCTION OF THE TREE STARTS WITH AN EMPTY TREE, AT THE ROOT

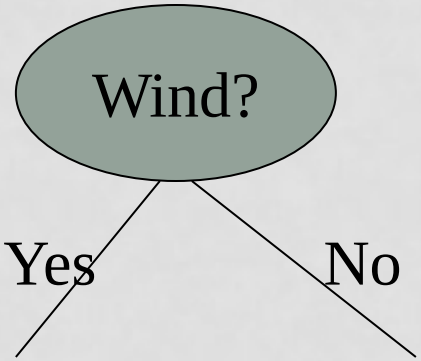


WHAT IS THE BEST ATTRIBUTE TO PUT IN THE ROOT OF THE TREE?





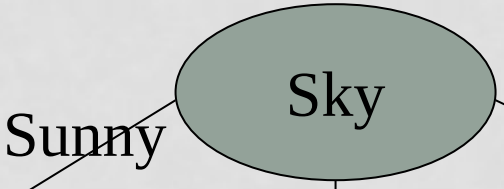




Let's try with attribute SKY

Sky	Temperature	Humidity	Wind	Tennis
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Overcast	83	86	No	Yes
Rainy	70	96	No	Yes
Rainy	68	80	No	Yes
Overcast	64	65	Yes	Yes
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Rainy	75	80	No	Yes
Sunny	75	70	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes
Rainy	71	91	Yes	No

Sky generates as many partitions as values (3: sunny, Overcast, rainy)



S	T	H	W	Ten
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Sunny	75	70	Yes	Yes

"3 No, 2 Yes"

"no" majority

S	T	H	W	Ten
Overcast	83	86	No	Yes
Overcast	64	65	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes

"0 No, 4 Yes"

Perfect partition

S	T	H	W	Ten
Rainy	70	96	No	Yes
Rainy	68	80	No	Yes
Rainy	75	80	No	Yes
Rainy	65	70	Yes	No
Rainy	71	91	Yes	No

"2 No, 3 Yes"

"yes" majority

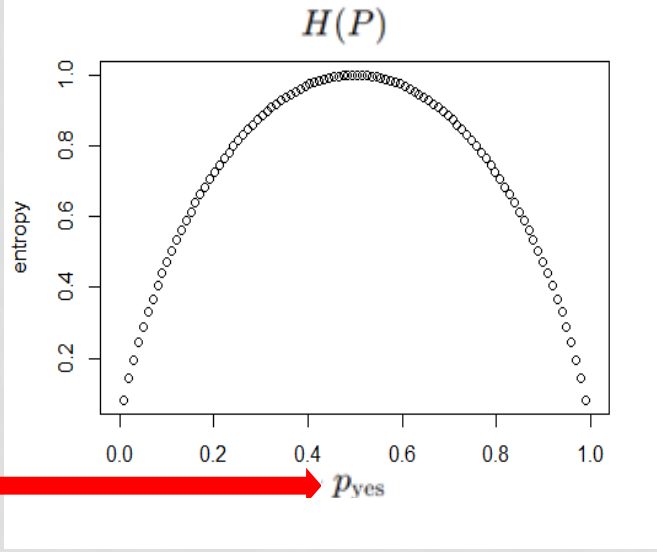
How do we know if SKY is a good attribute?

- Perfect partition (homogeneous):
  - 0% No, 100% Yes
  - 100% No, 0% Yes
- Worst partition: 50% No, 50% Yes (completely heterogeneous)
- Entropy measures partition quality (the larger, the worse)

$$H(P) = -\sum_{C_i} p_{C_i} \log_2(p_{C_i})$$

$$H(P) = -\left(p_{\text{yes}} \log_2(p_{\text{yes}}) + p_{\text{no}} \log_2(p_{\text{no}})\right)$$

$p_{\text{no}} = 1 - p_{\text{yes}}$ estimated prob = 2/5



Proportion of Yes

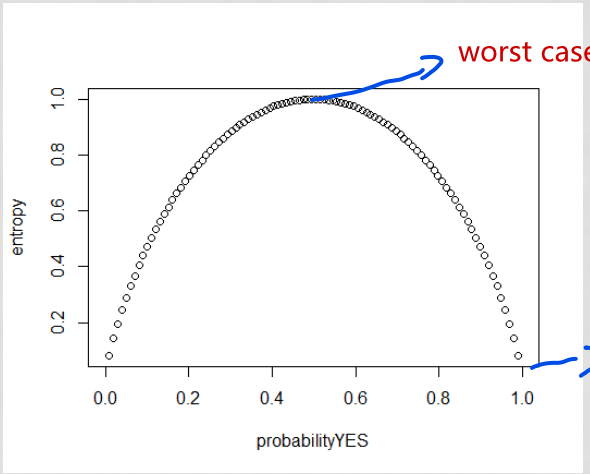
OTHER WAYS TO MEASURE PARTITION QUALITY

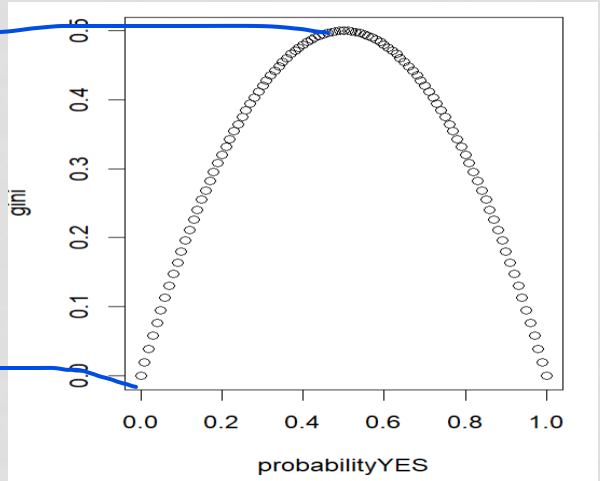
Entropy

$$H(P) = -\sum_{C_i} p_{C_i} \log_2(p_{C_i})$$

Gini

$$\text{Gini}(P) = \sum_{C_i} p_{C_i}(1 - p_{C_i})$$

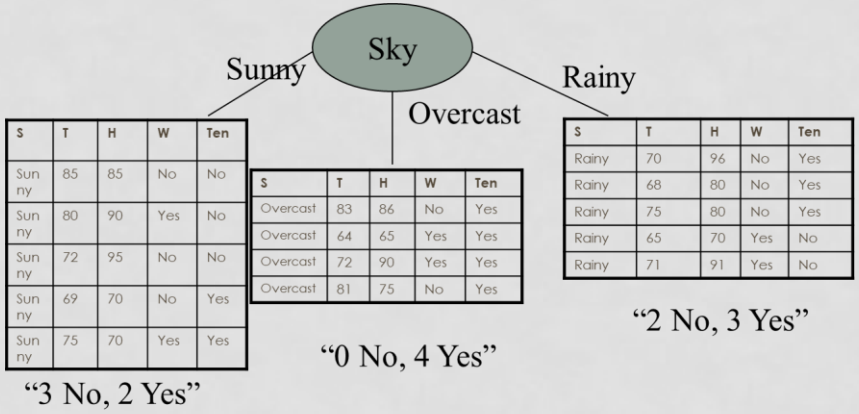




Minimize Entropy = Maximize Information Gain

Minimize Gini

Average entropy for Sky



S	T	H	W	Ten
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Sunny	75	70	Yes	Yes

S	T	H	W	Ten
Overcast	83	86	No	Yes
Overcast	64	65	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes

S	T	H	W	Ten
Rainy	70	96	No	Yes
Rainy	68	80	No	Yes
Rainy	75	80	No	Yes
Rainy	65	70	Yes	No
Rainy	71	91	Yes	No

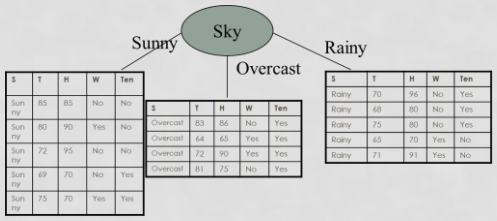
- Entropy for the three partitions of Sky:
  1. "3 No, 2 Yes": $H(P_{Sunny})=-((3/5)*\log_2(3/5)+(2/5)*\log_2(2/5)) = 0.97$
  2. "0 No, 4 Yes": $H(P_{Overcast})=-((0/4)*\log_2(0/4)+1*\log_2(1))=0$
  3. "2 No, 3 Yes": $H(P_{Rain})=-((2/5)*\log_2(2/5)+(3/5)*\log_2(3/5))= 0.97$
- (Weighted) Average Sky entropy:
  - $H_{Sky}=(5/14)*0.97+(4/14)*0+(5/14)*0.97 =$ **0.69**
  - Note: there are14 instances in the data set

ENTROPY AND INFORMATION GAIN

- Sometimes, instead of entropy (H) (to minimize), information gain (IG) is used (to be maximized)
- IG is the difference between the entropy of the original partition H(P) and the weighted average entropy after using the attribute (HP_{Sky}).
- Maximizing IG is equivalent to minimizing entropy.

P

Cielo	Temp	Hum	Viento	Tenis
sol	85	85	no	no
sol	80	90	si	no
nubes	83	86	no	si
lluvia	70	96	no	si
lluvia	68	80	no	si
lluvia	65	70	si	no
nubes	64	65	si	si
sol	72	95	no	no
sol	69	70	no	si
lluvia	75	80	no	si
sol	75	70	si	si
nubes	72	90	si	si
nubes	81	75	no	si
lluvia	71	91	si	no



P_1 P_2 P_3

$IG_{Sky} = H(P) - H_{Sky}(P_1, P_2, P_3)$

ENTROPY AND INFORMATION GAIN

- Choosing the attribute with highest IG is equivalent to choosing the attribute with smallest entropy, because H(P) is the same for all attributes.

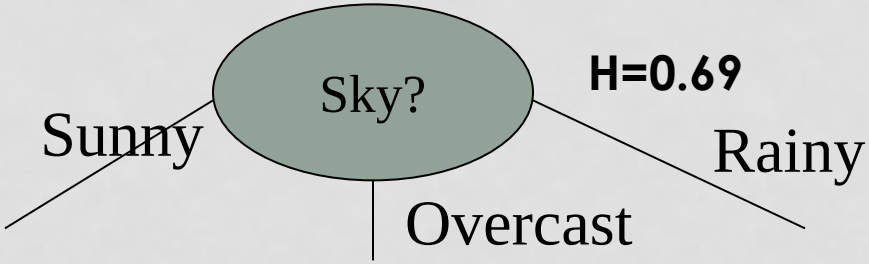
$IG_{Sky} = H(P) - H_{Sky}(P_1, P_2, P_3)$

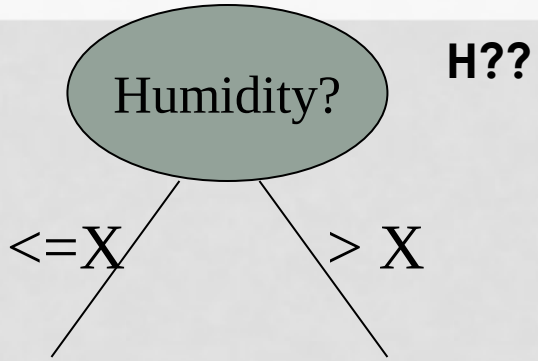
$IG_{Humidity} = H(P) - H_{Humidity}(P_1, P_2)$

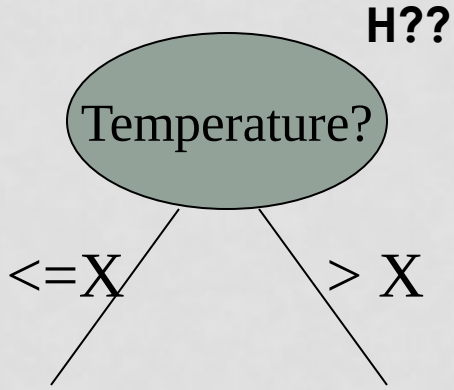
$IG_{Temperature} = H(P) - H_{Temperature}(P_1, P_2)$

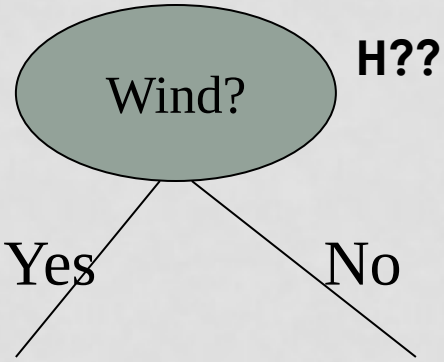
$IG_{Wind} = H(P) - H_{Wind}(P_1, P_2)$

WHAT IS THE BEST ATTRIBUTE TO PUT IN THE ROOT OF THE TREE?



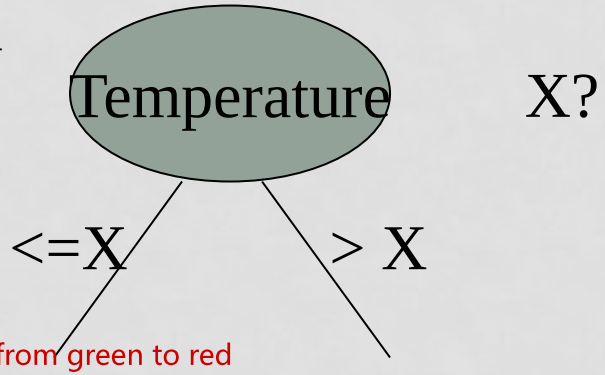






WHAT TO DO WITH CONTINUOUS ATTRIBUTES?

A binary (two-values) attribute is created by computing a threshold X



Note: only some thresholds are shown. The best one is X=84 with average entropy = 0.83

Thresholds to try: When there is a change from green to red

Sky	Temperature	Humidity	Windy	Play
sunny	85	85	FALSE	no
sunny	80	90	TRUE	no
overcast	83	86	FALSE	yes
rainy	70	96	FALSE	yes
rainy	68	80	FALSE	yes
rainy	65	70	TRUE	no
overcast	64	65	TRUE	yes
sunny	72	95	FALSE	no
sunny	69	70	FALSE	yes
rainy	75	80	FALSE	yes
sunny	75	70	TRUE	yes
overcast	72	90	TRUE	yes
overcast	81	75	FALSE	yes
rainy	71	91	TRUE	no

64 – Yes, 65-No, 68 – Yes, 69 – Yes, 70 – Yes, 71 – No, 72 – YesNo, 75 – YesYes, 80 – No, 81 – Yes, 83 – Yes, 85 - No

H = 0.83

4 No, 9 Yes

Select threshold with smallest entropy

X=84

1 No, 0 Yes

64 – Yes, 65-No, 68 – Yes, 69 – Yes, 70 – Yes, 71 – No, 72 – YesNo, 75 – YesYes, 80 – No, 81 – Yes, 83 – Yes, 85 - No

H = 0.93

2 No, 4 Yes

X=71.5

3 No, 5 Yes

64 – Yes, 65-No, 68 – Yes, 69 – Yes, 70 – Yes, 71 – No, 72 – YesNo, 75 – YesYes, 80 – No, 81 – Yes, 83 – Yes, 85 - No

H = 0.89

1 No, 4 Yes

X=70.5

4 No, 5 Yes

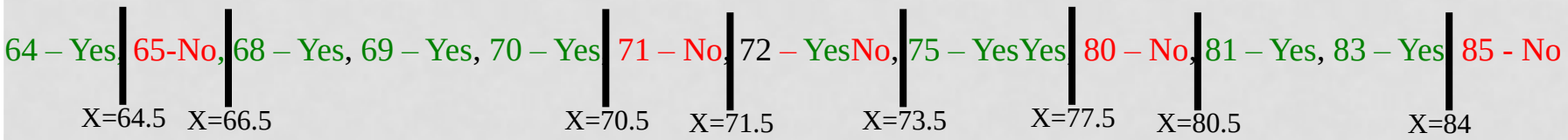
?

All possible threshold = n-1

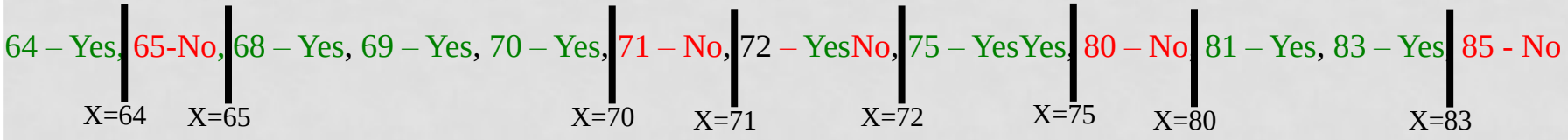
- Should **all** possible thresholds be actually tried? Or can we make the algorithm more efficient by ignoring some possible thresholds? Select just the change of colour

ALTERNATIVE POSSIBLE THRESHOLDS

Possible thresholds are transitions from Yes to No, or from No to Yes:

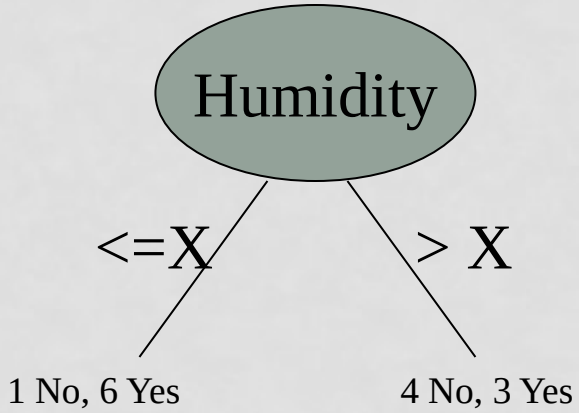


- The actual threshold may depend on the algorithm implementation. Some implementations use the average: Ej: 64.5 = (64+65)/2.
- Other implementations use the maximum of the left partition. In that case, the possible thresholds would have been:



- Notice that entropy computed with the training data is the same in both cases, because in the two cases data is partitioned in the same way.

HUMIDITY



65-Yes, 70-NoYesYes, 75–Yes, 80-YesYes, | 85-No, 86-Yes, 90-NoYes, 91-No, 95-No, 96-Yes

X=82.5

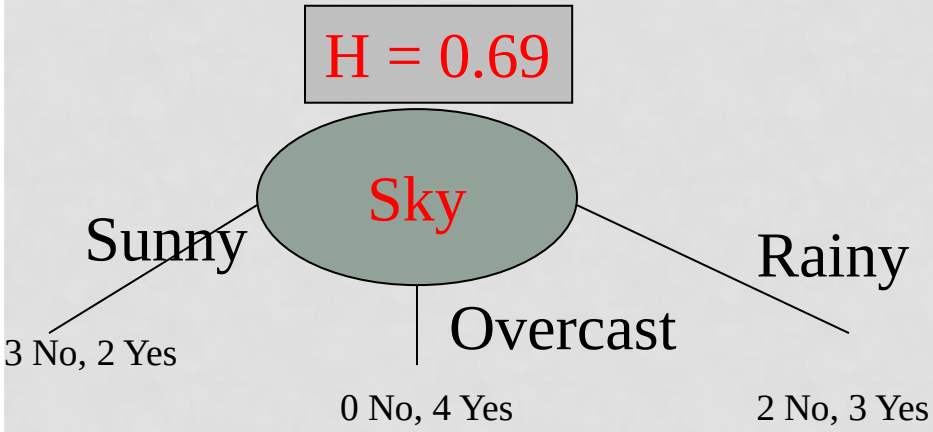
1 No, 6 Yes

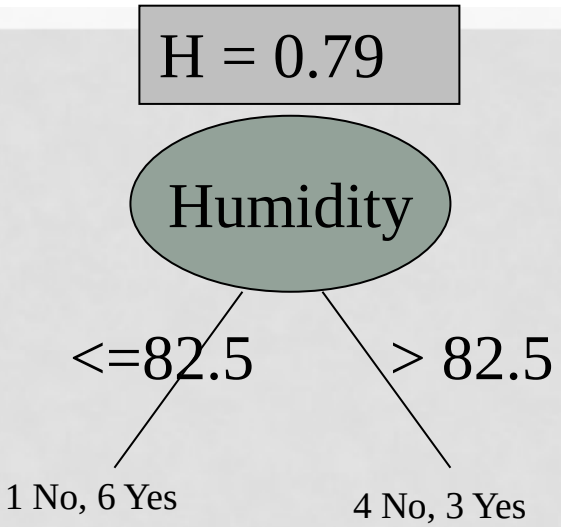
4 No, 3 Yes

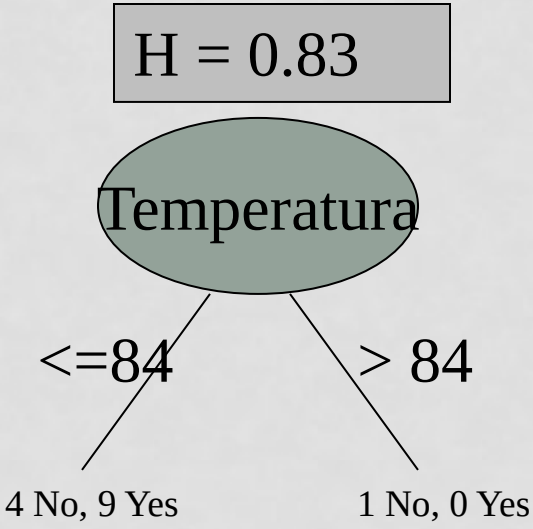
H = 0.79

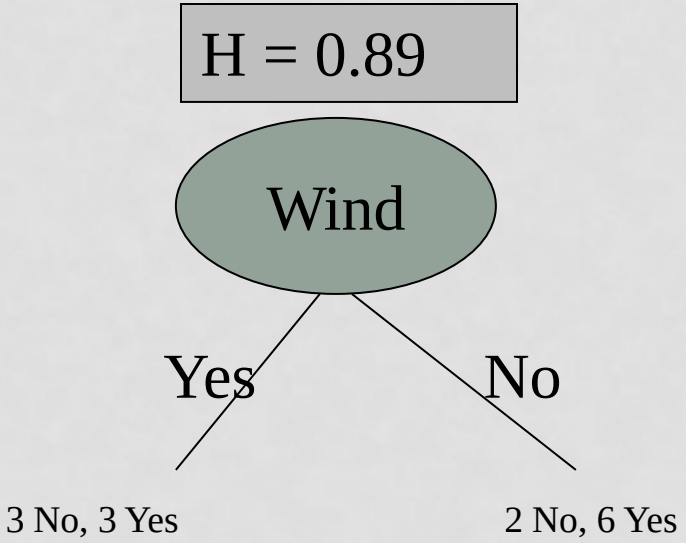
Note: there are other alternatives for the threshold, but this is the best one (minimum entropy)

WHAT IS THE BEST NODE TO PUT IN THE ROOT OF THE TREE?

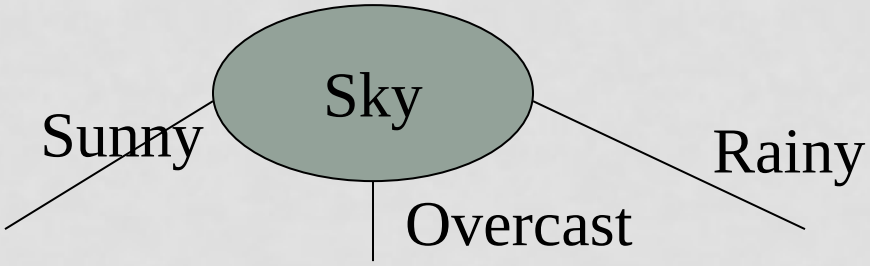






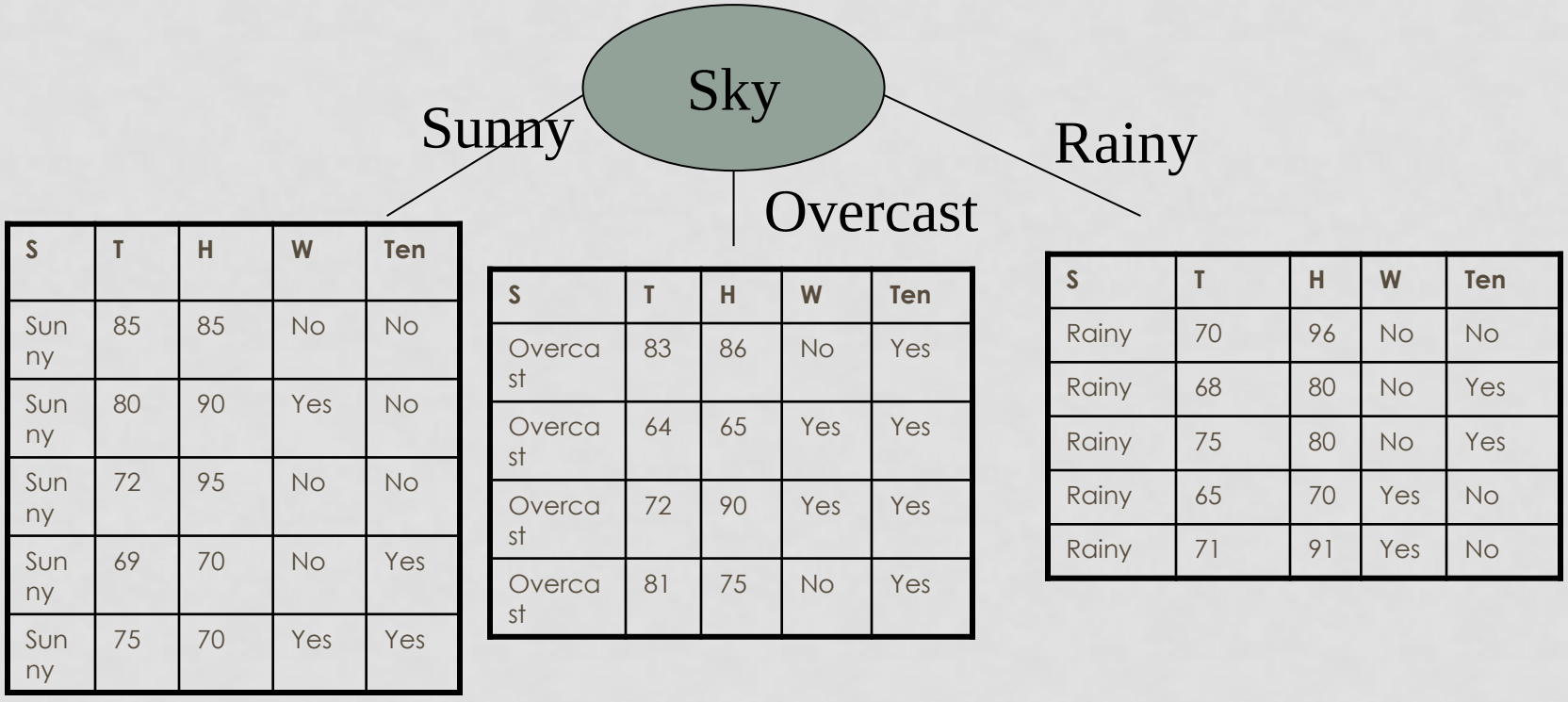


WHAT IS THE BEST NODE TO PUT IN THE ROOT OF THE TREE?



RECURSIVE TREE GROWTH

Now that the attribute for the root node has been determined, the process continues recursively. Now, the algorithm has to construct three new subtrees.



S	T	H	W	Ten
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Sunny	75	70	Yes	Yes

"3 No, 2 Yes"

S	T	H	W	Ten
Overcast	83	86	No	Yes
Overcast	64	65	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes

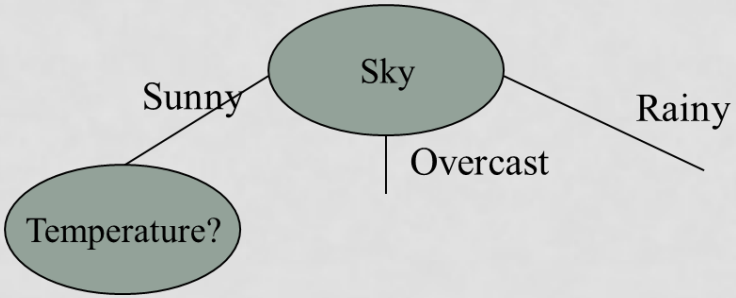
"0 No, 4 Yes"

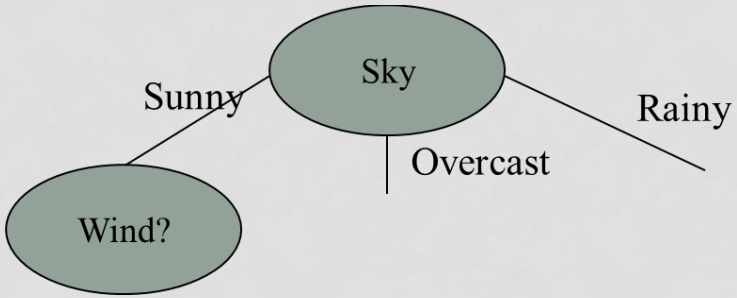
S	T	H	W	Ten
Rainy	70	96	No	No
Rainy	68	80	No	Yes
Rainy	75	80	No	Yes
Rainy	65	70	Yes	No
Rainy	71	91	Yes	No

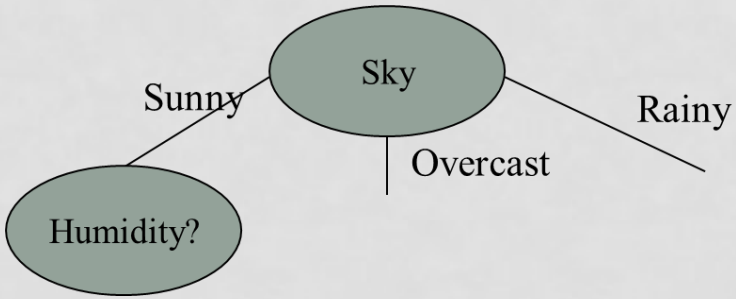
"2 No, 3 Yes"

RECURSIVE TREE GROWTH

Now that the attribute for the root node has been determined, the process continues recursively. Now, the algorithm has to construct three new subtrees.

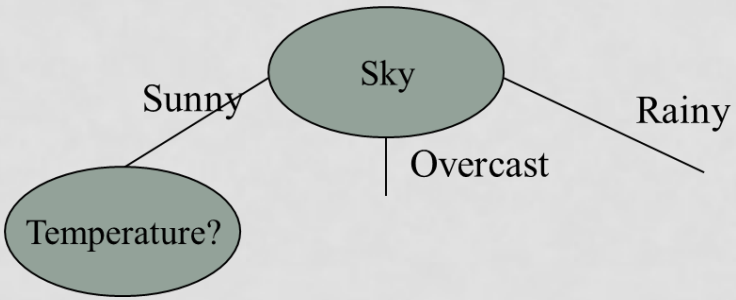


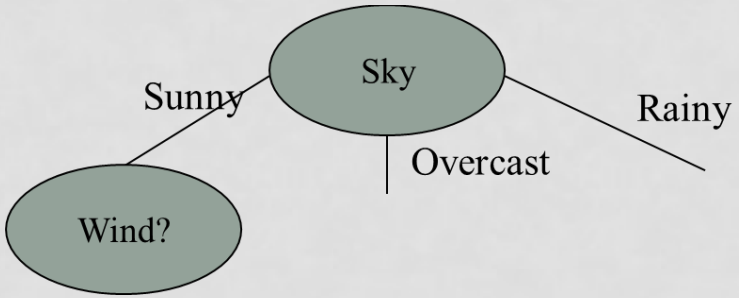


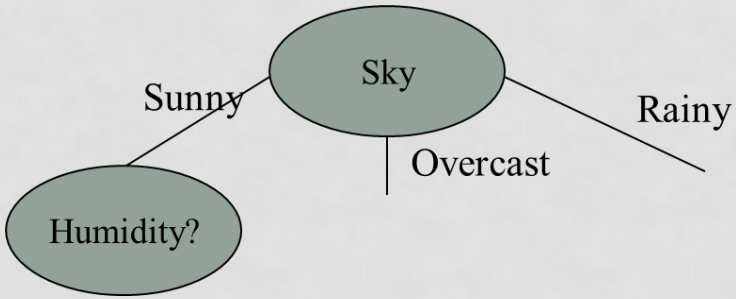


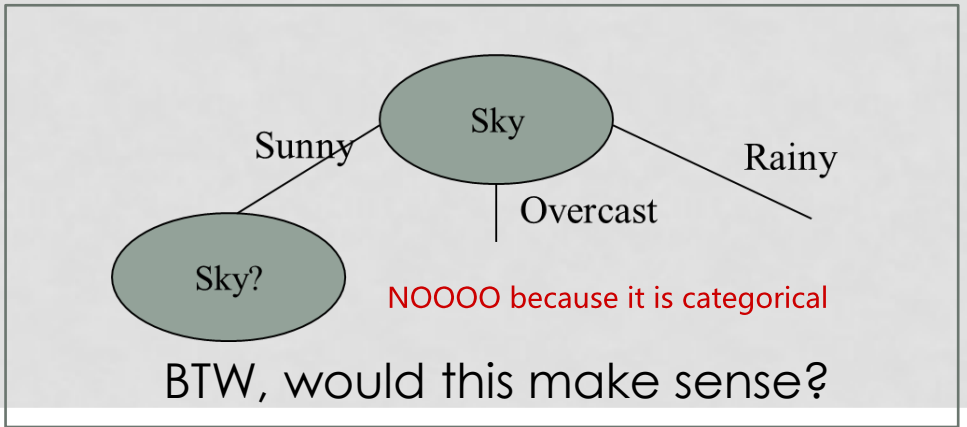
RECURSIVE TREE GROWTH

Now that the attribute for the root node has been determined, the process continues recursively. Now, the algorithm has to construct three new subtrees.





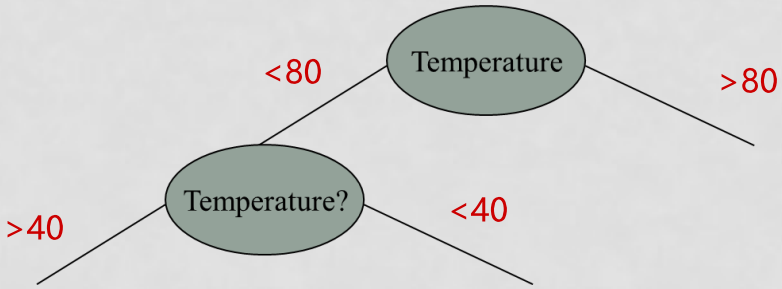




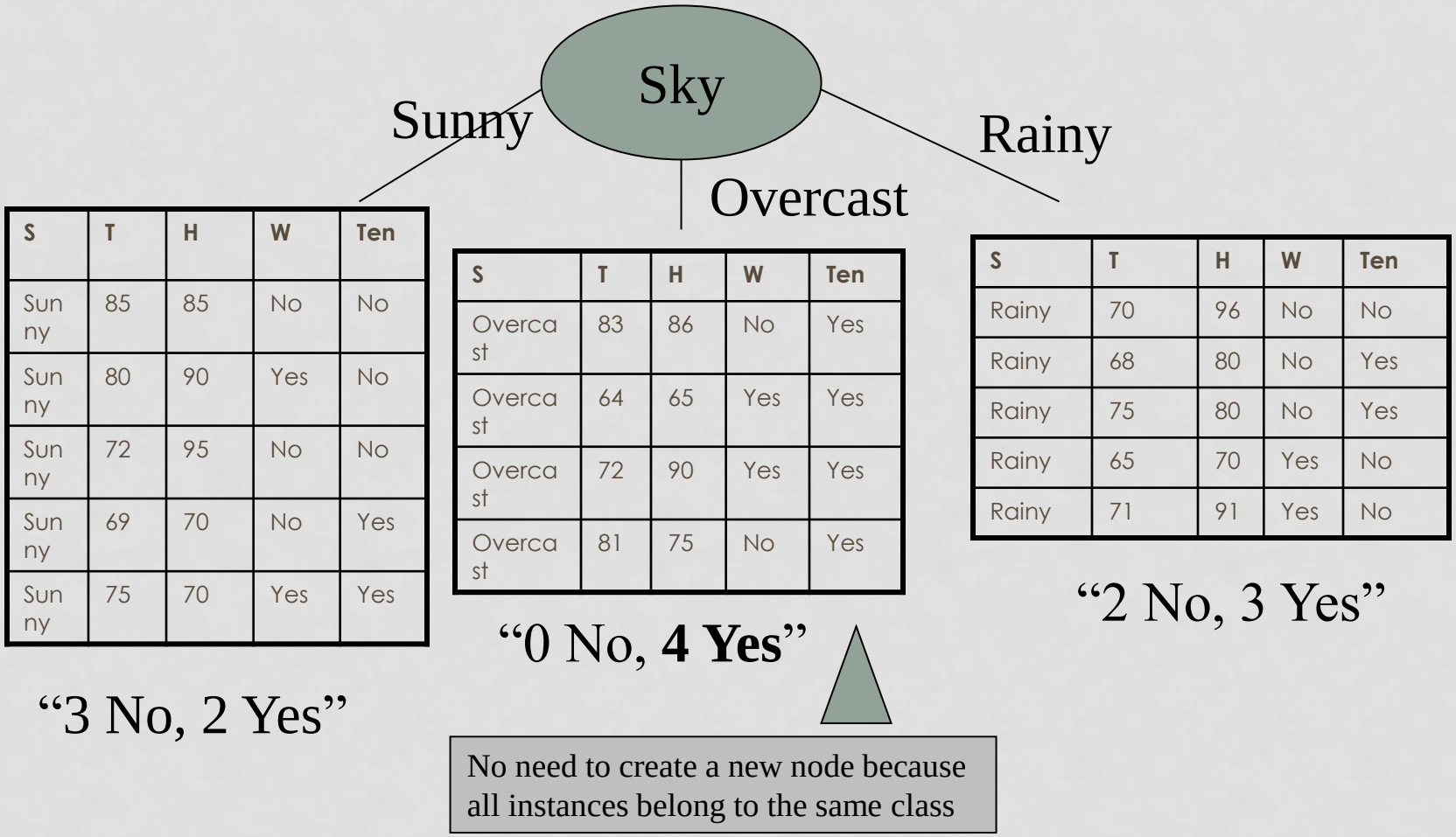
?

- If Temperature had been selected for the root, would it make sense to try (again) attribute Temperature?

YES because it is continuous and when we define a threshold, we are defining another categorical variable.



WHEN TO STOP SPLITTING PARTITIONS?



S	T	H	W	Ten
Sunny	85	85	No	No
Sunny	80	90	Yes	No
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Sunny	75	70	Yes	Yes

"3 No, 2 Yes"

S	T	H	W	Ten
Overcast	83	86	No	Yes
Overcast	64	65	Yes	Yes
Overcast	72	90	Yes	Yes
Overcast	81	75	No	Yes

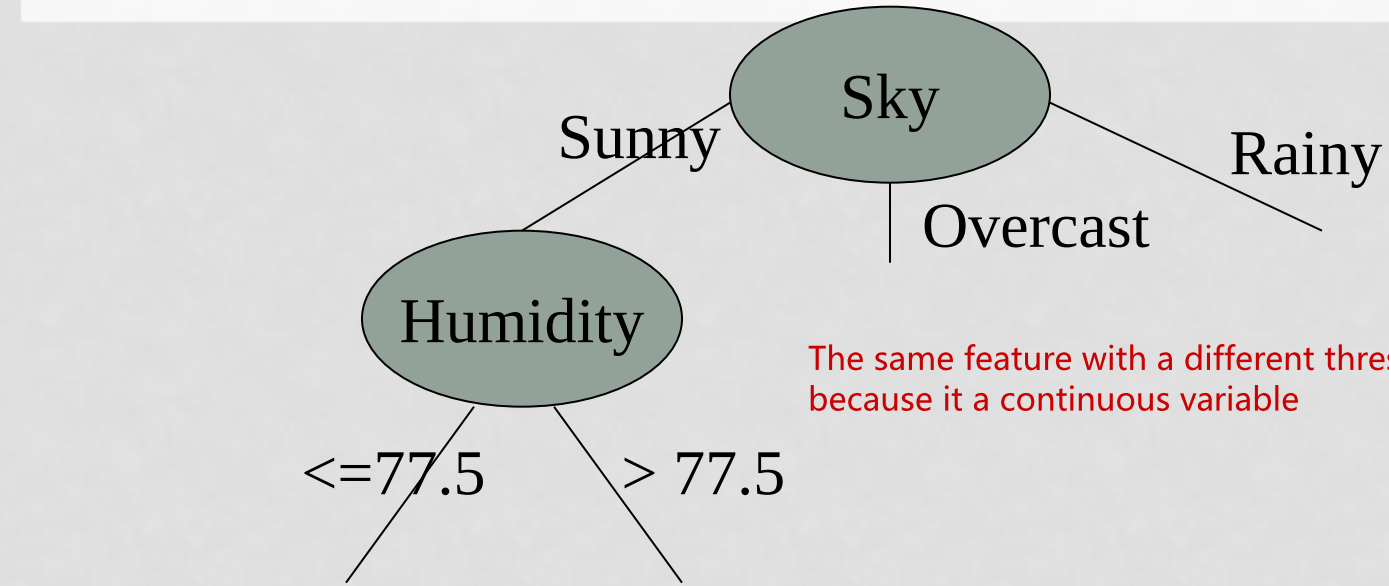
"0 No, **4 Yes**"

No need to create a new node because all instances belong to the same class

S	T	H	W	Ten
Rainy	70	96	No	No
Rainy	68	80	No	Yes
Rainy	75	80	No	Yes
Rainy	65	70	Yes	No
Rainy	71	91	Yes	No

"2 No, 3 Yes"

WHY TO STOP TREE GROWTH?



The same feature with a different threshold is a different feature because it a continuous variable

T	H	V	Ten
69	70	No	Yes
75	70	Yes	Yes

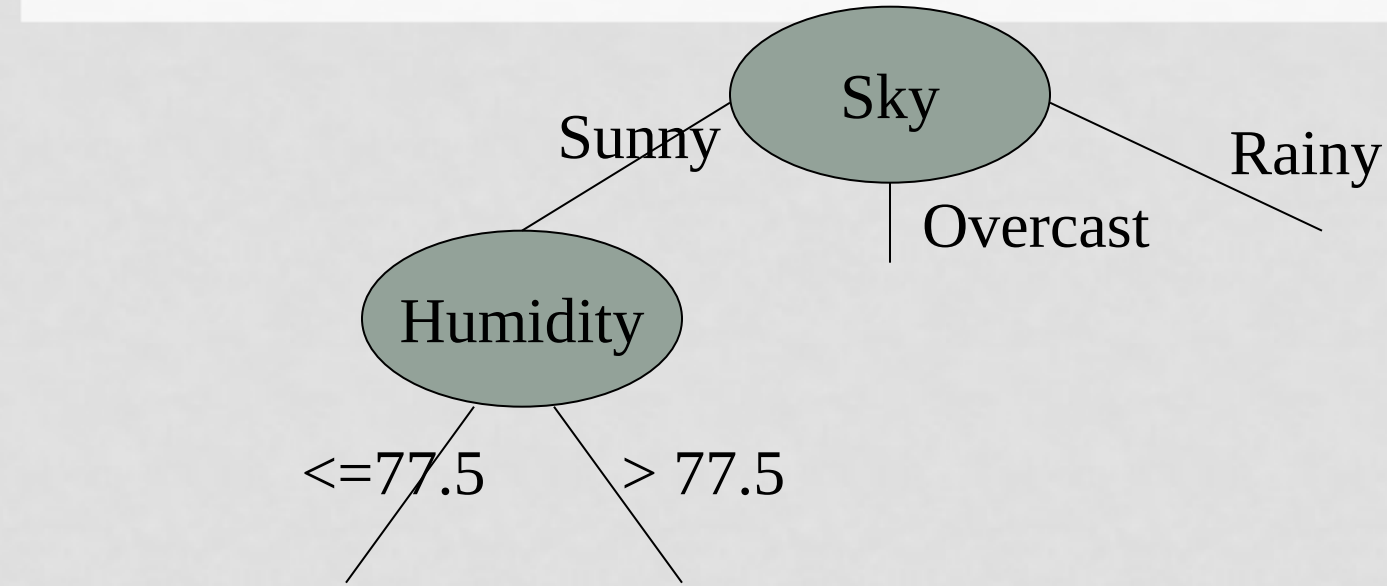
T	H	V	Ten
85	85	No	No
80	90	Yes	No
72	95	No	No

"**2 Yes,** 0 No"

"**3 No,** 0 Yes"

No need to create a new node because all instances belong to the same class

WHY TO STOP TREE GROWTH?



T	H	V	Ten
69	70	No	Yes
75	70	Yes	Yes

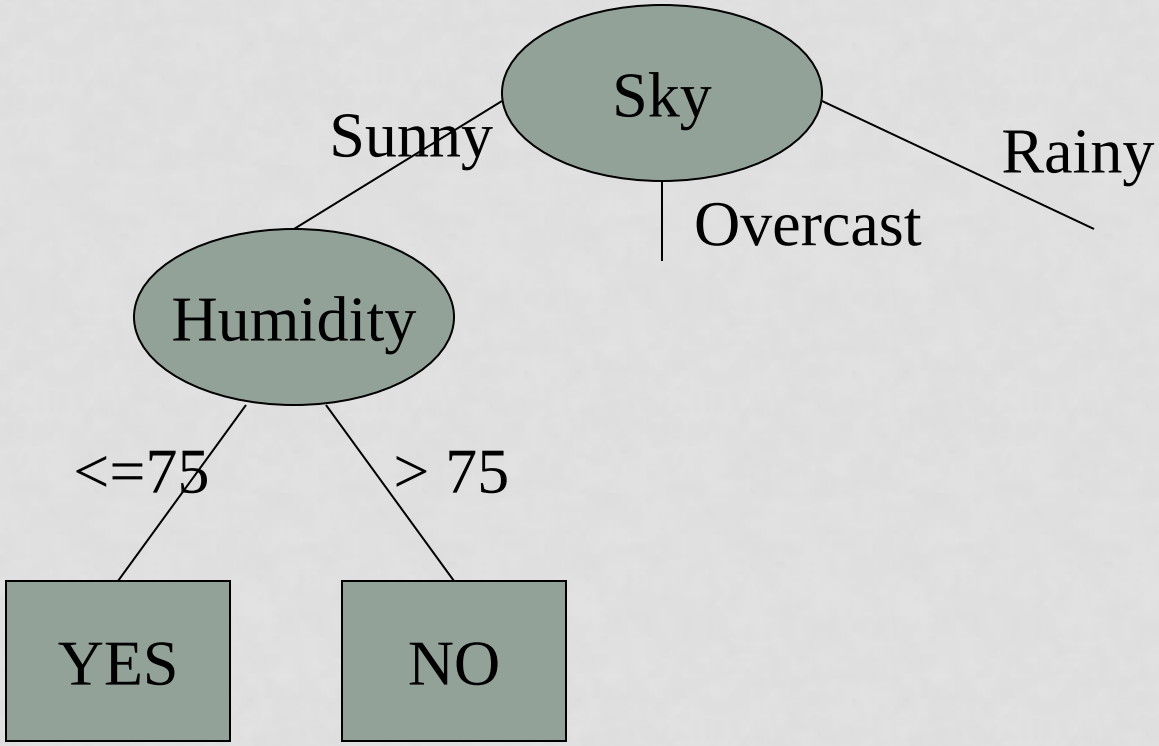
T	H	V	Ten
85	85	No	No
80	90	Yes	No
72	95	No	No

"**2 Yes,** 0 No"

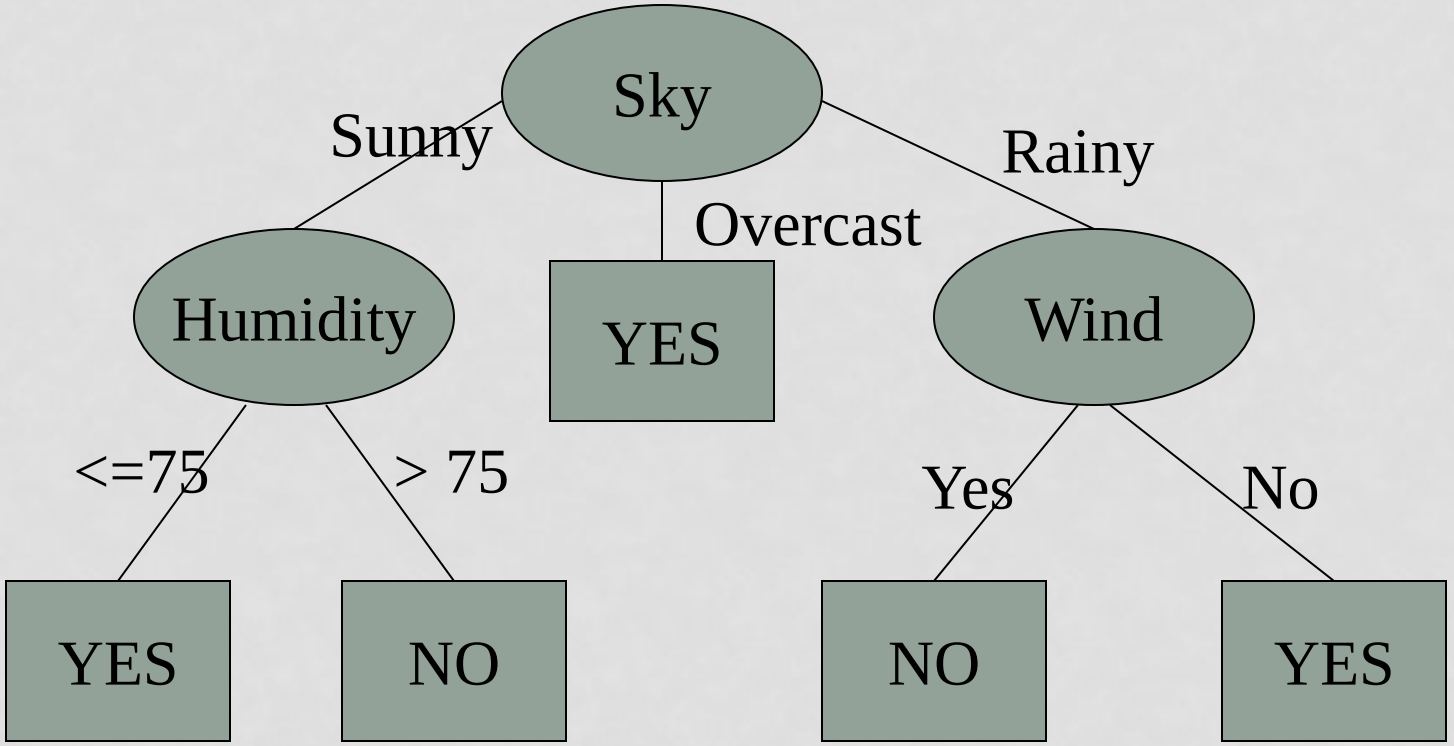
"**3 No,** 0 Yes"

No need to create a new node because all instances belong to the same class

RECURSIVE TREE GROWTH

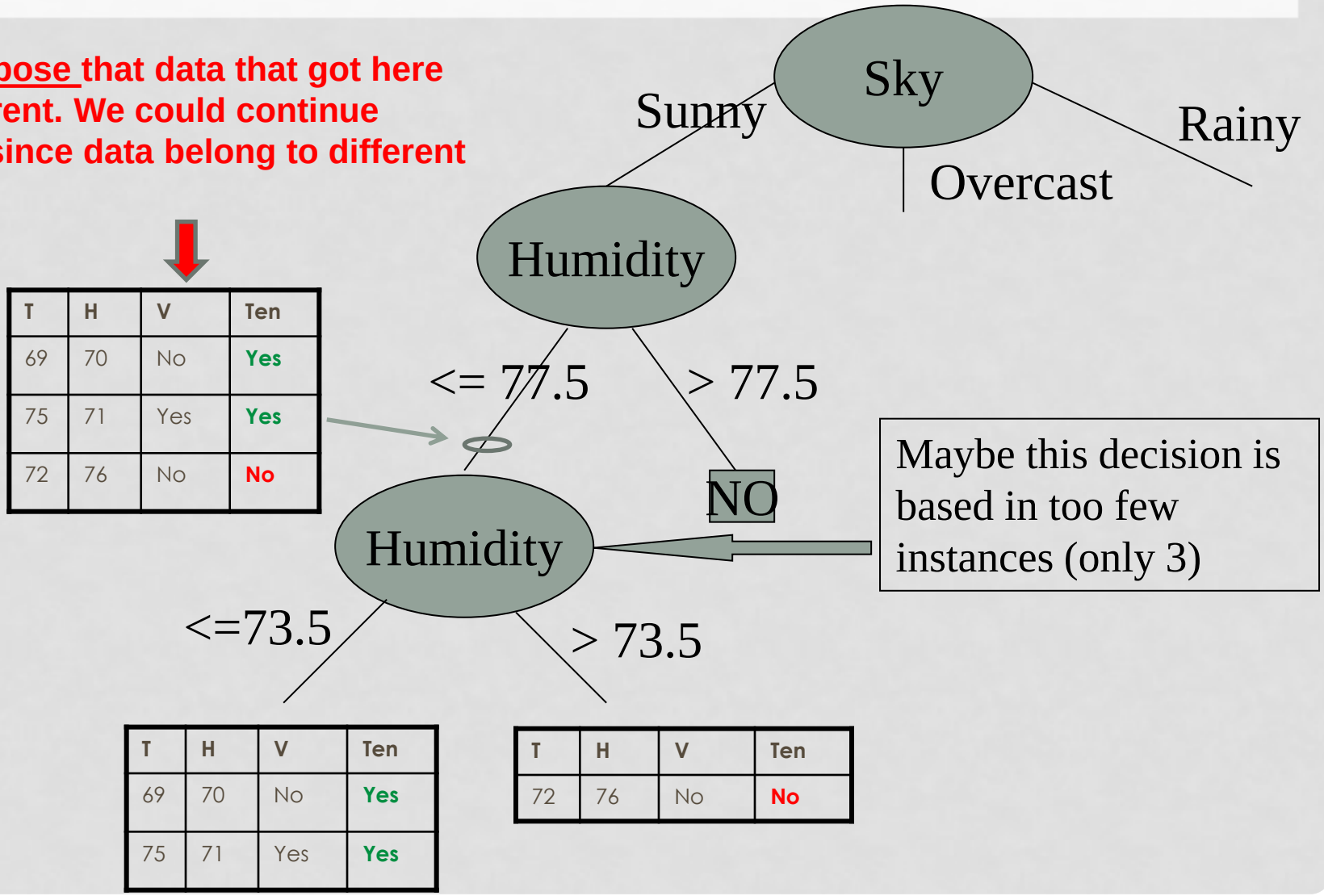


RECURSIVE TREE GROWTH



WHY TO STOP TREE GROWTH?

Let's suppose that data that got here was different. We could continue splitting since data belong to different classes.

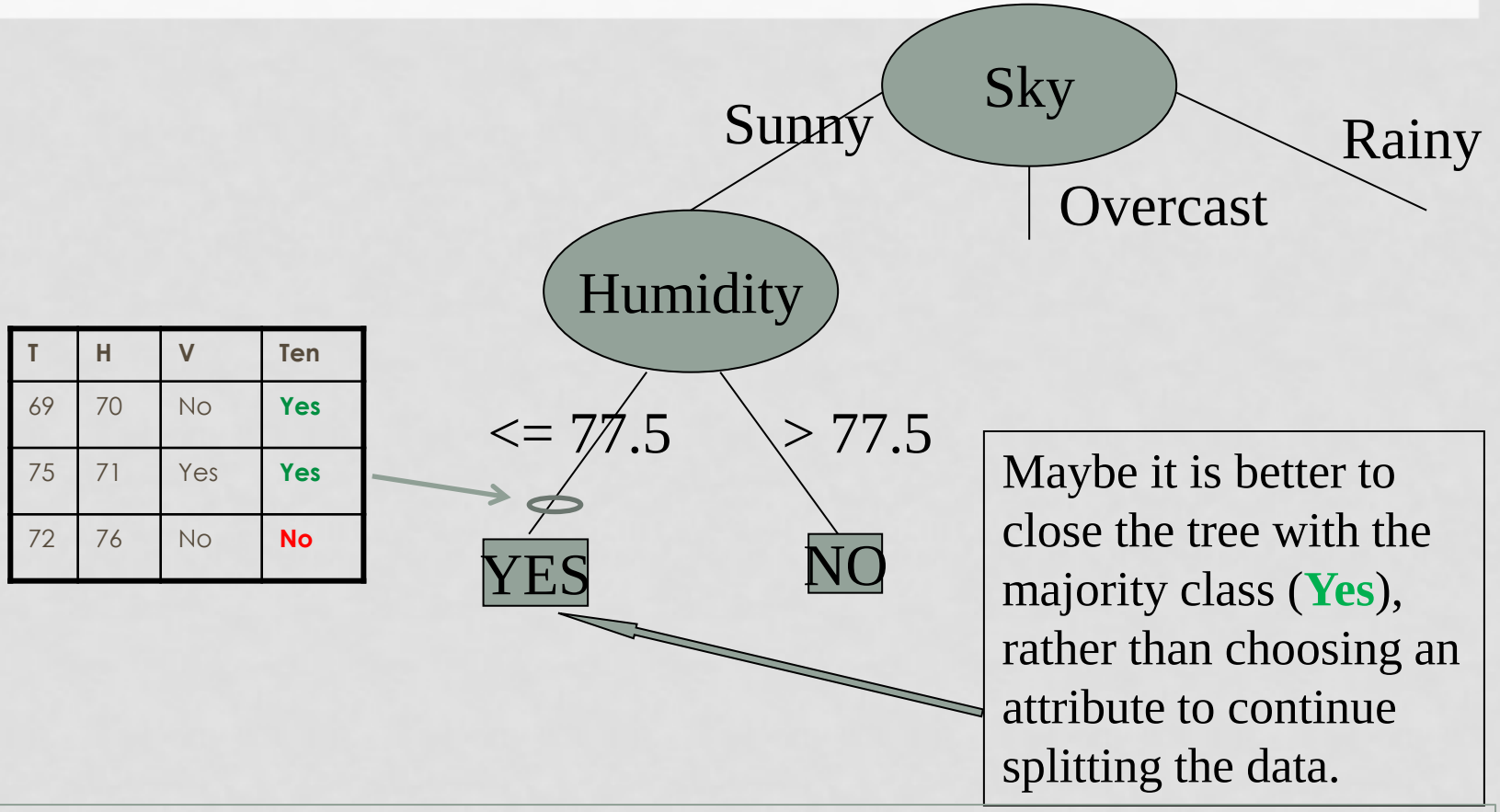


T	H	V	Ten
69	70	No	Yes
75	71	Yes	Yes
72	76	No	No

T	H	V	Ten
69	70	No	Yes
75	71	Yes	Yes

T	H	V	Ten
72	76	No	No

WHY TO STOP TREE GROWTH?



T	H	V	Ten
69	70	No	Yes
75	71	Yes	Yes
72	76	No	No

- The algorithm may use a statistical criterion in order to determine whether it is worth to continue tree growth, whether the sample is too small, etc.
- But stopping tree growth is usually controlled with the **min-samples** hyperparameter (or **max-depth**).

minimum number of instances for continuing splitting the tree

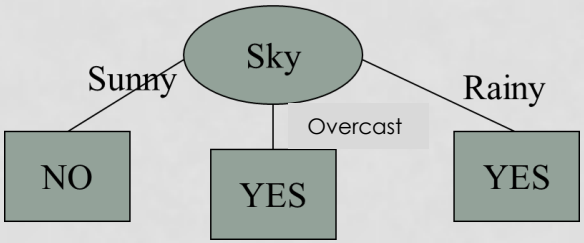
MAIN HYPER-PARAMETERS OF DECISION TREES

- **max_depth**: maximum depth of the tree
- **min_samples_split**: minimum number of instances in order to continue subdividing the tree

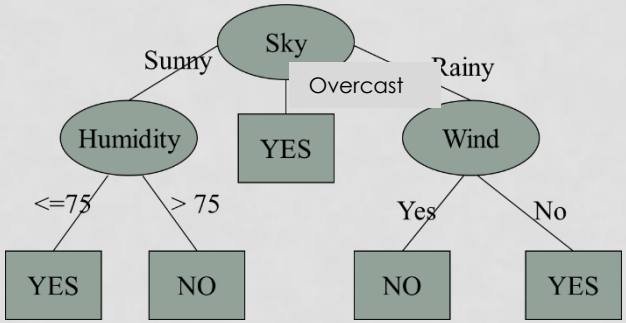
MAIN HYPER-PARAMETERS OF DECISION TREES

- **max_depth**: maximum depth of the tree

max_depth = 1



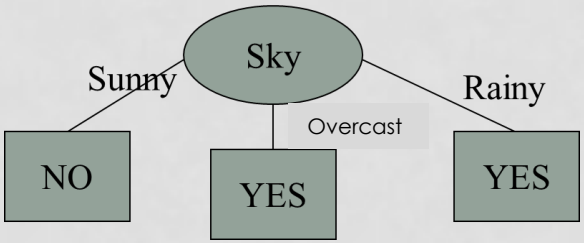
max_depth = 2



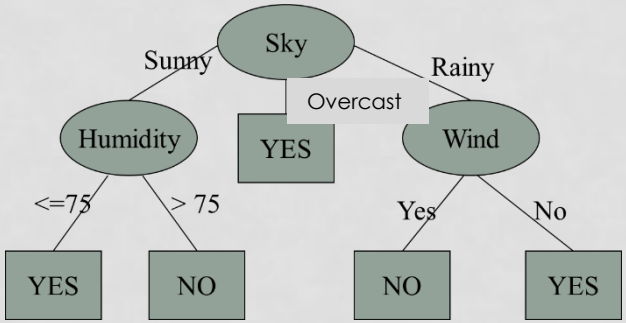
MAIN HYPER-PARAMETERS OF DECISION TREES

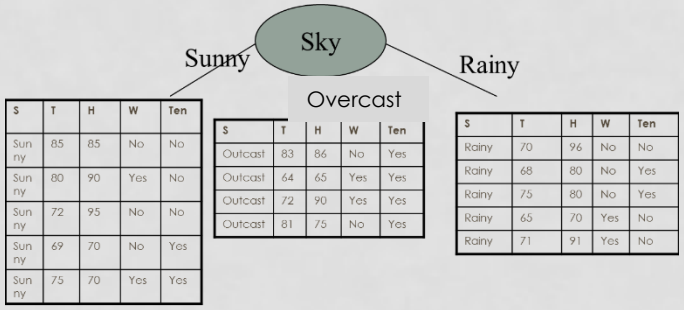
- **min_samples_split**: minimum number of instances in order to continue subdividing the tree

min_samples_split = 6



min_samples_split = 5





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Sunny	80	90	Yes	No
Sunny	72	95	No	No
Sunny	69	70	No	Yes
Sunny	75	70	Yes	Yes

S	T	H	W	Ten
Outcast	83	86	No	Yes
Outcast	64	65	Yes	Yes
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Outcast	81	75	No	Yes

S	T	H	W	Ten
Rainy	70	96	No	No
Rainy	68	80	No	Yes
Rainy	75	80	No	Yes
Rainy	65	70	Yes	No
Rainy	71	91	Yes	No

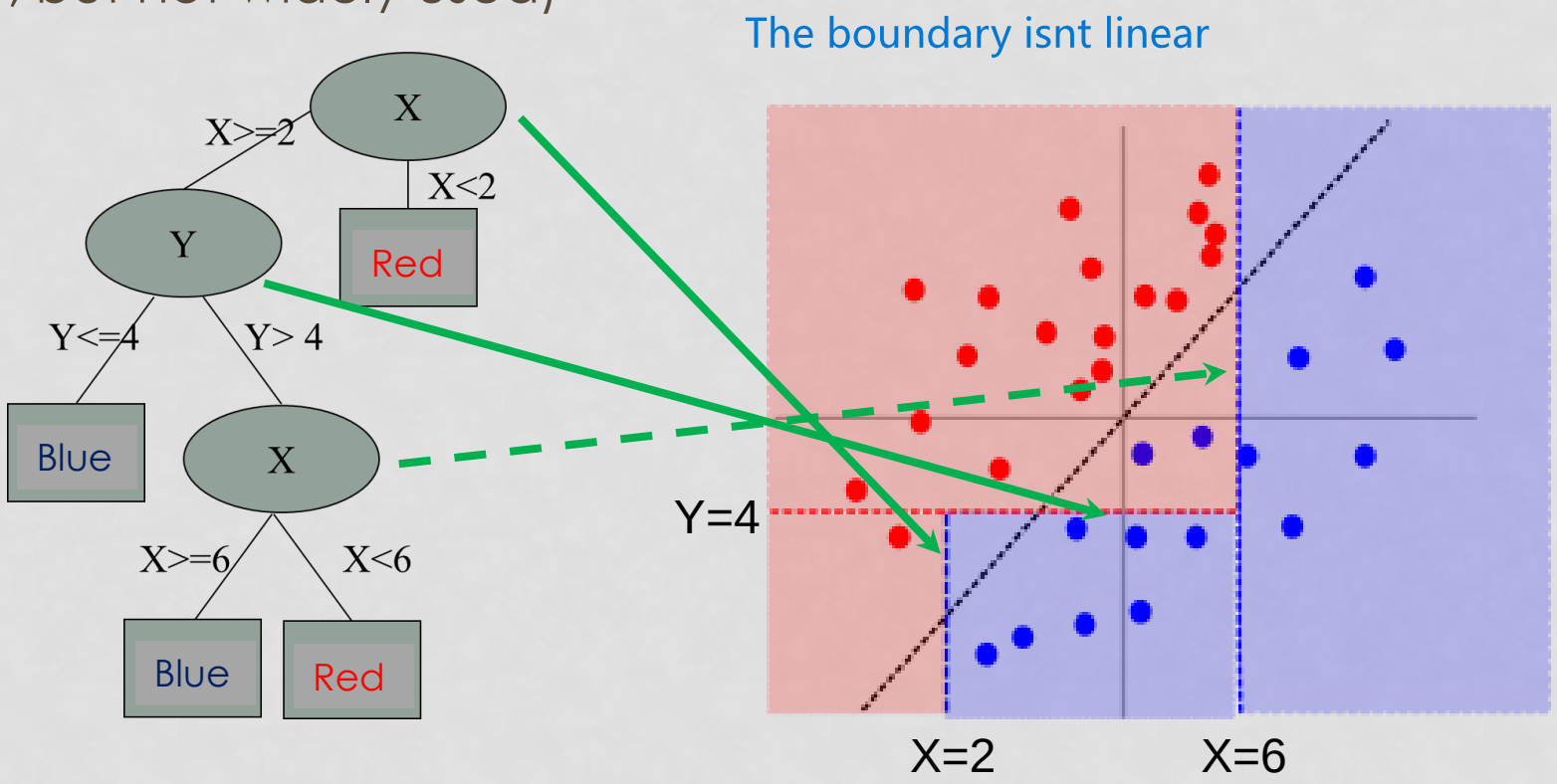
MAIN HYPER-PARAMETERS OF DECISION TREES

- **max_depth**: maximum depth of the tree
- **min_samples_split**: minimum number of instances in order to continue subdividing the tree

- Both hyper-parameters (and hyper-parameters in general) control the complexity of the model (in feature-space, the complexity of the boundary)

TREE BOUNDARIES IN FEATURE SPACE

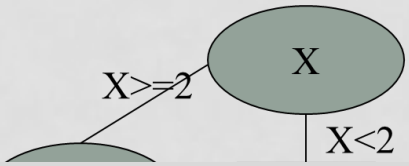
- Decision trees are non-linear. Boundary is made of piece-wise linear segments parallel to axis.
- Therefore, not very good for oblique boundaries (there are "oblique trees", but not widely used)

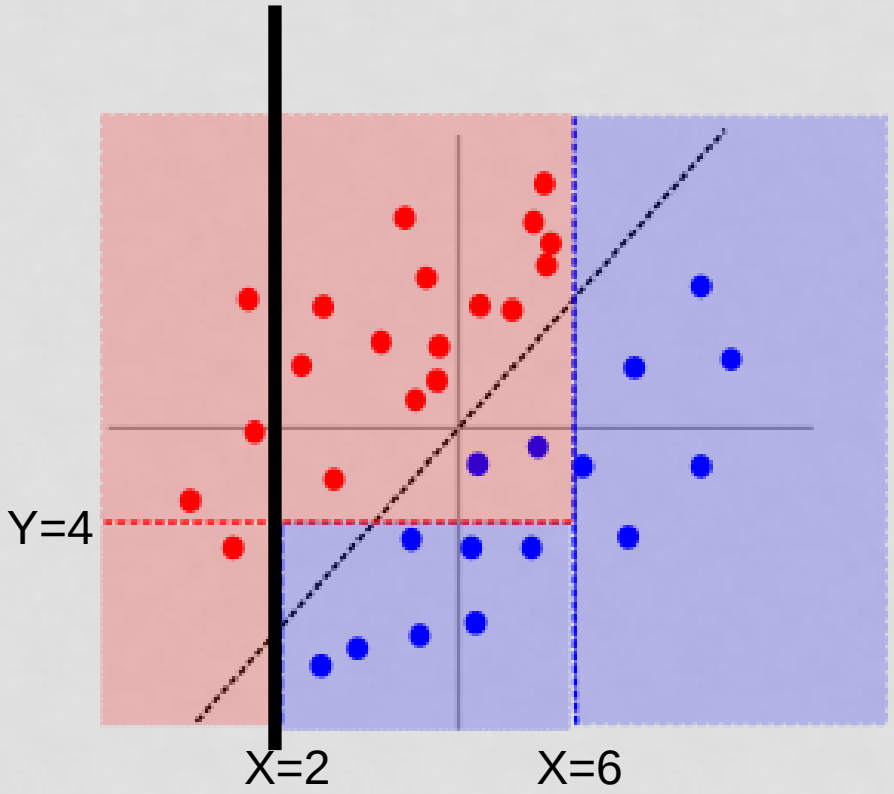


MAX-DEPTH HYPER-PARAMETER FOR DECISION TREES

The complexity of the model is the complexity of the boundary

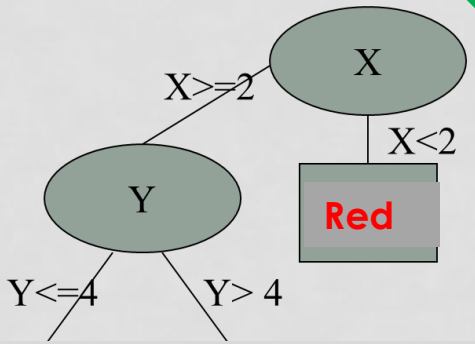
- With max_depth = 1, boundary is a line.

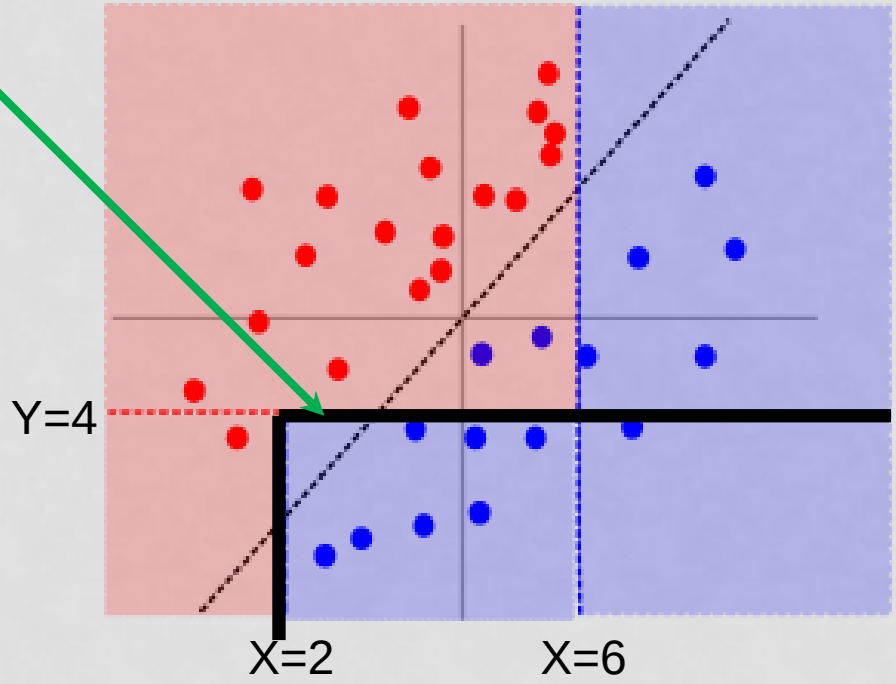




MAX-DEPTH HYPER-PARAMETER FOR DECISION TREES

- With max_depth = 2, boundary is non-linear

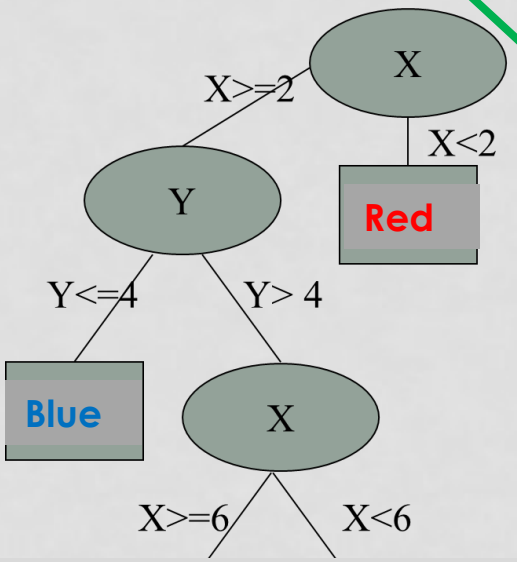




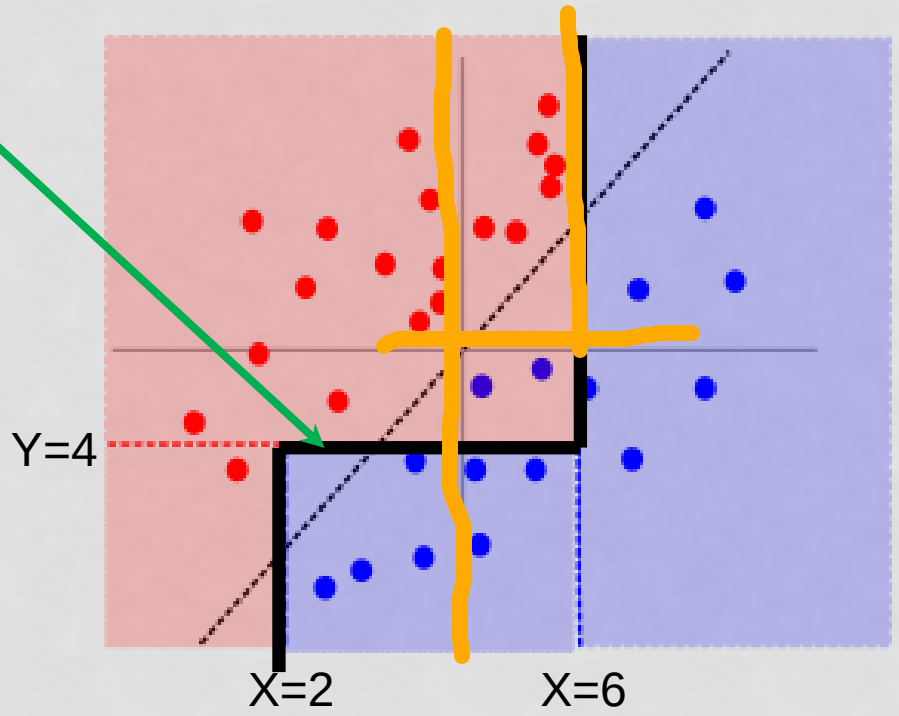
MAX-DEPTH HYPER-PARAMETER FOR DECISION TREES

Decision trees can just generate horizontal and vertical boundaries

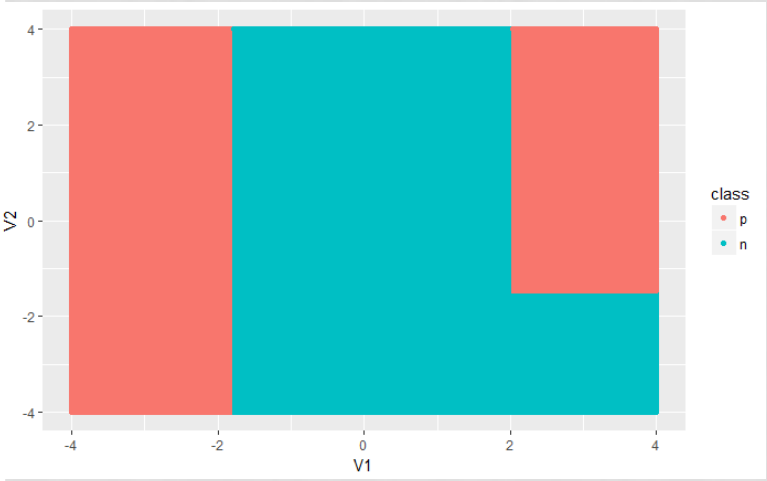
- With max_depth = 3, boundary is non-linear and more complex than with max_depth = 2
- And so on



For including the blue instances:
X=4 ,Y=6 , X=6

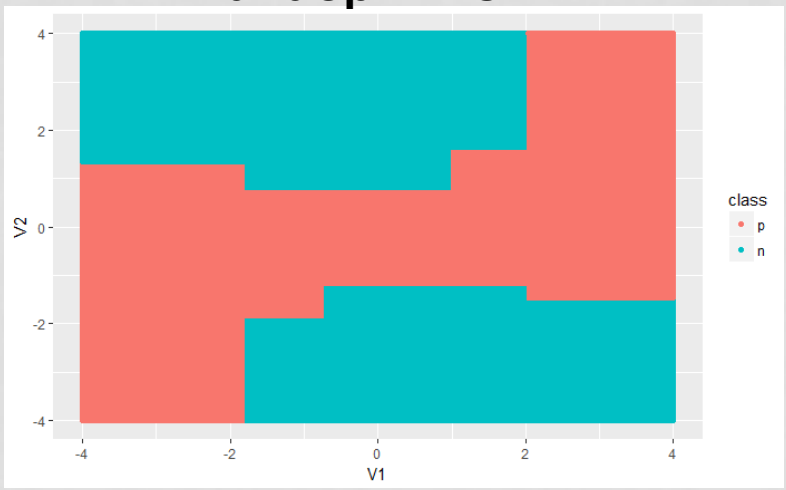


Maxdepth = 2



Maxdepth = 8

Most complex model



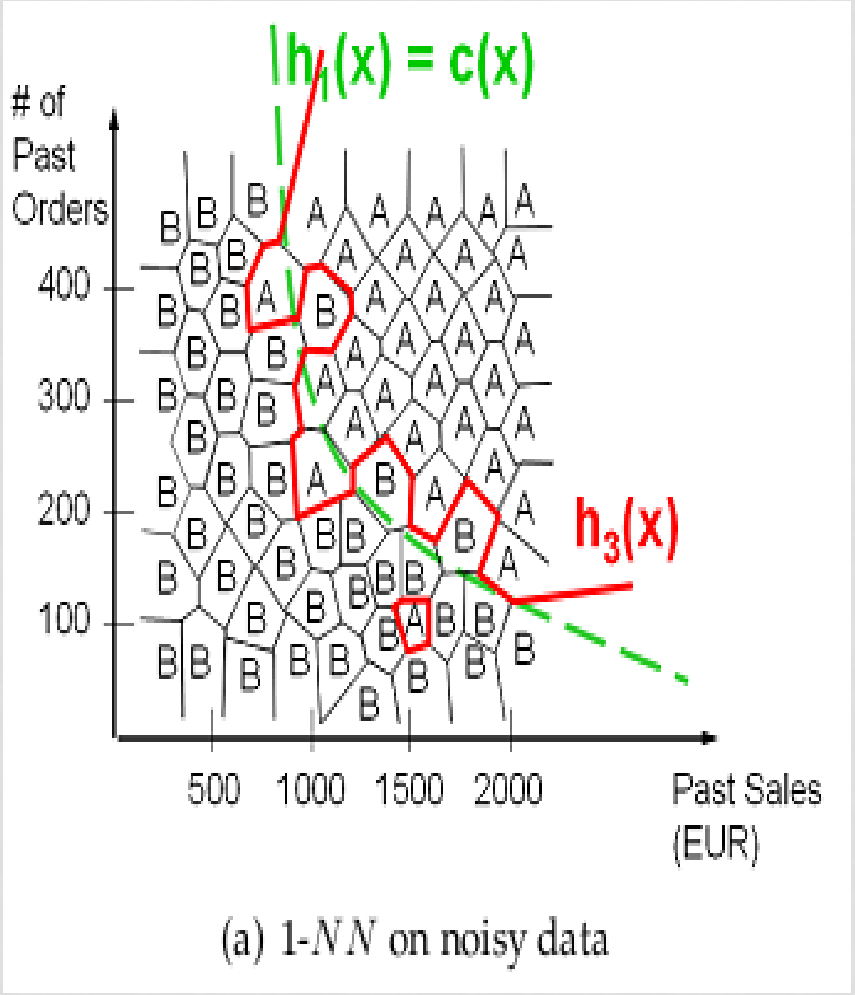
V1>=2.02897 “red”
V2>=-1.474671 “red”
V2< -1.474671 “blue”
V1< 2.02897 “blue”
6) V1< -1.797563 “red”
7) V1>=-1.797563 “blue”

Usually, huper-parameters control the **complexity** of the model

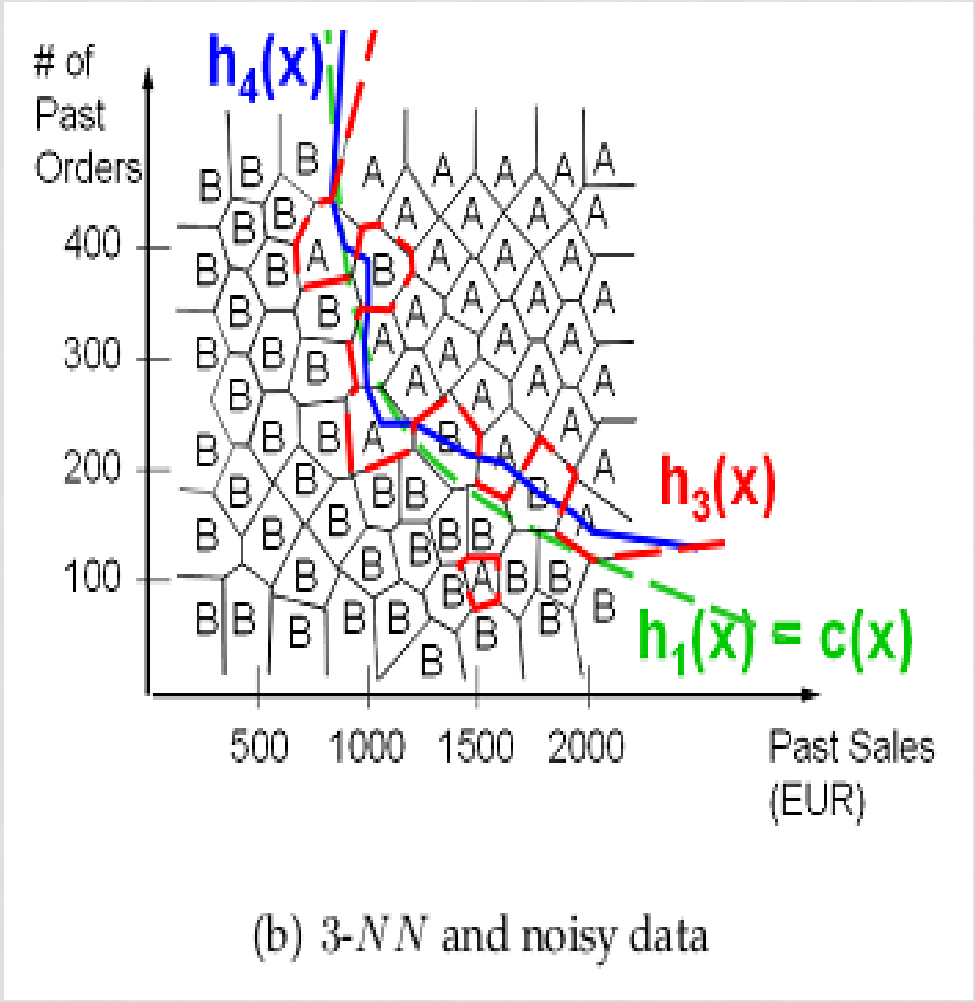
It is the opposite to trees

FOR KNN, LARGE K = SIMPLER MODEL

The boundary is less complex



(a) 1-NN on noisy data



(b) 3-NN and noisy data

Rules (created from the decision tree)

Obtain one rule from each path from the root to the leaves

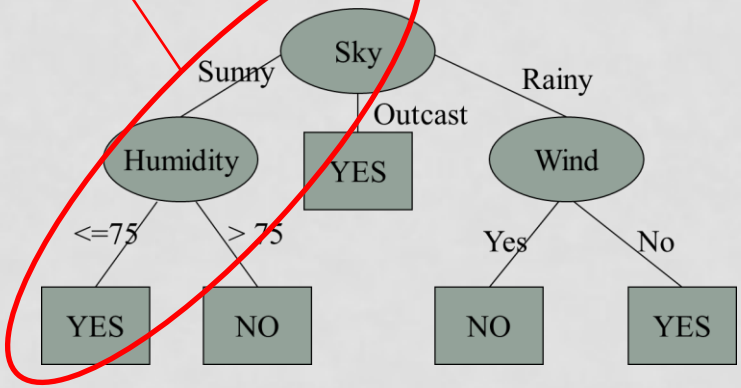
IF Sky = Sunny **AND** Humidity <= 75 **THEN** Tennis = Yes

ELSE IF Sky = Sunny AND Humidity > 75 **THEN** Tennis = No

ELSE IF Sky = Overcast **THEN** Tennis = Yes

ELSE IF Sky = Rainy AND Wind = Yes **THEN** Tennis = Yes

ELSE Tennis = No

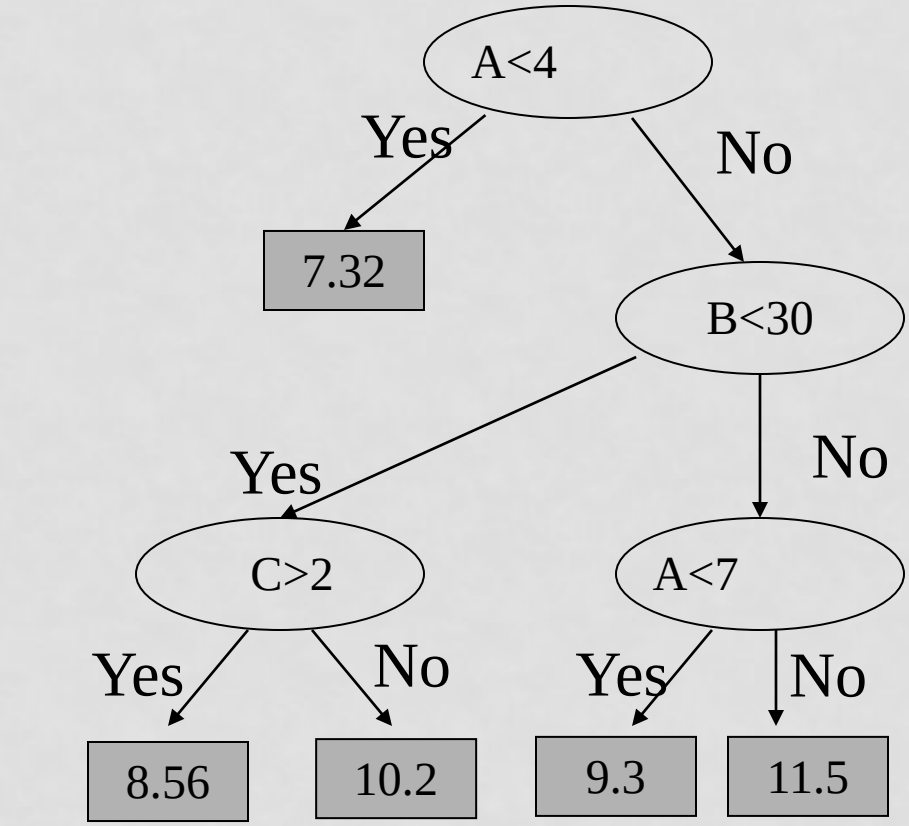


But there are algorithms that build rules directly from data

TREES FOR REGRESSION

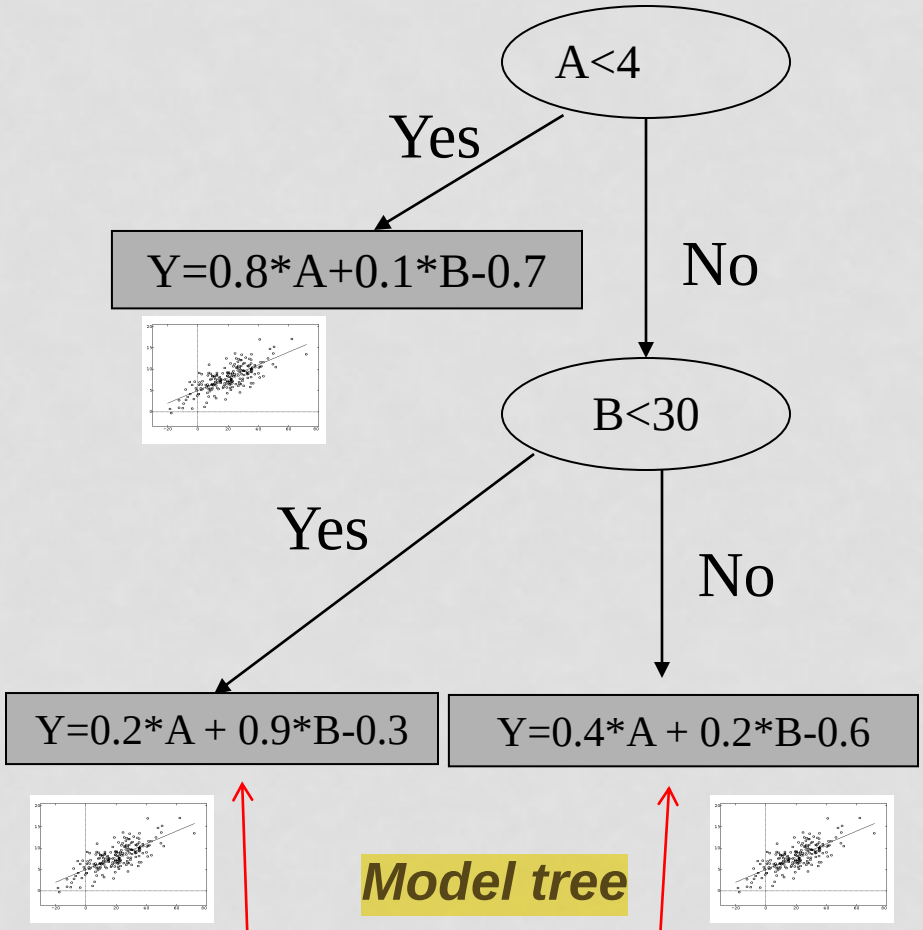
- What to do if the "class" (response variable) is continuous (rather than categorical)?
  - Answer: variance reduction (instead of entropy reduction)
- Two types:
  - Model trees
  - Regression trees

TREES FOR REGRESSION: TWO TYPES



Regression tree

Constants



Model tree

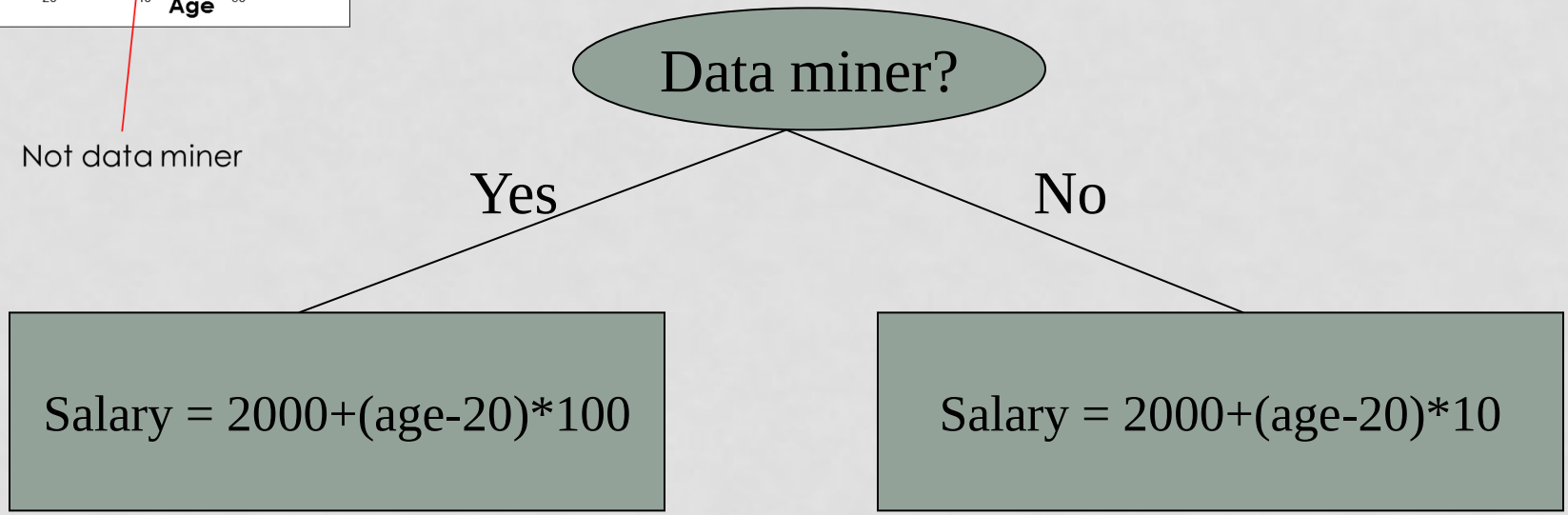
Linear models in the leaves

EXAMPLE

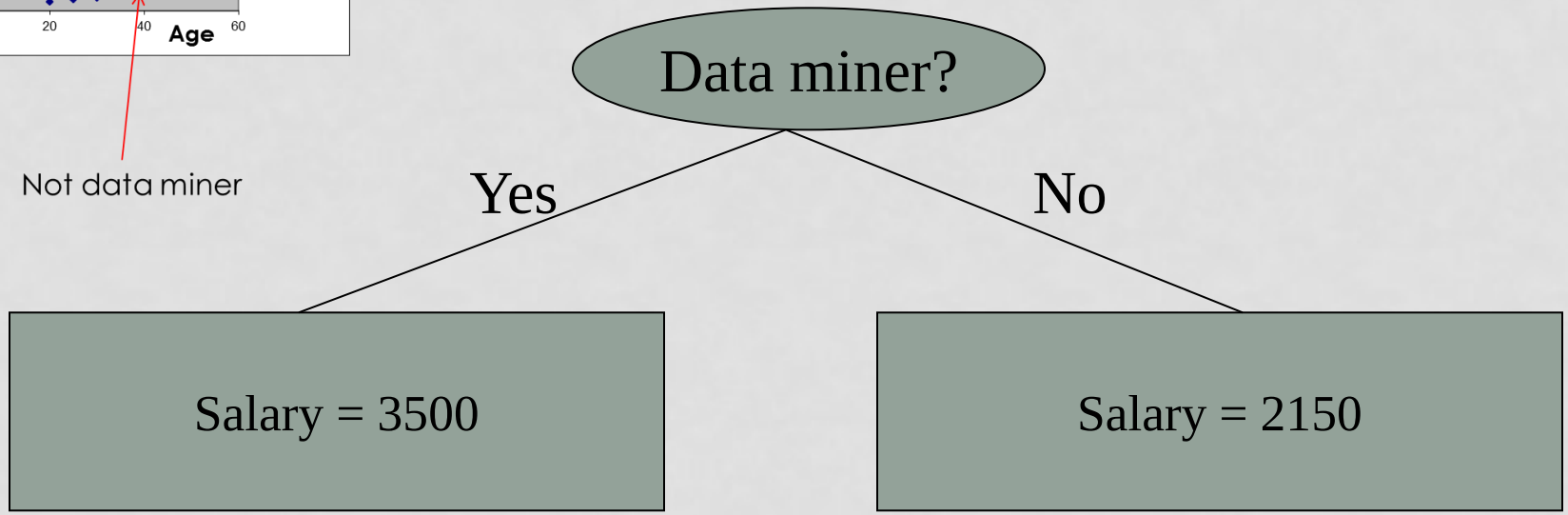
Training data

Data Miner?	Age	Salary
Yes	20	2000
Yes	25	2500
Yes	30	3000
Yes	35	3500
Yes	40	4000
Yes	45	4500
Yes	50	5000
No	20	2000
No	25	2050
No	30	2100
No	35	2150
No	40	2200
No	45	2250
No	50	2300

MODEL TREES. EXAMPLE

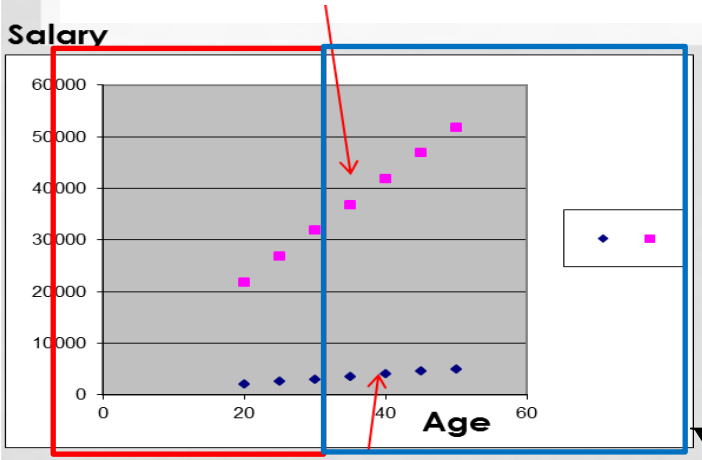


REGRESSION TREES. EXAMPLE

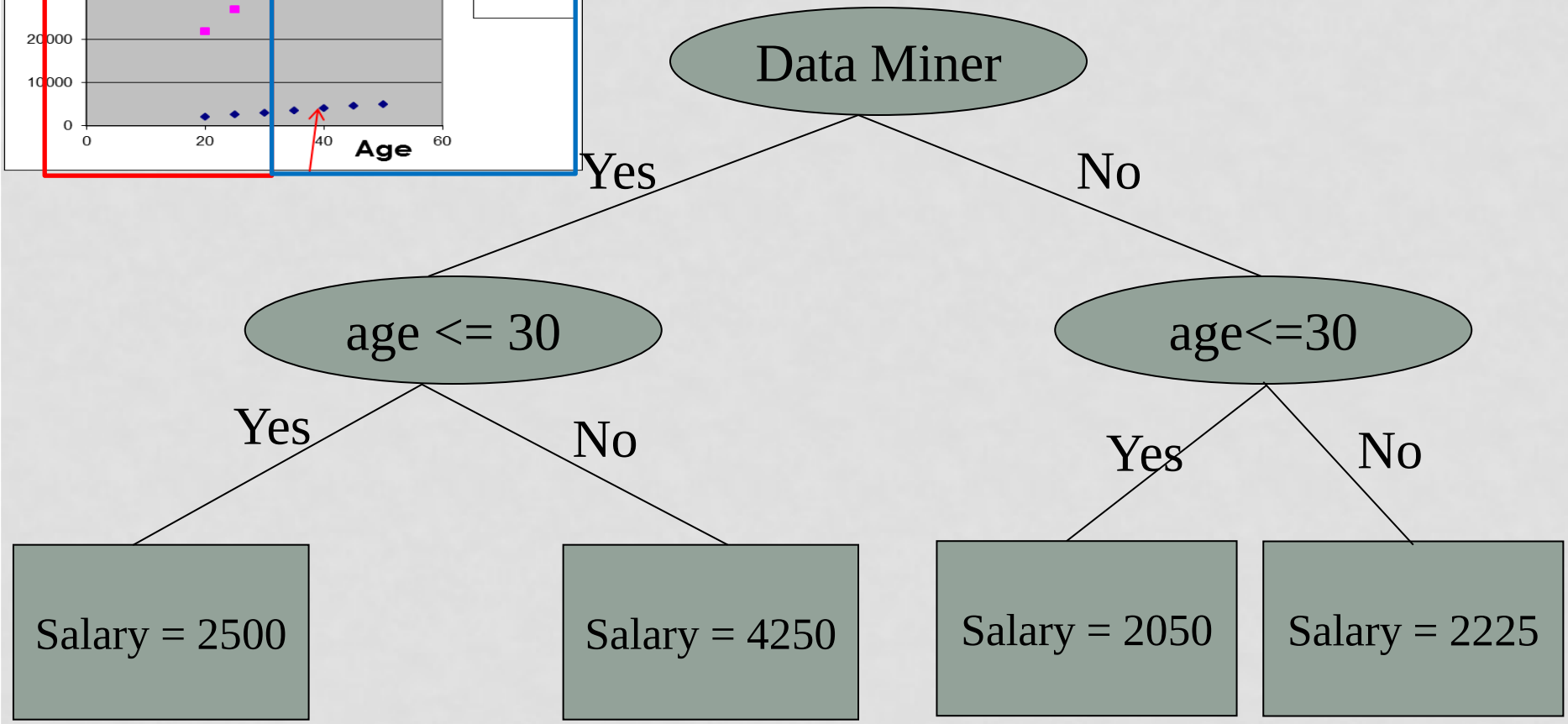


In the leaves, we can see the average salary for data miners (3500 euros) and the average salary for non-data miners (2150 euros)

REGRESSION TREES. EXAMPLE



A larger depth and using *age* allows the regression tree to approximate the problema, piece-wise.



TREES FOR REGRESSION

Instead of minimizing entropy, we minimize variance

- Regression and model trees are built similarly, except that in the leaves:
  - For regression trees, the average output value is computed
  - For model trees, a linear model is constructed (M5 (Quinlan, 93))
- Trees for regression are built similarly than trees for classification (decision trees), except that **standard deviation / variance** is reduced (instead of entropy)
- The tree is built recursively until a stopping condition is reached (max_depth, minsplit, …)

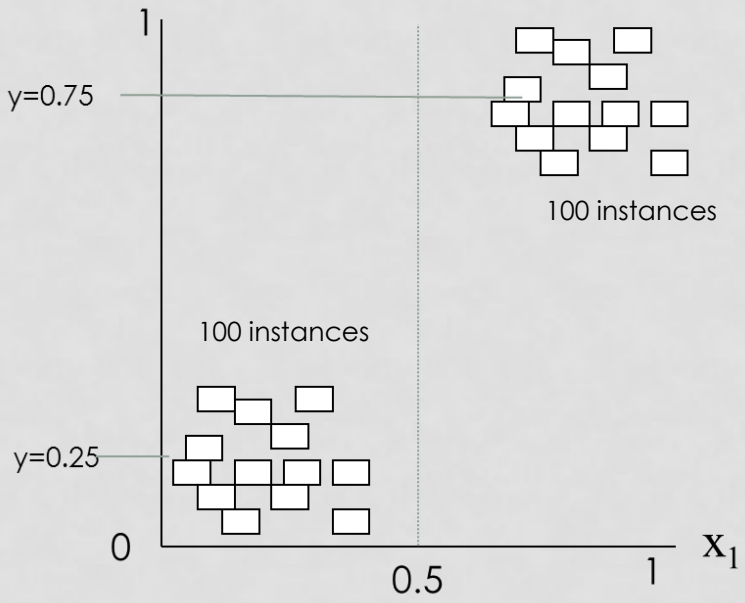
WHAT IS THE BEST NODE TO PUT IN THE ROOT OF THE TREE?

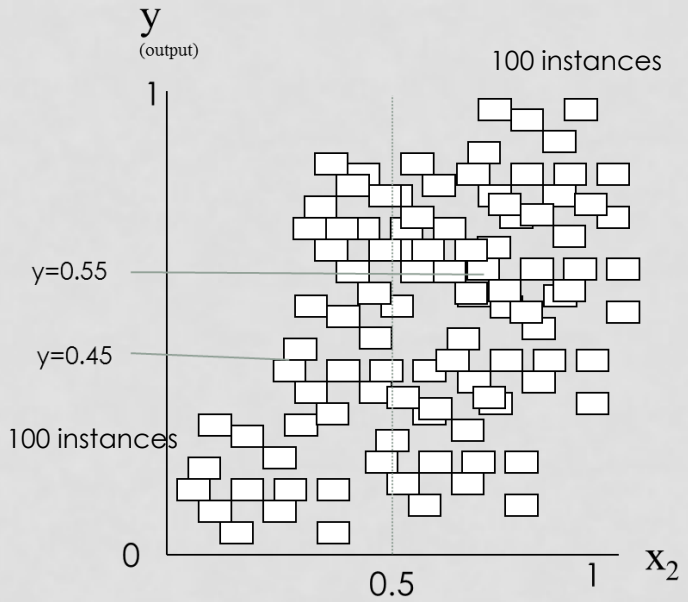
Which attribute is better?

x_1 or x_2?

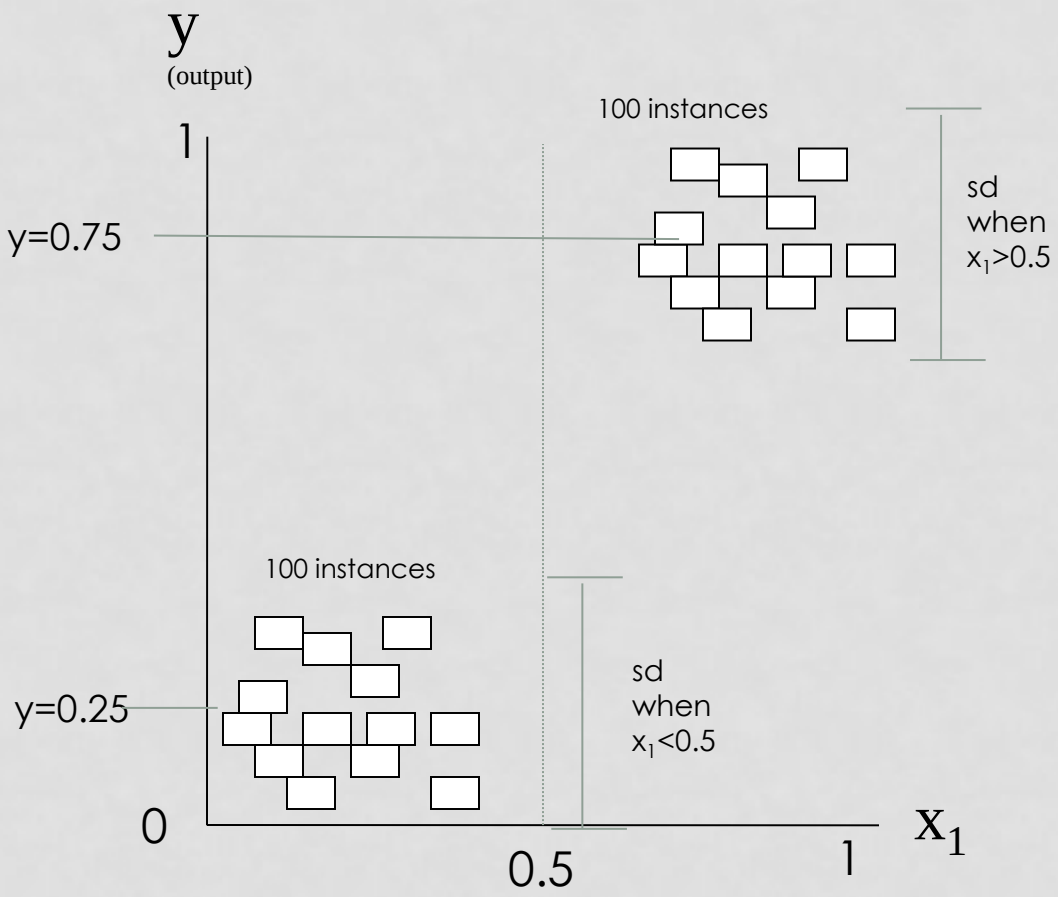
We will choose the attribute for which the average standard deviation (sd) **after the partition** is small:

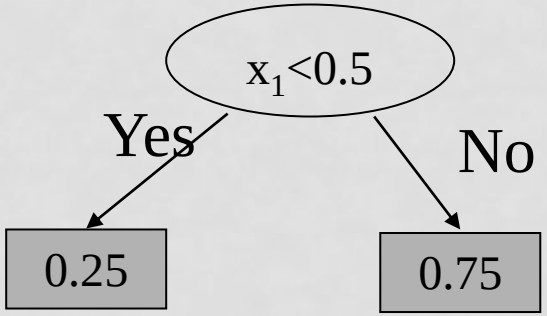
$$100/200 * sd(x_i<0.5) + 100/200 * sd(x_i>0.5)$$





WHAT IS THE BEST NODE TO PUT IN THE ROOT OF THE TREE?



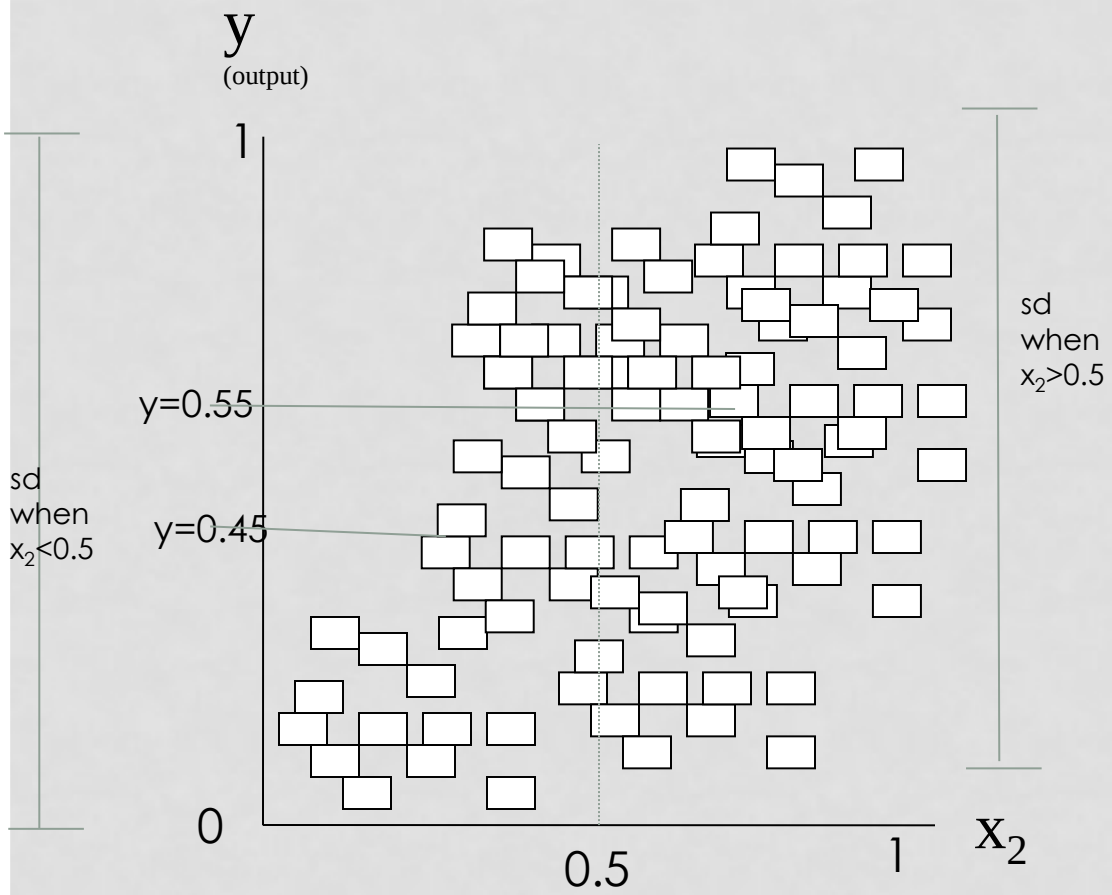


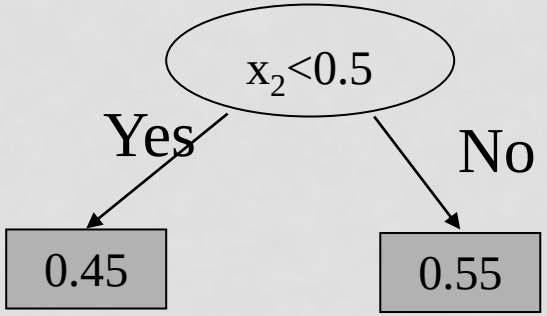
It can be noticed that x_1 is quite predictive

Instances after doing the partitions are not spread

½*sd(x_1<0.5) + ½* sd(x_1>0.5) is small

WHAT IS THE BEST NODE TO PUT IN THE ROOT OF THE TREE?



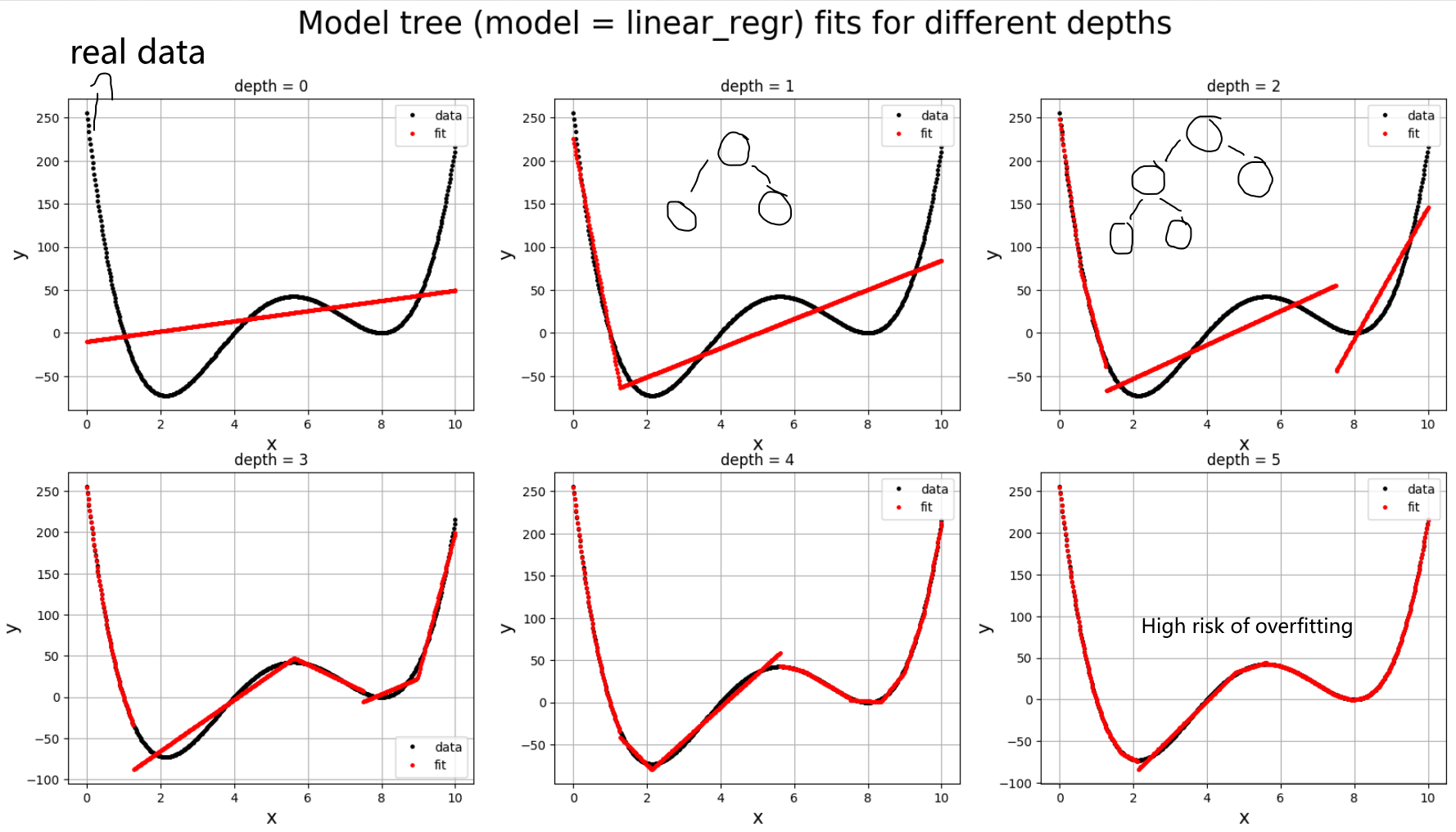


It can be noticed that x_2 is not predictive

Instances after the partition are very spread

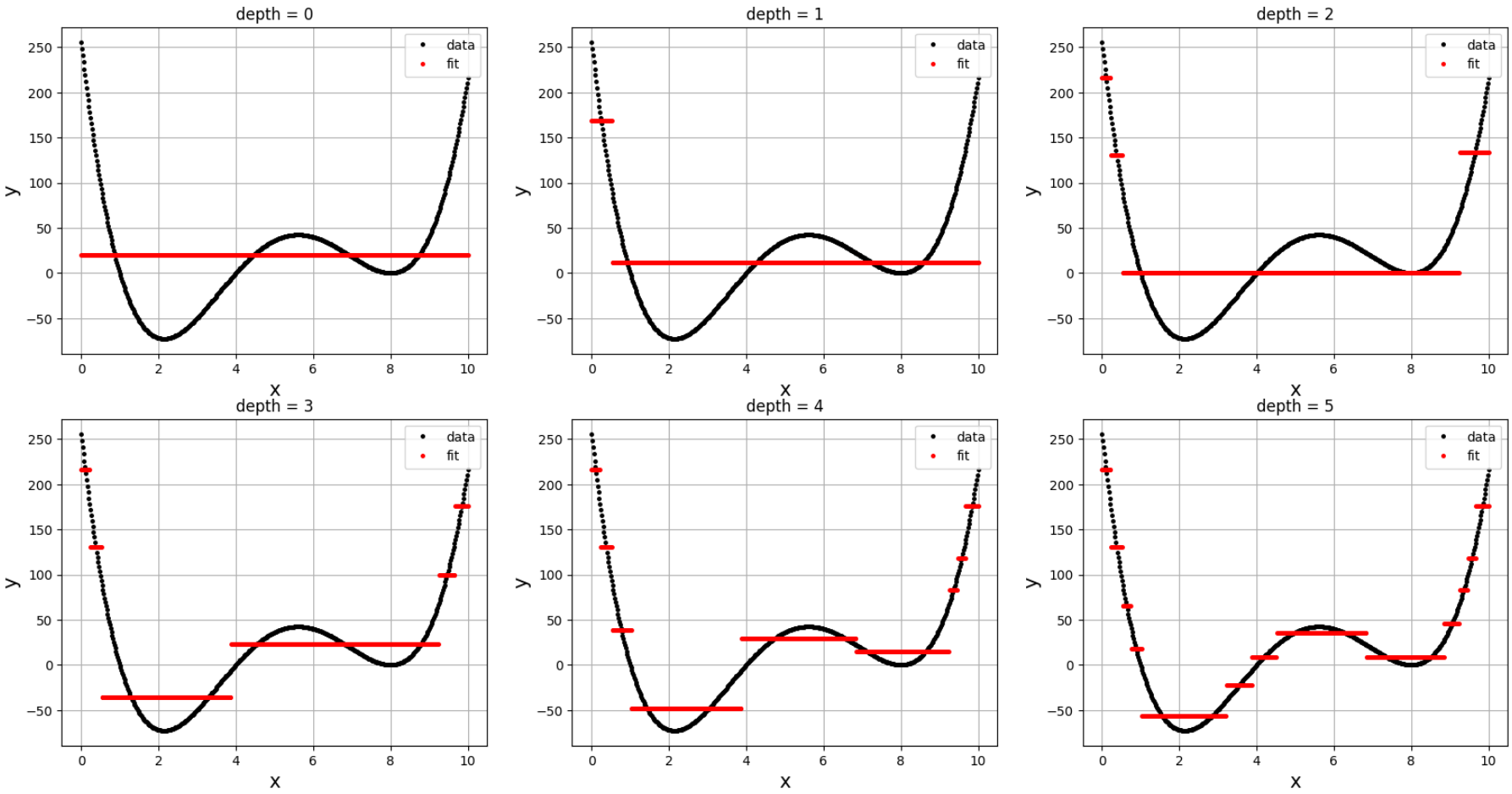
½* sd(x_2<0.5) + ½* sd(x_2>0.5) is very large

MODEL TREE


Model tree (model = linear_regr) fits for different depths
real data
depth = 0
depth = 1
depth = 2
depth = 3
depth = 4
depth = 5
data
fit
x
y
High risk of overfitting

REGRESSION TREE

Model tree (model = mean_regr) fits for different depths

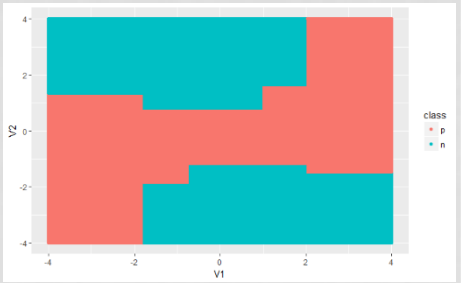


ACTUAL METHODS

- Classification and regression trees: C4.5, C5.0, CART
- Model trees: M5P, Cubist

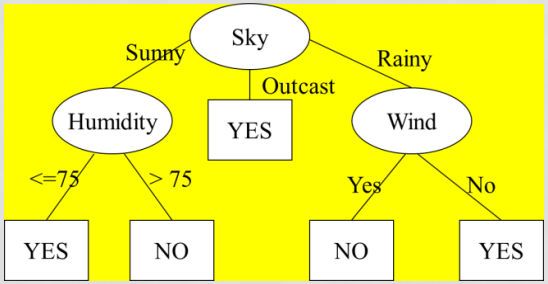
DISADVANTAGES OF TREES

- Boundaries too simple for some problems (parallel to axes)
  - However, trees are the elements of advanced methods, such as Random Forests and Gradient Tree Boosting (ensembles).
- Hyper-parameters must be tuned carefully (maxdepth, ..), otherwise (deep) trees are prone to overfitting (bad generalization). HIGH RISK OF OVERFITTING



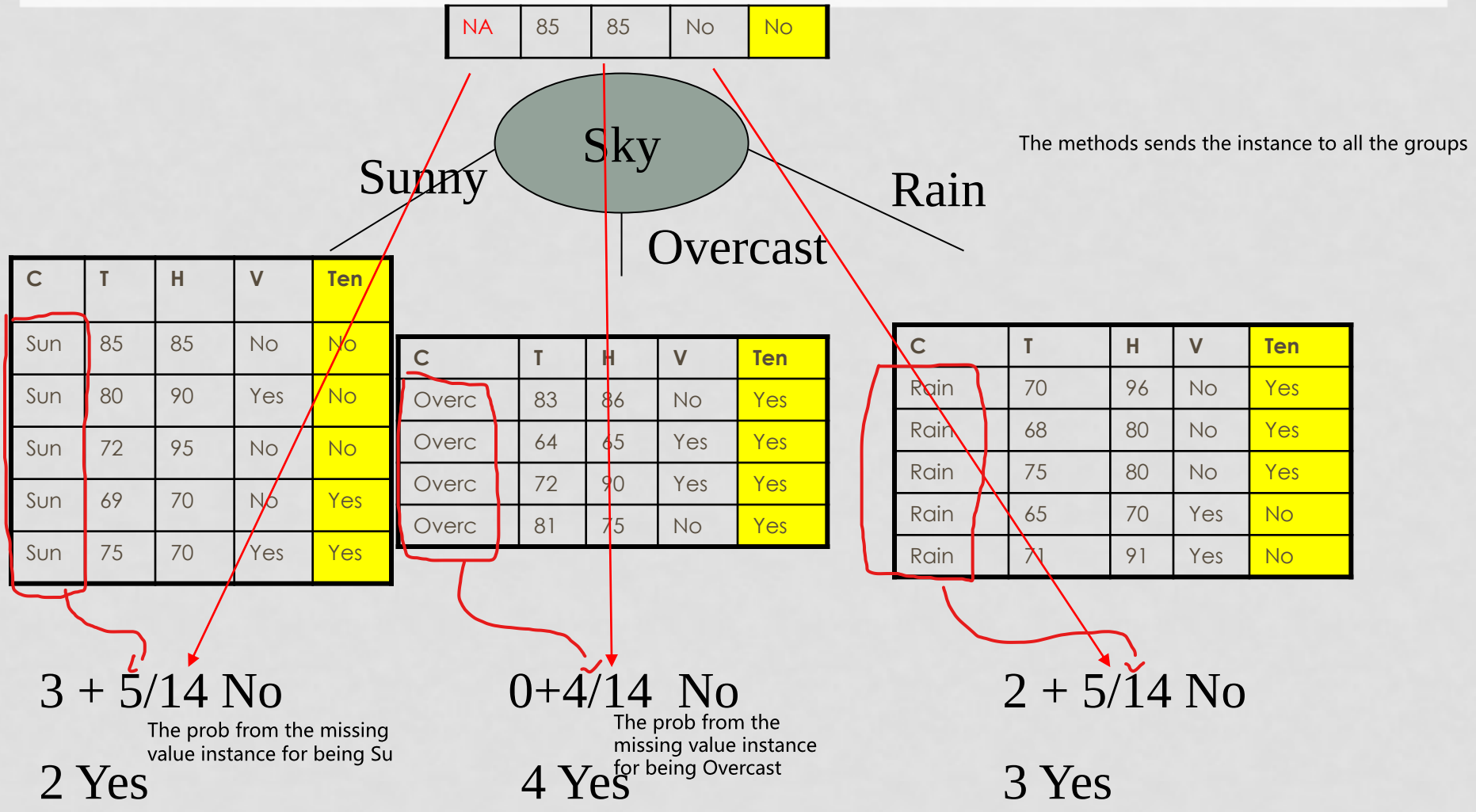
ADVANTAGES OF TREES

- Interpretable.
  - Attributes closer to the root are the most relevant.
- They can handle naturally categorical attributes (no need for one-hot-encoding variables)
  - But not in scikit-learn ☹ For Scikit-learn you need to do one-hot encoding
- Training is fast (compared to other methods)
- They can handle multiple classes naturally.
- They can handle missing values



HANDLING "MISSING VALUES"

This method doesnt work for sckit learn



HANDLING "MISSING VALUES“ IN SCIKIT-LEARN TREES

- Unfortunately, the previous approach is not available in scikit-learn.
- Before version 1.3, the way of dealing with missing values (np.nan) in scikit-learn was **imputation** : replacing the missing value by some other value (mean, median, mode). This can still be used, and belongs to “preprocessing”.
- Since versión 1.3, sklearn decisión trees are able to deal with missing values in this manner:

NATIVE WAY SCIKIT-LEARN MANAGES MISSING VALUES

  - For each potential threshold on the non-missing data, the splitter will evaluate the split with all the missing values going to the left node or the right node. That is, the algorithm determines what is the best branch to send instances with a missing value for that particular feature.
  - When making predictions for new instances, the tree will remember which way the missing values should go.
- Yet another way is **to consider the missing value just like another value**: if feature A has possible values ‘red’, ‘green’, ‘blue’, but some values are missing, then the actual set of values is: ‘red’, ‘green’, ‘blue’, NA