Machine Learning for econometrics

Flexible models for tabular data

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February 18th, 2025

Reminder from previous session

- Statistical learning 101: bias-variance trade-off
- Regularization for linear models: Lasso, Ridge, Elastic Net
- Transformation of variables: polynomial regression
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Reminder from previous session

- Statistical learning 101: bias-variance trade-off
- Regularization for linear models: Lasso, Ridge, Elastic Net
- Transformation of variables: polynomial regression
- 🤔 But… How to select the best model? the best hyper-parameters?

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Model evaluation and selection with cross-validation

Example with the Wage dataset

- Raw dataset: (N=534, p=11)

EDUCATION	SOUTH	SEX	EXPERIENCE	UNION	WAGE	AGE	RACE	OCCUPATION	SECTOR	MARR
8	no	female	21	not_member	5.10	35	Hispanic	Other	Manufacturing	Married
9	no	female	42	not_member	4.95	57	White	Other	Manufacturing	Married
12	no	male	1	not_member	6.67	19	White	Other	Manufacturing	Unmarried
12	no	male	4	not_member	4.00	22	White	Other	Other	Unmarried
12	no	male	17	not_member	7.50	35	White	Other	Other	Married

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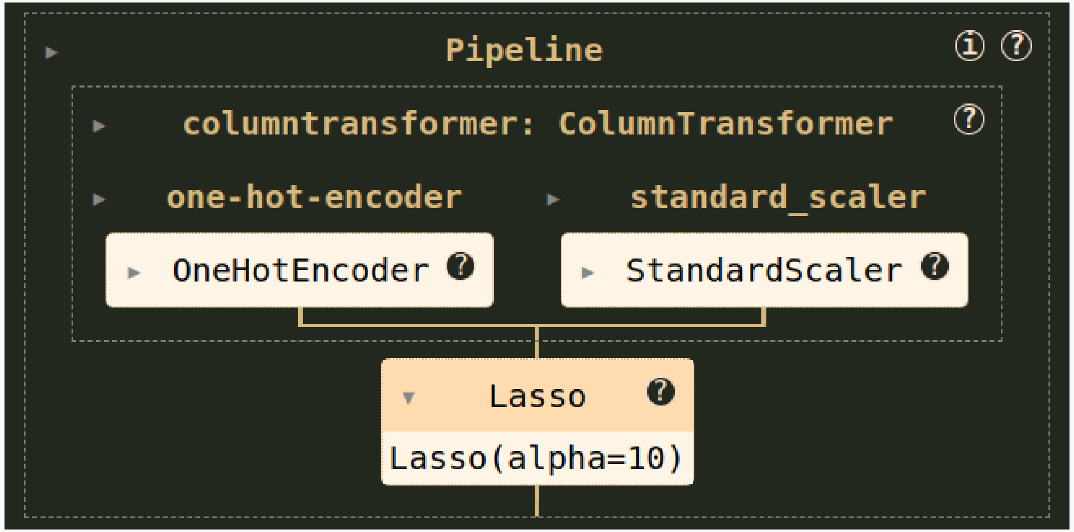
Example with the Wage dataset

- Raw dataset: (N=534, p=11)
- Transformation: encoding categorical data, scaling numerical data: (N=534, p=23)

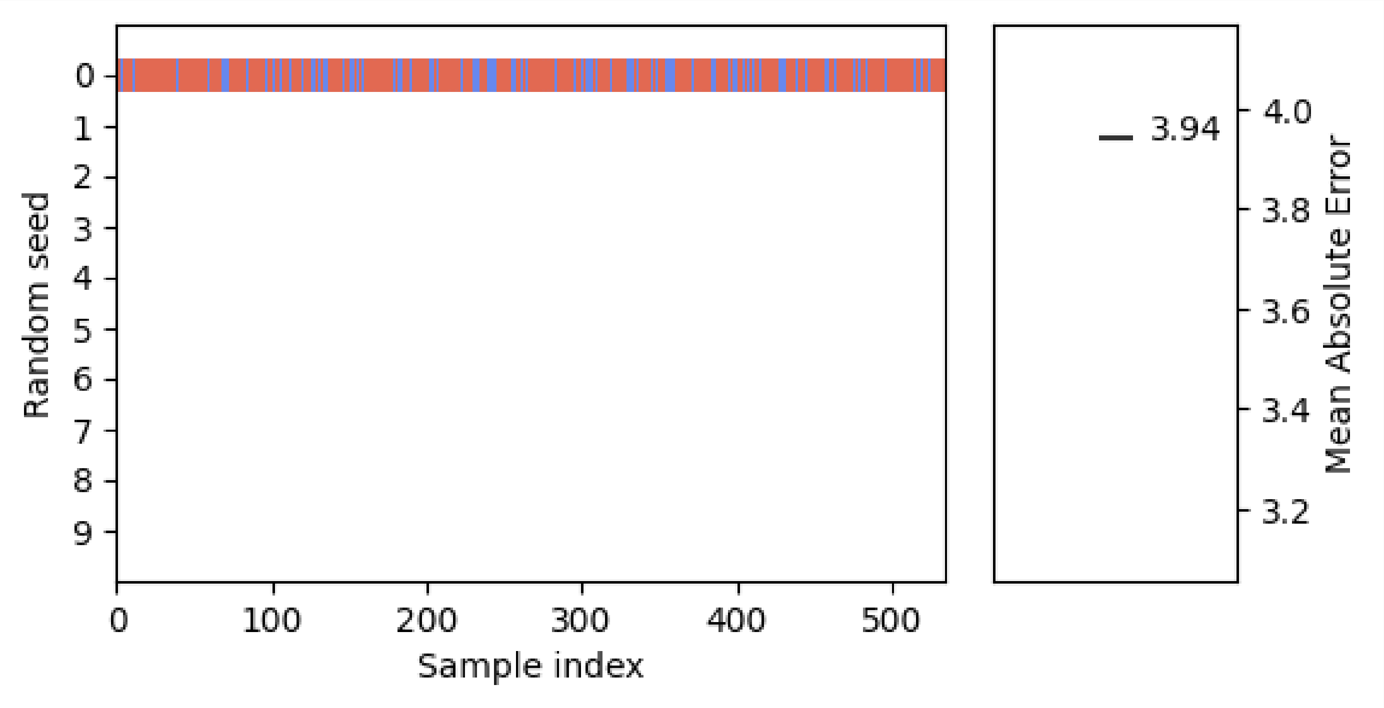
one-hot-encoder__SOUTH_no	one-hot-encoder__SOUTH_yes	one-hot-encoder__SEX_female	one-hot-encoder__SEX_male	one-hot-encoder__UNION_member	encoder__UNION_not
1.0	0.0	1.0	0.0	0.0	
1.0	0.0	1.0	0.0	0.0	
1.0	0.0	0.0	1.0	0.0	
1.0	0.0	0.0	1.0	0.0	
1.0	0.0	0.0	1.0	0.0	

Example with the Wage dataset

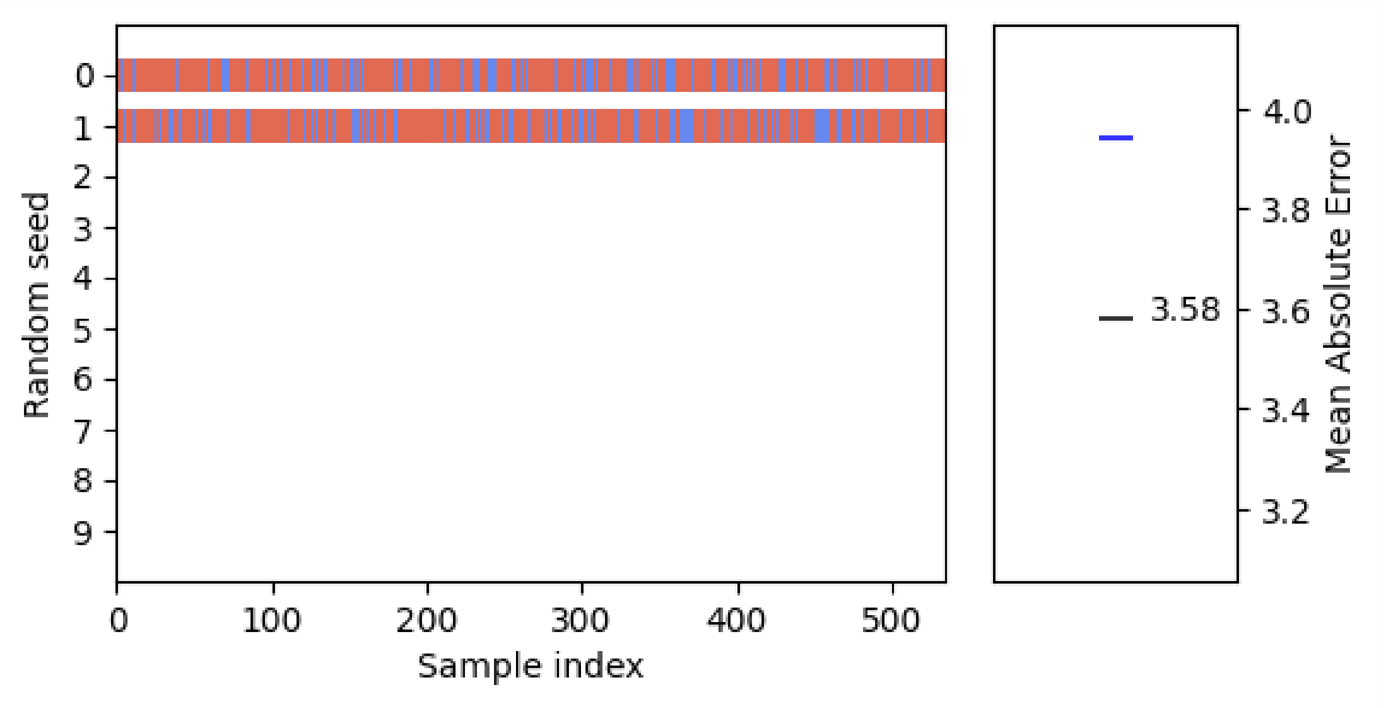
- Raw dataset: (N=534, p=11)
- Transformation: encoding categorical data, scaling numerical data: (N=534, p=23)
- Regressor: Lasso with regularization parameter ($\alpha = 10$)



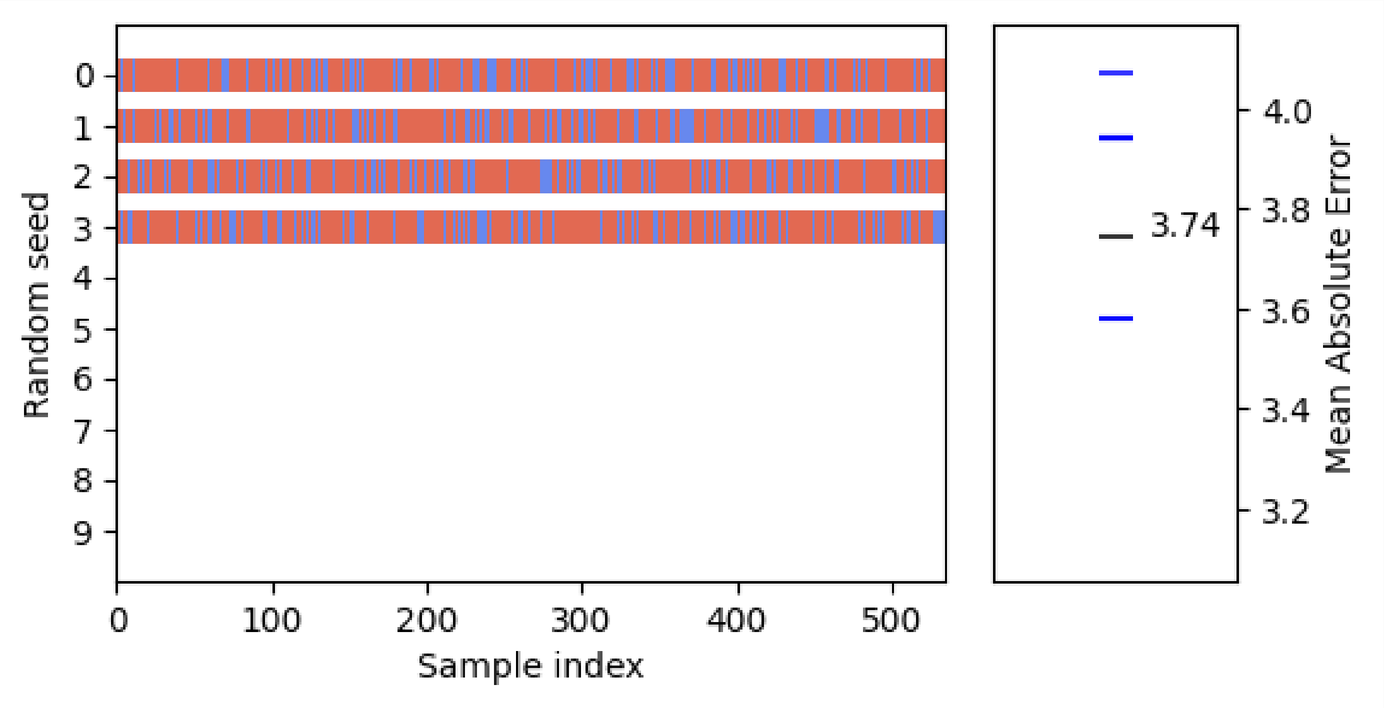
Splitting once: In red, the training set, in blue, the test set



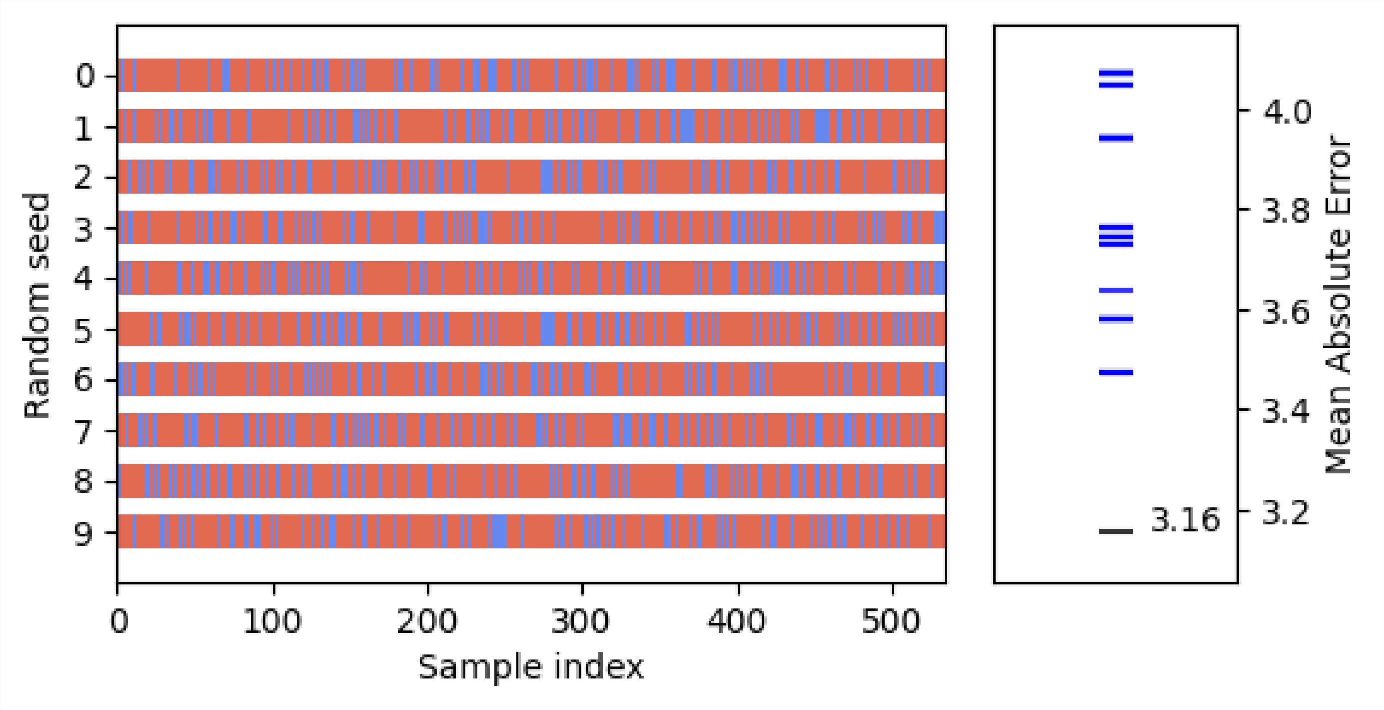
But we could have chosen another split ! Yielding a different MAE



And another split...



Splitting ten times



🎉 **Distribution of MAE:** 3.71 ± 0.26

Cross-validation

- In sklearn, it can be instantiated with `cross_validate`.

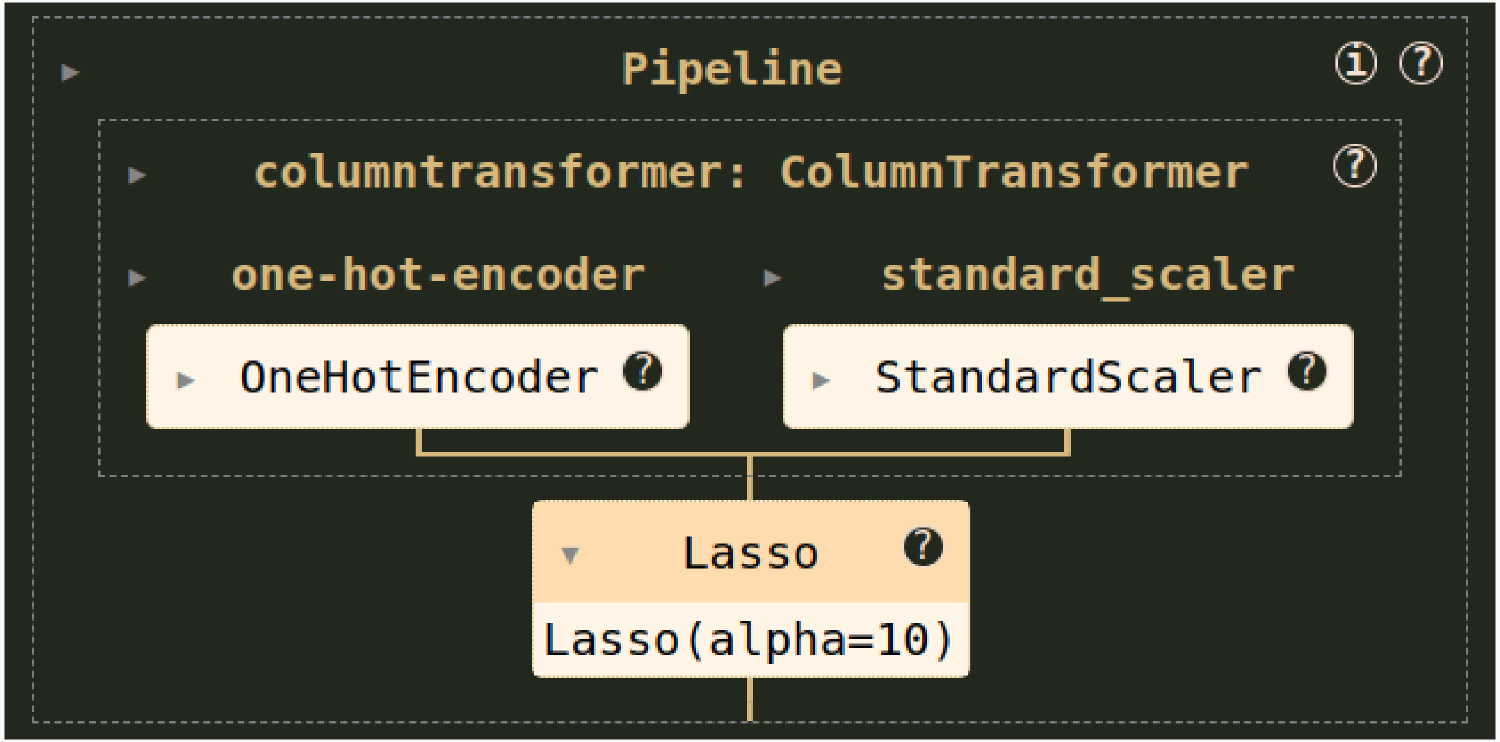
```python
from sklearn.model_selection import cross_validate
from sklearn.model_selection import ShuffleSplit

cv = ShuffleSplit(n_splits=40, test_size=0.3, random_state=0)
cv_results = cross_validate(
    regressor, data, target, cv=cv, scoring="neg_mean_absolute_error"
)
```

Cross-validation

- In sklearn, it can be instantiated with `cross_validate`.
- 🙂 Robustly estimate generalization performance
- 🤩 Estimate variability of the performance: similar to bootstrapping (but different).
- 🚀 Let's use it to select the best models among several canditates!
- Proof that it selects the best model (averaging on the folds): (Lecué & Mitchell, 2012)

Cross-validation for model selection: choose best α for lasso

- Wage pipeline



Cross-validation for model selection: choose best α for lasso

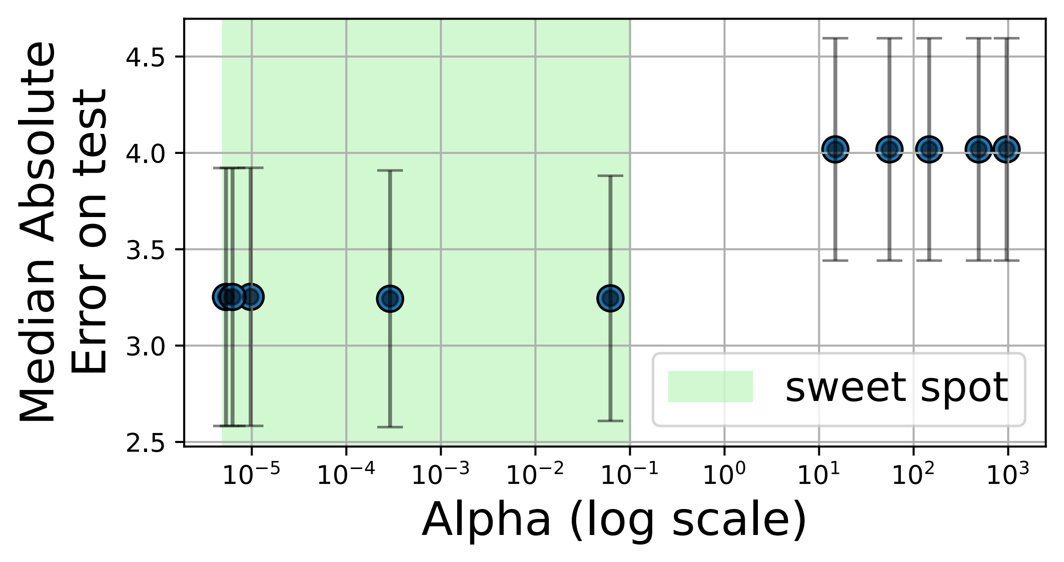
- Wage pipeline
- Random search over a distribution of α values

Python

```
param_distributions = {"lasso__alpha": loguniform(1e-6, 1e3)}
model_random_search = RandomizedSearchCV(
    pipeline,
    param_distributions=param_distributions,
    n_iter=10, # number of hyper-parameters sampled
    cv=5, # number of folds for the cross-validation
    scoring="neg_mean_absolute_error", # score to optimize
)
model_random_search.fit(X, y)
```

Cross-validation for model selection: choose best α for lasso

- Wage pipeline
- Random search over a distribution of α values
- Identify the best α value(s)



What final model to use for new prediction?

- Either refit on full data the model with the best hyper-parameters on the full data
- Or use the aggregation of outputs from the cross-validation of the best model:

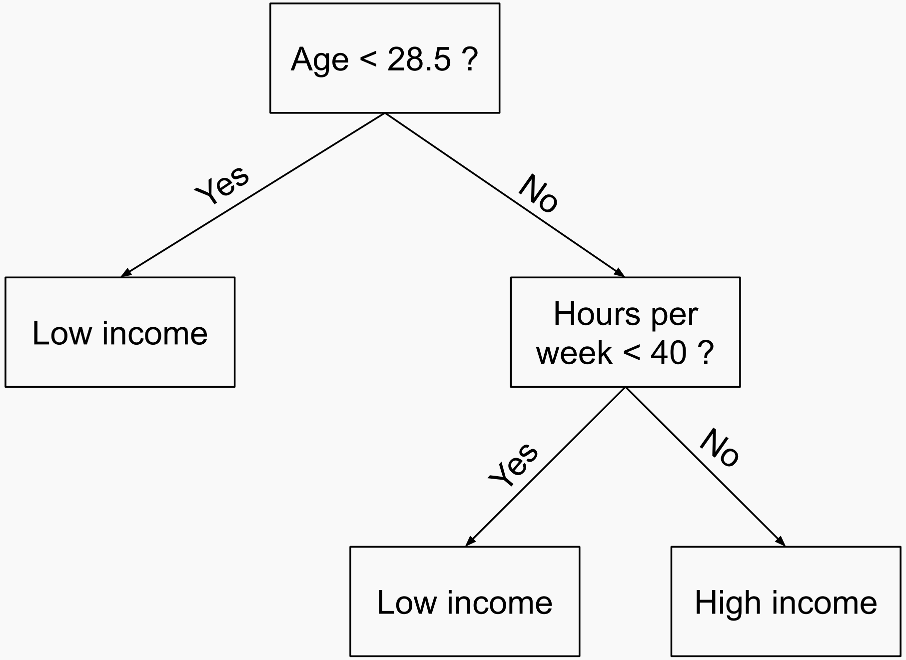
$\hat{y} = \frac{1}{K} \sum_{k=1}^{K} \hat{y}_k$ where $\hat{y}_k$ is the prediction of the model trained on the k-th fold

Naive cross-validation to select AND estimate the best performances

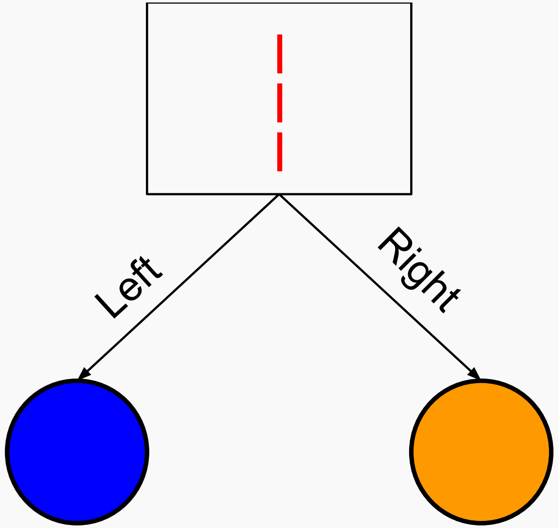
Nested cross-validation to select the best model

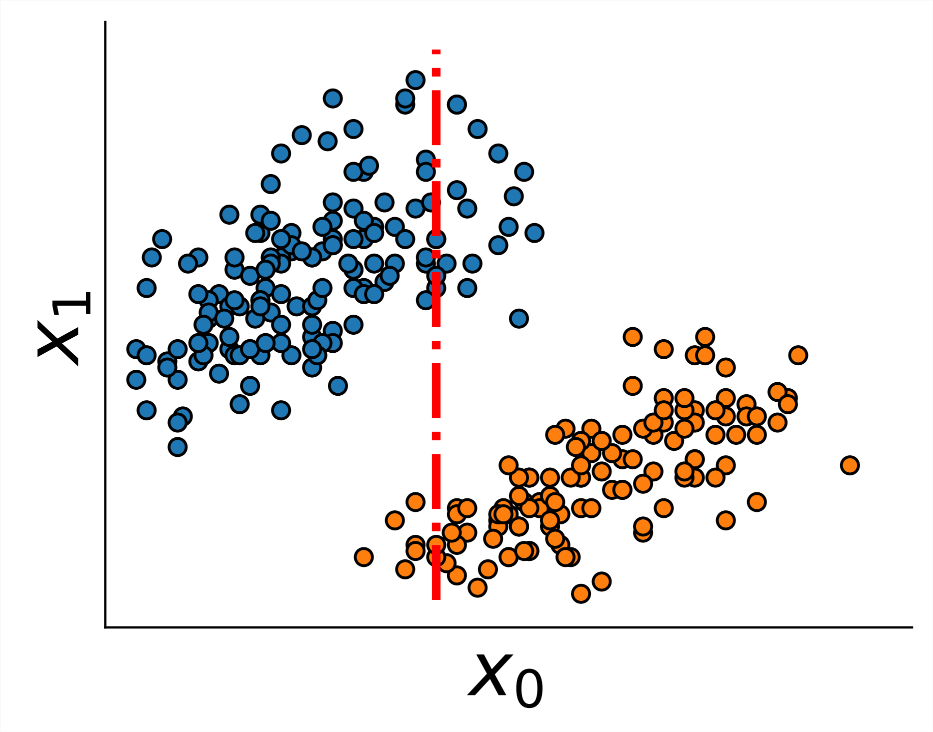
Flexible models: Tree, random forests and boosting

What is a decision tree? An example.

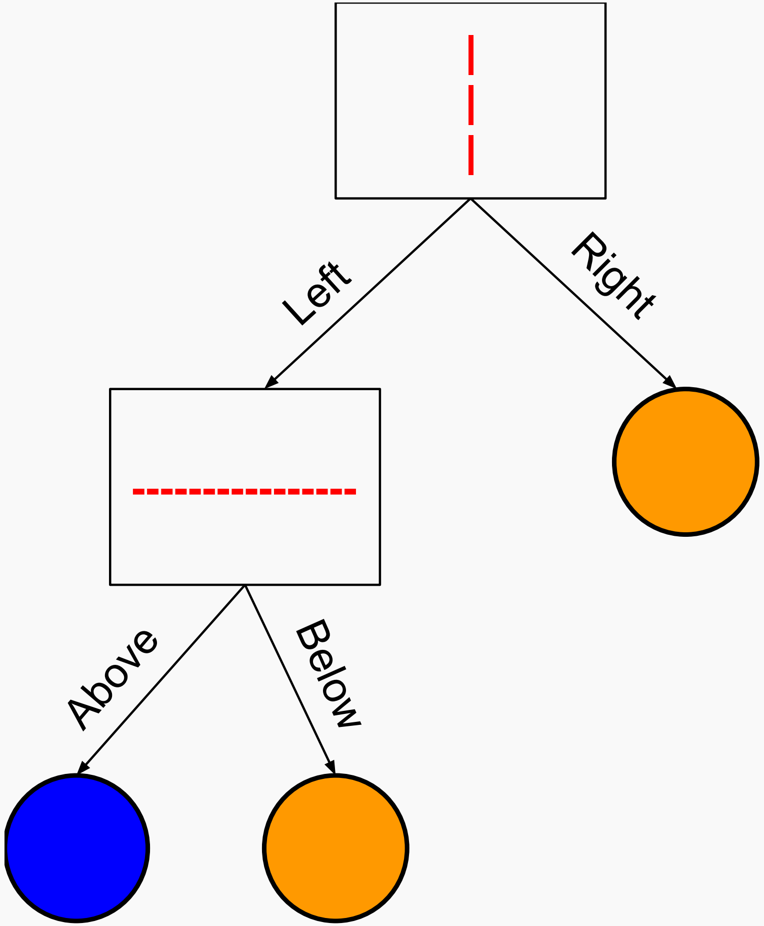


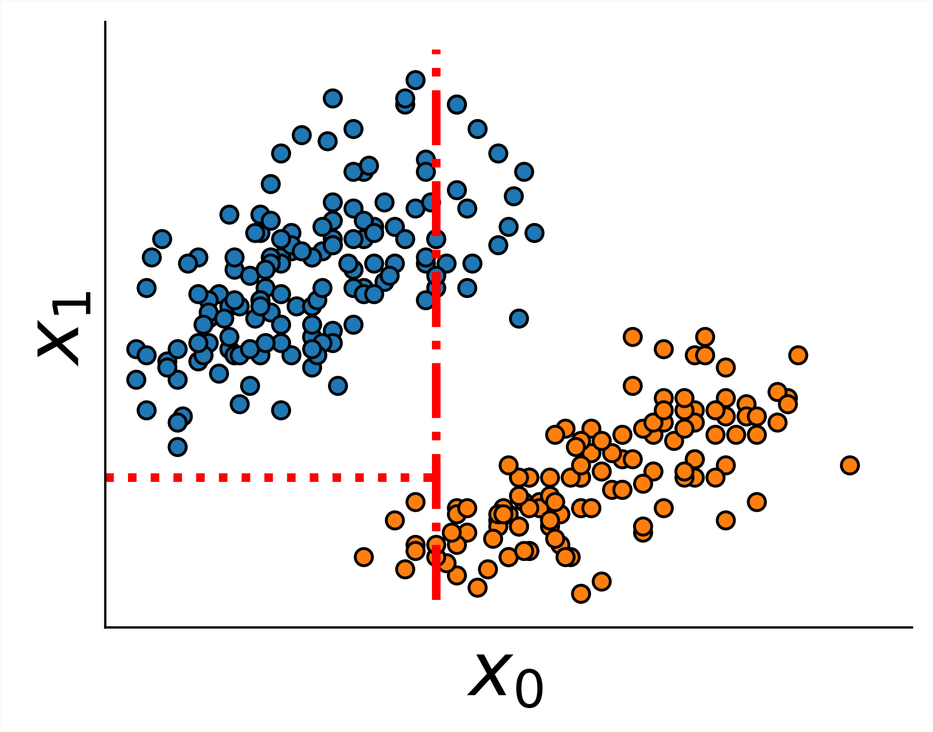
Growing a classification tree



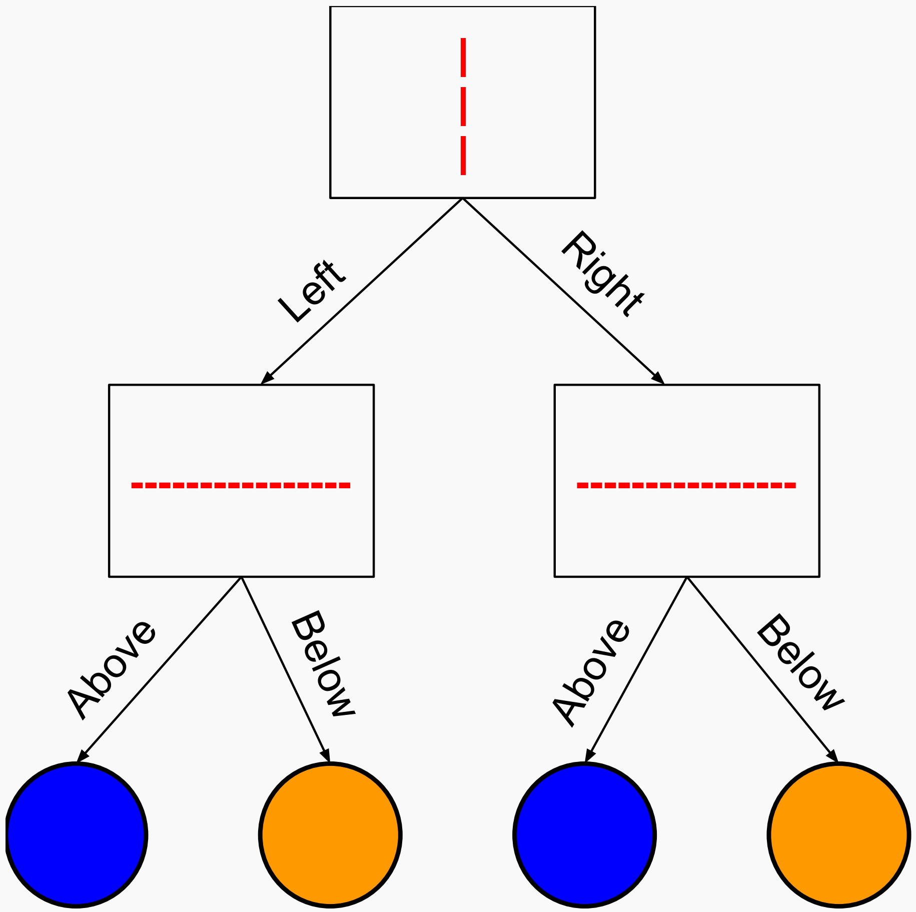


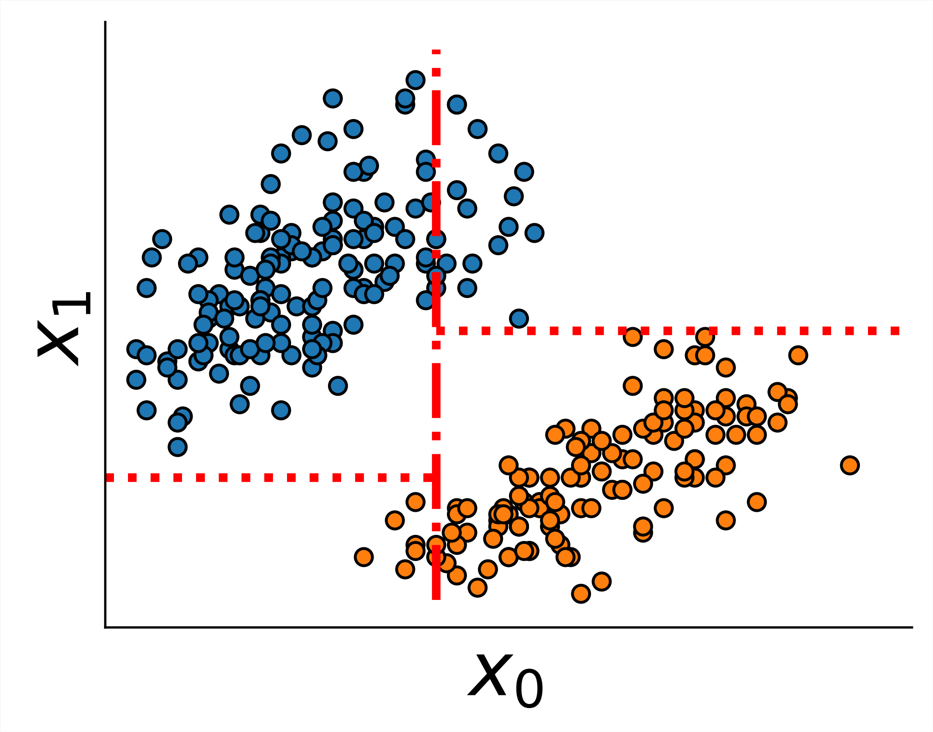
Growing a classification tree



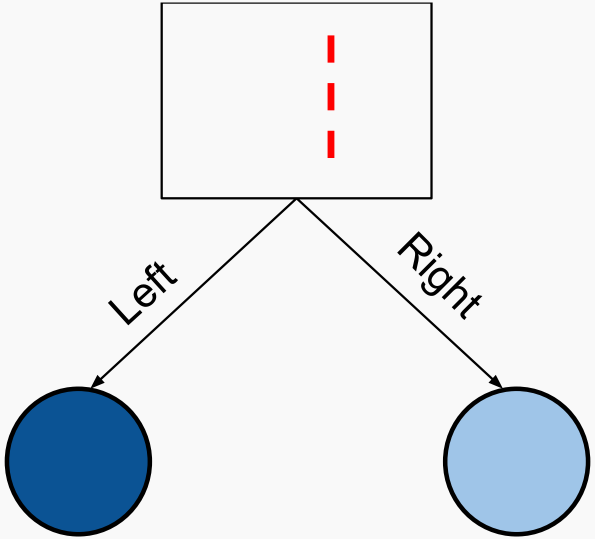


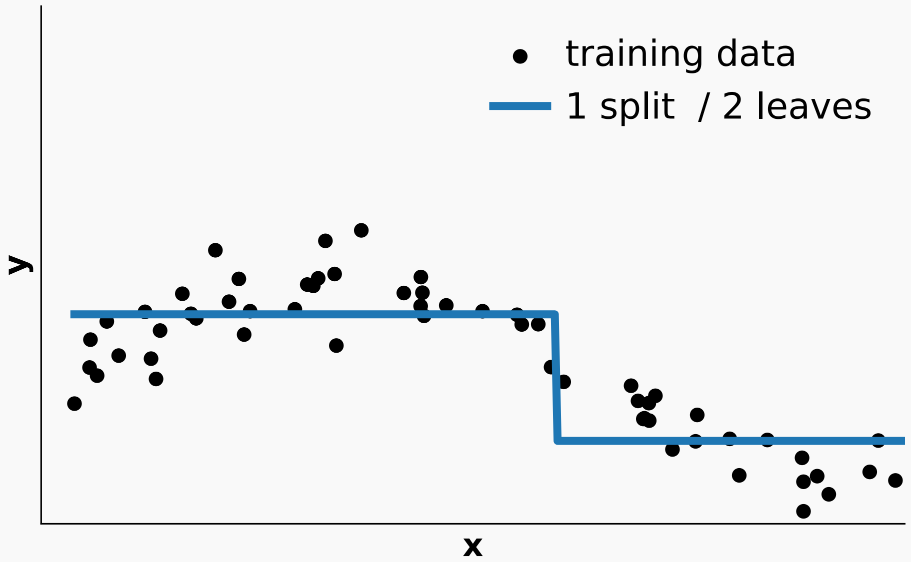
Growing a classification tree



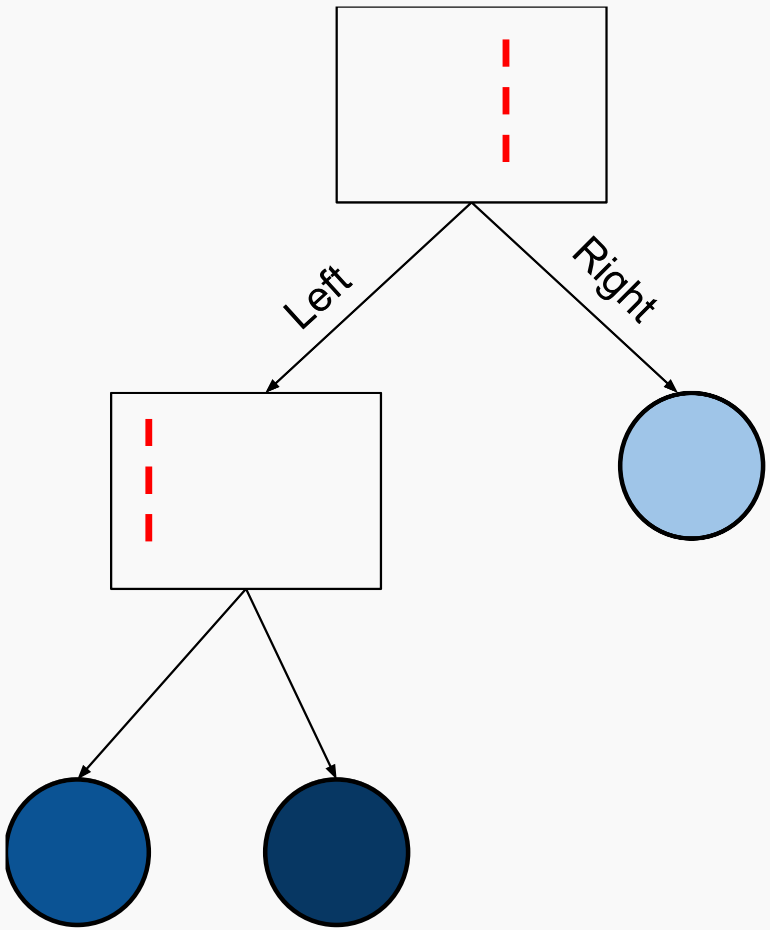


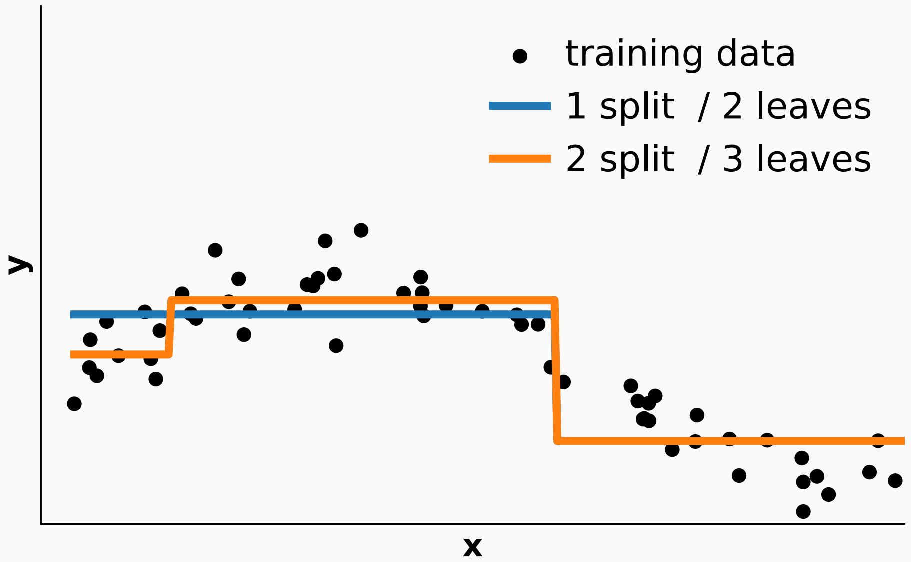
Growing a regression tree



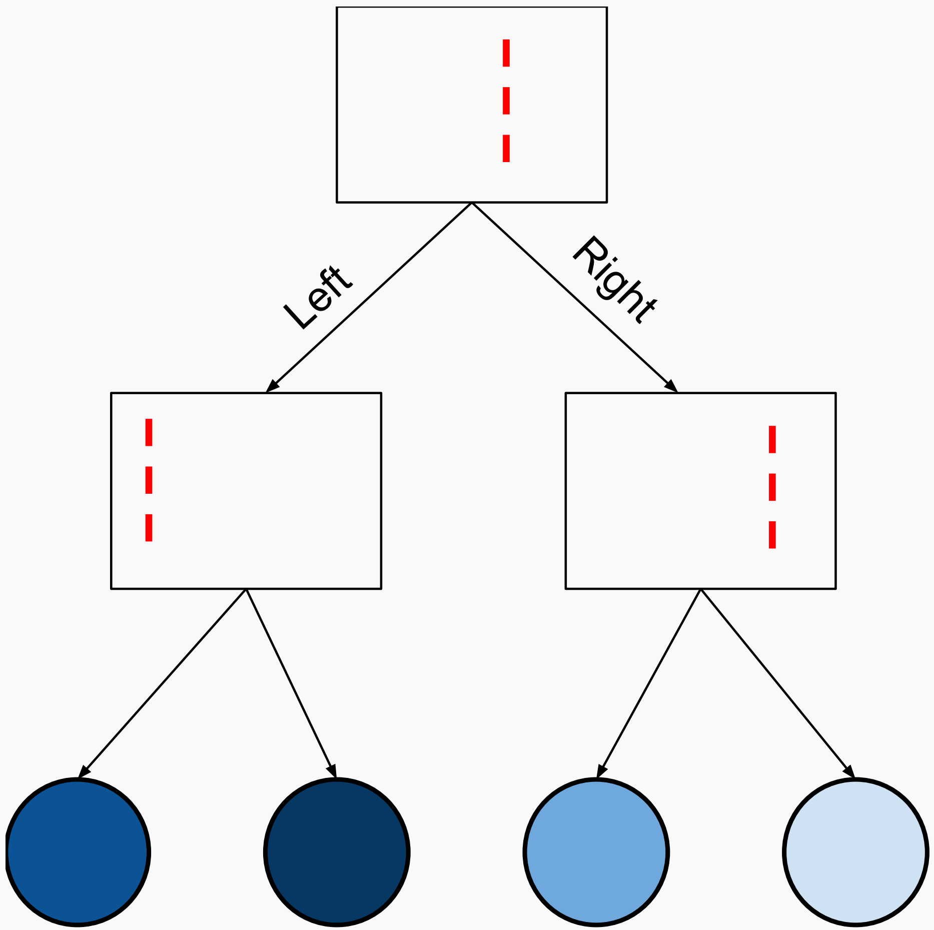


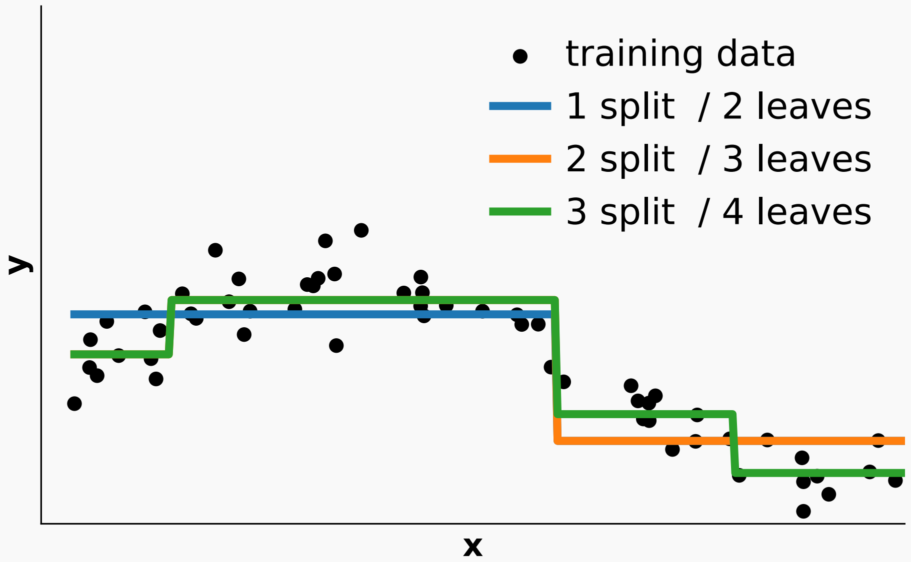
Growing a regression tree





Growing a regression tree





How the best split is chosen?

The best split minimizes an impurity criteria

- for the next left and right nodes
- over all features
- and all possible splits

Formally

Let the data at node m be Q_m with n_m samples. For a candidate split on feature j and threshold t_m $\theta = (j, t_m)$, the split yields:

$Q_m^{\text{left}}(\theta) = \left\{(x, y) | x_j \leq t_m\right\}$ and $Q_m^{\text{right}}(\theta) = Q_m \setminus Q_m^{\text{left}}(\theta)$

Then θ is chosen to minimize the impurity criteria averaged over the two children nodes:

$\theta^* = \operatorname{argmin}_{j, t_m} \left[\frac{n_m^{\text{left}}}{n_m} H\left(Q_m^{\text{left}}(\theta)\right) + \frac{n_m^{\text{right}}}{n_m} H\left(Q_m^{\text{right}}(\theta)\right)\right]$ with H the impurity criteria.

Impurity criteria

For classification

Gini impurity

$H(Q_m) = \sum_k p_{mk}(1 - p_{mk})$ with $p_{mk} = \frac{1}{n_m} \sum_{y \in Q_m} I(y = k)$

Cross-entropy

$H(Q_m) = -\sum_{k \in K} p_{mk} \log(p_{mk})$

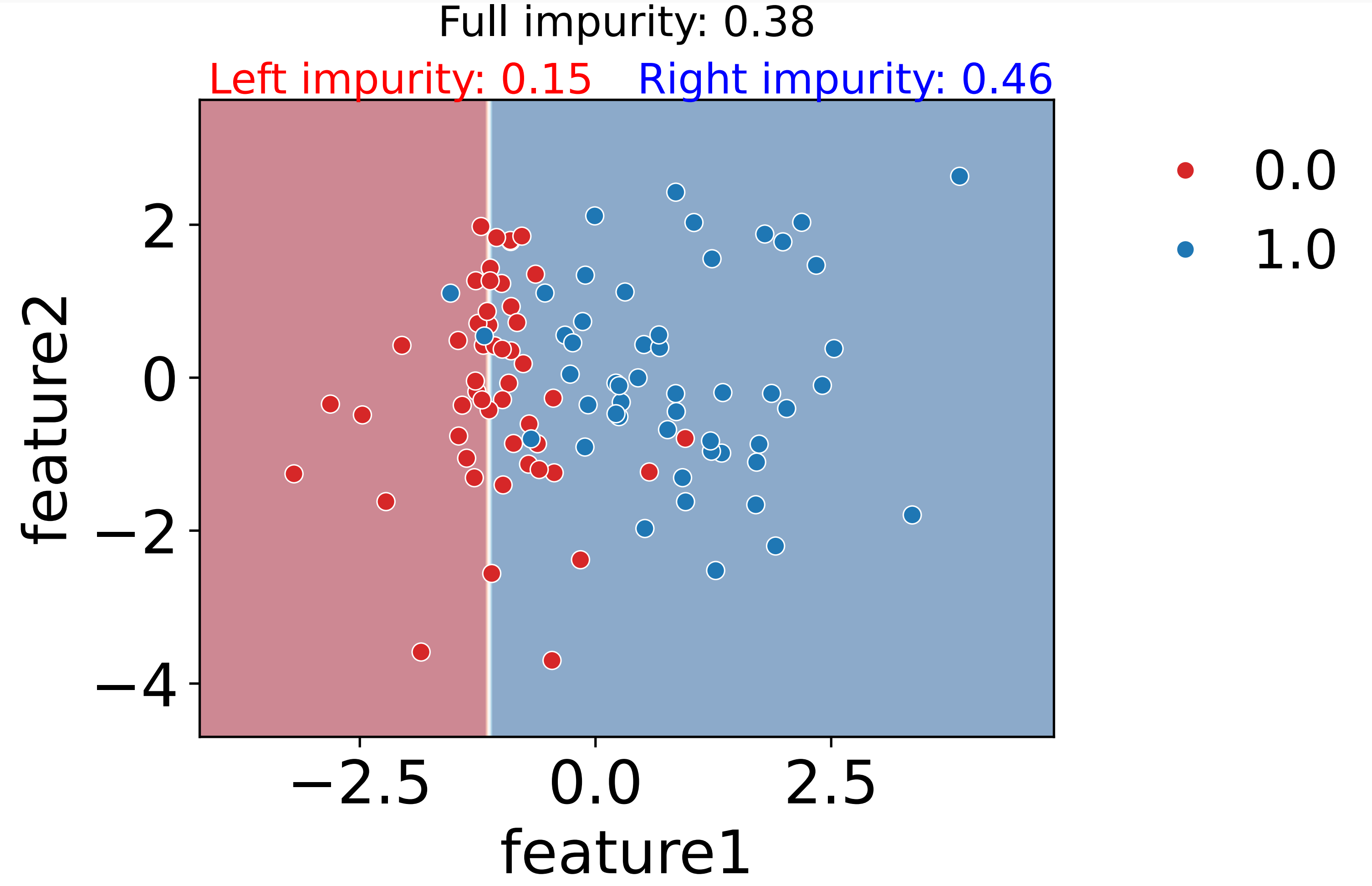
For regression

Mean squared error

$H(Q_m) = \frac{1}{n_m} \sum_{y \in Q_m} (y - \overline{y_m})^2$ where $\overline{y_m} = \frac{1}{n_m} \sum_{y \in Q_m} y$

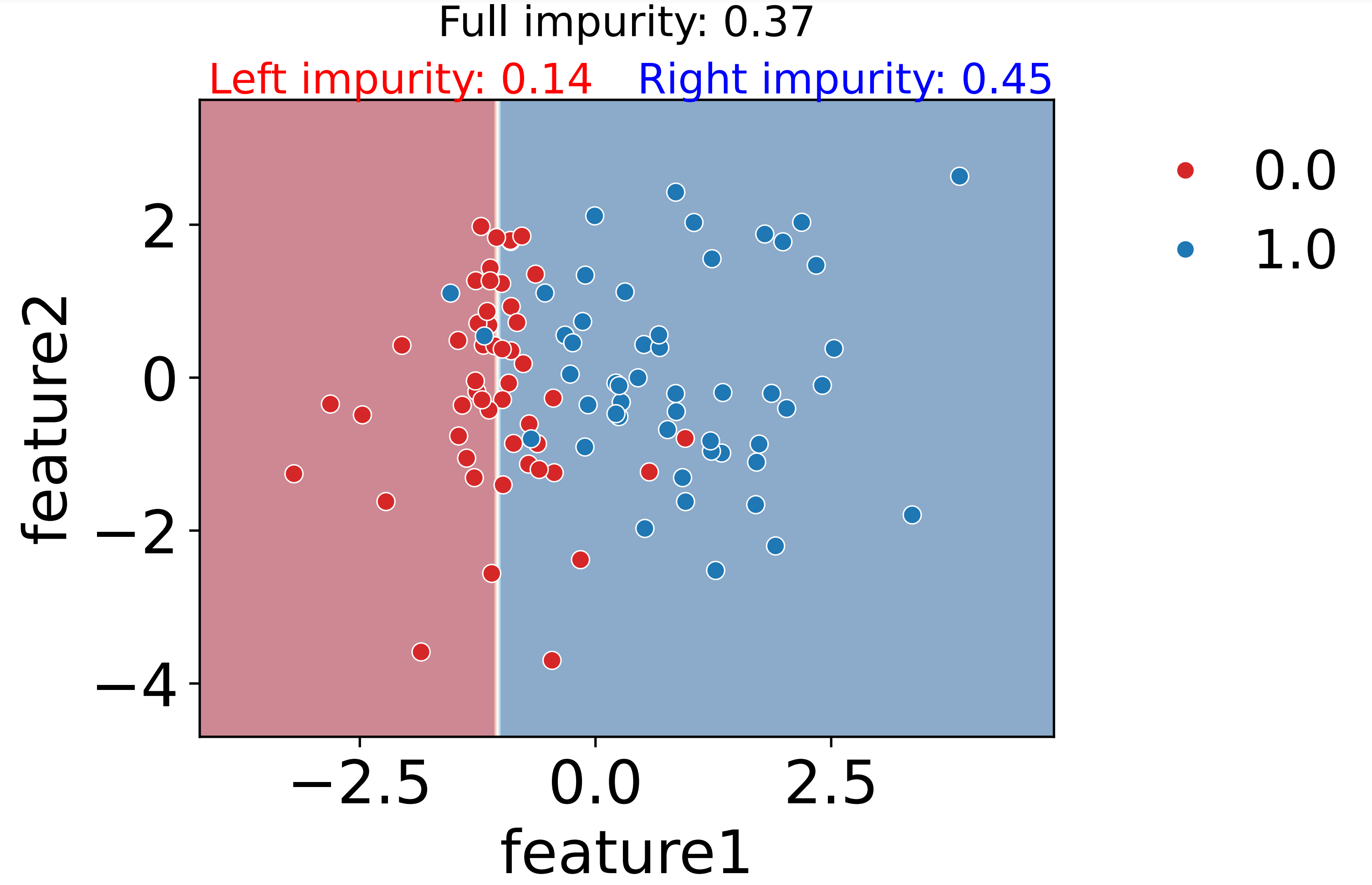
Chose the best split: example

Random split



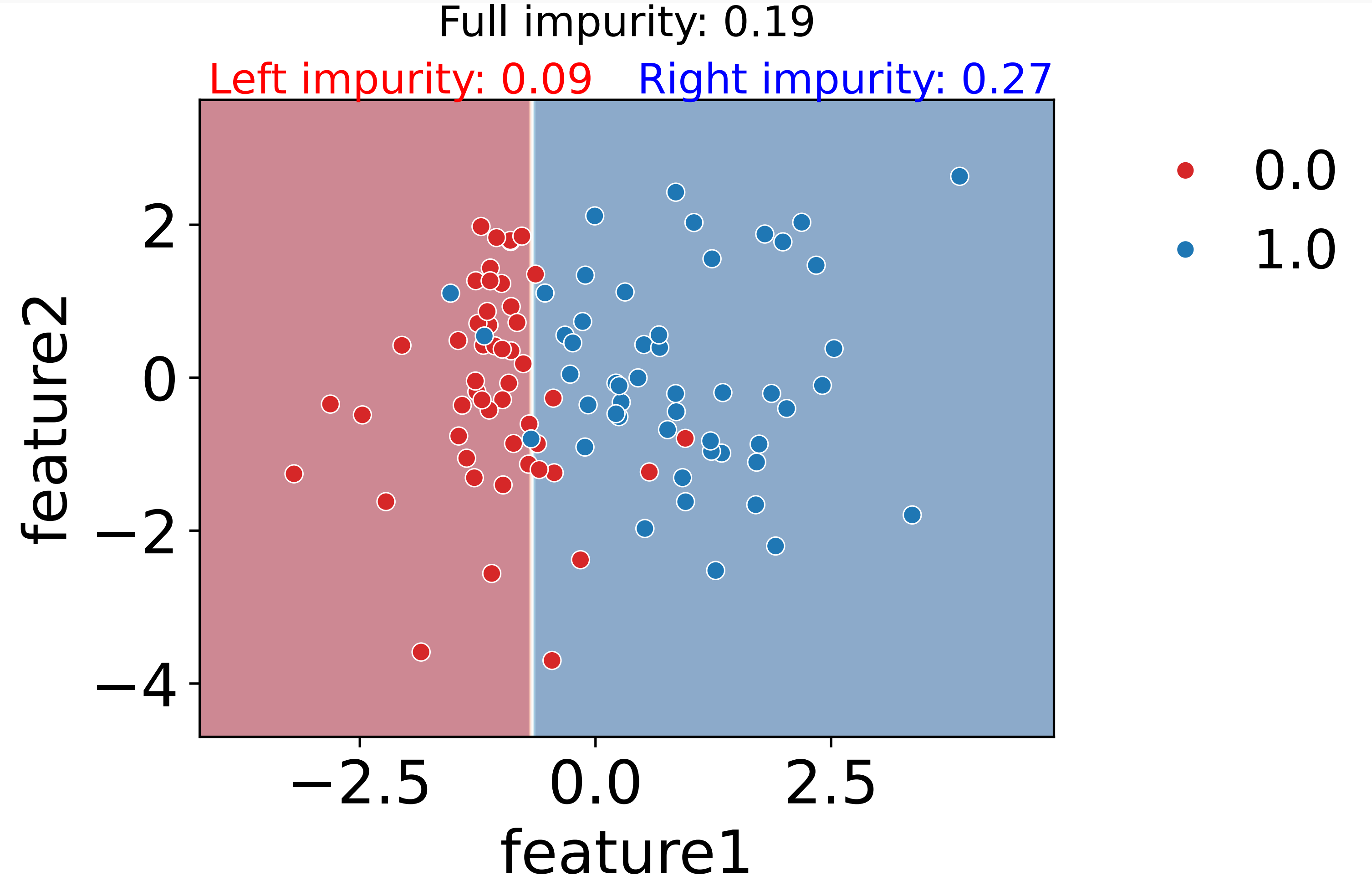
Chose the best split: example

Moving the split to the right from one point



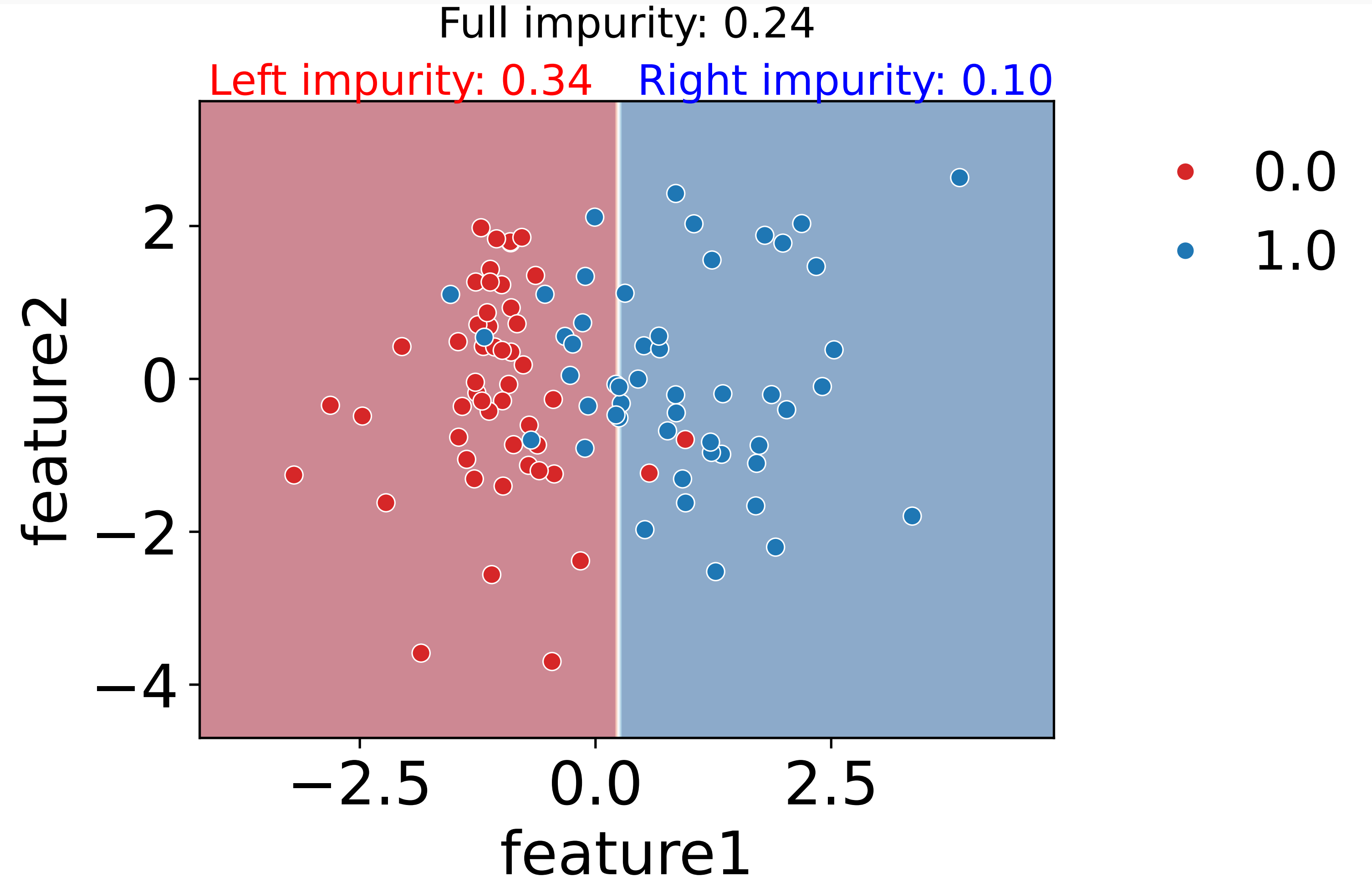
Chose the best split: example

Moving the split to the right from 10 points



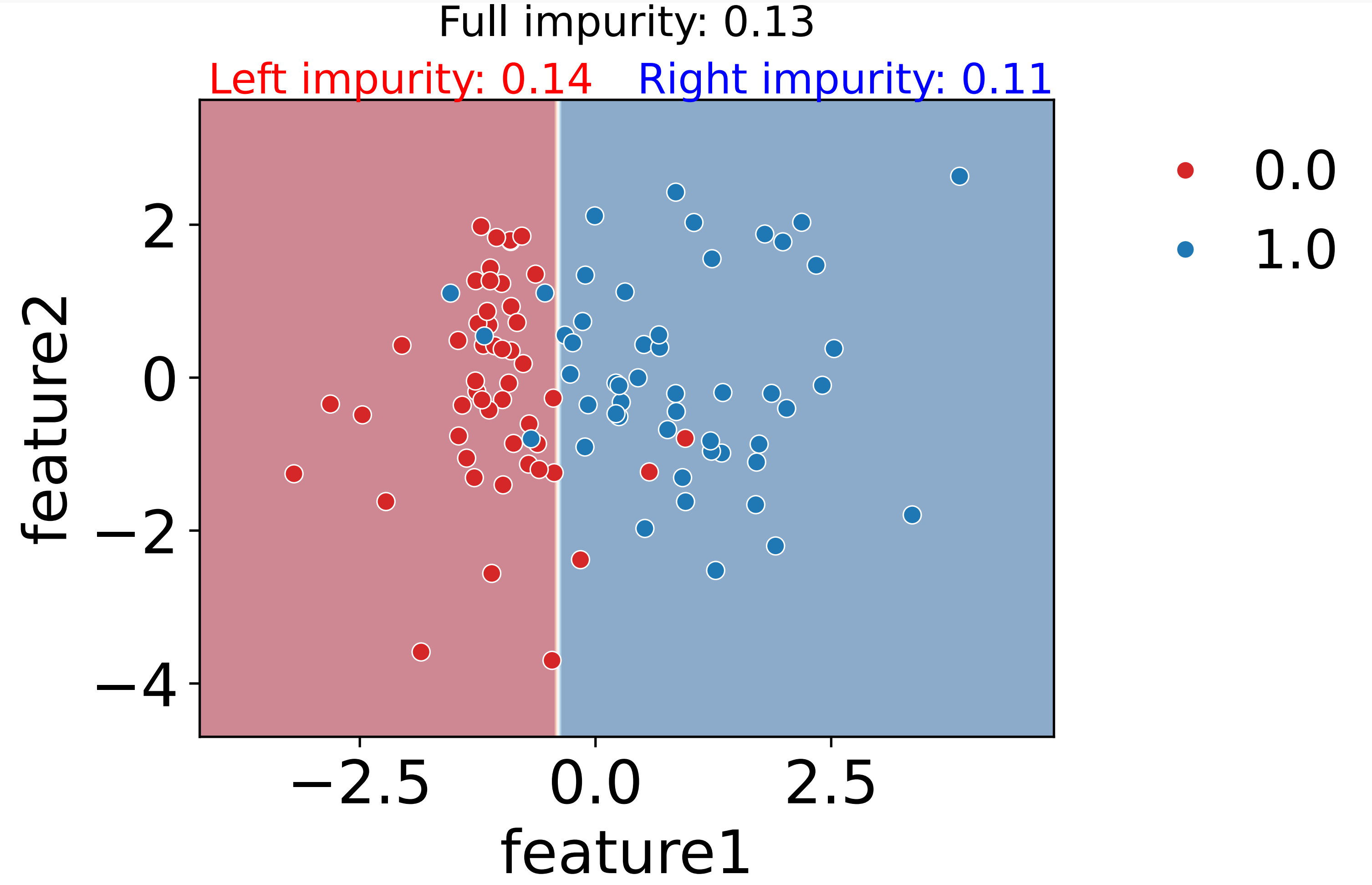
Chose the best split: example

Moving the split to the right from 20 points

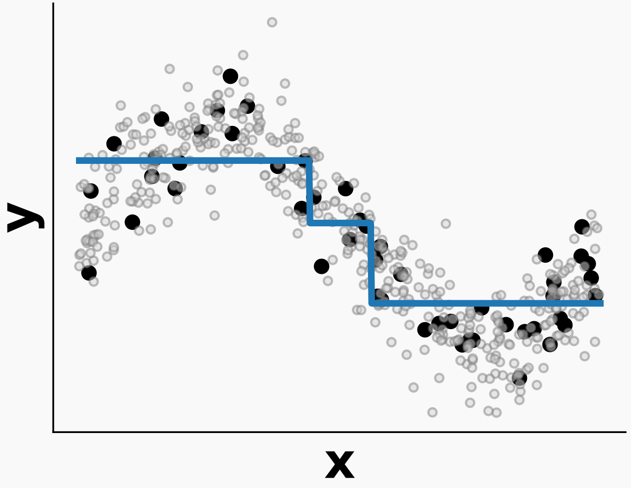


Chose the best split: example

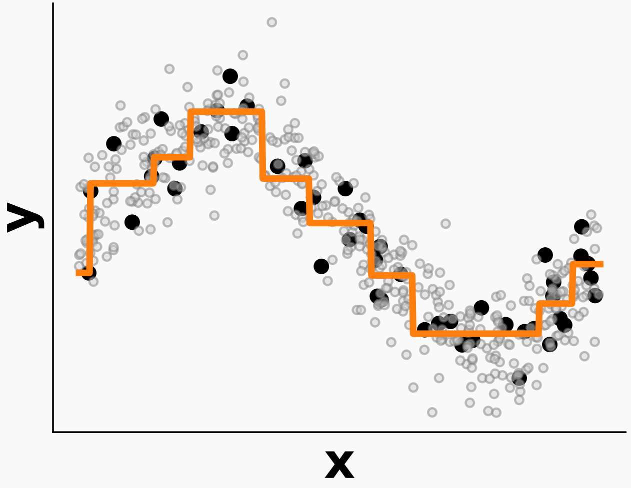
Best split



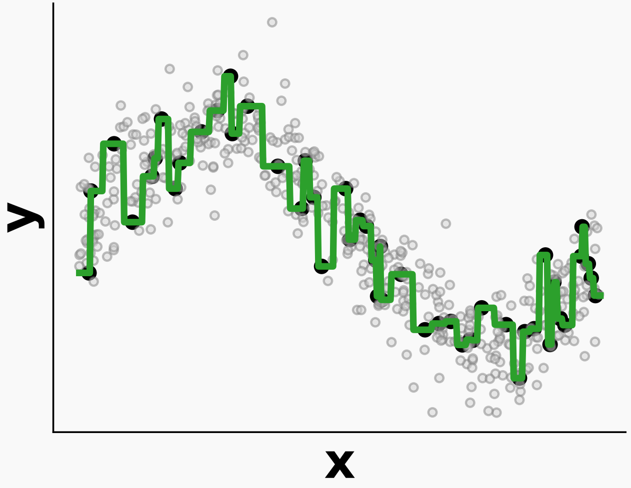
Tree depth and overfitting



Underfitting
max depth or
max_leaf_nodes
too small



Best trade-off



Overfitting
max depth or
max_leaf_nodes
too large

Main hyper-parameters of tree models

```python
DecisionTreeRegressor(
	criterion="mse",
	max_depth=None, # control tree depth (assume symetric trees)
	min_samples_split=2, # control tree depth (allowing asymetric trees)
	min_samples_leaf=1, # control tree depth (allowing asymetric trees)
	max_leaf_nodes=None, # control tree depth (allowing asymetric trees)
	min_impurity_decrease=0.0, # control tree depth (allowing asymetric trees)
)
```

Pros and cons of trees

Pros

- Easy to interpret
- Handle mixed types of data: numerical, categorical and missing data
- Handle interactions
- Fast to fit

Cons

- Prone to overfitting
- Unstable: small changes in the data can lead to very different trees
- Mostly useful as a building block for ensemble models: random forests and boosting trees

Ensemble principle: average the predictions of multiple predictors

Boosting

Ensemble models

A word on other families of models

Other well known families of models

Generalized linear models

Kernel methods: Support vector machines, Gaussian processes

Deep neural networks

Why not use deep learning everywhere?

- Success of deep learning (aka deep neural networks) in image, speech recognition and text
- 🤔 Why not so used in econometrics?

Why not use deep learning everywhere?

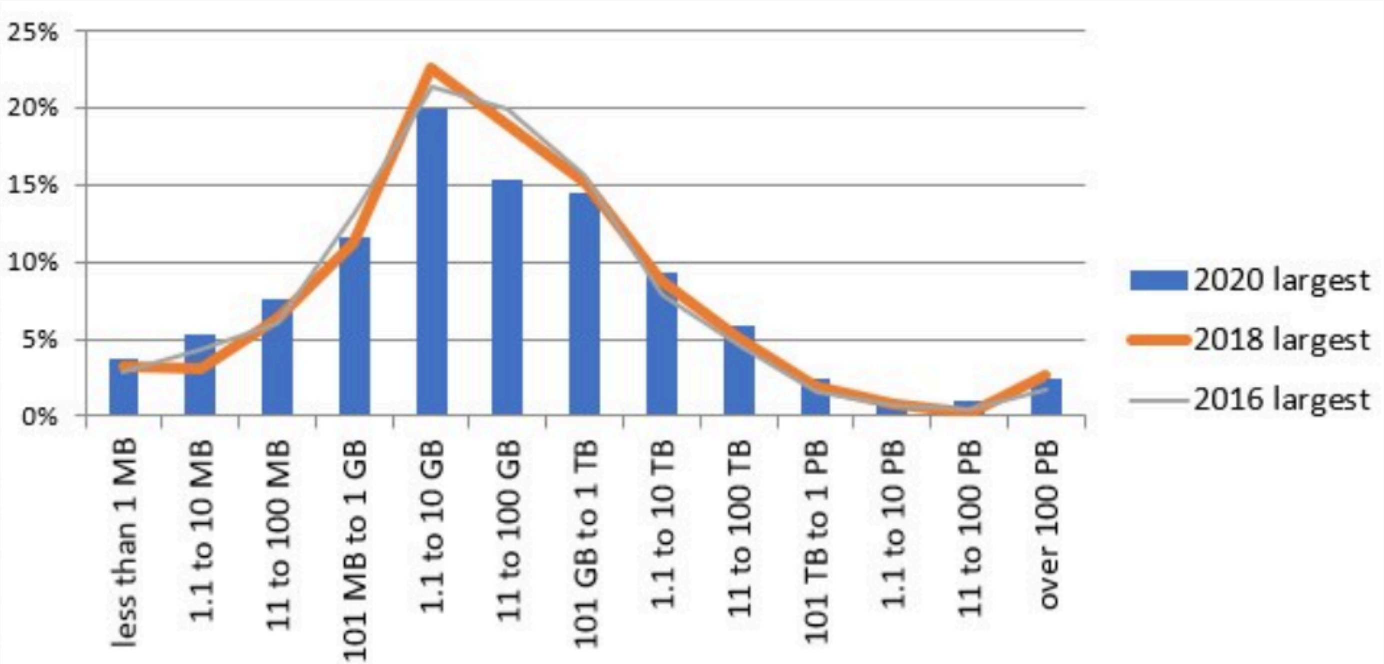
- Success of deep learning (aka deep neural networks) in image, speech recognition and text
- 🤔 Why not so used in econometrics?

Deep learning needs a lot of data (typically $N \approx 1$ million)

Do we have this much data in econometrics?

Answer 1: Limited data settings

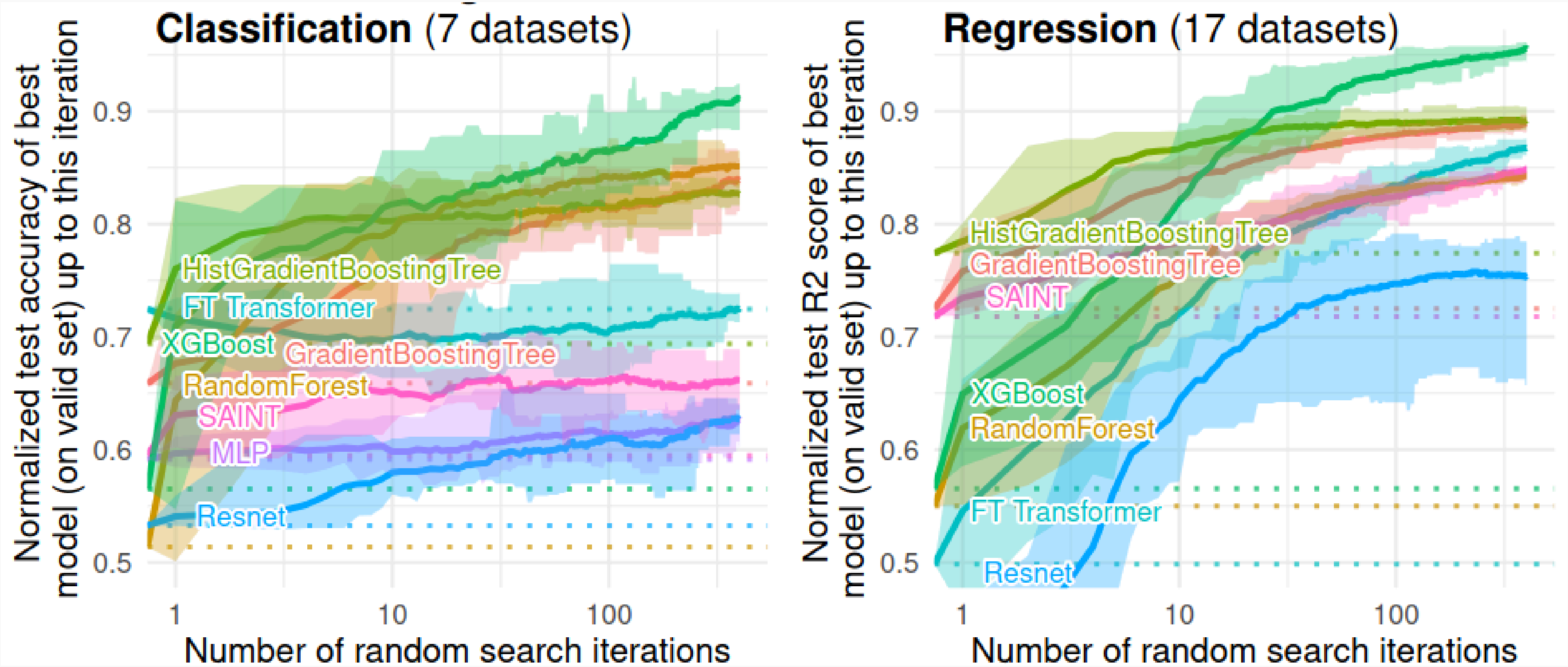
- Typically in economics (but also everywhere), we have a limited number of observations



Typical dataset are mid-sized. This does not change with time.[1]

[1]https://www.kdnuggets.com/2020/07/poll-largest-dataset-analyzed-results.html

Tree-based methods outperform tailored deep learning architectures (Grinsztajn et al., 2022)



Nuance: recent work on LLM and pre-trained techniques for tabular learning

Some references:

- Skrub python library: data-wrangling and encoding (same people than sklearn)
- (Kim et al., 2024): CARTE: pretraining and transfer for tabular learning
- (Grinsztajn et al., 2023) : Vectorizing string entries for data processing on tables: when are larger language models better?

Bibliography

Grinsztajn, L., Oyallon, E., & Varoquaux, G. (2022). *Why do tree-based models still outperform deep learning on typical tabular data?*. Advances in Neural Information Processing Systems, 35, 507–520.

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