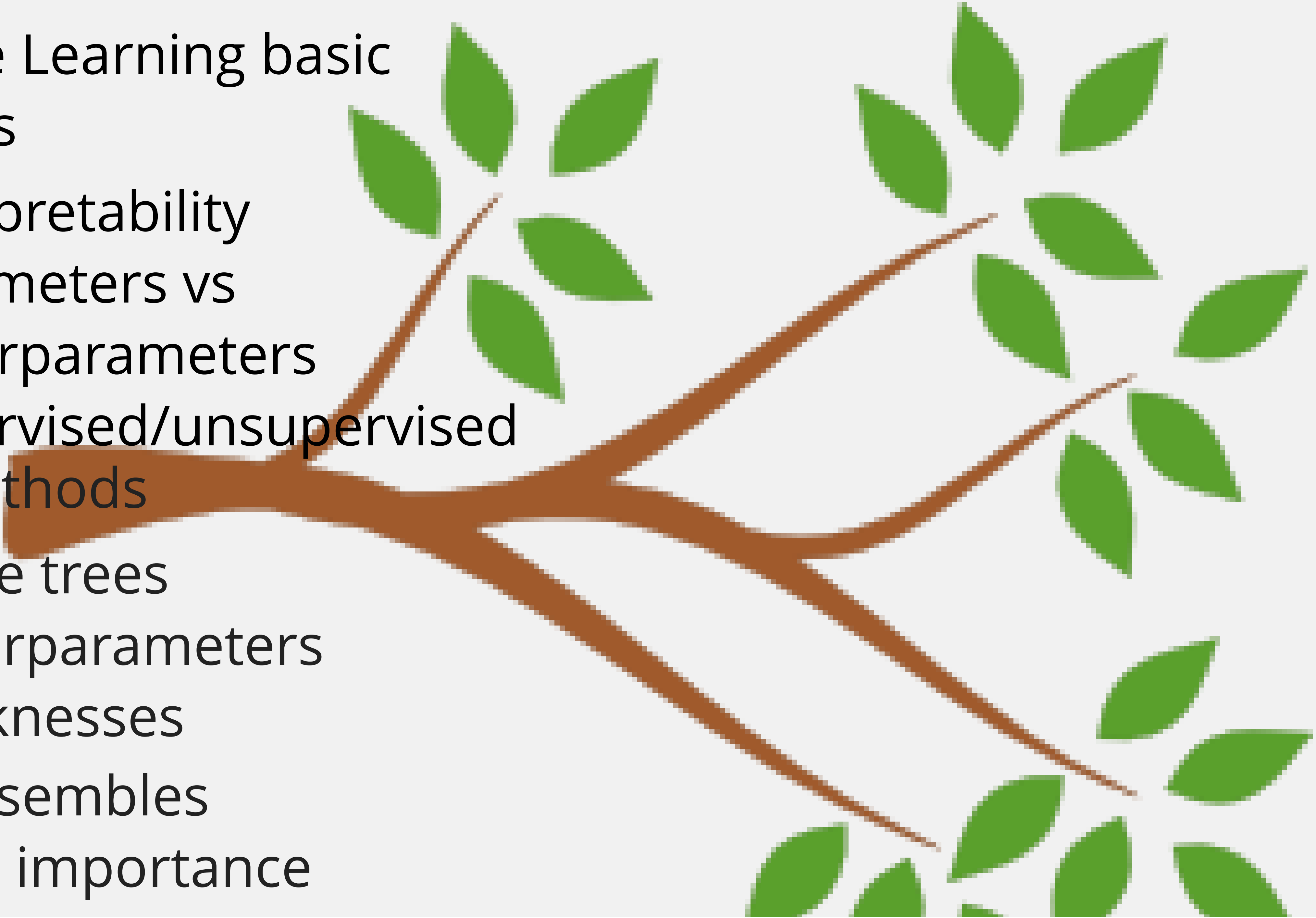
data science for (physical) scientists VIII

Tree methods

dr.federica bianco | fbb.space | fedhere | fedhere

this slide deck: http://bit.ly/dspsVIII

- Machine Learning basic concepts
  - interpretability
  - parameters vs hyperparameters
  - supervised/unsupervised
- Tree methods
  - single trees
  - hyperparameters
  - weaknesses
- Tree ensembles
- Feature importance

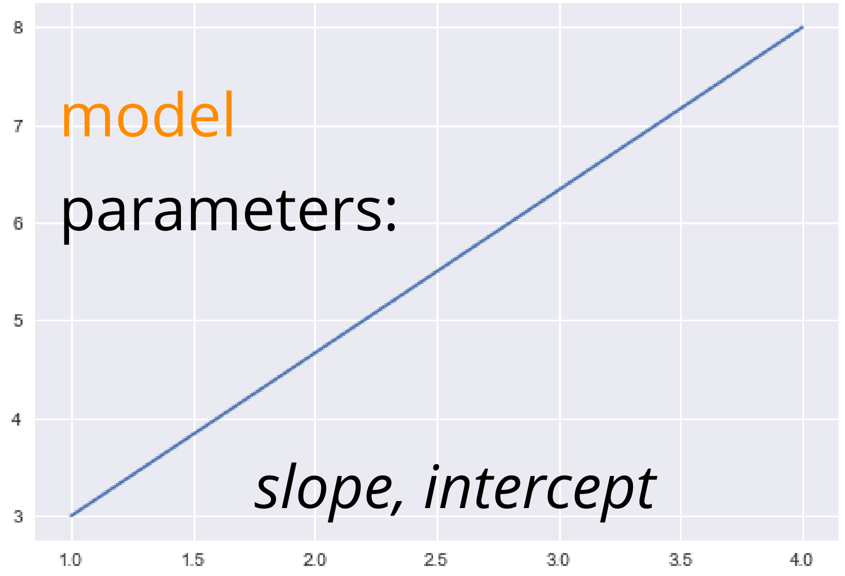


recap

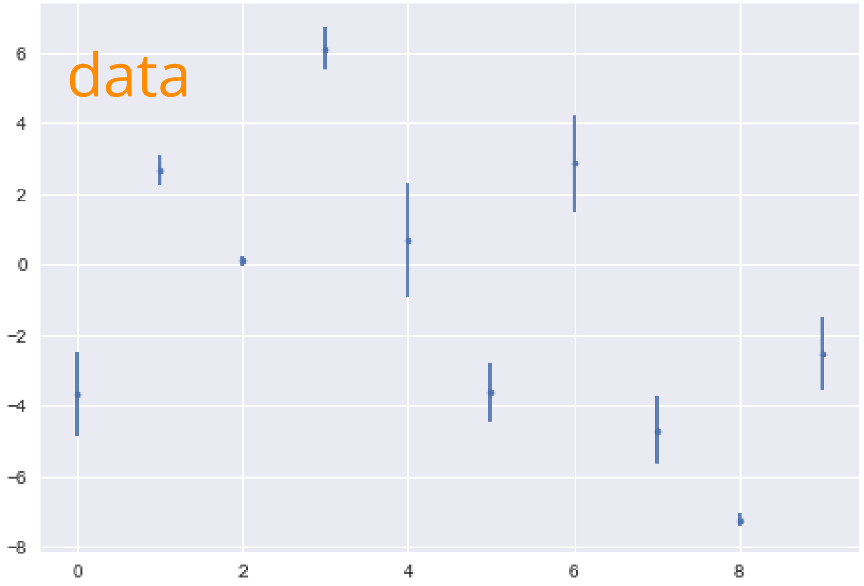
what is machine learning

what is machine learning?

[Machine Learning is the] field of study that gives computers the ability to learn without being explicitly programmed. Arthur Samuel, 1959



ML: any model with parameters learnt from the data



what is machine learning?

supervised learning

classification

prediction

feature selection

unsupervised learning

understanding structure

organizing/compressing data

anomaly detection

dimensionality reduction

what is machine learning?

supervised learning

k-Nearest Neighbors
Regression
Support Vector Machines
Classification/Regression Trees
Neural networks

classification
prediction
feature selection

unsupervised learning

understanding structure
organizing/compressing data
anomaly detection
dimensionality reduction

clustering
PCA
Apriori

general ML points

used to:

understand structure of feature space

classify based on examples,

regression (classification with infinitely small classes)

general ML points

should be interpretable: why?

ethical implications

predictive policing,

selection of conference participants.

general ML points

should be interpretable: why?

ethical implications

prective policing,

selection of conference participants.

causal connection

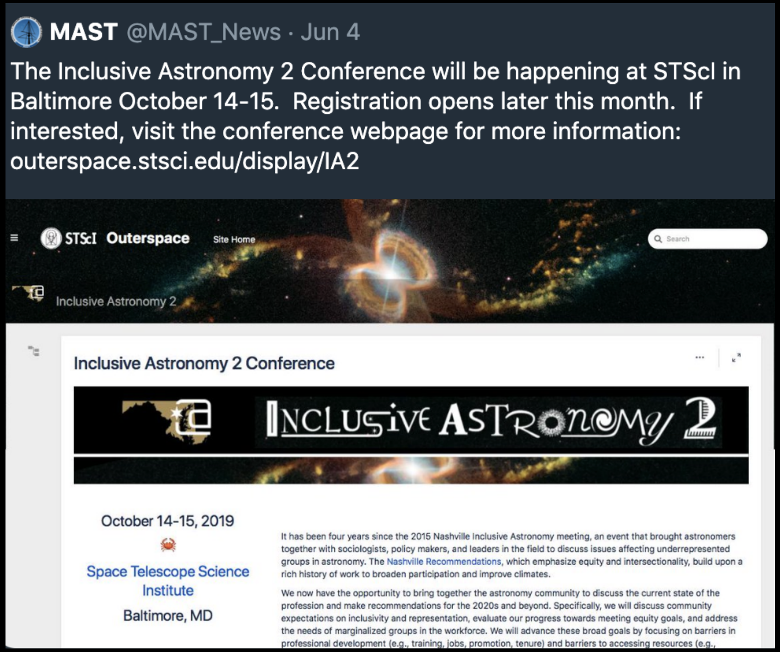
why the model made a choice?

which feature mattered?

general ML points

should be interpretable:

ethical implications



general ML points

ML model have *parameters* and *hyperparameters*

parameters: the model optimizes based on the data

hyperparameters: chosen by the model author, could be based on domain knowledge, other data, guessed (?!).

e.g. the shape of the polynomial

1

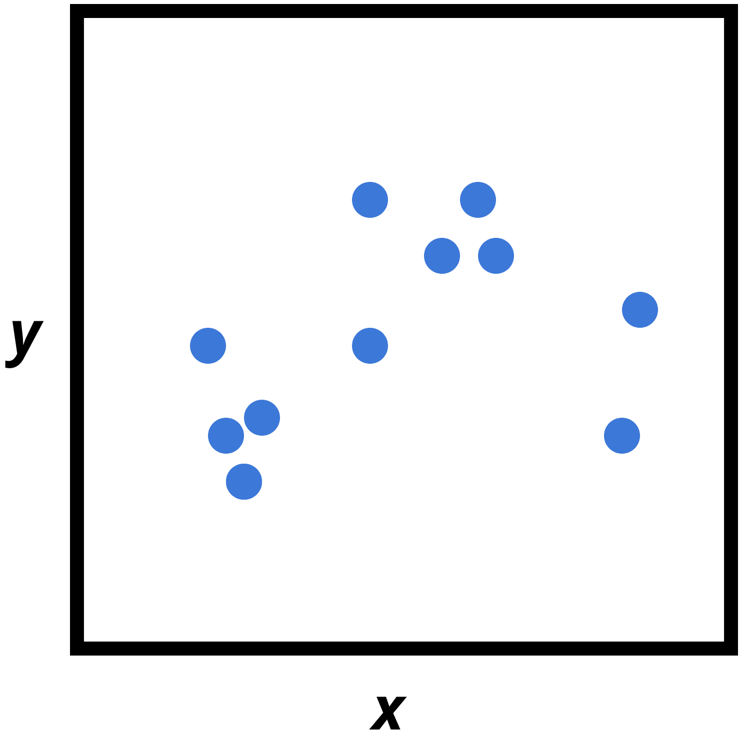
classification vs clustering

clustering vs classifying

unsupervised

observed features:

$(\vec{x}, \vec{y})$

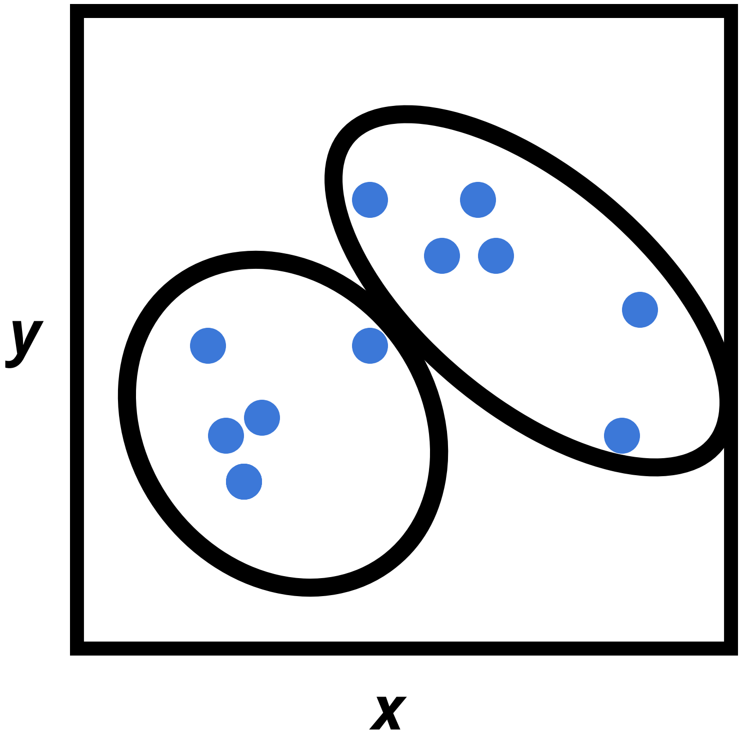


clustering vs classifying

unsupervised

observed **features:**

$(\vec{x}, \vec{y})$



clustering vs classifying

unsupervised

goal is to partition the space so that the **observed** variables are

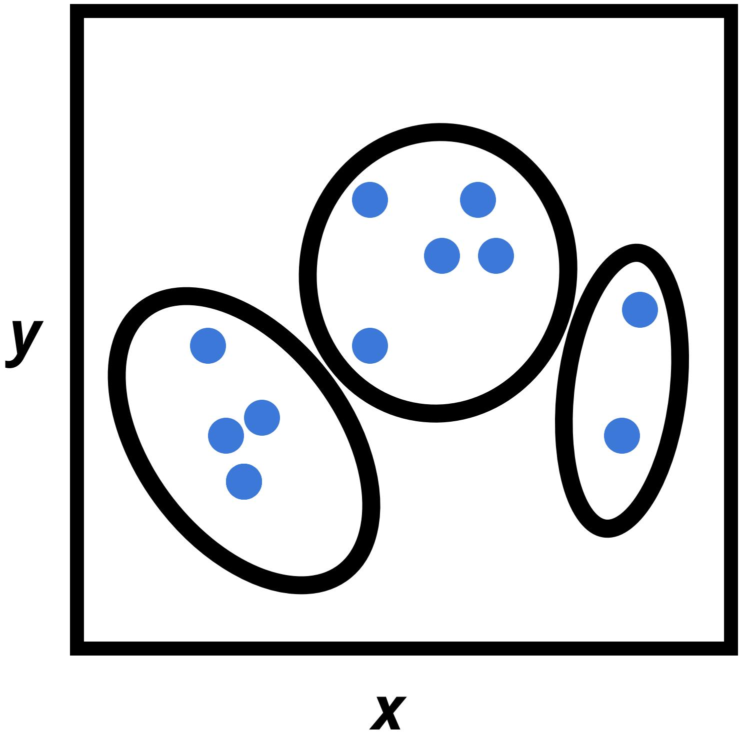
separated into

maximally homogeneous

maximally distinguishable groups

observed features:

$(\vec{x}, \vec{y})$



models typically return a cluster label by object

clustering vs classifying

unsupervised *supervised*

goal is to partition the space so that the **unobserved** variables are

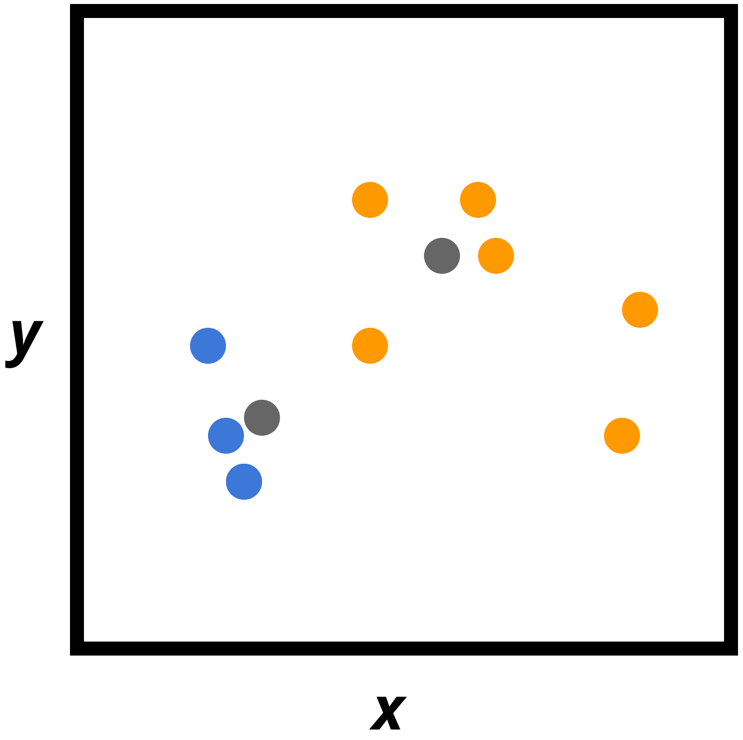
separated in groups

consistently with

an observed subset

observed features:

$(\vec{x}, \vec{y})$



target features:

$(\overrightarrow{color})$

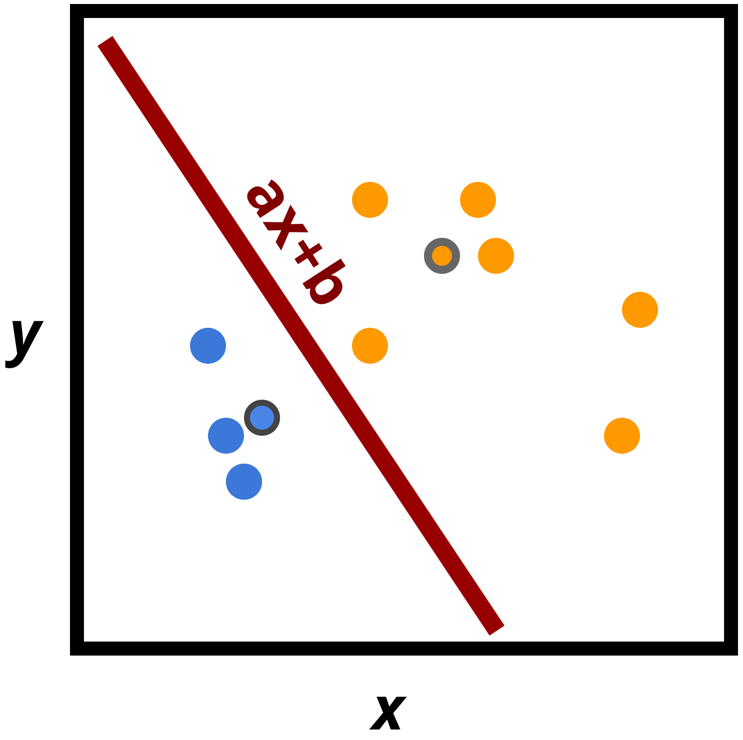
models typically return a partition of the space

clustering vs classifying

unsupervised *supervised*

observed features:

$(\vec{x}, \vec{y})$



target features:

$(\overrightarrow{color})$

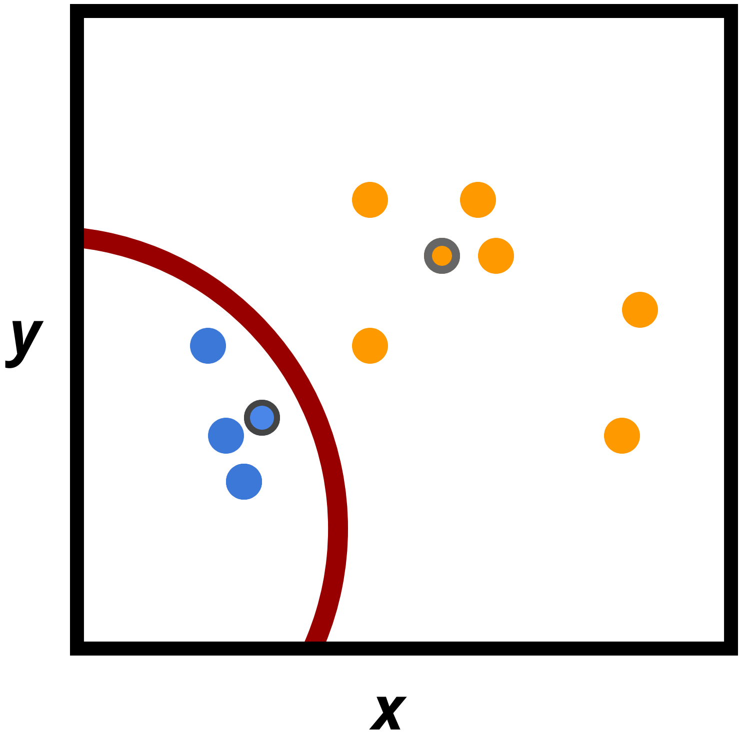
```
if y <= a*x + b :
        return blue
else:
        return orange
```

clustering vs classifying

unsupervised *supervised*

observed **features:**

$(\vec{x}, \vec{y})$



target **features:**

$(\overrightarrow{color})$

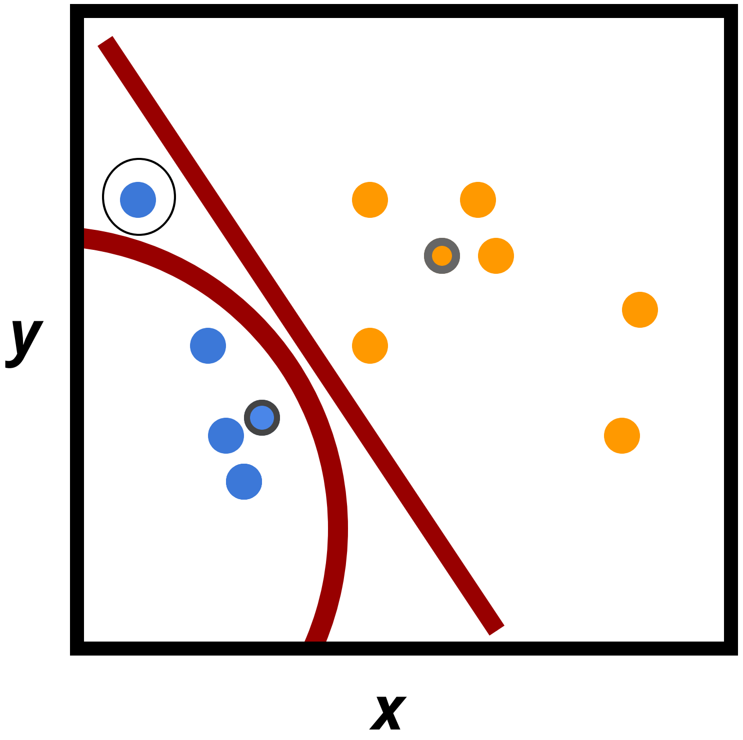
```
if x**2 + y**2 <= (x-a)**2 + (y-b)**2 :
        return blue
else:
        return orange
```

clustering vs classifying

unsupervised *supervised*

observed **features:**

$(\vec{x}, \vec{y})$



target **features:**

$(\overrightarrow{color})$

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if x**2 + y**2 <= (x-a)**2 + (y-b)**2 :
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clustering vs classifying

unsupervised *supervised*

observed **features:**

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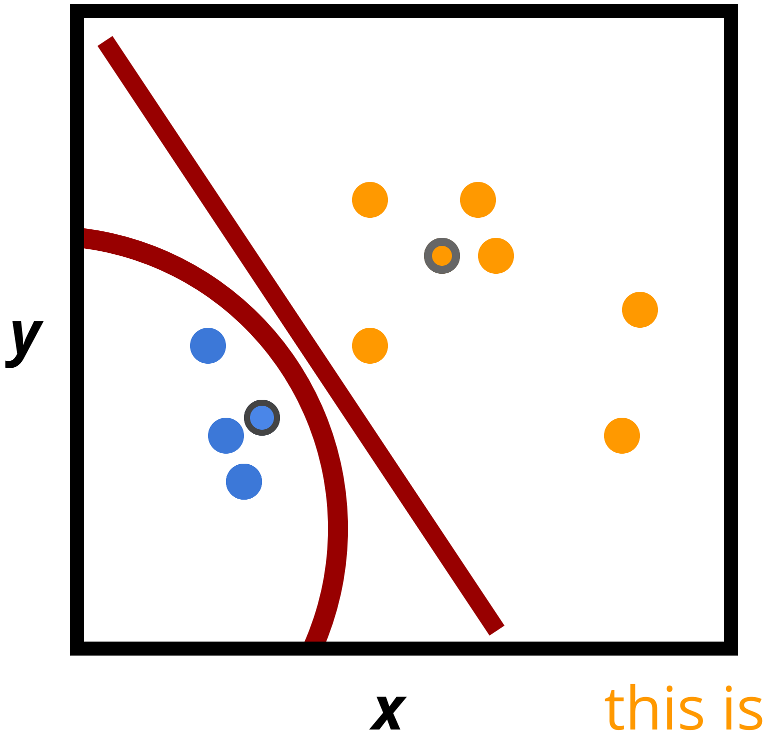


target **features:**

$(\overrightarrow{color})$

this is a solution SVM would provide:

Support Vector Machine

supervised ML: classification

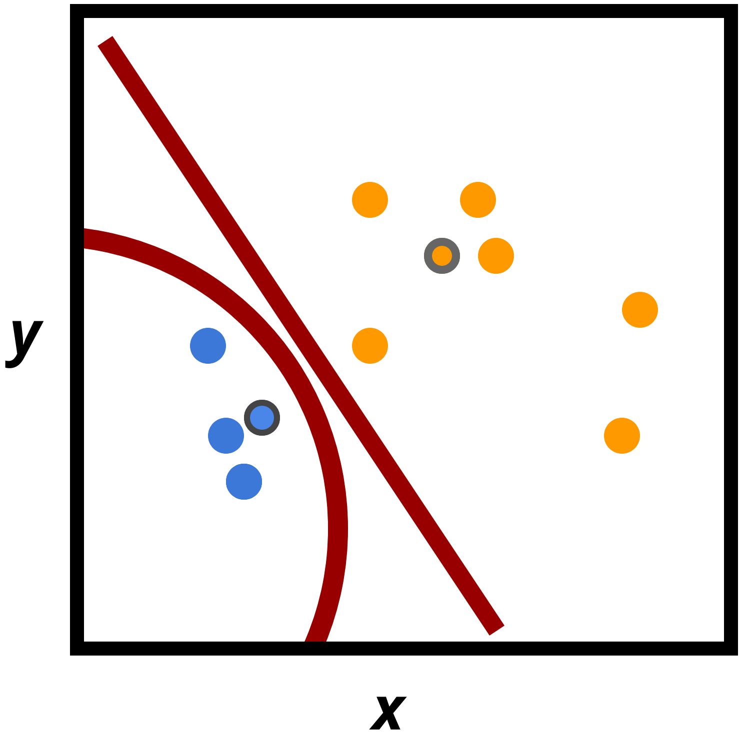
A subset of variables has class labels.
Guess the label for the other variables

Support Vector Machine:

finds a hyperplane that partitions the space

observed features:

$(\vec{x}, \vec{y})$



target features:

$(\overrightarrow{color})$

supervised ML: classification

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Support Vector Machine:

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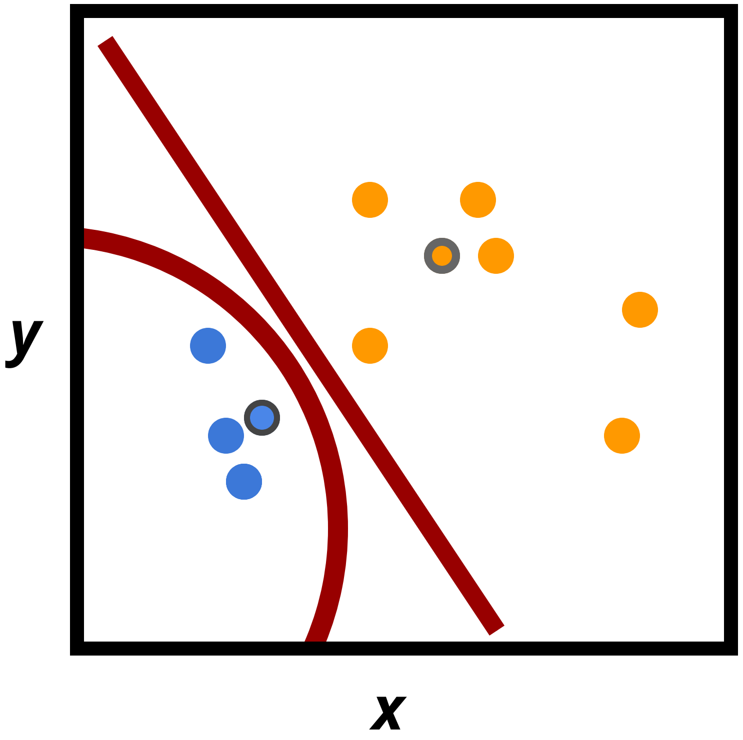


2d hyperplane: line (curve)

3d hyperplane: surface

4d hyperplane: volume

...

target features:

$(\overrightarrow{color})$

supervised ML: classification

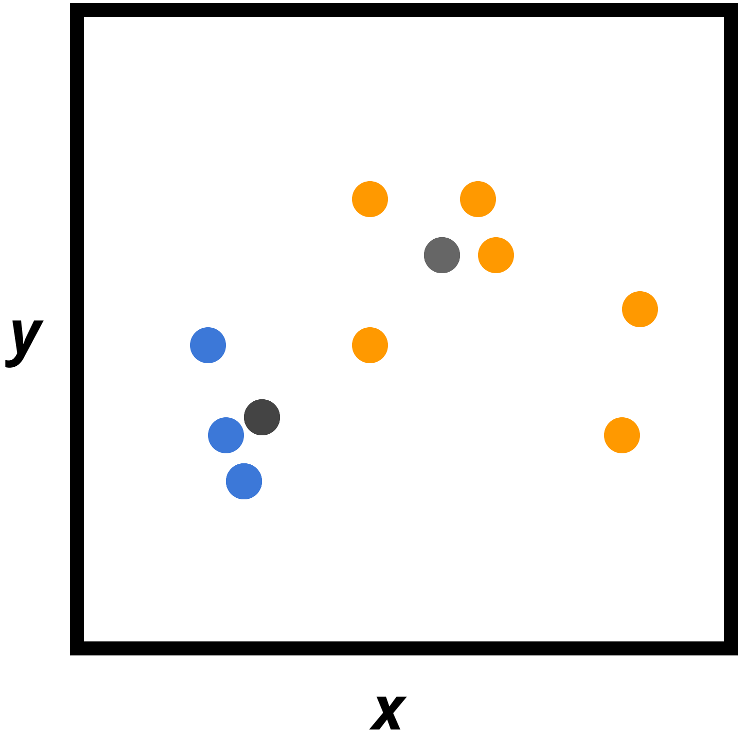
A subset of variables has class labels.
Guess the label for the other variables

Tree Methods

split spaces along each axis separately

observed features:

$(\vec{x}, \vec{y})$



target features:

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Tree Methods

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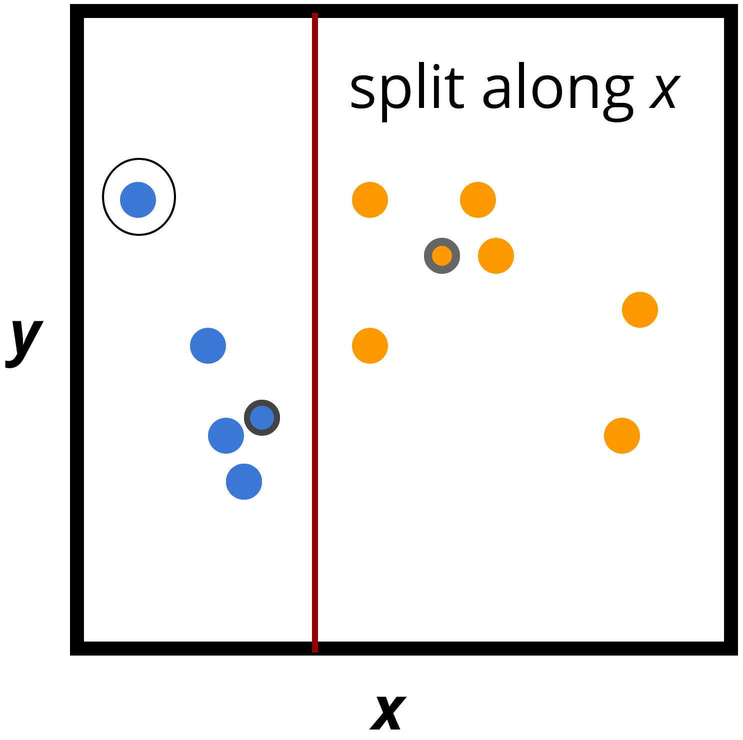

observed features:
$(\vec{x}, \vec{y})$

target features:
$(\overrightarrow{color})$

```
if x <= a :
        return blue
else:
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```

supervised ML: classification

A subset of variables has class labels.
Guess the label for the other variables

Tree Methods

split spaces along each axis separately

observed features:

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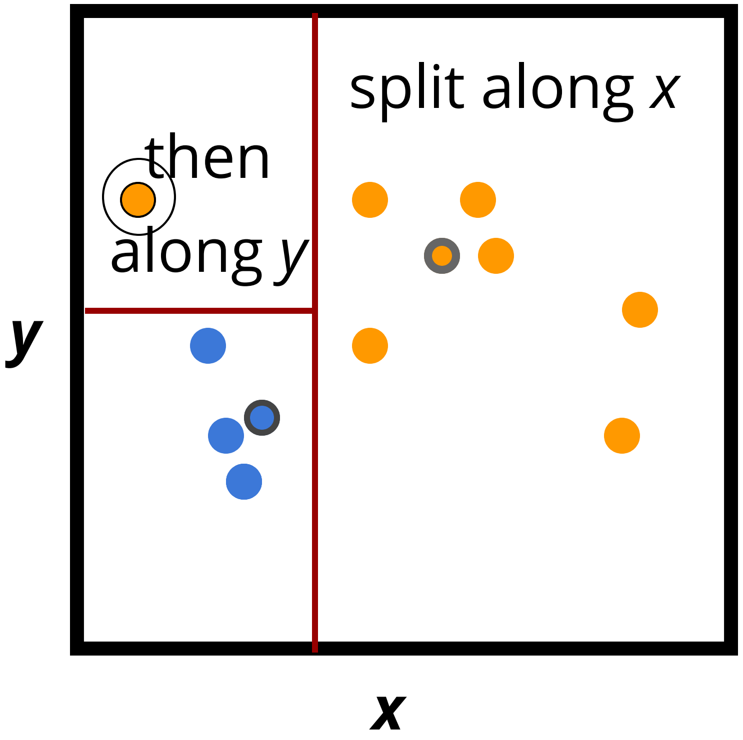


target features:

$(\overrightarrow{color})$

```
if x <= a :
        if y <= b:
                return blue
return orange
```

Tree Methods

supervised learning method

partitions feature space along each feature separately

The good

- Non-Parametric
- White-box: can be easily interpreted
- Works with any feature type and mixed feature types
- Works with missing data
- Robust to outliers

The bad

- High variability (-> use ensamble methods)
- Tendency to overfit
- (not really easily interpretable after all...)

single tree

1

Application:

a robot to predict surviving the Titanic

(Kaggle)

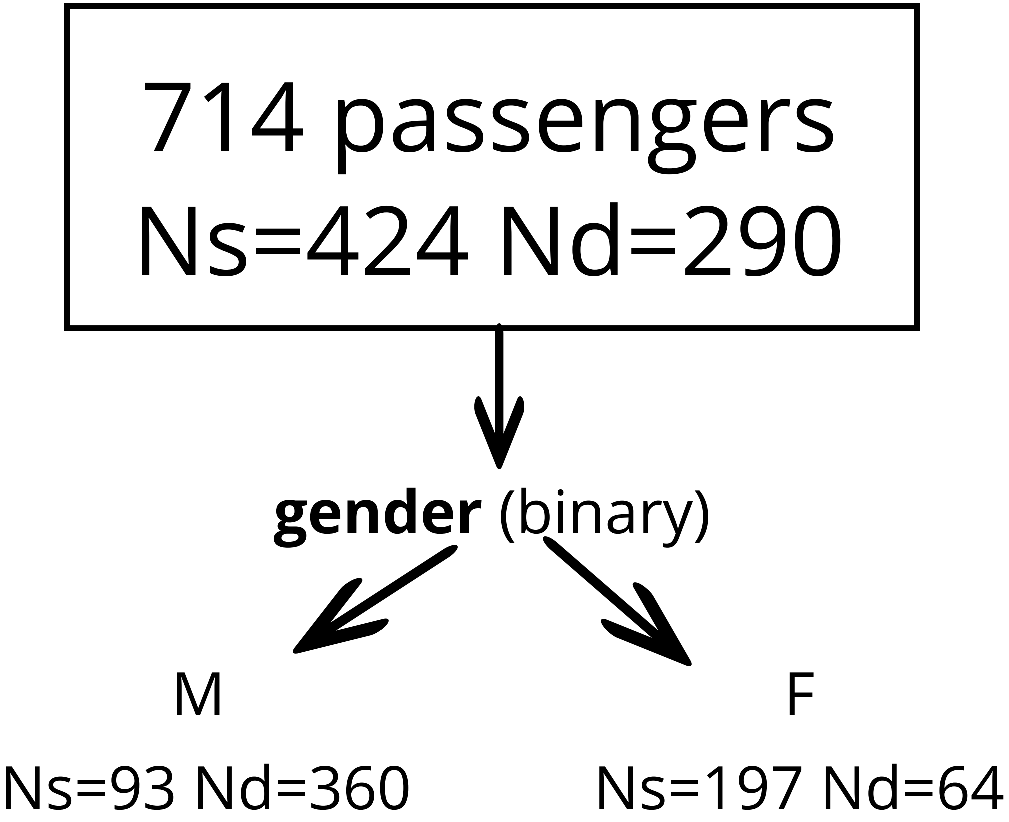
https://www.kaggle.com/c/titanic

features:

- gender
- ticket class
- age

target variable:

-> survival (y/n)



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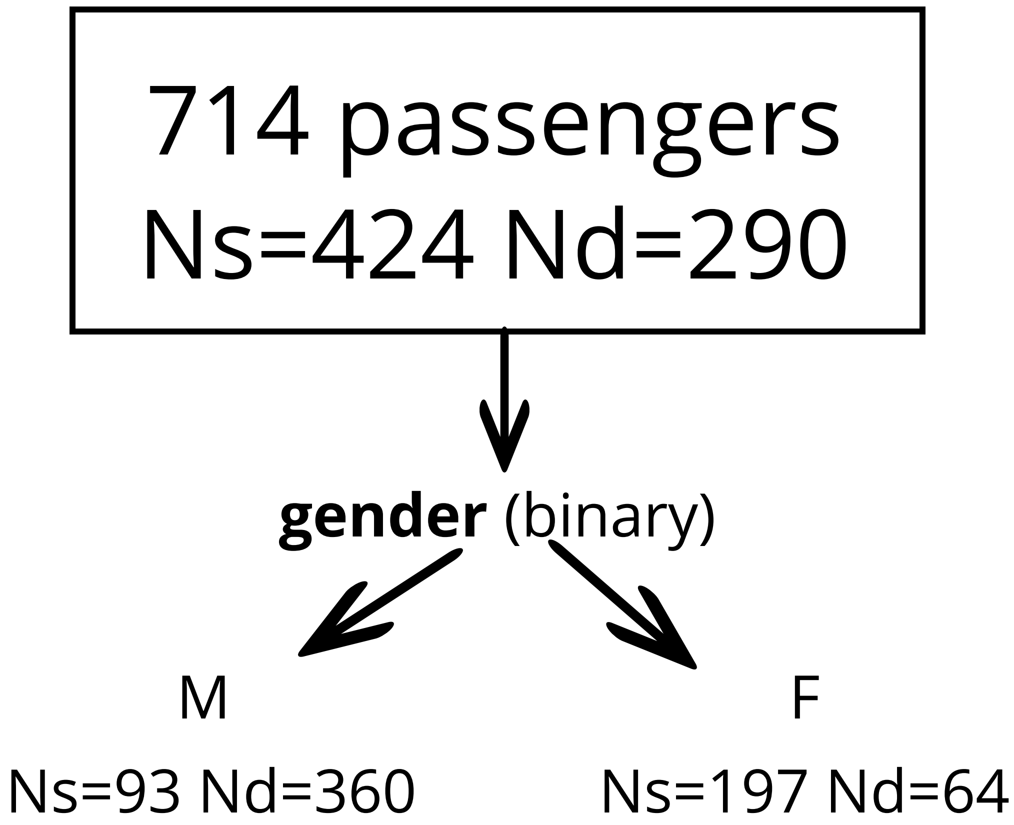

optimize over purity:

$$p = \frac{N_{largest\ class}}{N_{total}}$$

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features:

- gender
- ticket class
- age

target variable:

-> survival (y/n)

714 passengers
Ns=424 Nd=290

gender (binary)

M

Ns=93 Nd=360

$$p = \frac{360}{360+93}$$

F

Ns=197 Nd=64

$$p = \frac{197}{197+64}$$

optimize over purity:

$$p = \frac{N_{largest\ class}}{N_{totalset}}$$

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features:

- gender
- ticket class
- age

target variable:

-> survival (y/n)

714 passengers
Ns=424 Nd=290

gender (binary)

M

Ns=93 Nd=360

$p = 79\%$

F

Ns=197 Nd=64

$p = 75\%$

optimize over purity:

$$p = \frac{N_{largest\ class}}{N_{totalset}}$$

Application:

a robot to predict surviving the Titanic

(Kaggle)

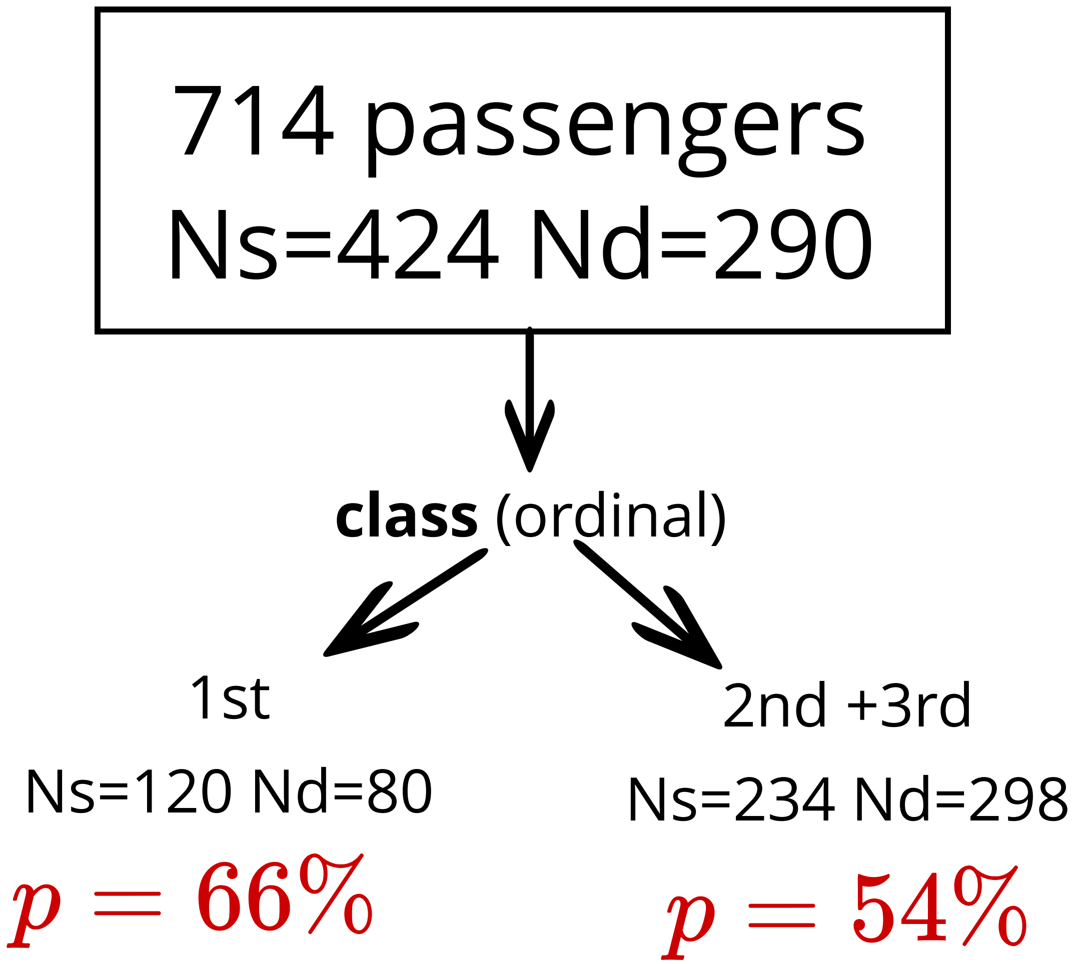
https://www.kaggle.com/c/titanic

features:

- gender 79%|75%
- ticket class 66 | 54%
- age

target variable:

-> survival (y/n)



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a robot to predict surviving the Titanic

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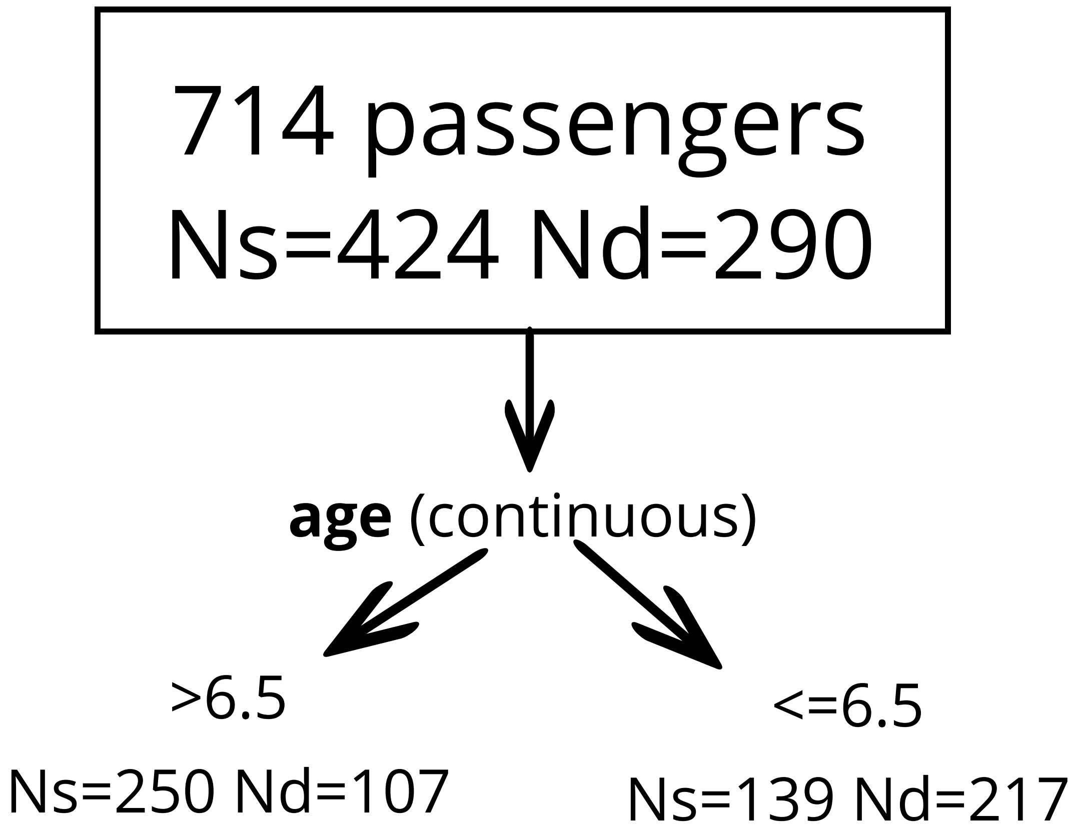
features:

- gender 79%|75%
- ticket class 66% | 54%
- age 66% | 61%

target variable:

-> survival (y/n)



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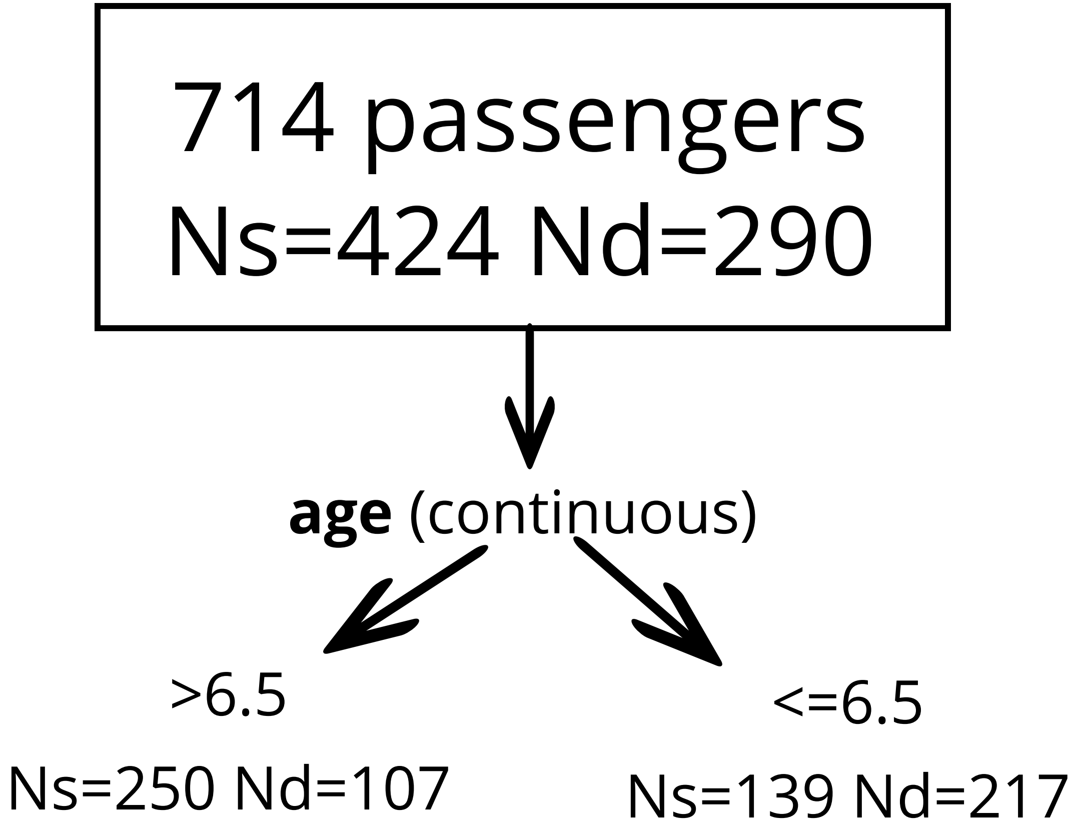
- gender 79%|75%
- ticket class 66% | 44%
- age 66% | 61%

target variable:

-> survival (y/n)



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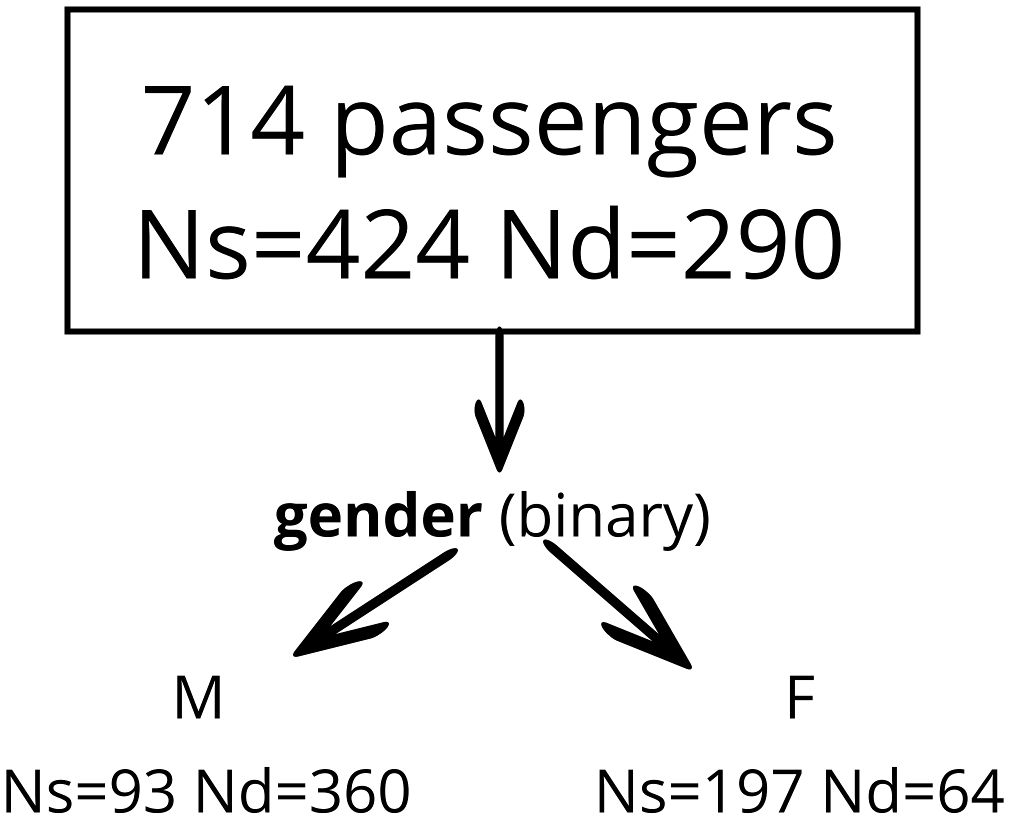
features:

- gender 79|75%
- ticket class *M* 60|85% *F* 96|65%
- age *M* 74|67% *F* 66|60%

target variable:

-> survival (y/n)



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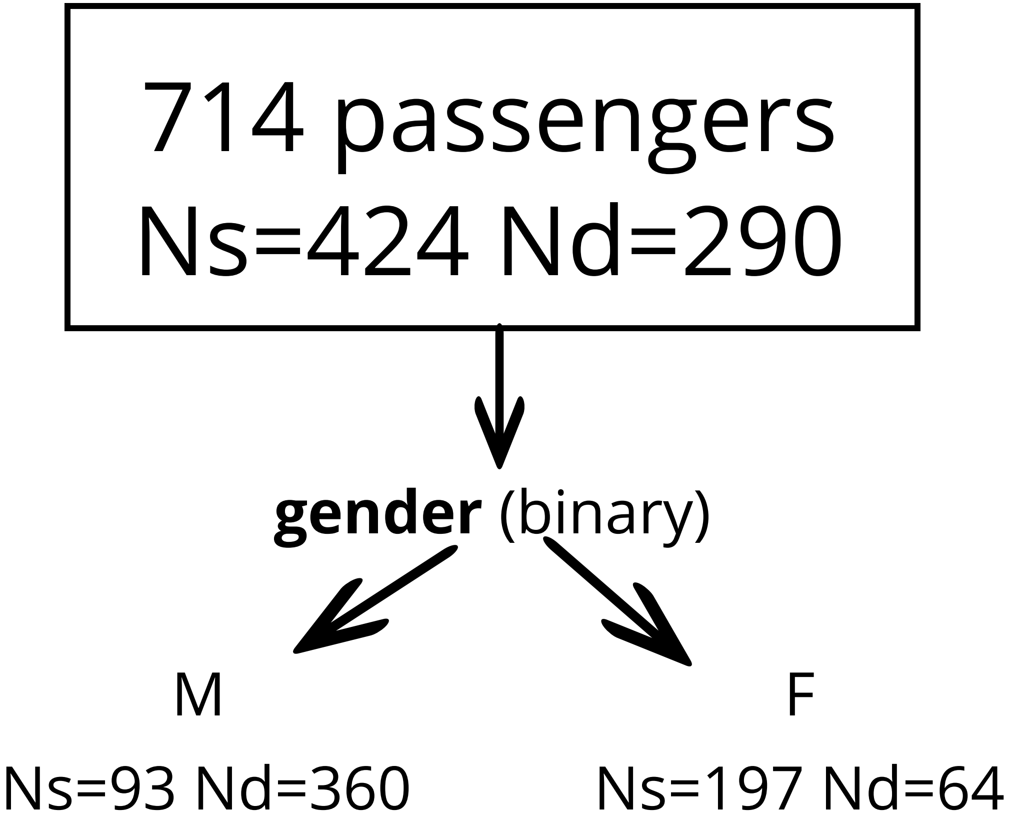

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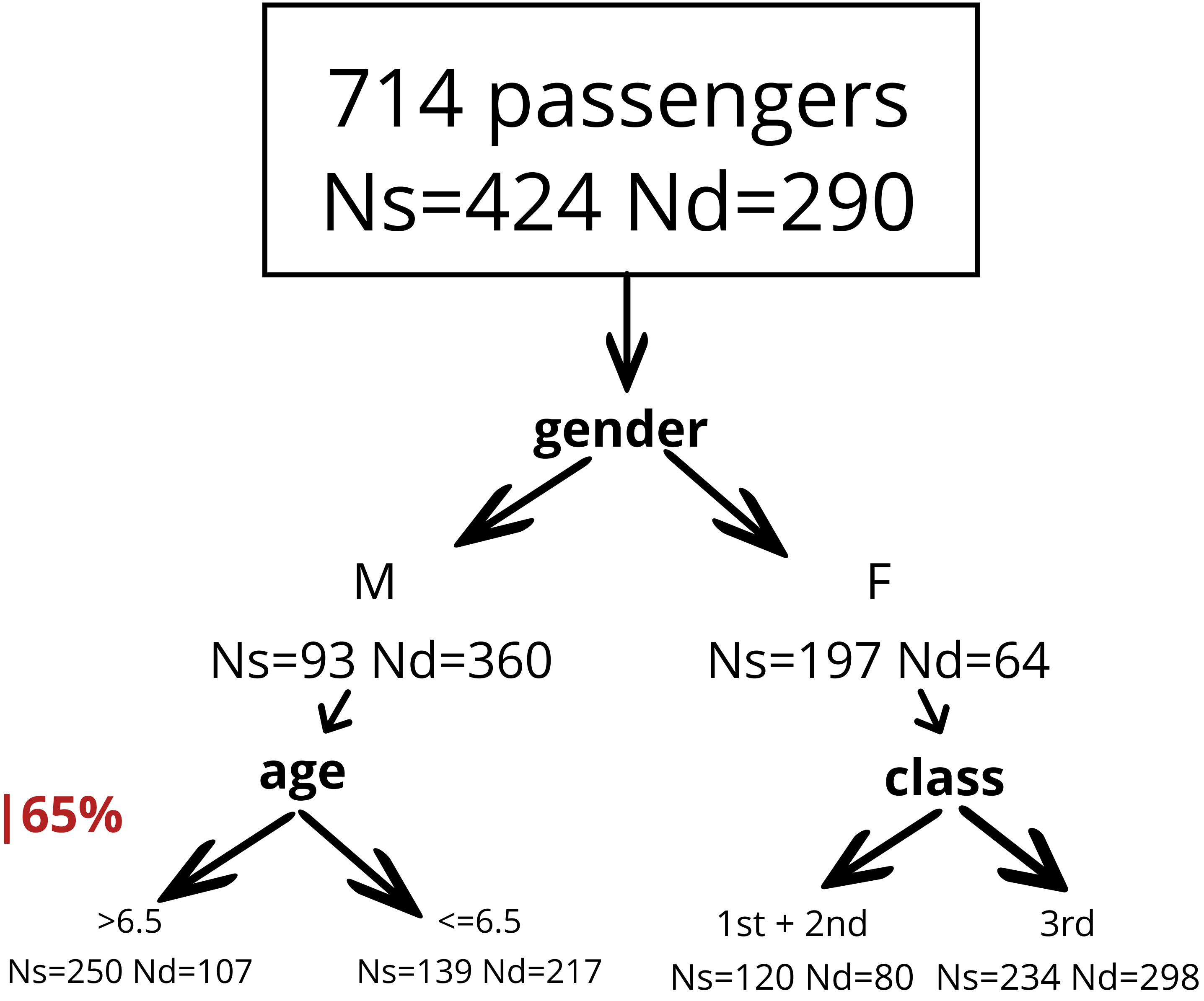

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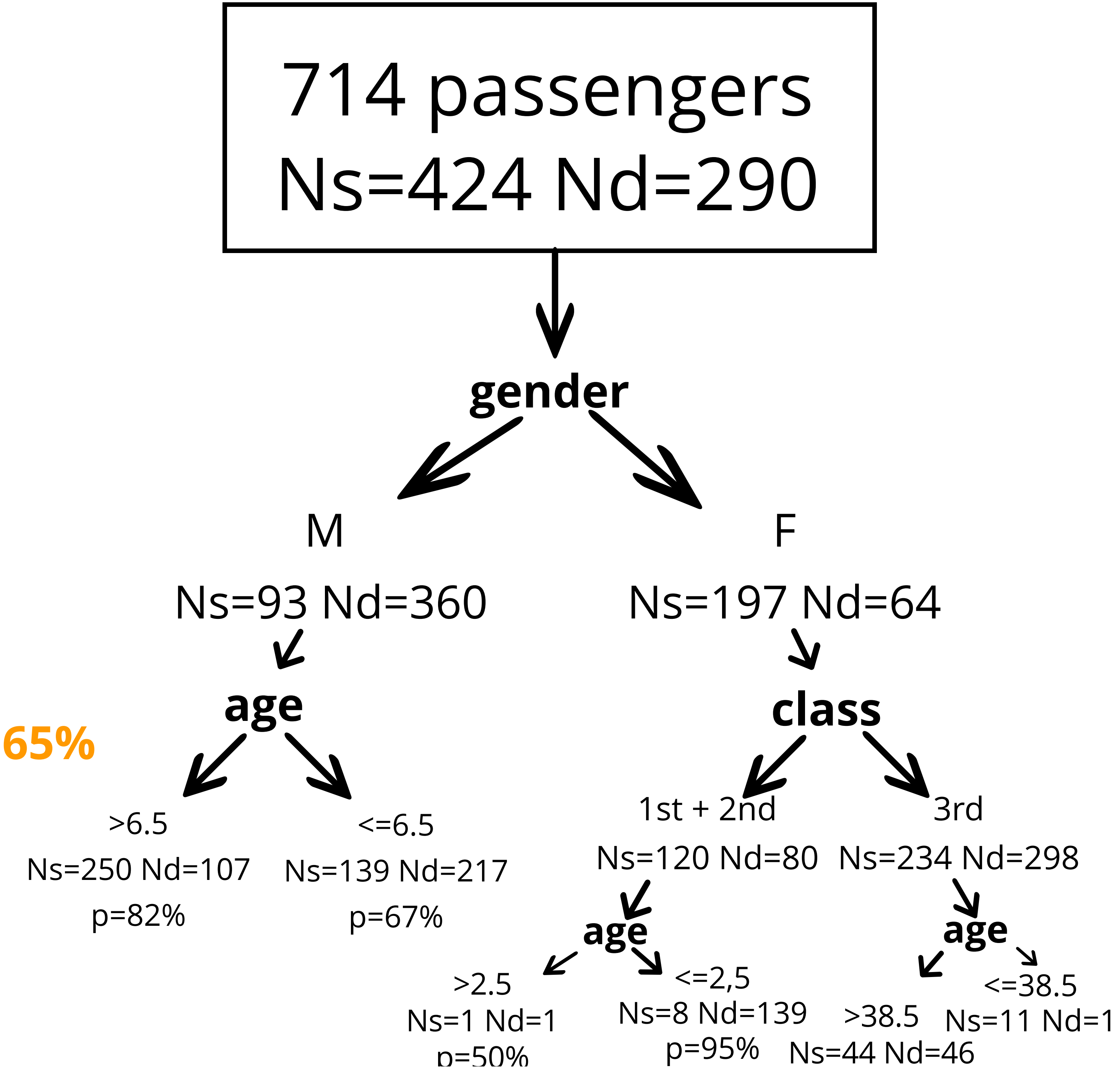


Application:

a robot to predict surviving the Titanic

(Kaggle)

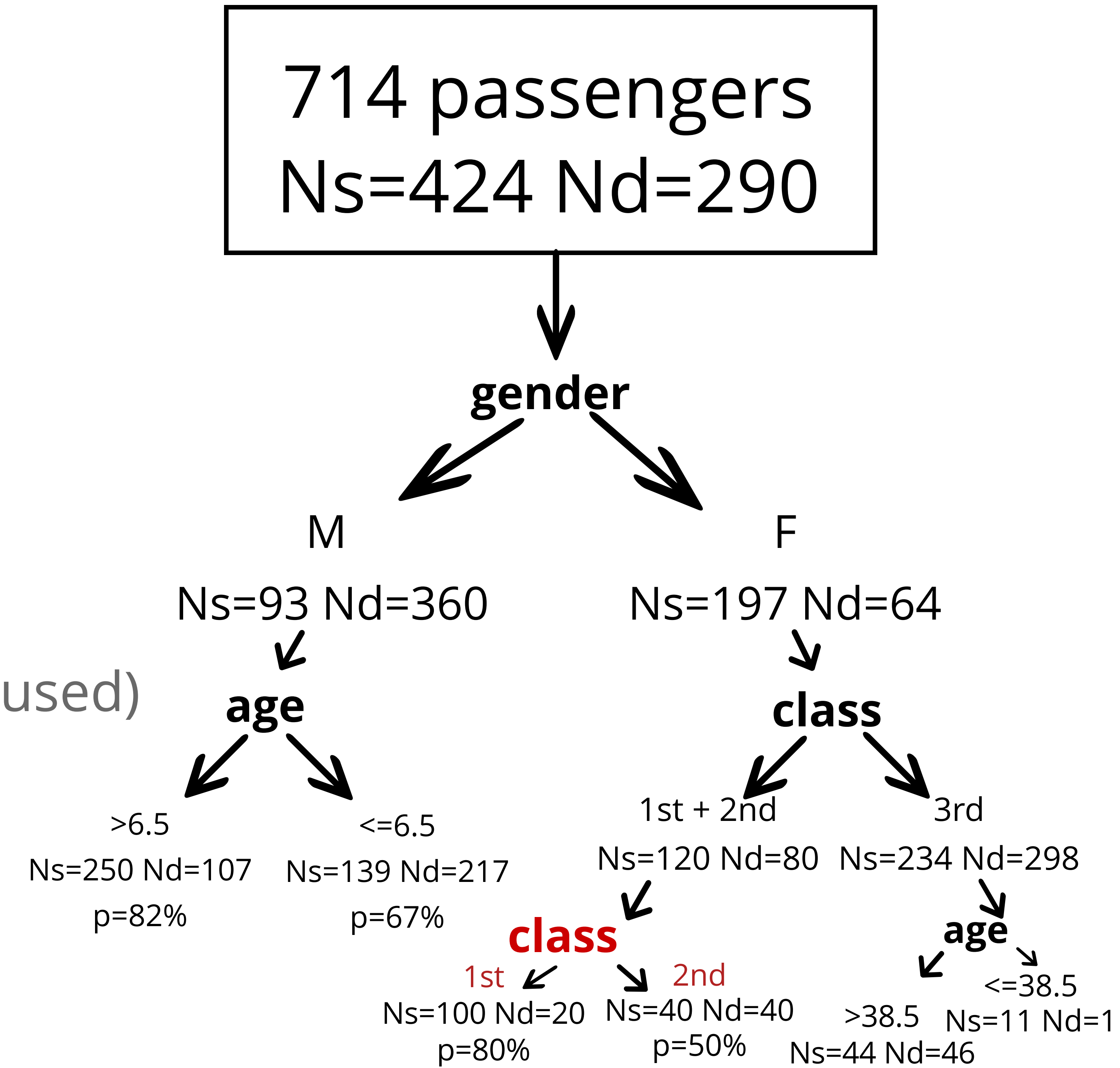
https://www.kaggle.com/c/titanic

features:

- gender (binary already used)
- ticket class (*ordinal*)
- age (continuous)

target variable:

-> survival (y/n)

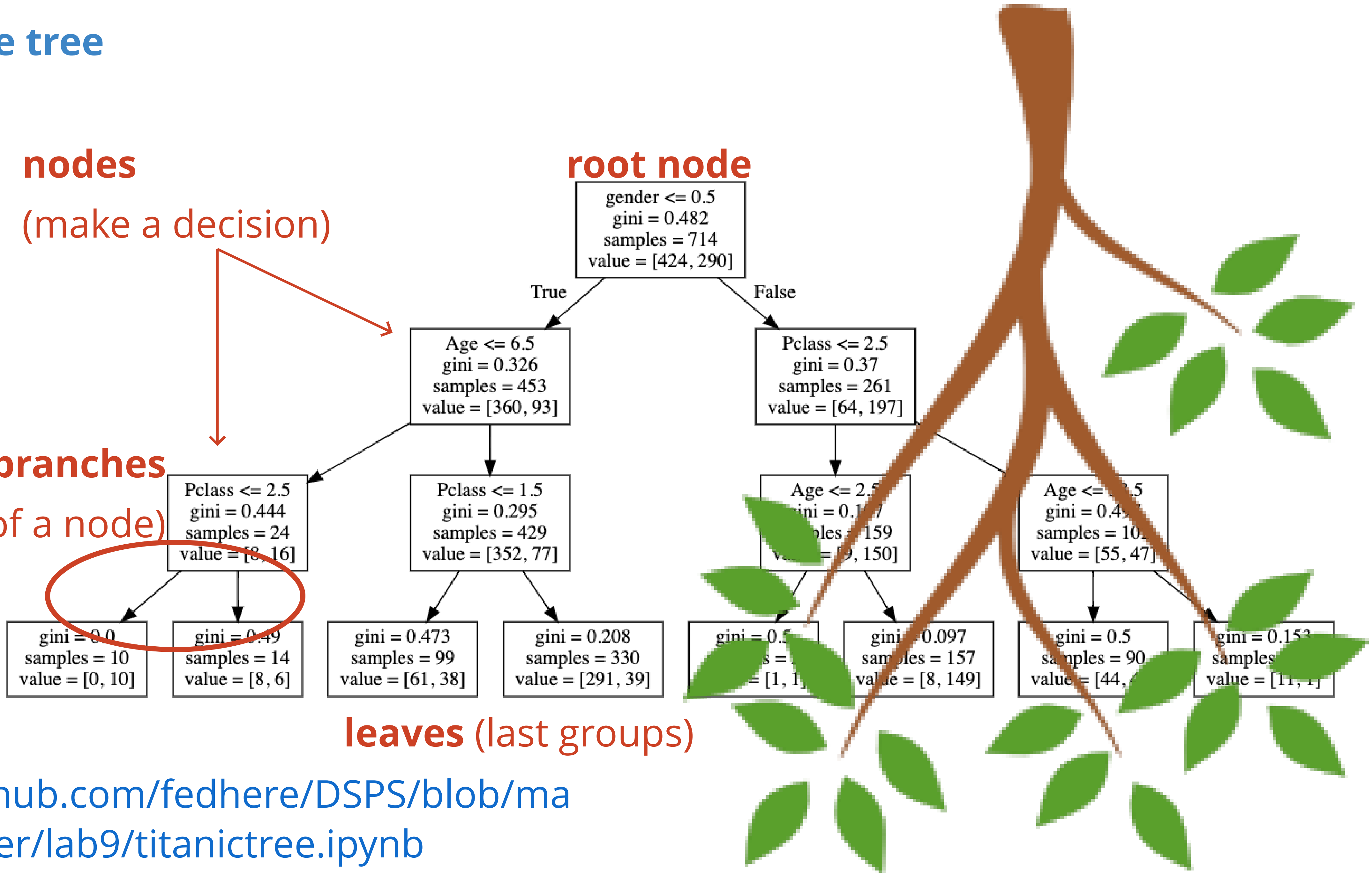


A single tree

nodes

(make a decision)

root node



branches

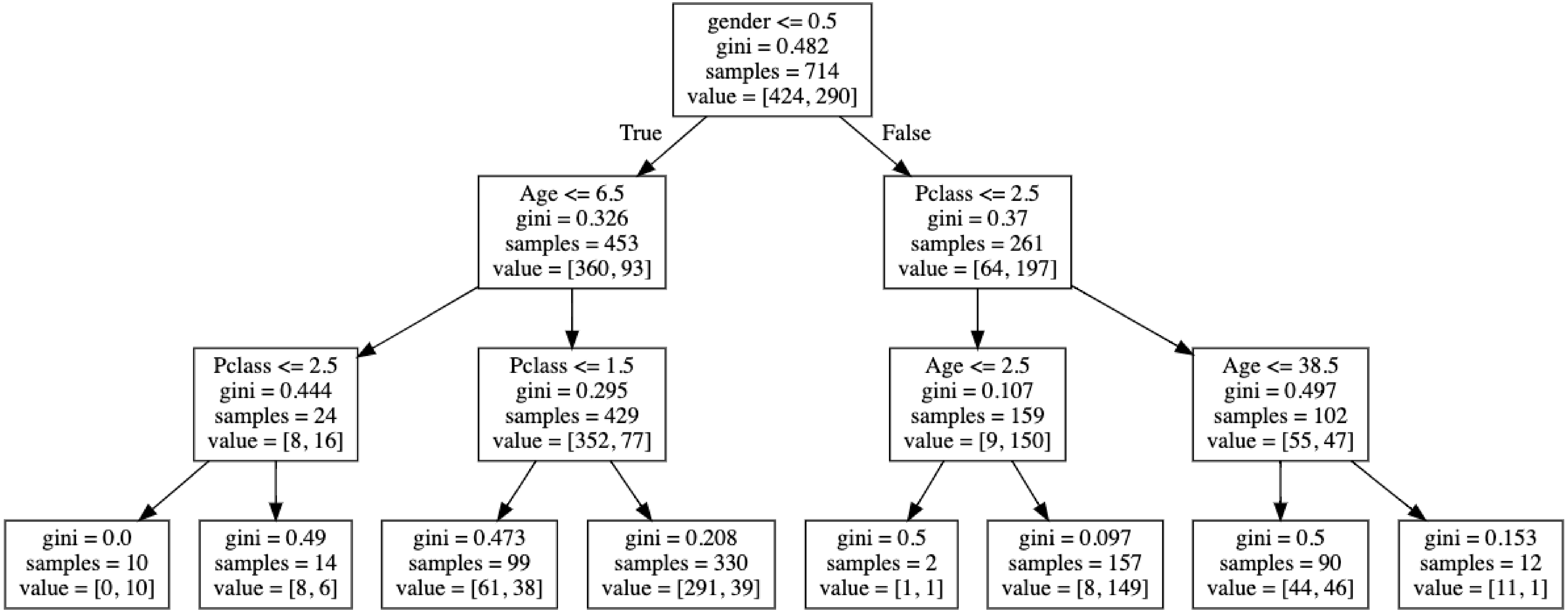
(split off of a node)

leaves (last groups)

https://github.com/fedhere/DSPS/blob/master/lab9/titanictree.ipynb

A single tree

this visualization is called a "dendrogram"



tree hyperparameters

2

tree hyperparameters

sklearn.tree.DecisionTreeClassifier ¶

class `sklearn.tree.` **`DecisionTreeClassifier`** (*criterion='gini', splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, class_weight=None, presort=False*)

[source]

A single tree: hyperparameters

criterion : ***string, optional (default=”gini”)***

The function to measure the quality of a split. Supported criteria are “gini” for the Gini impurity and “entropy” for the information gain.

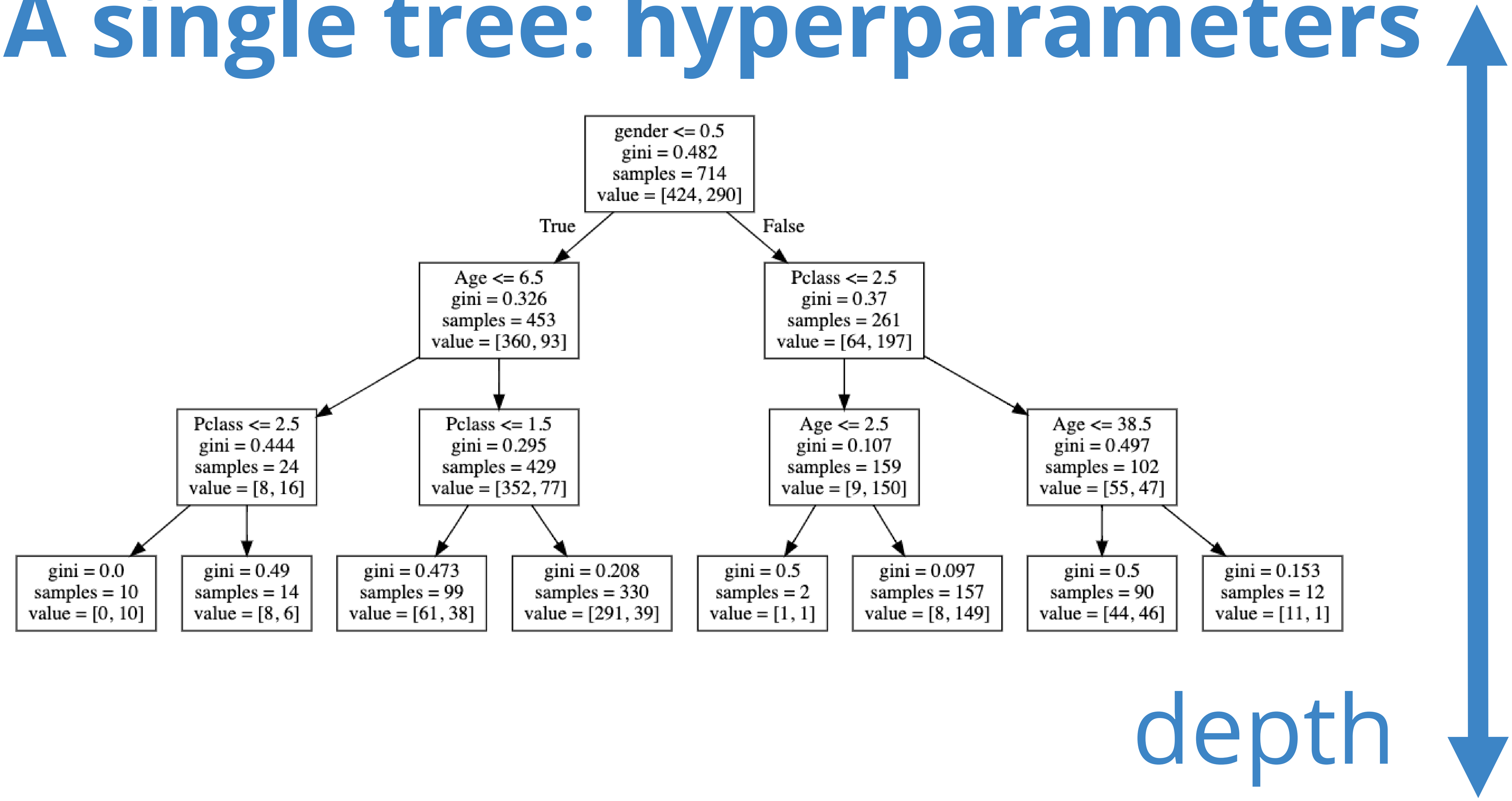
gini impurity

$$\mathrm{I}_G(p) = 1 - \sum_{i=1}^{J} {p_i}^2$$

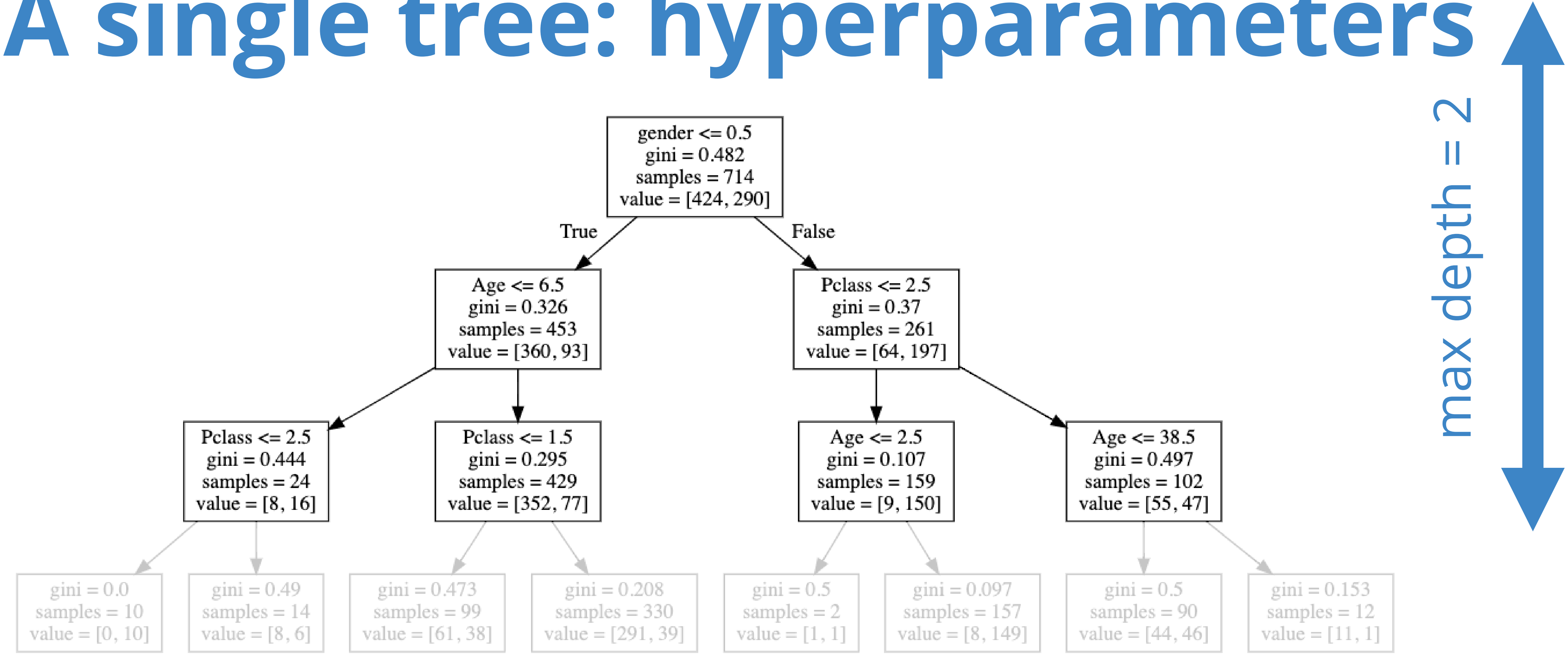
information gain (entropy)

$$\mathrm{H}(T) = - \sum_{i=1}^{J} p_i \log_2 p_i$$

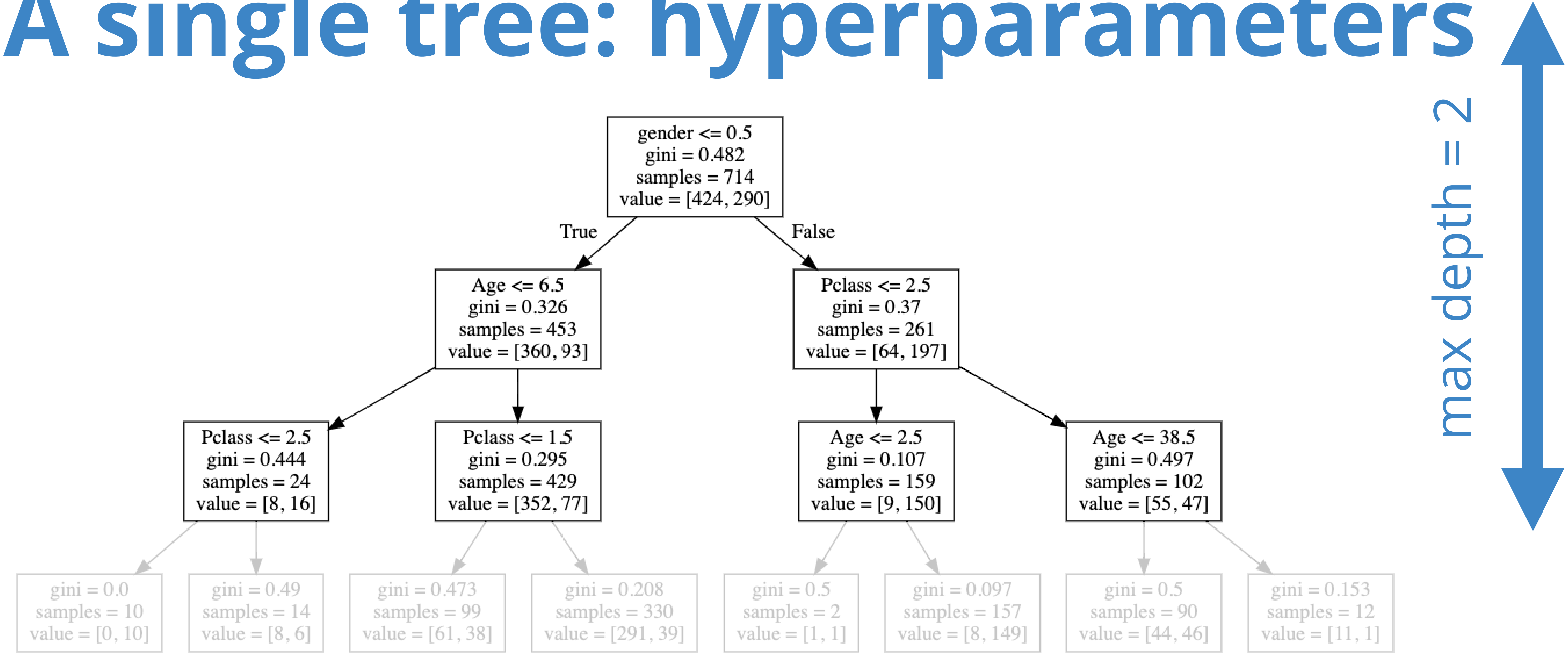
A single tree: hyperparameters



A single tree: hyperparameters

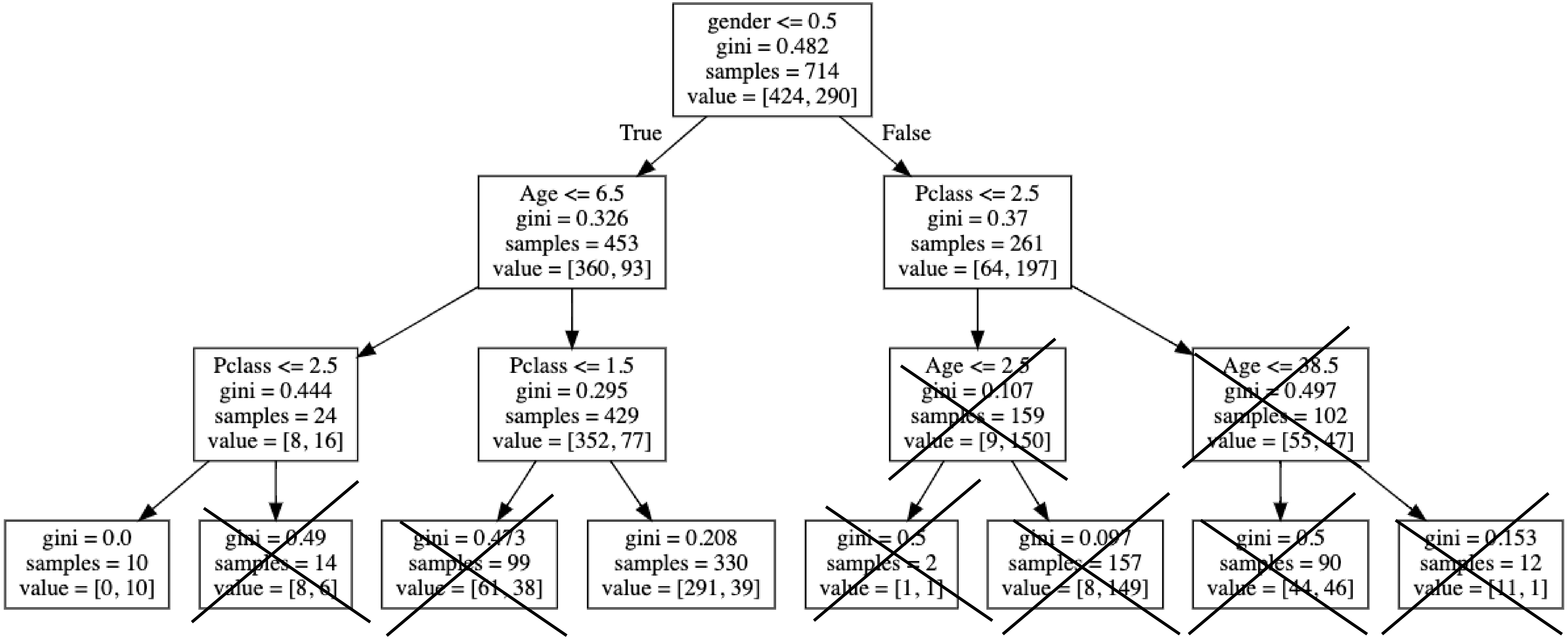


A single tree: hyperparameters



PREVENTS OVERGFITTING

A single tree: hyperparameters



alternative: tree pruning

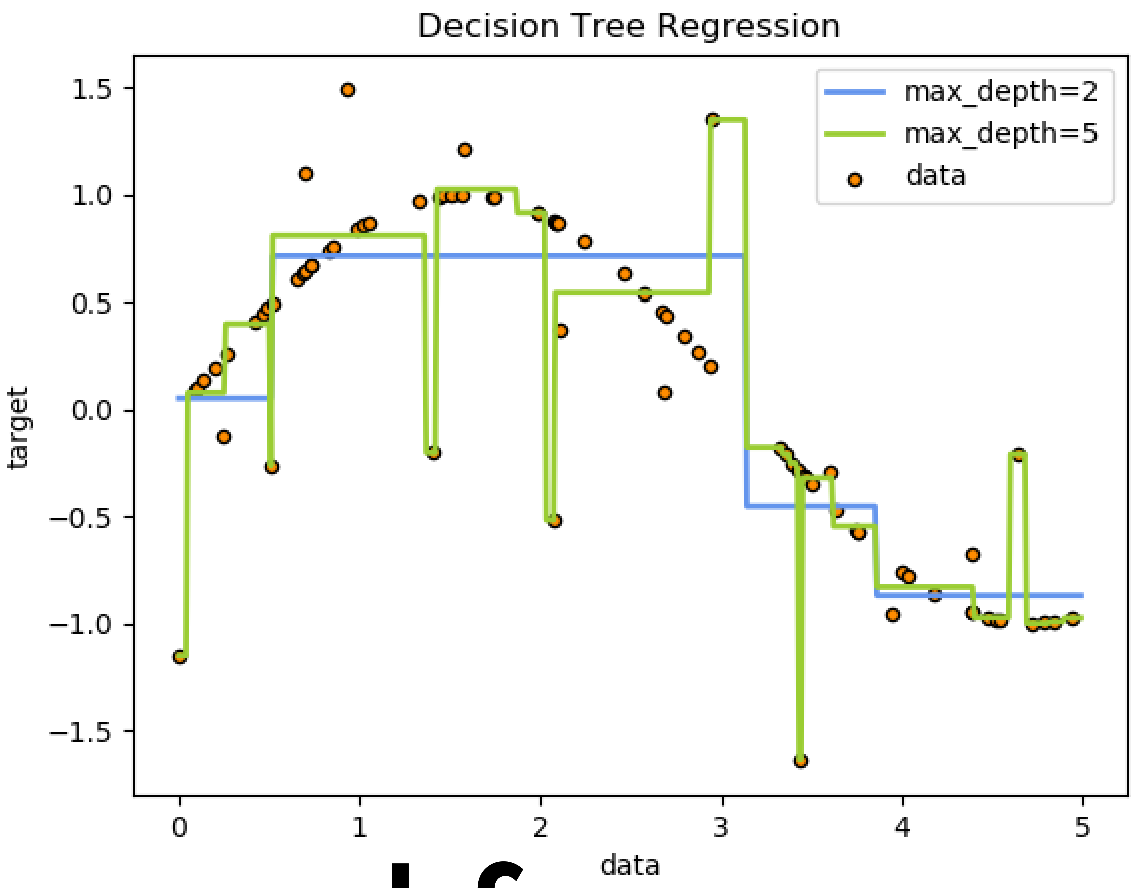
regression with trees

3

CART: Classification and Regression Trees

Trees can be used for regression

(think about it as very many small classes) https://scikit-learn.org/stable/auto_examples/tree/plot_tree_regression.html



Trees can be used for regression

(think about it as very many small classes)

sklearn.tree.DecisionTreeRegressor

class `sklearn.tree.` **`DecisionTreeRegressor`** (*criterion='mse', splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features=None, random_state=None, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, presort=False*) ¶ [source]

https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeRegressor.html

A single tree: hyperparameters

criterion : *string, optional (default="mse")*

The function to measure the quality of a split. Supported criteria are "mse" for the mean squared error, which is equal to variance reduction as feature selection criterion and minimizes the L2 loss using the mean of each terminal node, "friedman_mse", which uses mean squared error with Friedman's improvement score for potential splits, and "mae" for the mean absolute error, which minimizes the L1 loss using the median of each terminal node.

mean square error

$$L_2 = (y_{true} - y_{predicted})^2$$

mean absolute error

$$L_1 = |y_{true} - y_{predicted}|$$

issues with trees

4

issues with trees

variance:

different trees lead to different results

issues with trees

variance:

different trees lead to different results

why?

because calculating the criterion for every split and every mote is an untractable problem!

e.g. 2 coutinuous variables would be a problem of order ∞^2

issues with trees

variance:

different trees lead to different results

solution

run many trees and take an "ensamble" decision!

Random Forests

a bunch of parallel trees

Gradient Boosted Trees

a series of trees

5

ensemble methods

ensemble methods

run multiple versions of the same model with some small (stochastic or progressive) variation and learn from the emsemble of methods

tree ensemble methods

Random forest:

trees run in parallel (independently of each other)

each tree uses a random subset of observations/features (boostrap - bagging)

class predicted by majority vote:

what class do most trees think a point belong to

Gradient boosted trees:

trees run in series (one after the other)

each tree uses different *weights* for the features learning the weighs from the previous tree

the last tree has the prediction

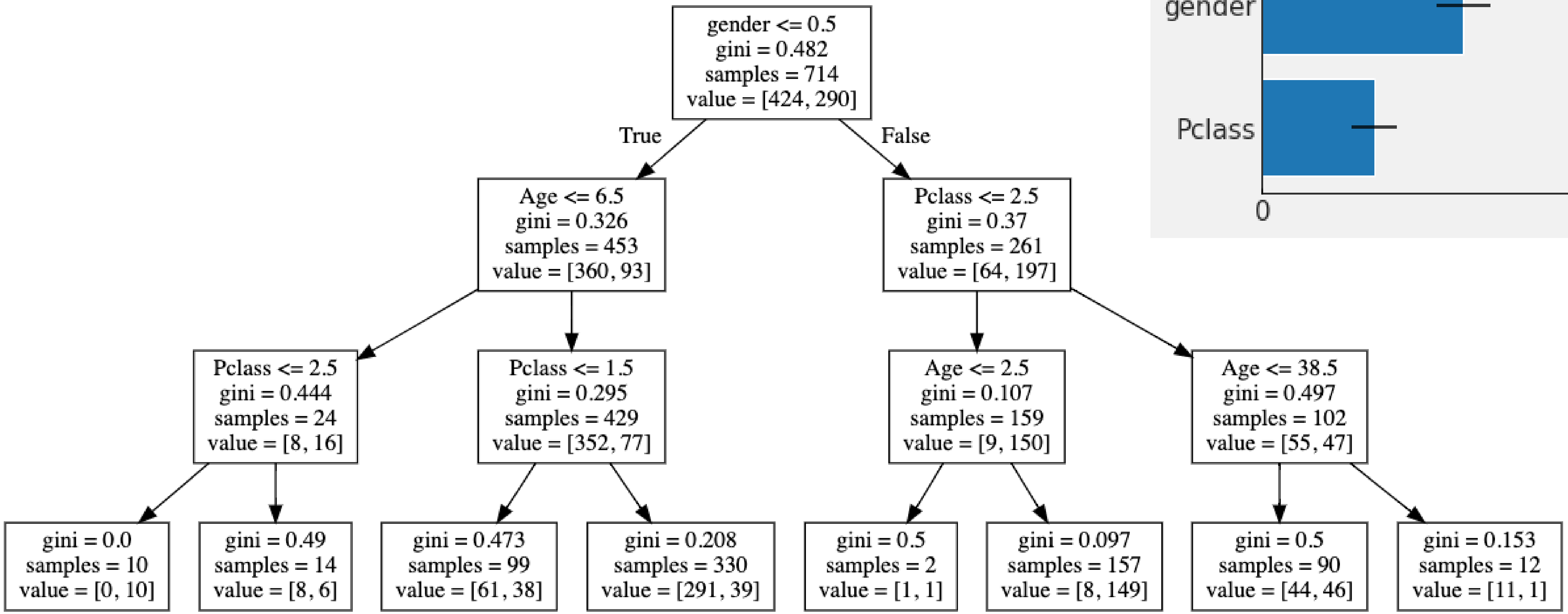
feature importance

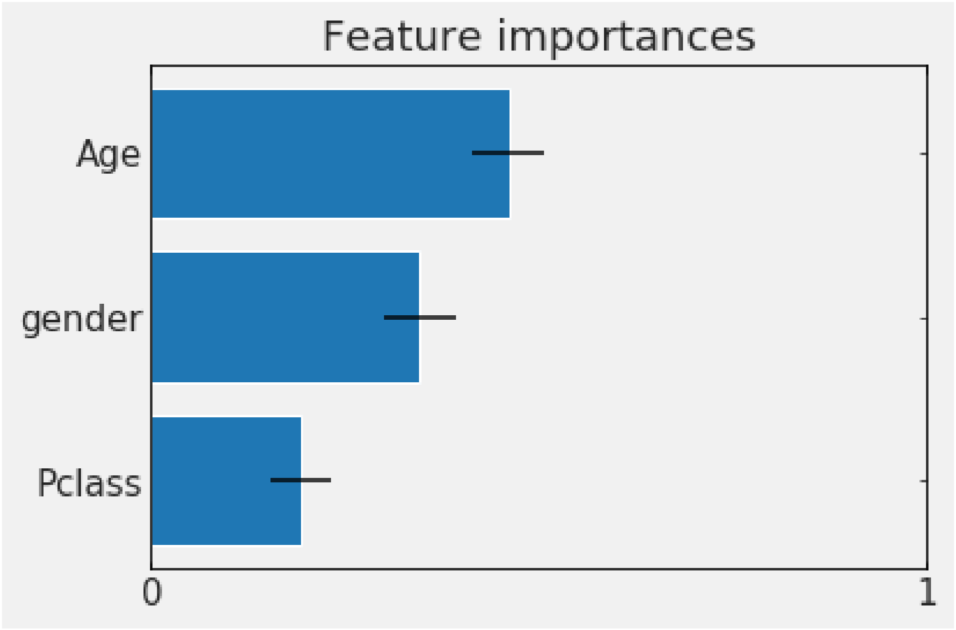
6

feature importance

In principle CART methods are interpretable

you can measure the influence that each
feature has on the decision : feature importance





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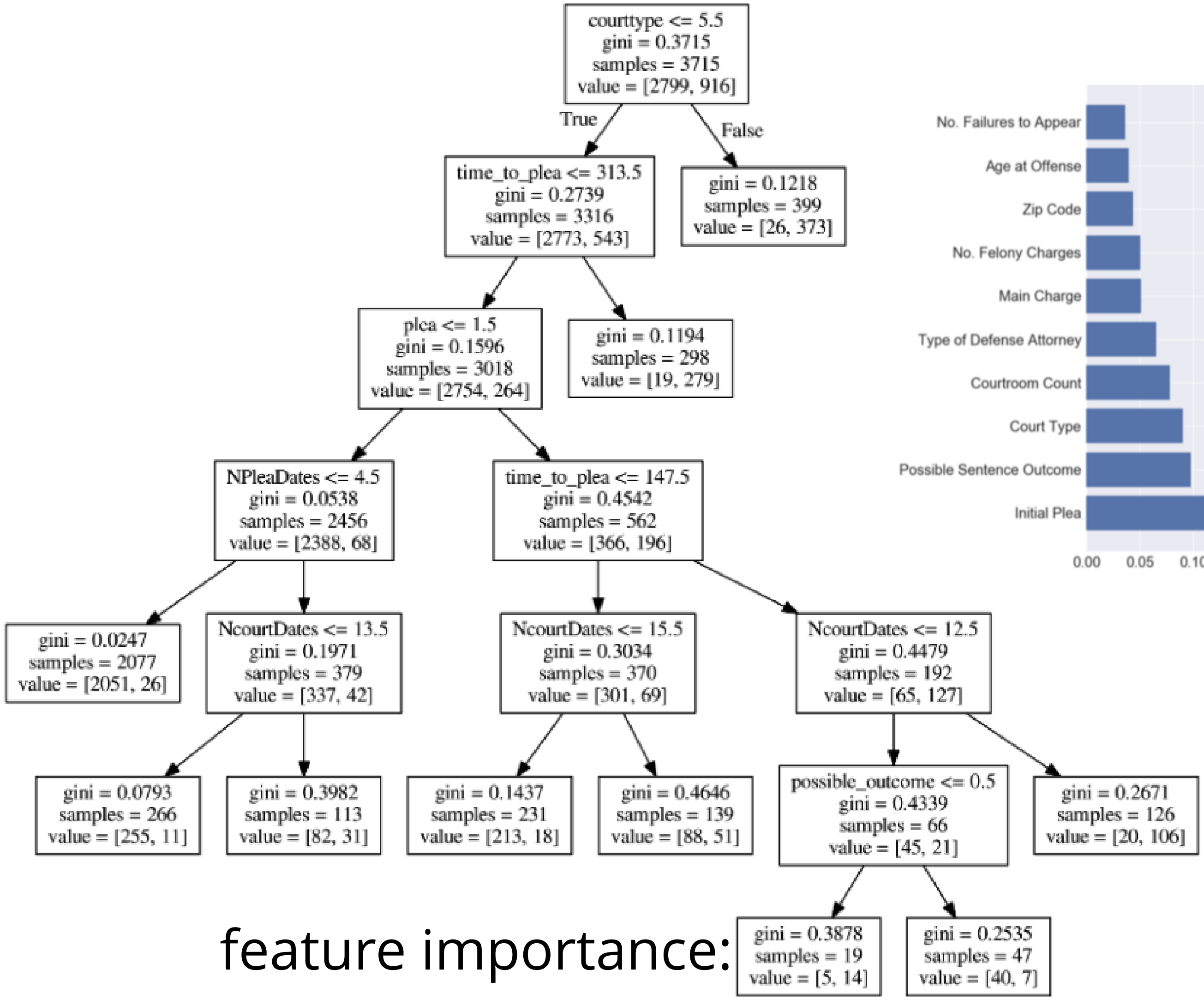

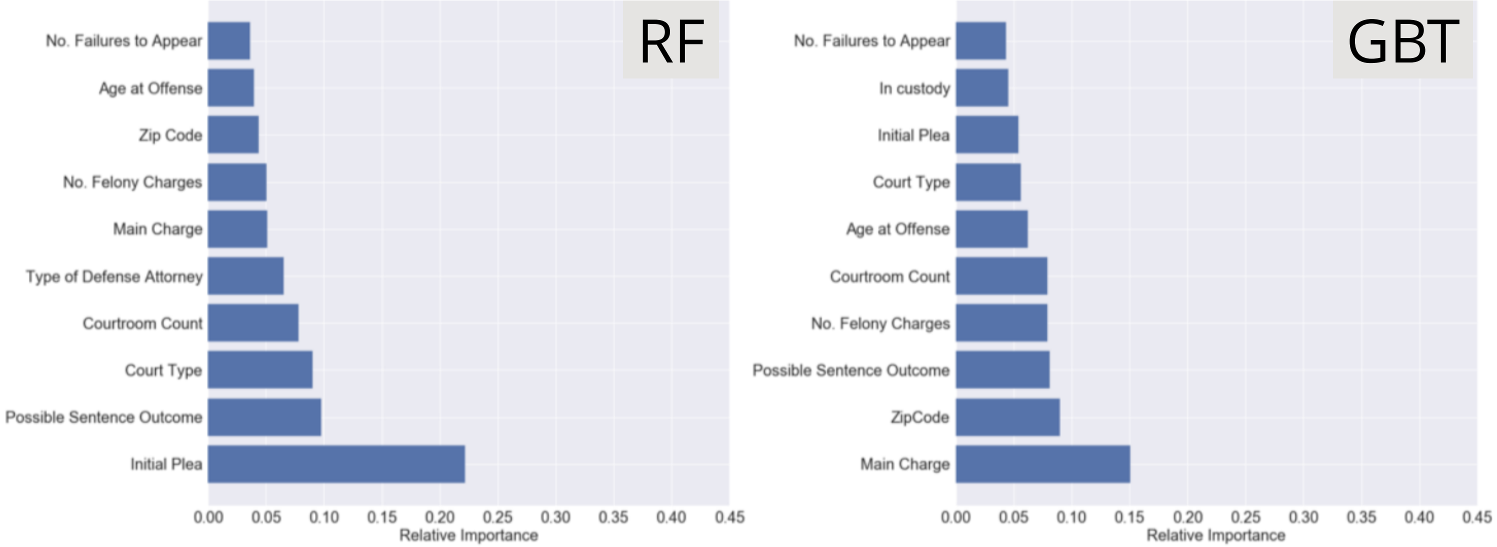

feature importance:

how soon was a feature chosen,

how many times was it used...

https://explained.ai/rf-importance/

A Data-Driven Evaluation of Delays in Criminal Prosecution

https://doi.org/10.22541/au.155535549.97131926

feature importance

In principle CART methods are interpretable

you can measure the influence that each
feature has on the decision : feature importance

In practice the interpretation is complicated by covariance of features

7

encoding categorical variables

Categorical Variable

variable that can take a finite number of values.

spicies	age	weight
dog	7	32.3
bird	1	0.3
cat	3	8.1

Categorical Variable

variable that can take a finite number of values.

spicies	age	weight
dog	7	32.3
bird	1	0.3
cat	3	8.1

continuous

Categorical Variable

variable that can take a finite number of values.

ordinal

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numerical encoding

change categorical to (integer) numerical

spicies	**age**	**weight**
1	7	32.3
2	1	0.3
3	3	8.1

one-hot encoding

change each category to a binary

cat	**bird**	**dog**	**age**	**weight**
0	0	1	7	32.3
0	1	0	1	0.3
1	0	0	3	8.1

numerical encoding

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implies an order that does not exist

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ignores covariance between features

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implies an order that does not exist

one-hot encoding

Definitely

change each category to a binary

Preferred!

cat	**bird**	**dog**	**age**	**weight**
0	0	1	7	32.3
0	1	0	1	0.3
1	0	0	3	8.1

ignores covariance between features

problematic if you are interested in feature importance

numerical encoding one-hot encoding

https://github.com/fedhere/DSPS/blob/master/lab9/LocationLocationLocation.ipynb

ML model performance

8

ML model performance

Accuracy, Recall, Precision

$$LR = \frac{\text{False Negative}}{\text{True Negative}}$$

	H0 is True	**H0 is False**
H0 is falsified	Type I Error False Positive	True Positive
H0 is not falsified	True Negative	Type II Error False Negative

ML model performance

Accuracy, Recall, Precision

$$LR = \frac{\text{False Negative}}{\text{True Negative}}$$

	H0 is True	**H0 is False**
H0 is falsified	**important message spammed**	True Positive
H0 is not falsified	True Negative	**spam in your inbox**

ML model performance

Accuracy, Recall, Precision

$$\textbf{Precision} = \frac{TP}{TP + FP}$$

$$\textbf{Recall} = \frac{TP}{TP + FN}$$

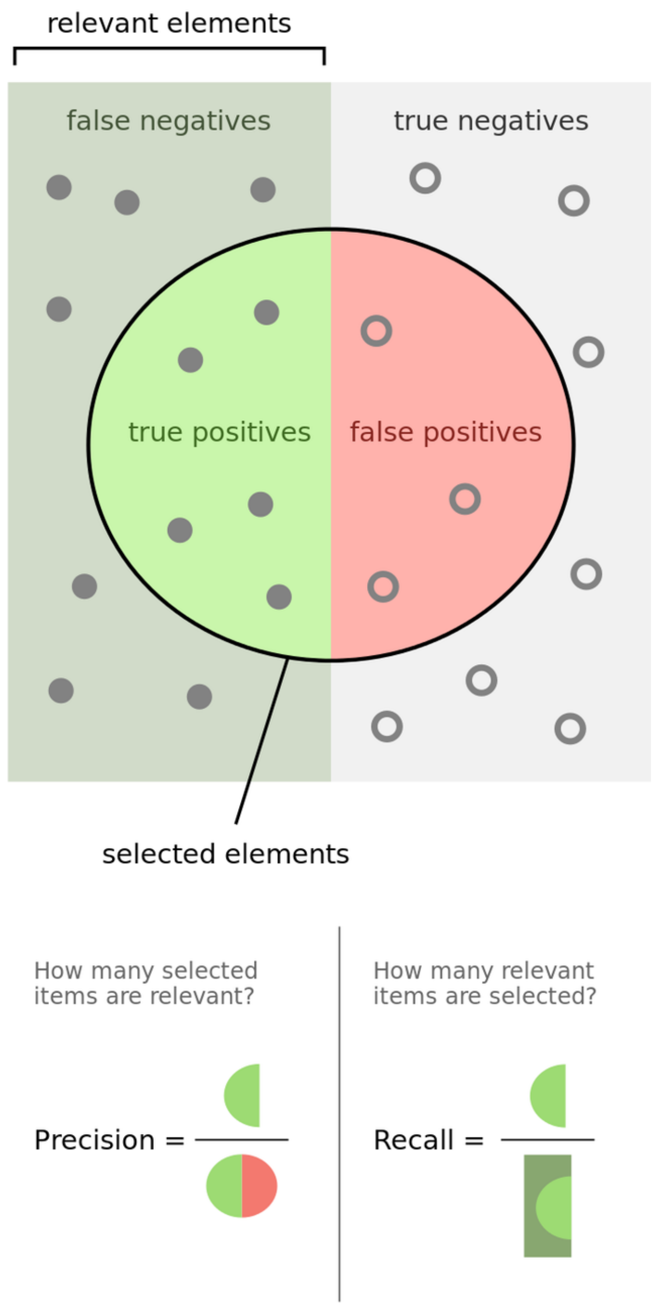
$$\textbf{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

TP=True Positive

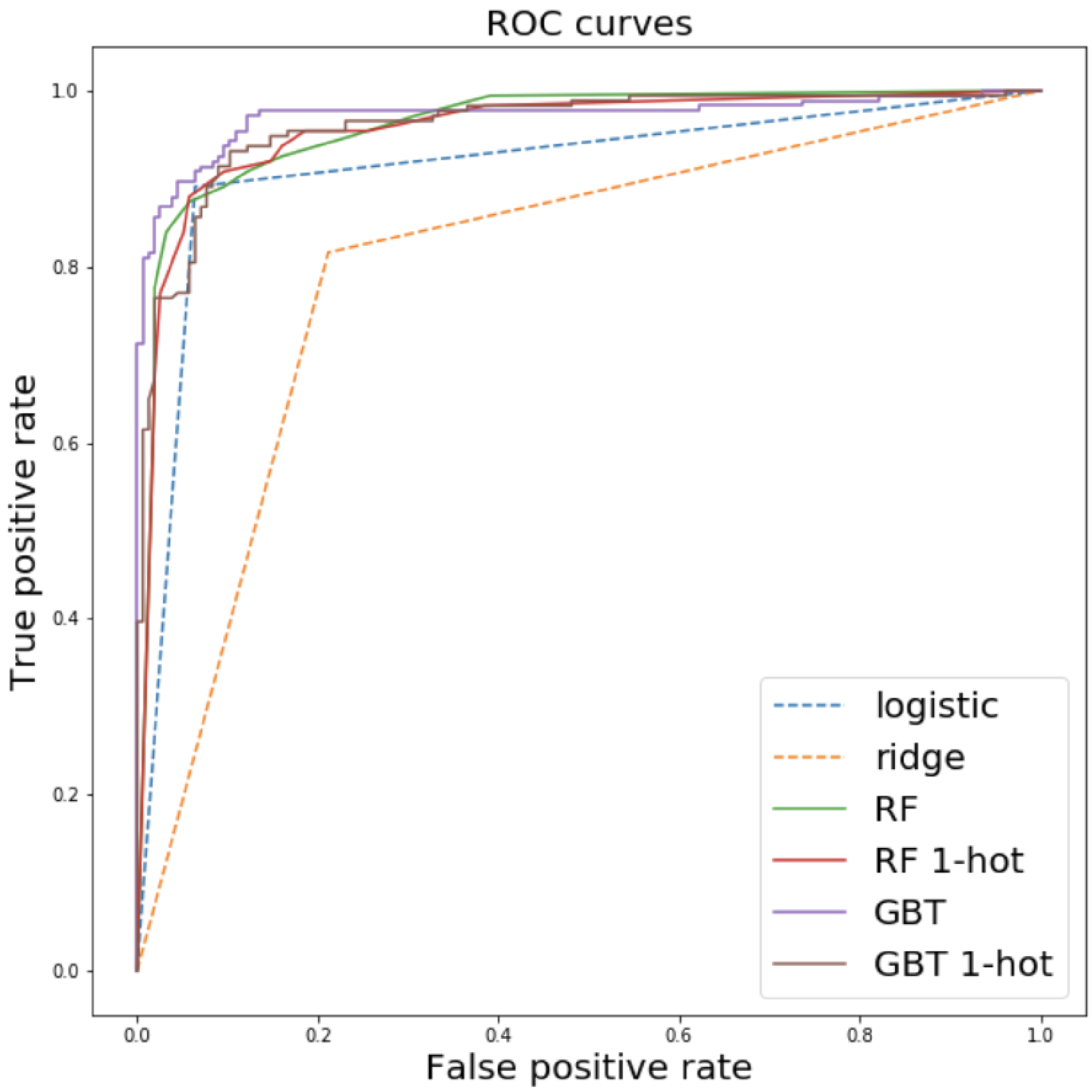
FP=False Positive

TN=True Negative

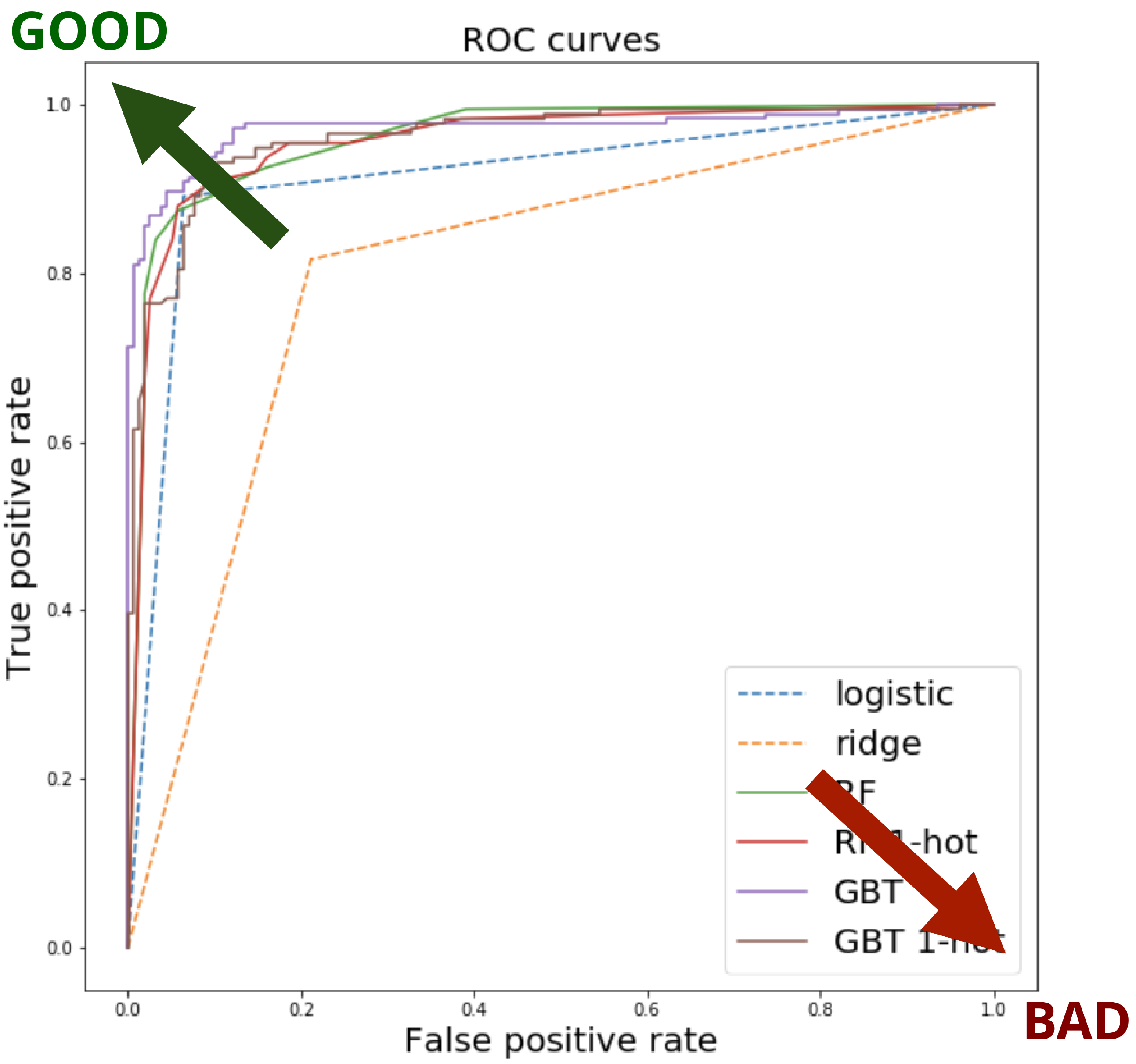
FN=False Positive



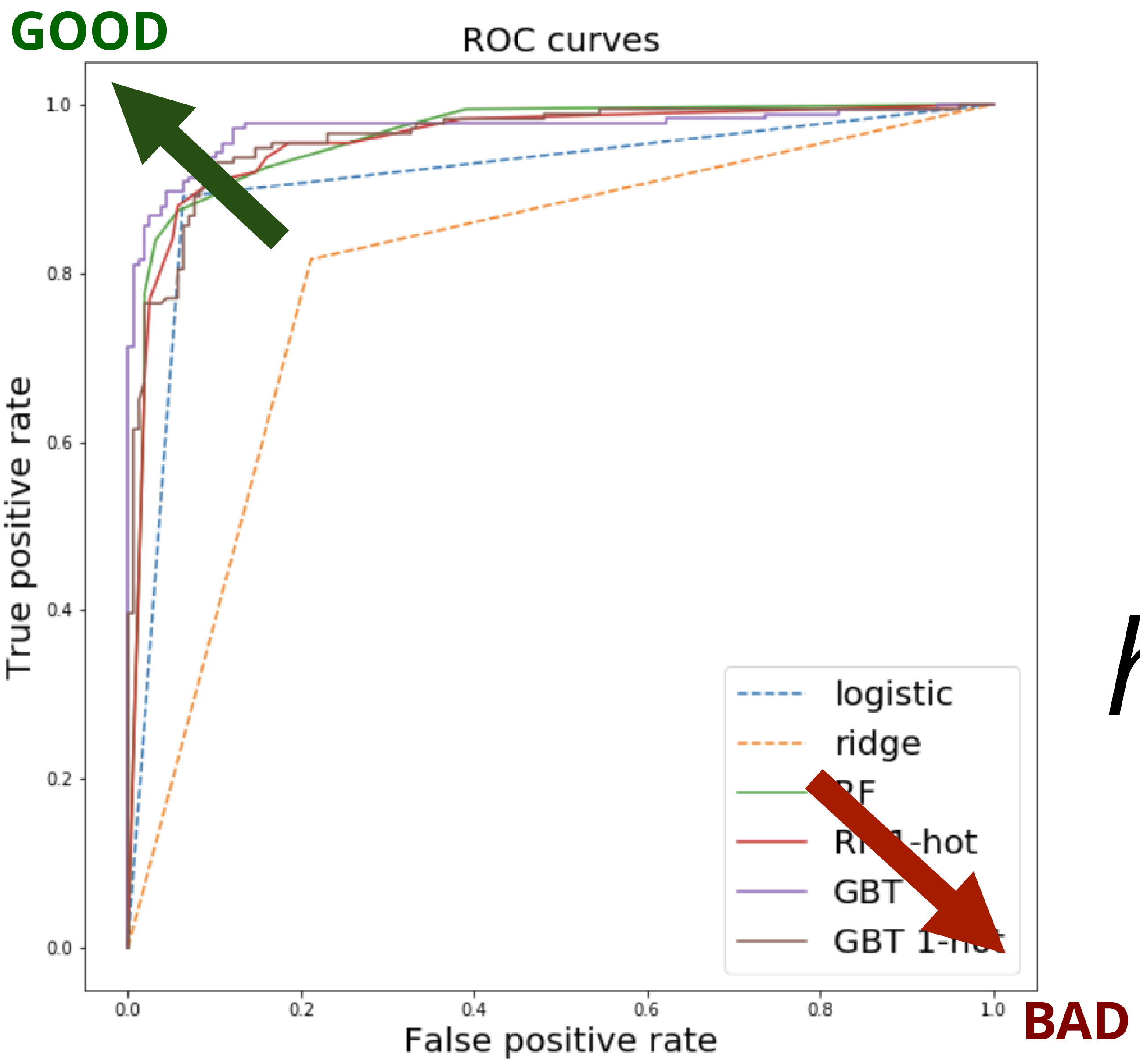
https://en.wikipedia.org/wiki/Precision_and_recall



Receiver operating characteristic



Receiver operating characteristic



tuning by changing *hyperparameters*

Receiver operating characteristic

Machine Learning includes models that learn parameters from data

ML models have parameters learned from the data and **hyperparameters** assigned by the user.

Unsupervised learning:

- all variables observed for all data points
- learns the structure of the features space from the data
- predicts a label (group of belonging) based on similarity of all features

Supervised learning:

- a target feature is observed only for a subset of the data
- learns target feature for data where it is not observed based on similarity of the other features
- predicts a class/value for each datum without observed label

Tree methods:

- partition the space one feature at a time with binary choices
- prone to overfitting
- can be used for regression

key concepts

single trees have high variance as the optimization has to be local

ensemble methods solve variance issue by running multiple trees and making an ensemble decision

random forest: trees run in parallel with a random subset of features and the decision scheme is "majority" decision

gradient boosted trees: trees run in series with feature weighted learning the weights from the outcome of the previous tree. The last tree has the division

feature importance: the importance of each feature can be extracted. In presence of covariance the feature importance may be hard to interpret

encoding categorical variables:

variables have to be encoded as numbers for computers to understand them. You can encode categorical variables with integers or floating point but you implicitly impart an order. The standard is to ***one-hot-encode*** which means creating a binary (True/False) feature (column) for each category of a categorical variables but this *increases the feature space and generated covariance.*

model diagnostics for classifiers: Fraction of True Positives and False Positives are the metrics to evaluate classifiers. Combinations of those numbers include Accuracy (TP/ (TP+FP)), Precision (TP/(TP+FN)), Recall ((TP+TN)/(TP+TN+FP+FN)).

ROC curve: (TP vs FP) is a holistic metric of a model. It can be used to guide the choice of hyperparameters to find the "sweet spot" for your problem http://what-when-how.com/artificial-intelligence/decision-tree-applications-for-data-modelling-artificial-intelligence/

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4466856/

resources

actually a video: watching not reading (~1 hour)

https://www.youtube.com/watch?v=Trar7GZOPl8&feature=youtu.be&utm_medium=email&utm_source=intercom&utm_campaign=modular-code-event

reading

Higgs Boson Search

- Download the Higgs boson data from Kaggle (programmatically within the notebook)
- Split the provided training data into a training and a test set. For each model calculate and discuss the training and test score results.
- Use a Random Forest and a Gradiend Boosted Tree *Classifier model* to predict the label of the particles.
- Produce a confusion matrix for each model and compare them
- Use a Random Forest and a Gradiend Boosted Tree *Regressor model* to predict the weight of the particles.
- Calculate the L1 and L2 metrics of each model and compare them.
- For the Random Forest classifier, explore the parameter space with the sklearn module sklearn.model_selection.RandomizedSearchCV
- Generate an ROC curve plot and discuss it
- EC and 667
    - ---- Download the script provided in the kaggle challenge to validate your model.
    - ---- Generate an output file as required by this script for your best model
    - ---- Report on the result

Higgs Boson Search

- Work on this alone

You will recieve an email with 2 names and github handles of classmates. Review their plots according to the things we discussed last lecture. You can discuss your review with others but each of you should submit a review for each of the plots

There will be detailed instructions in the email on how to review, what structure the review should have, what to focus on, etc. Please comply to the instructions. Upload the review on your github DSPS HW9 repo AND ALSO in your classmate's HW8 repo, forking and submitting a pull request, NOT JUST your fork of their repo! Please note the numbers: I will grade what is in your HW9 repo and check that it is also in your classmate HW8 repo.

Each review will be reviewed and graded by me. (Please take this homework seriously: one sentence generic reviews will be graded 0)