

Machine Learning for econometrics

Flexible models for tabular data

Matthieu Doutreligne

A lot of today's content is taken from the excellent [sklearn mooc](#) (Estève et al., 2022)

Reminder from previous session

- Statistical learning 101: bias-variance trade-off
- Regularization for linear models: Lasso, Ridge, Post Lasso
- Transformation of variables: polynomial regression

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

Contents

Model evaluation and selection with cross-validation	3
Flexible models: Tree, random forests and boosting	14
A quick word on other families of models	42
Python hands-on	51
Bibliography	53

Model evaluation and selection with cross-validation

A closer look at model evaluation: Wage example

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

A closer look at model evaluation: Wage example

Example with the Wage dataset

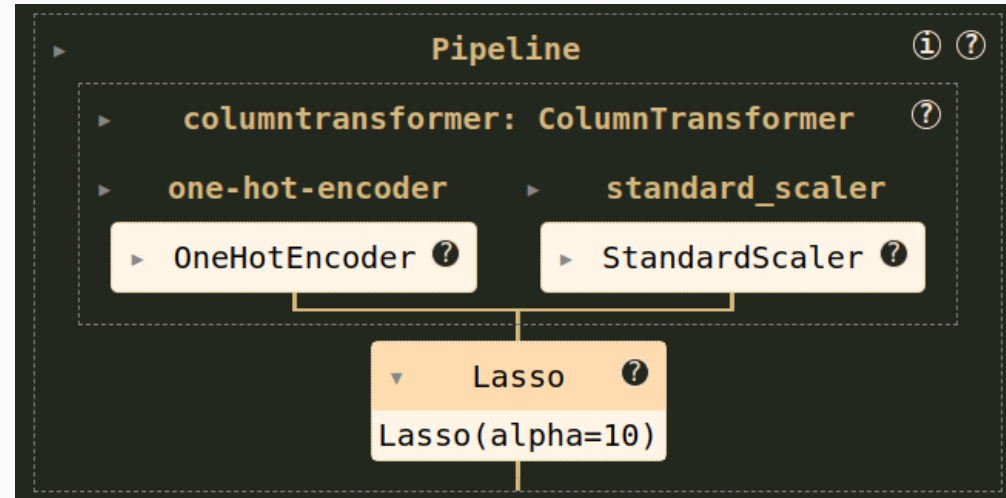
- Raw dataset: (N=534, p=11)
- Transformation: encoding categorical data, scaling numerical data: (N=534, p=23)

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	one-hot- 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	

A closer look at model evaluation: Wage example

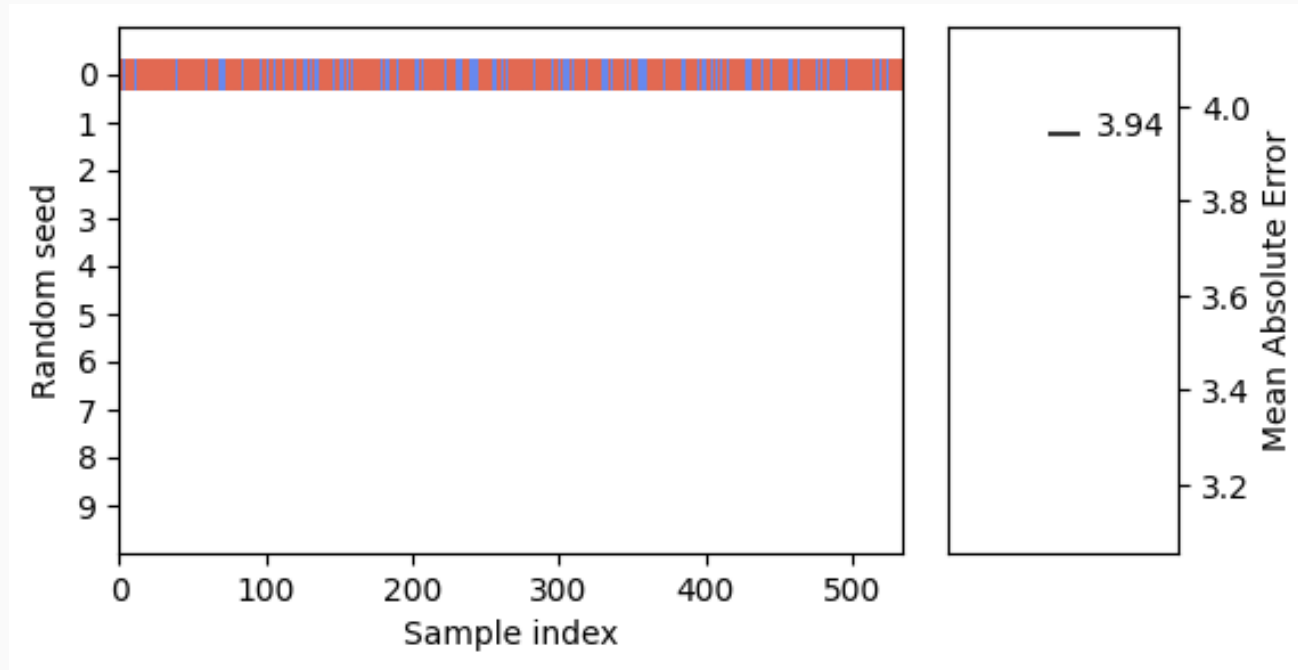
Example with the Wage dataset

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

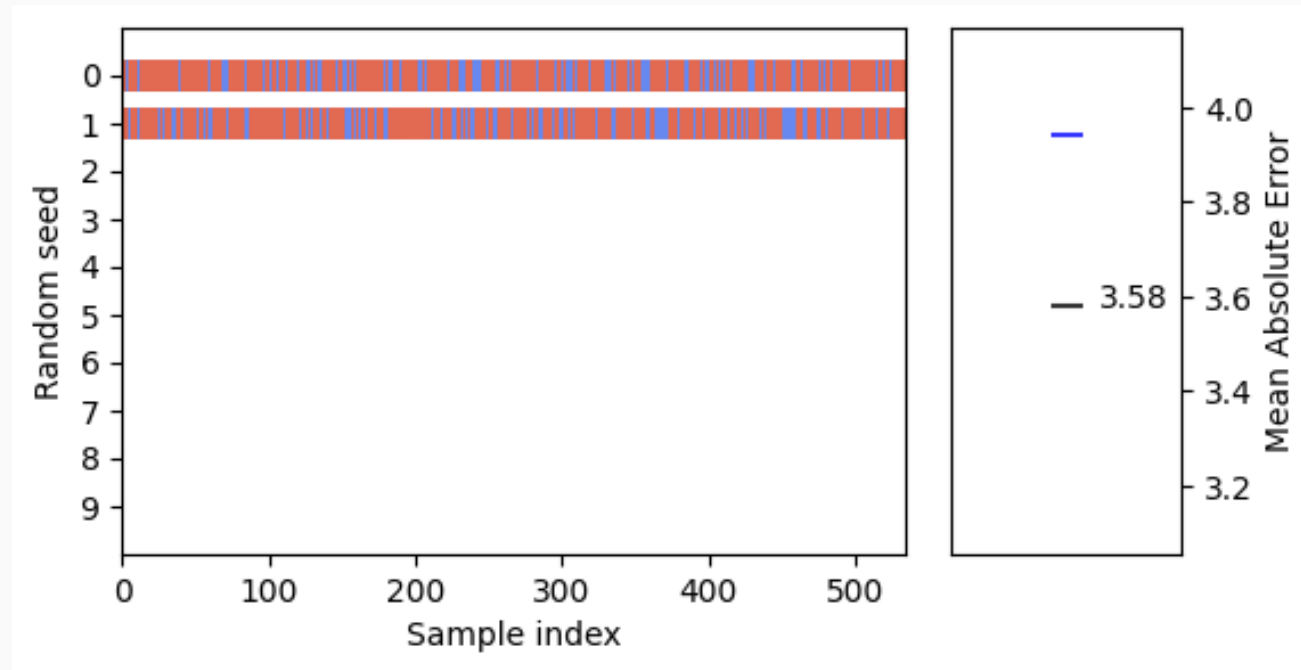


Repeated train/test splits

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

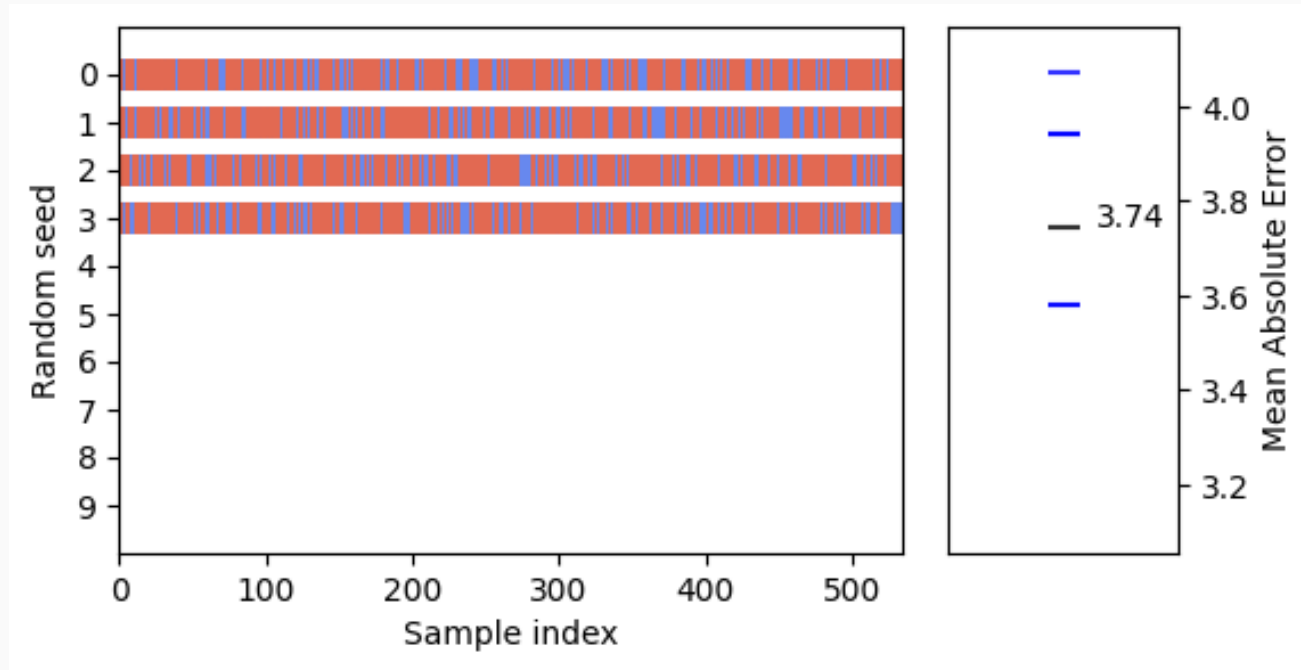


But we could have chosen another split ! Yielding a different MAE



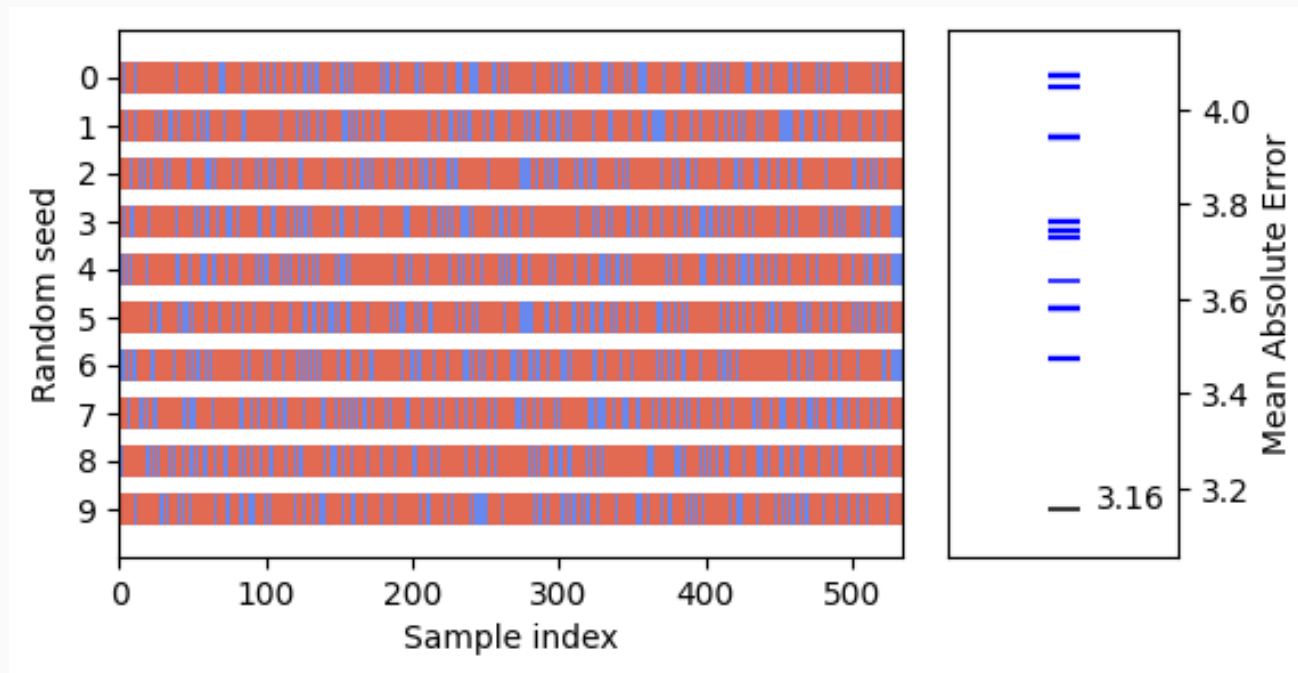
Repeated train/test splits

And another split...



Repeated train/test splits

Splitting ten times



Distribution of MAE: 3.71 ± 0.26

Repeated exclusive train/test splits = Cross-validation

Practical usage with sklearn: `cross_validate`.

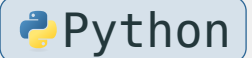
```
1 from sklearn.model_selection import cross_validate
2 cv_results = cross_validate(
3     pipeline, X, y, cv=5, scoring="neg_mean_absolute_error"
4 )
```



Repeated exclusive train/test splits = Cross-validation

Practical usage with sklearn: `cross_validate`.

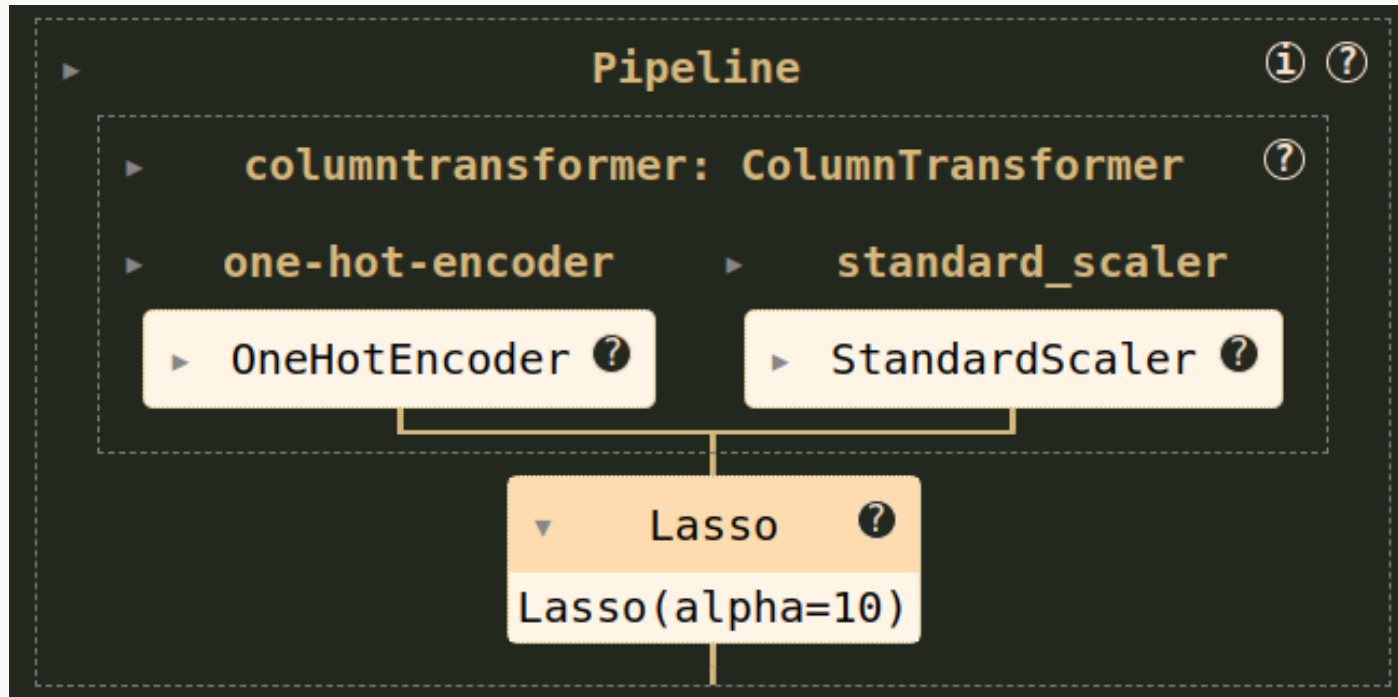
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1 from sklearn.model_selection import cross_validate
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3     pipeline, X, y, cv=5, scoring="neg_mean_absolute_error"
4 )
```



- 😊 Robustly estimate generalization performance.
- 🤪 Estimate data variability of the performance : bigger source of variation in ML (Bouthillier et al., 2021).
- 🚀 Let's use it to select the best models among several candidates!

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

Wage pipeline



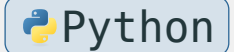
What is the best α value for the Lasso regularization?

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

Wage pipeline

Random search over a distribution of α values

```
1 param_distributions = {"lasso__alpha": loguniform(1e-6, 1e3)}
2 model_random_search = RandomizedSearchCV(
3     pipeline,
4     param_distributions=param_distributions,
5     n_iter=10, # number of hyper-parameters sampled
6     cv=5, # number of folds for the cross-validation
7     scoring="neg_mean_absolute_error", # score to optimize
8 )
9 model_random_search.fit(X, y)
```

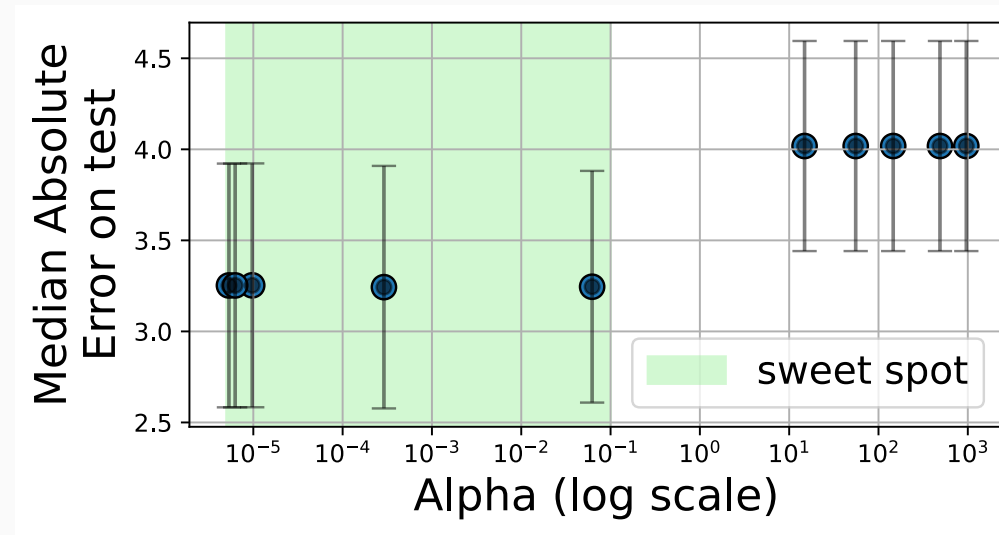


Cross-validation for model selection: choose best α for lasso

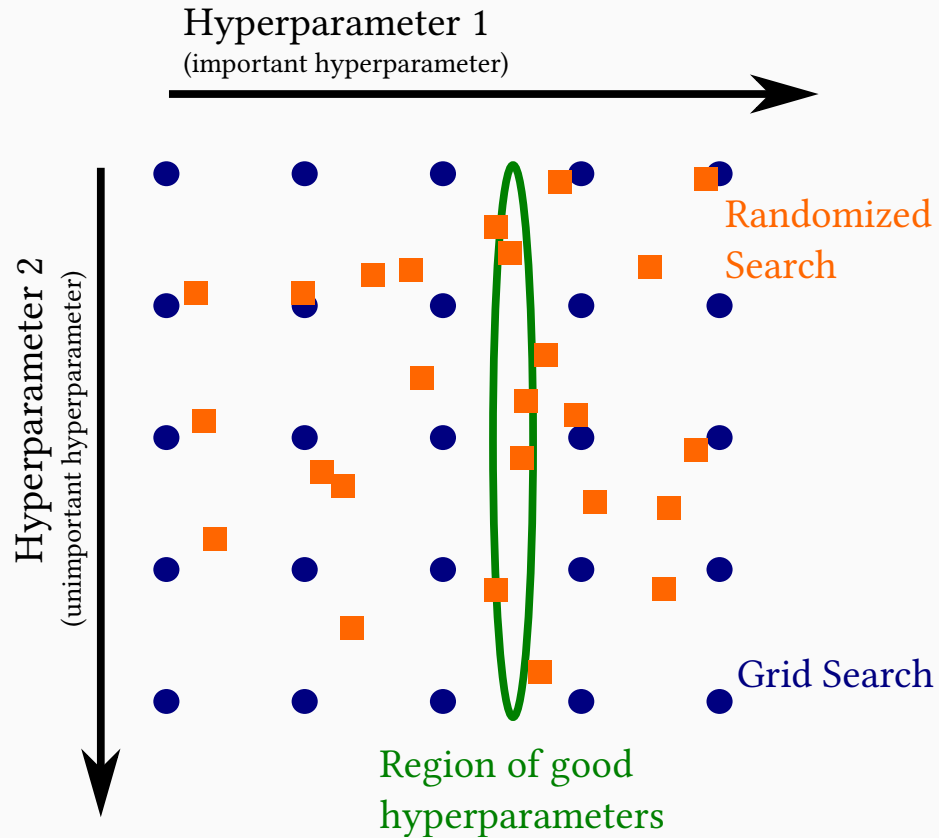
Wage pipeline

Random search over a distribution of α values

Goal: Identify the best α value(s)



Random search more efficient than grid search (Bergstra & Bengio, 2012)



- Grid search: Explores HP along all fixed directions (waste of time if one parameter is not important)
- Grid search: good HP may fall between grid points
- Random search: explores hyper-parameters in every direction

What final model to use for new prediction?

- Often used in practice: **refit on the full data** the model with the best hyper-parameters.

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- Often used in practice: **refit on the full data** the model with the best hyper-parameters.
- Theoretically motivated: Aggregate outputs from the cross-validate estimators 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.

What final model to use for new prediction?

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- **Averaging the estimators of the best model** selected by cross-validation select the best model for generalization performances (Van der Laan et al., 2007).

Hyper-parameters selection is a kind of model fitting

Using a single loop of cross-validation, the **full dataset** is used to:

- **Select** the best hyper-parameters
- **Estimate** the generalization performance of the selected model

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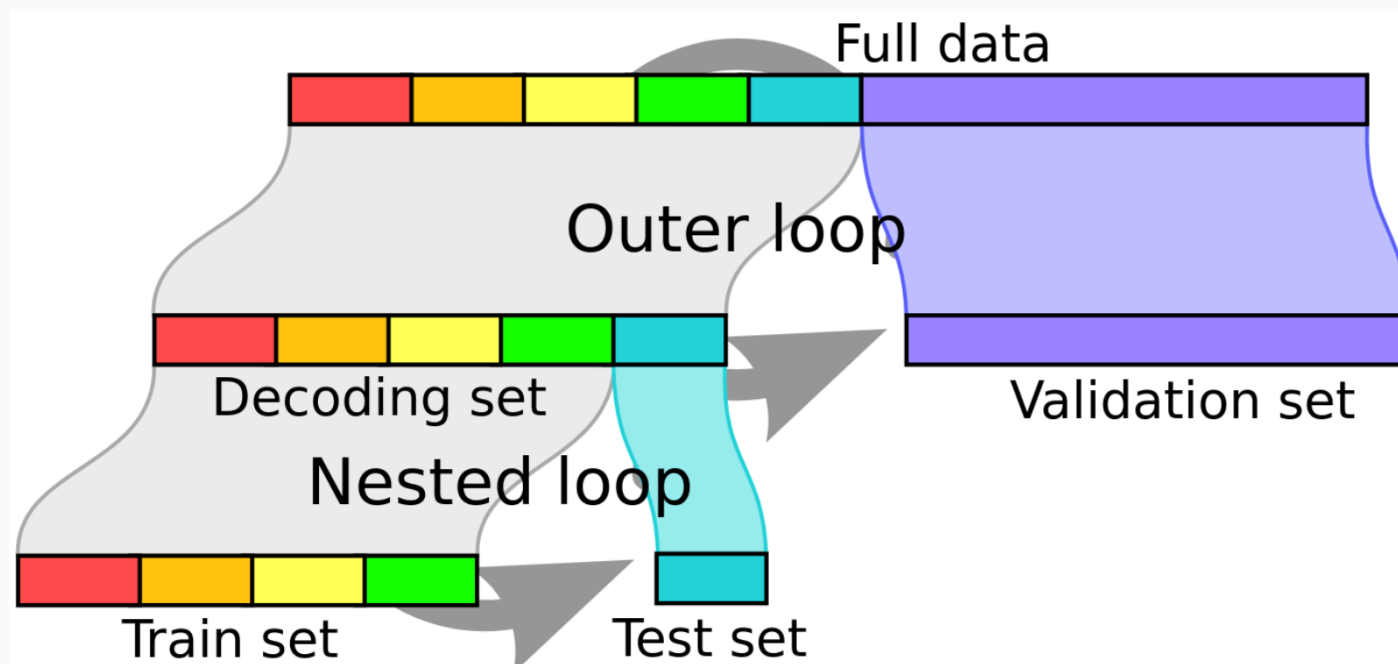
- **Select** the best hyper-parameters
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 **Naive cross-validation can lead to overfitting and over-optimistic performance estimation**

 **Solution: Nested cross-validation (Varoquaux et al., 2017)**

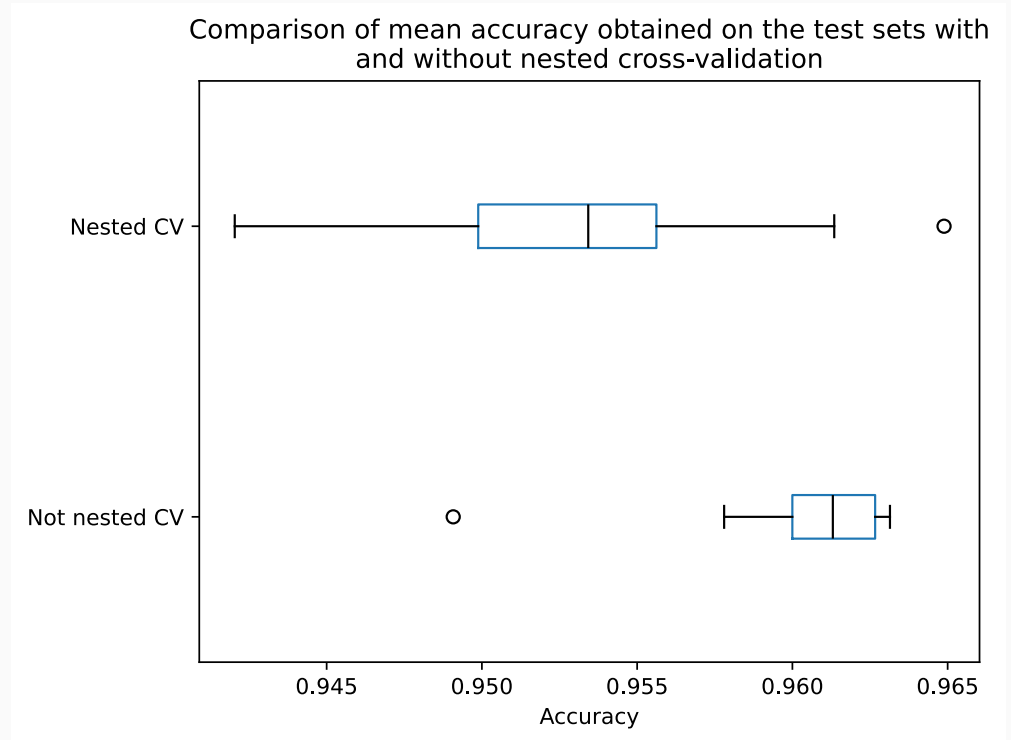
Nested cross-validation to select and estimate the best performances

- Inner CV loop to select the best hyper-parameters
- Outer loop to estimate the generalization performance of the selected model

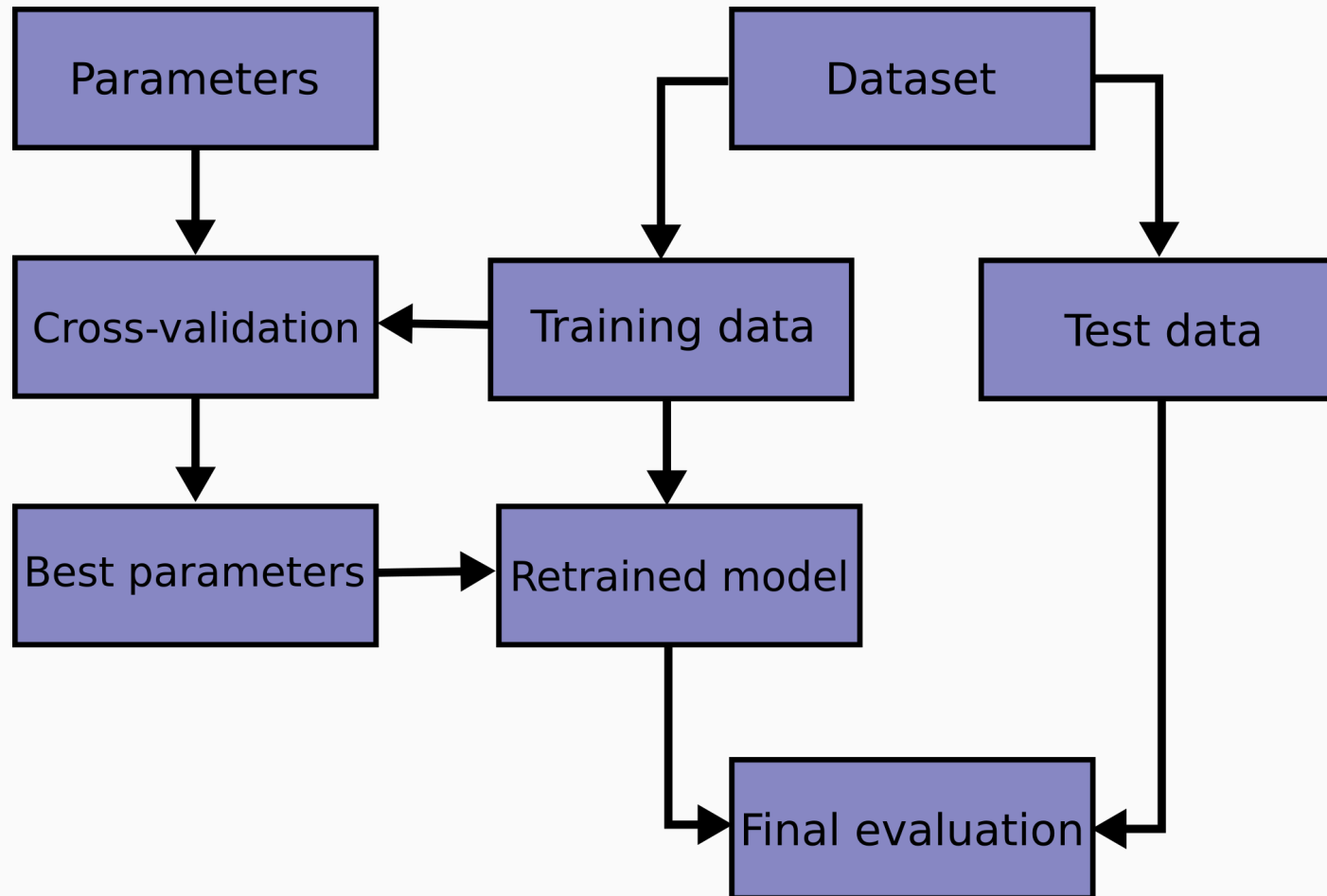


Over-optimistic performance estimation: Toy example

- Dataset: Breast cancer (N, p) = (569, 30)
- Classifier: RandomForestClassifier with multiple choices of hyper-parameter

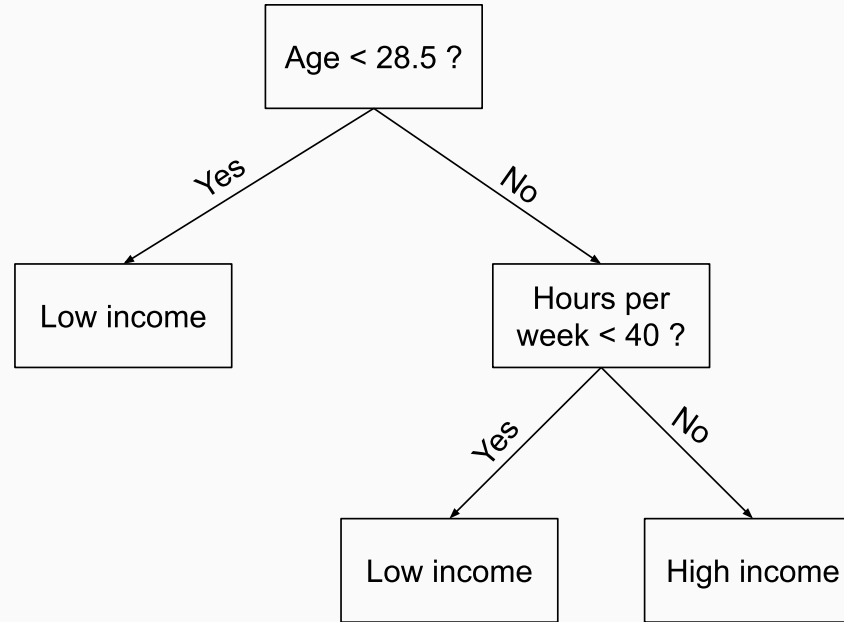


Nested cross-validation : An overview of the full procedure

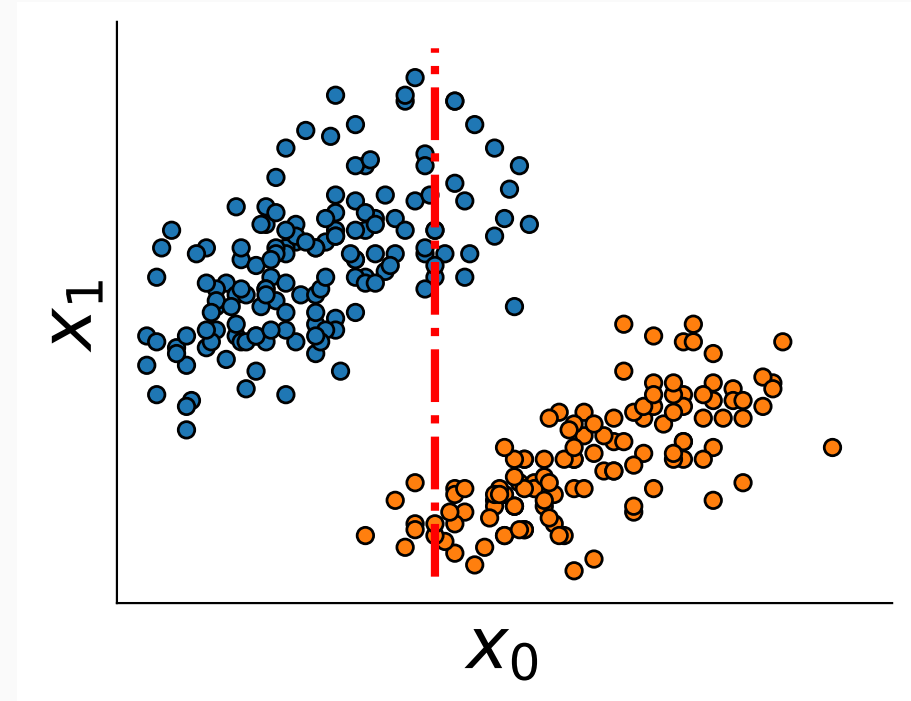
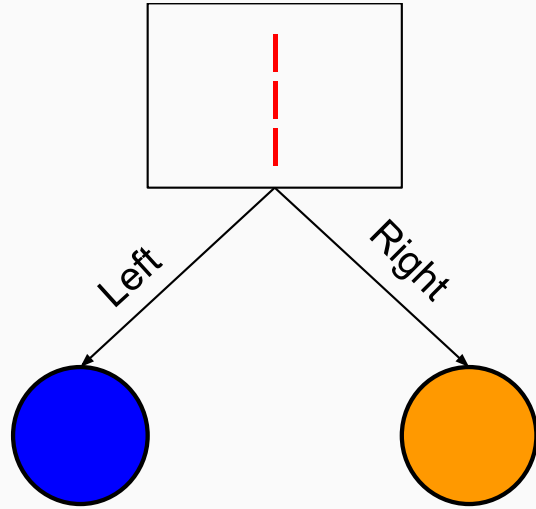


Flexible models: Tree, random forests and boosting

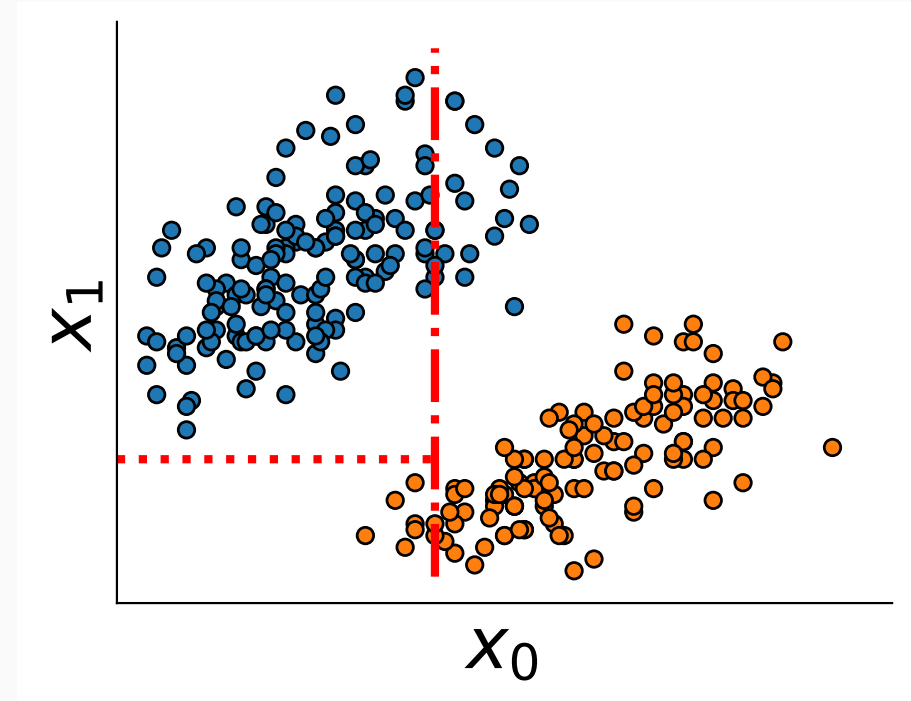
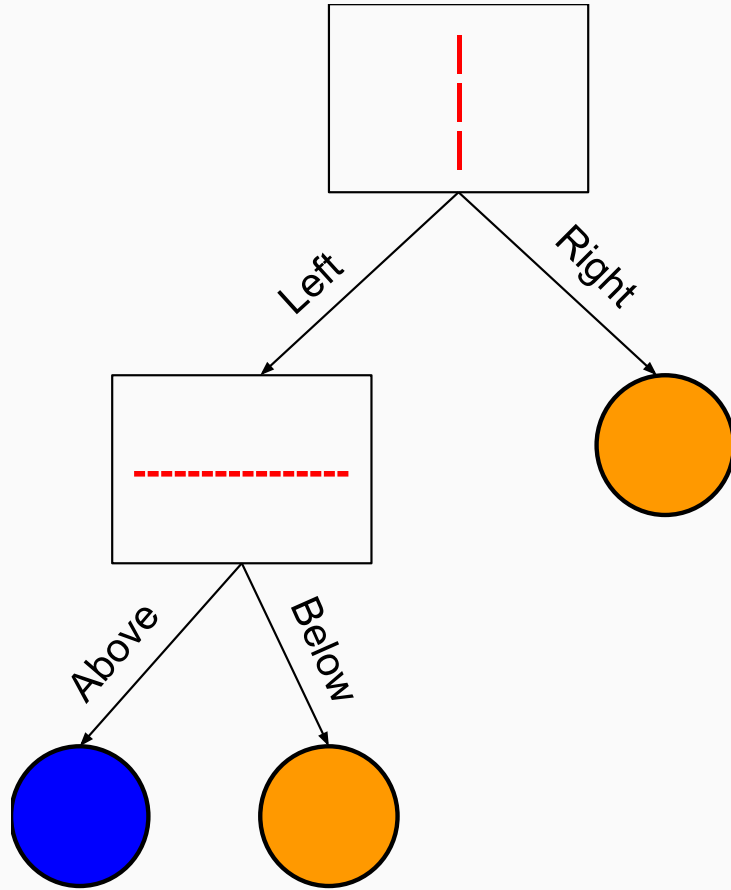
What is a decision tree? An example.



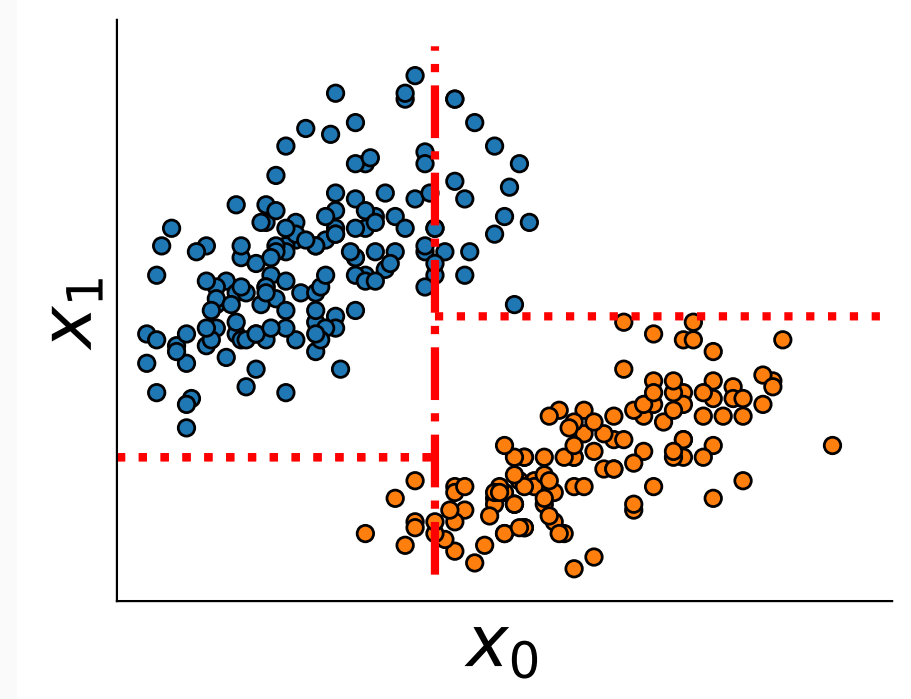
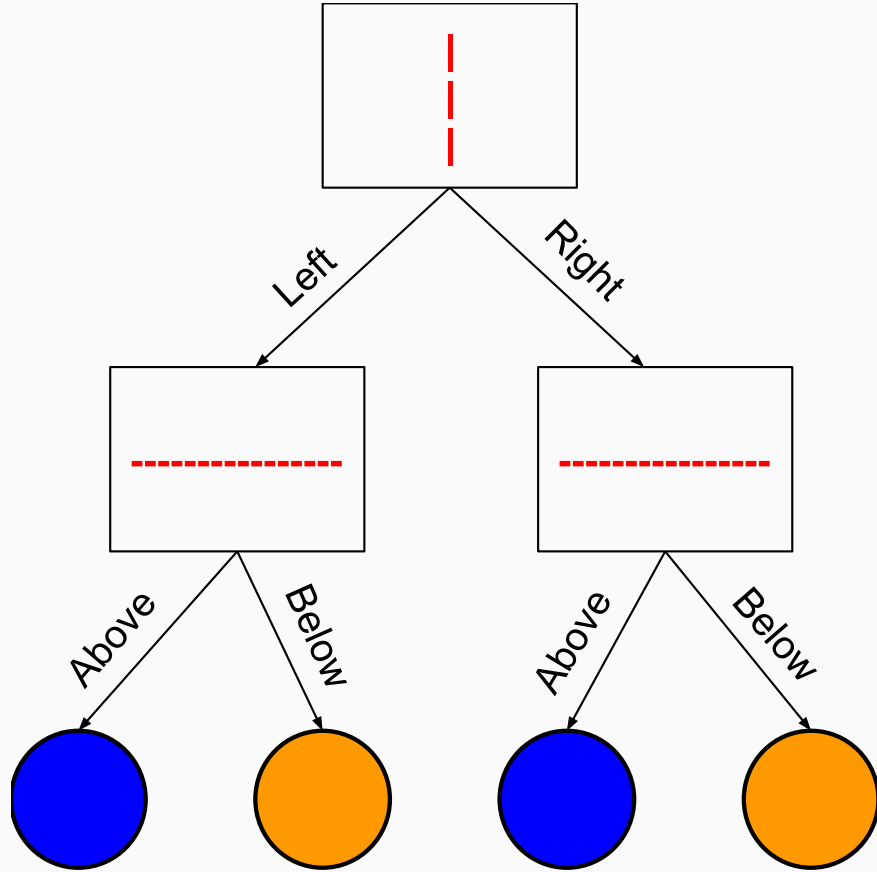
Growing a classification tree



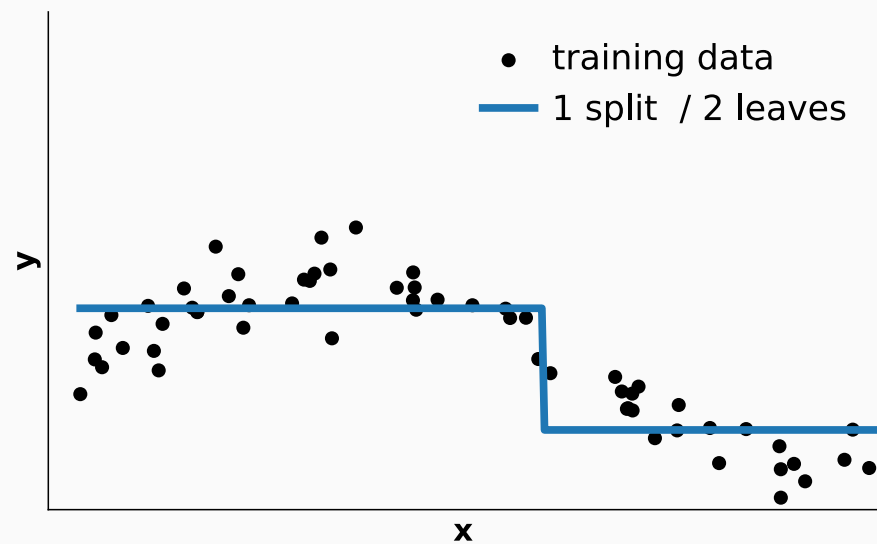
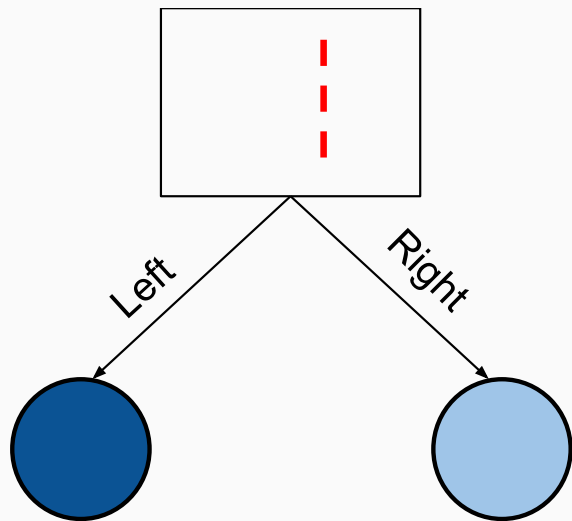
Growing a classification tree



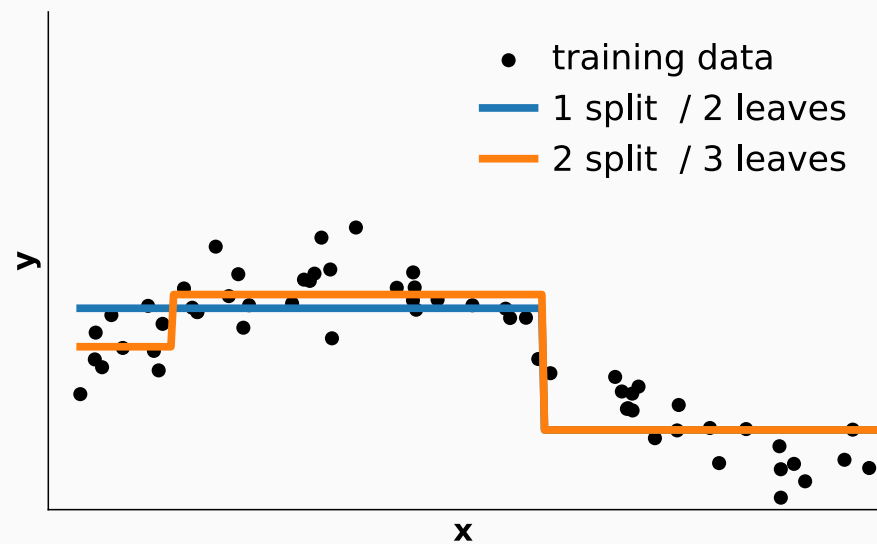
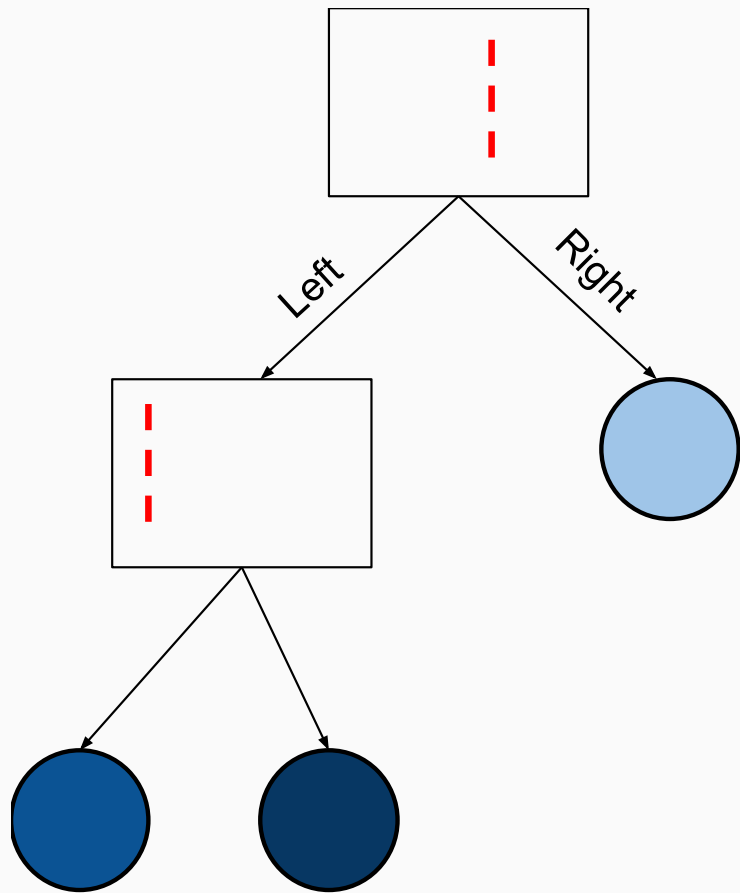
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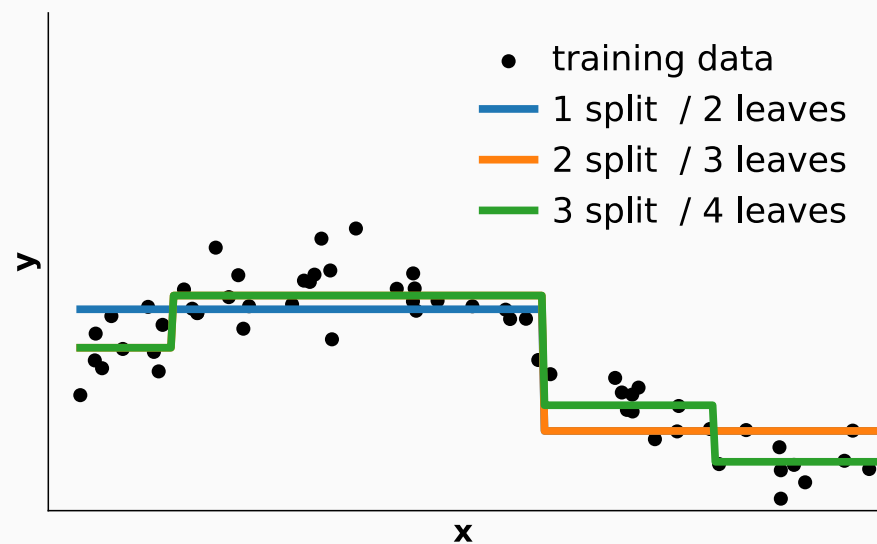
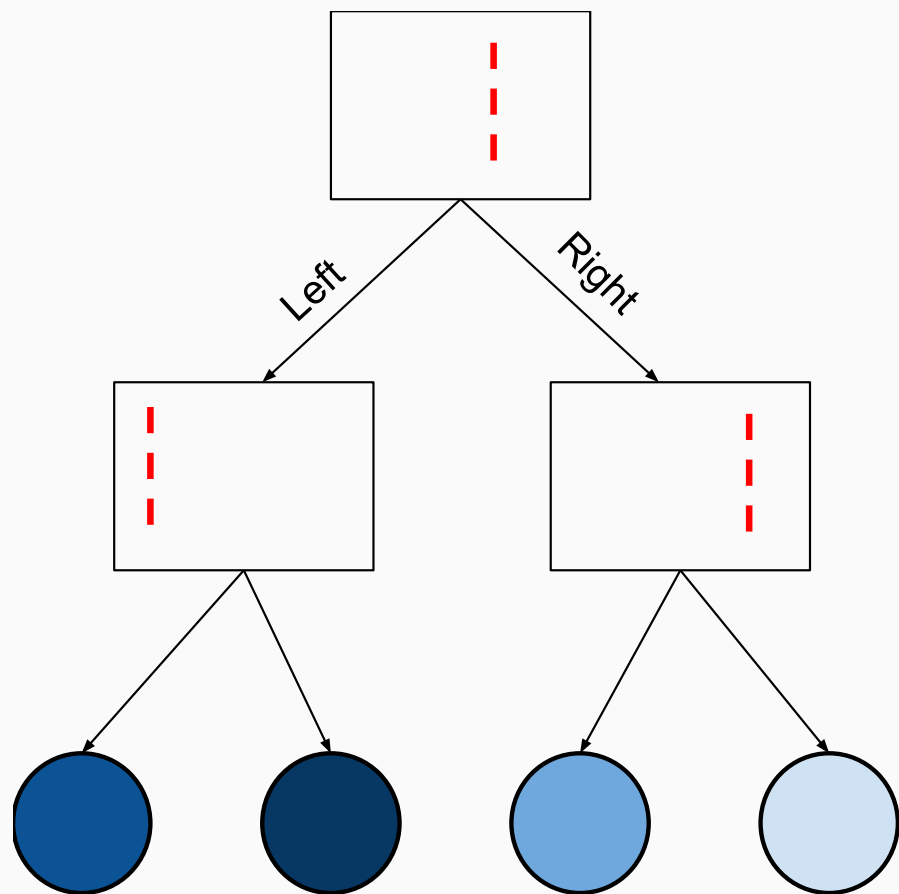
Growing a regression tree



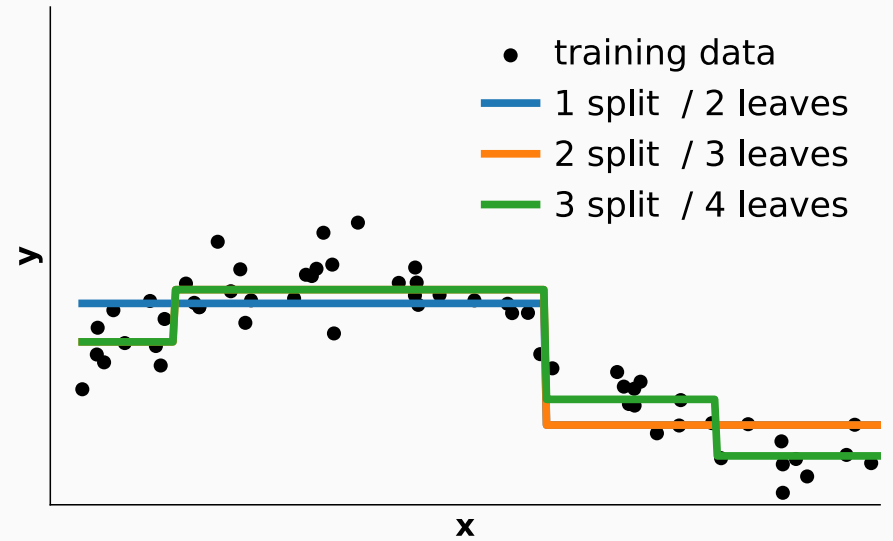
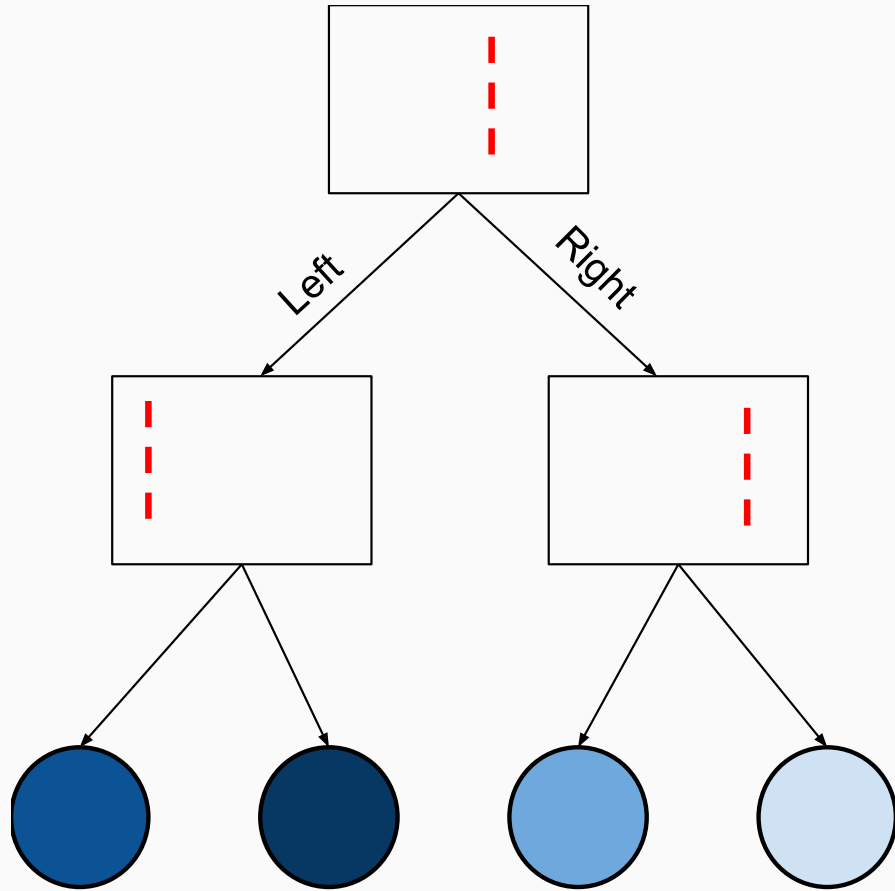
Growing a regression tree



Growing a regression tree



Growing a regression tree



Remark: Trees don't extrapolate outside training data

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

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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:

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

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

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

Classification

Gini impurity

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

Classification

Gini impurity

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Classification

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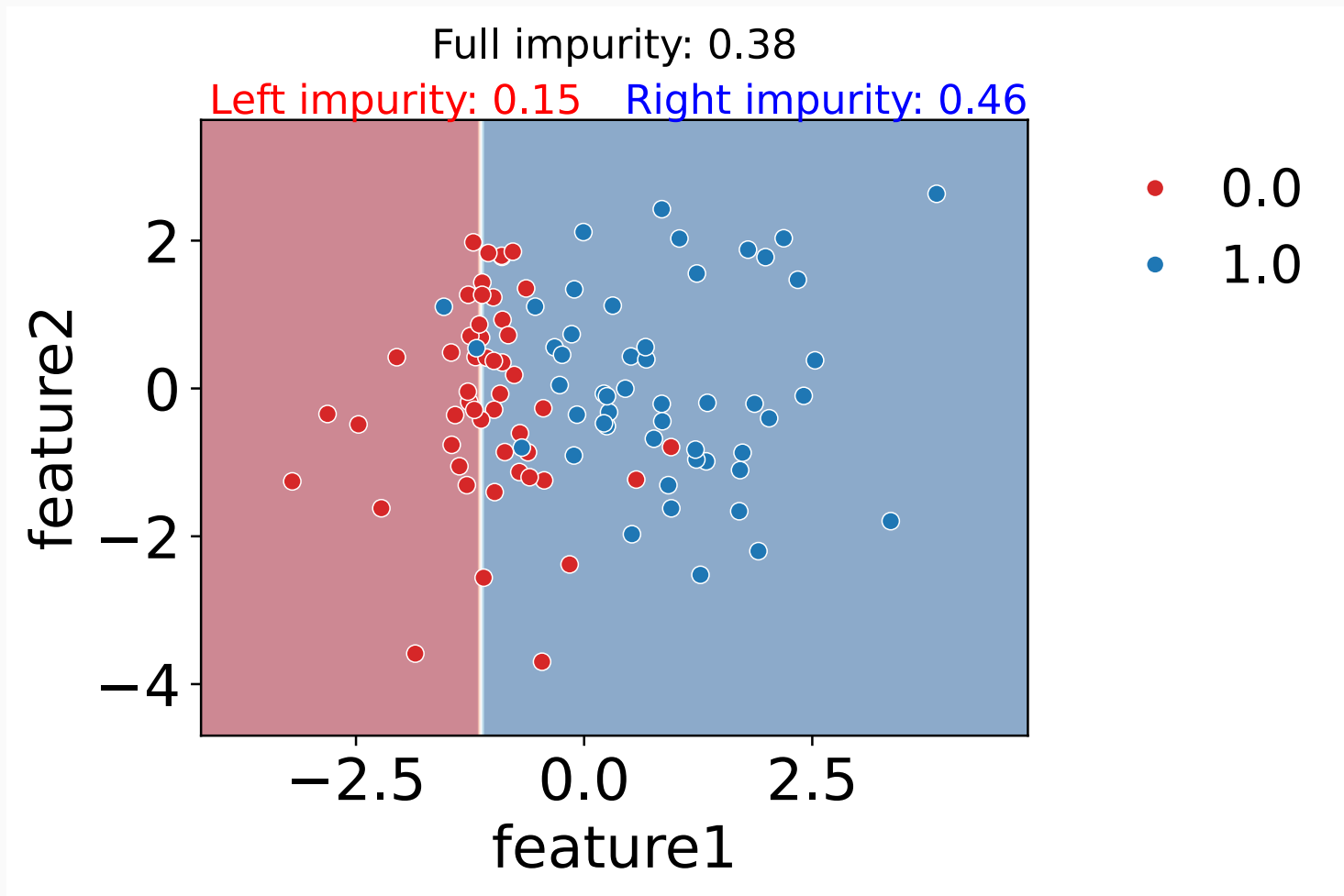
Regression

Mean squared error

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

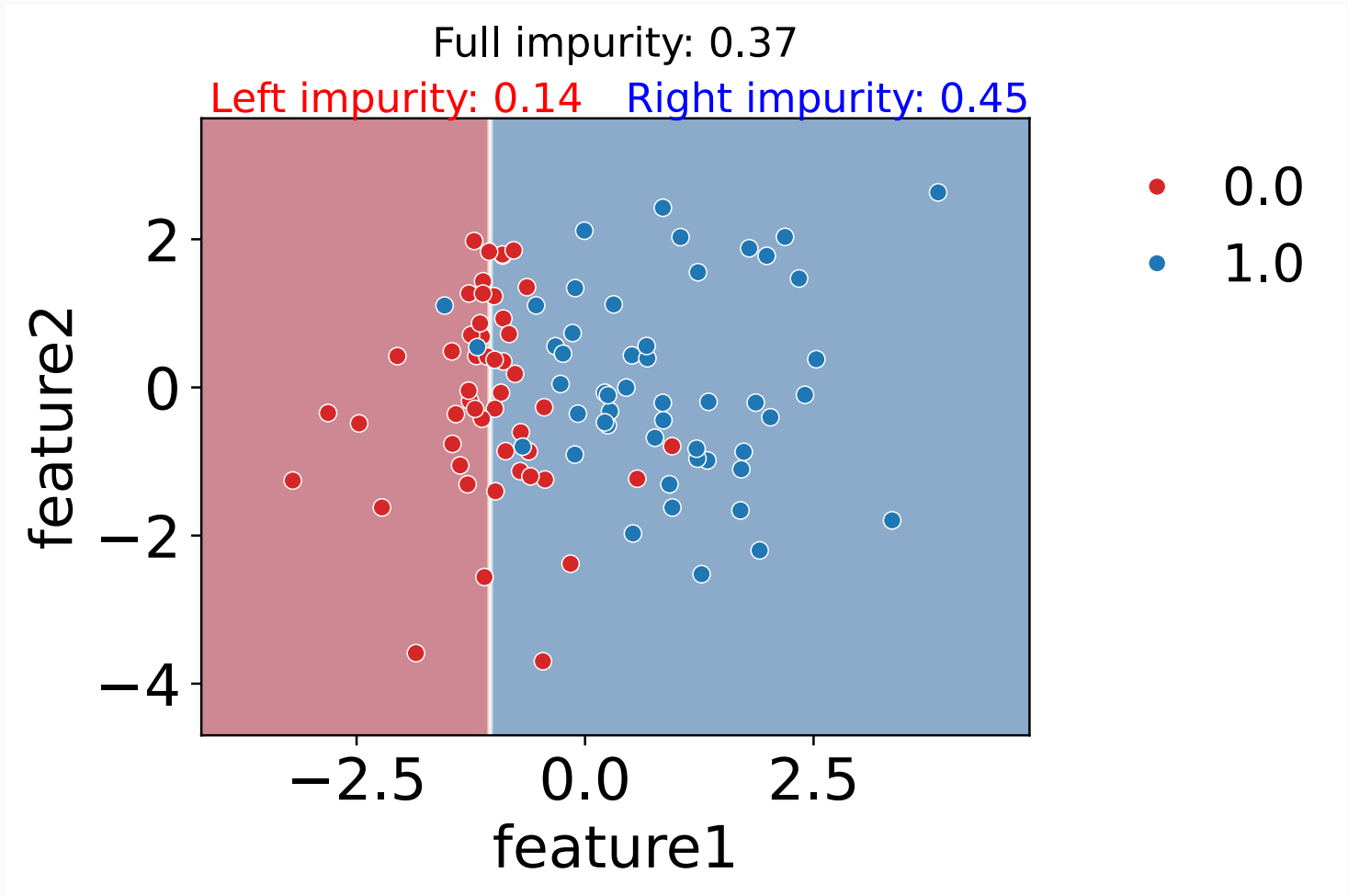
Chose the best split: example

Random split



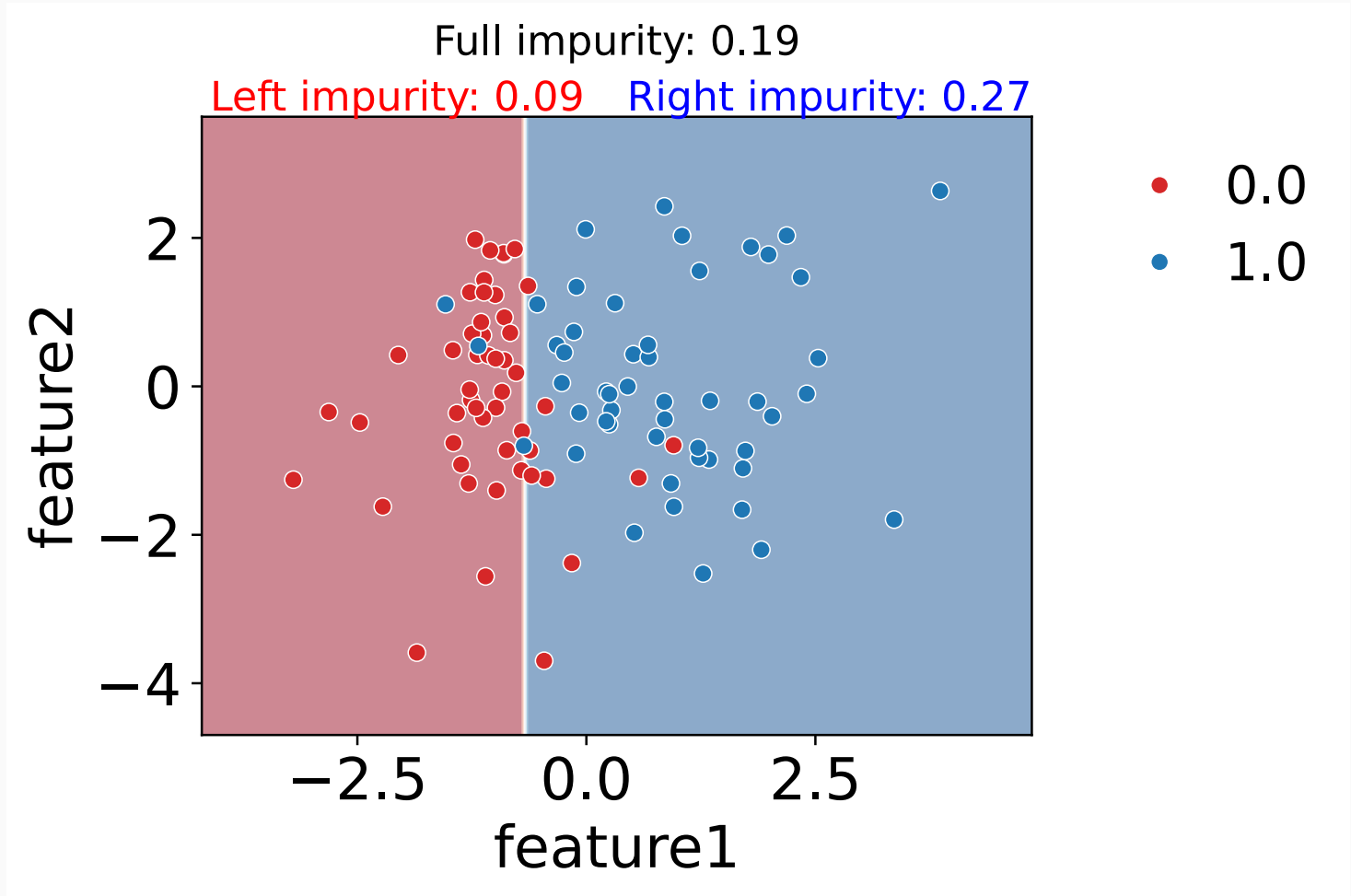
Chose the best split: example

Moving the split to the right from one point



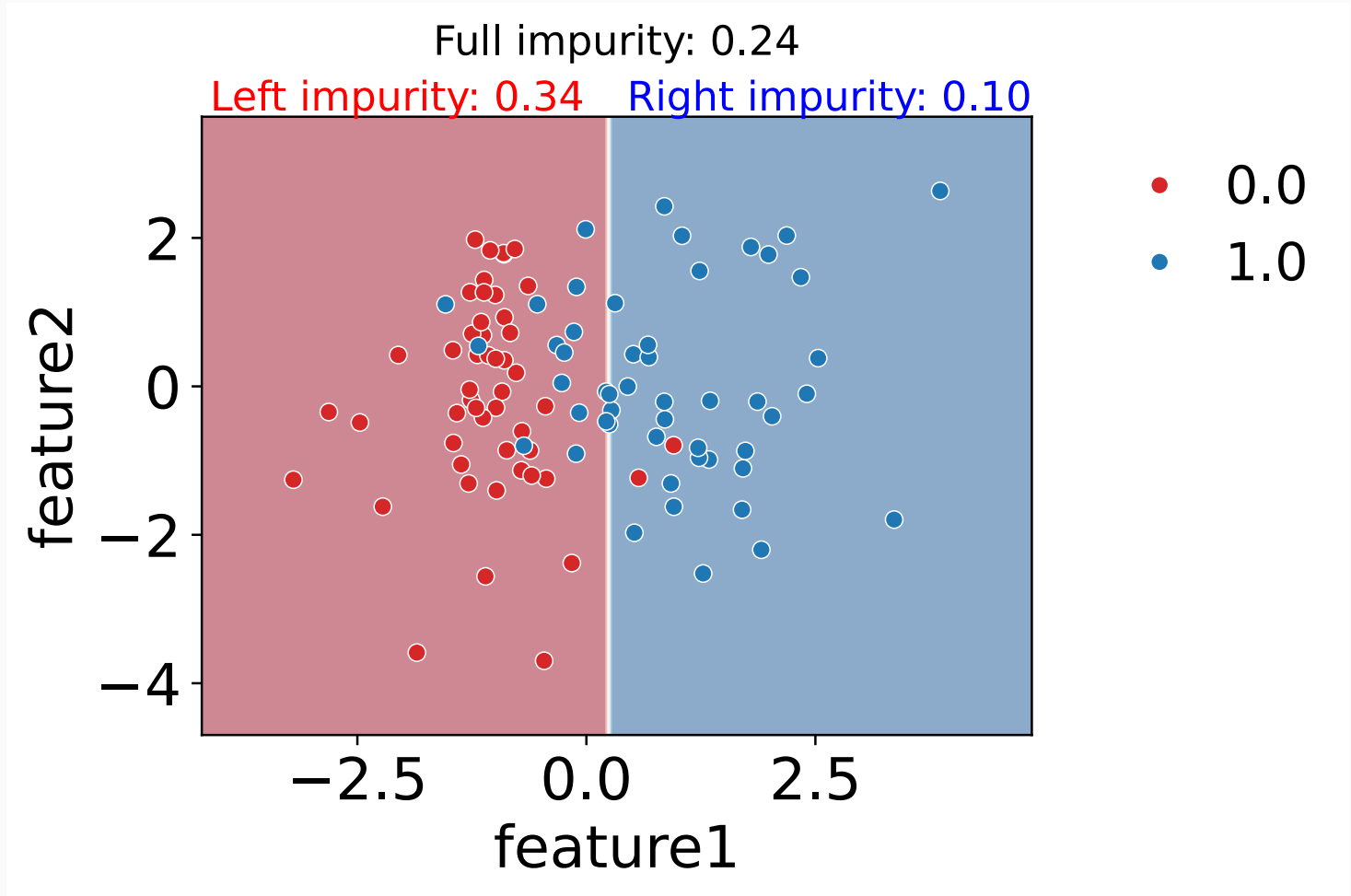
Chose the best split: example

Moving the split to the right from 10 points



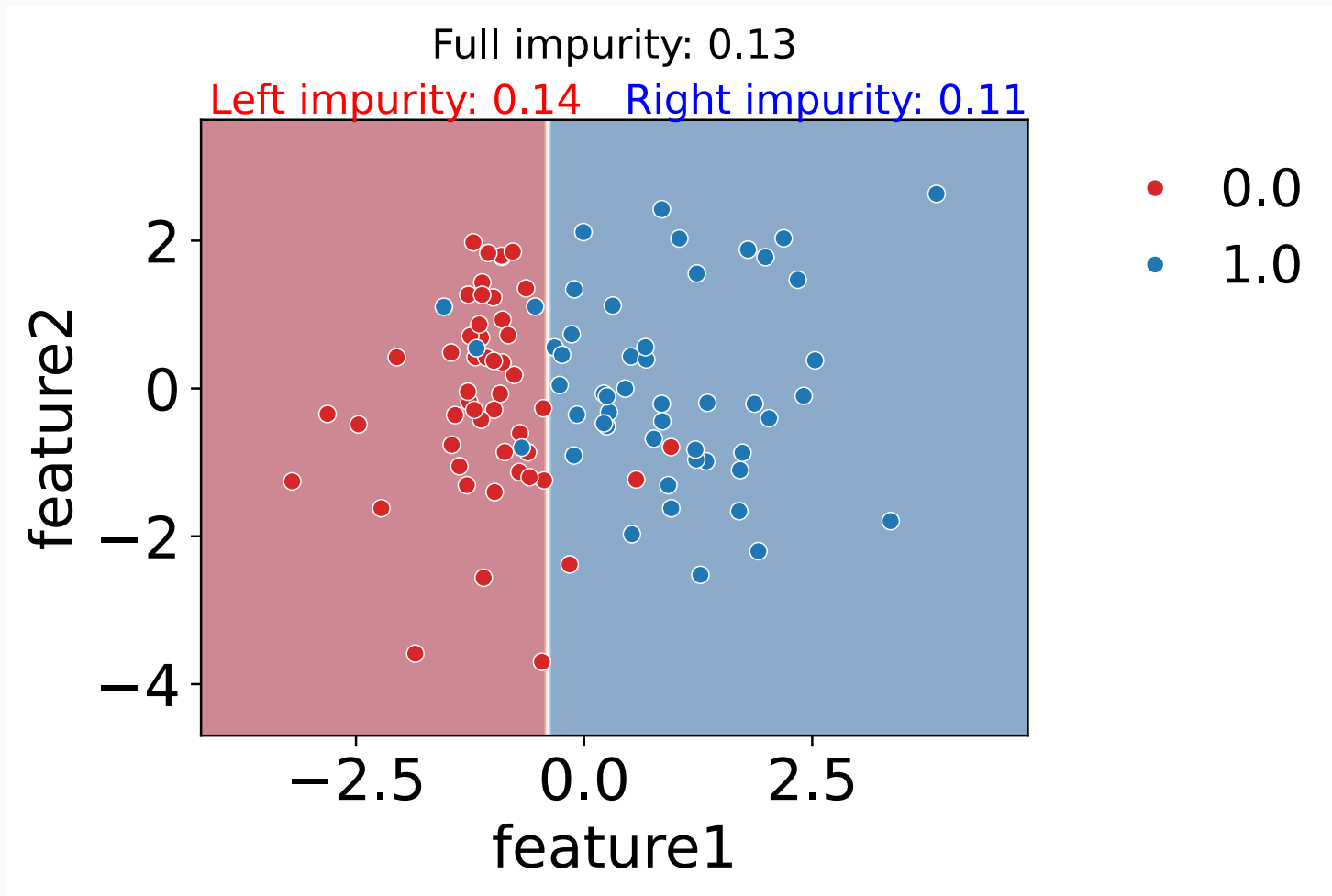
Chose the best split: example

**Moving the split to
the right from 20
points**

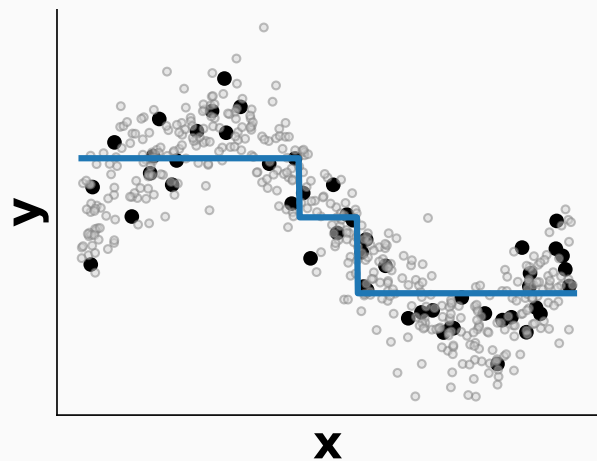


Chose the best split: example

Best split

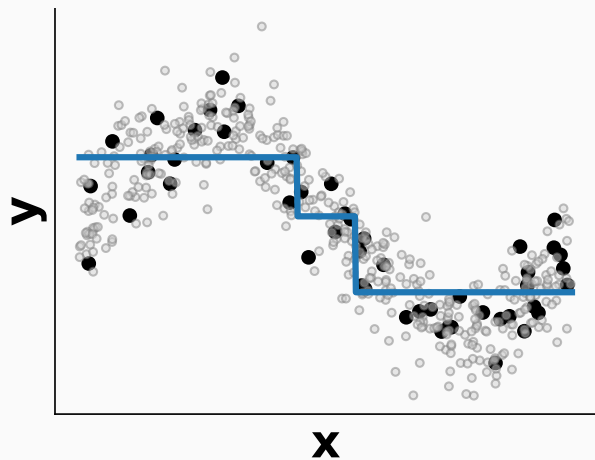


Tree depth and overfitting

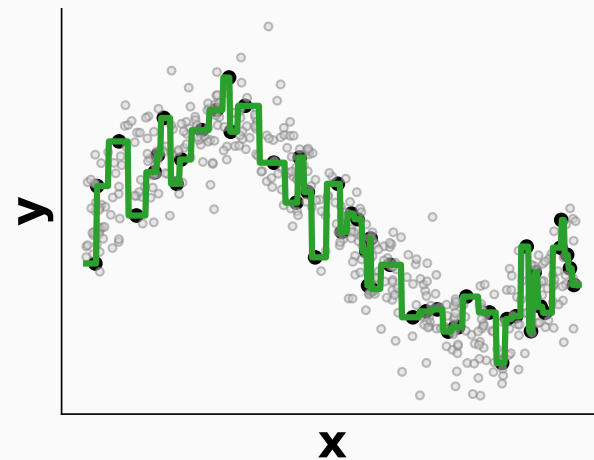


Underfitting
max_depth or
max_leaf_nodes
too small

Tree depth and overfitting

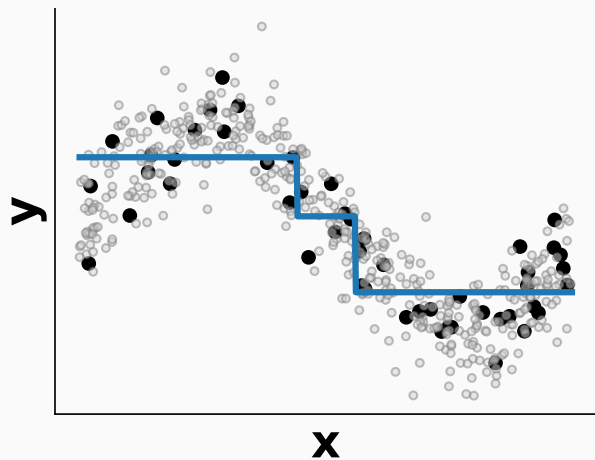


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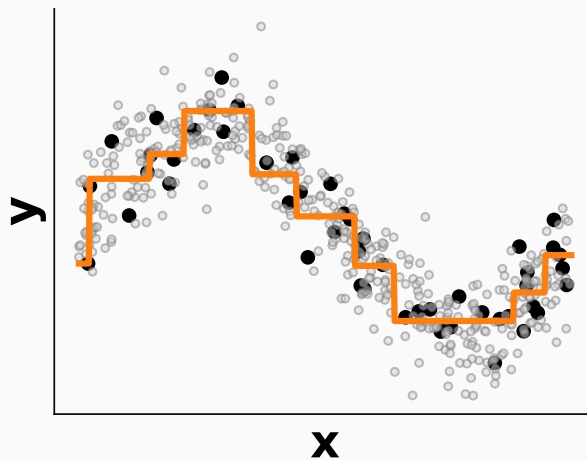


Overfitting
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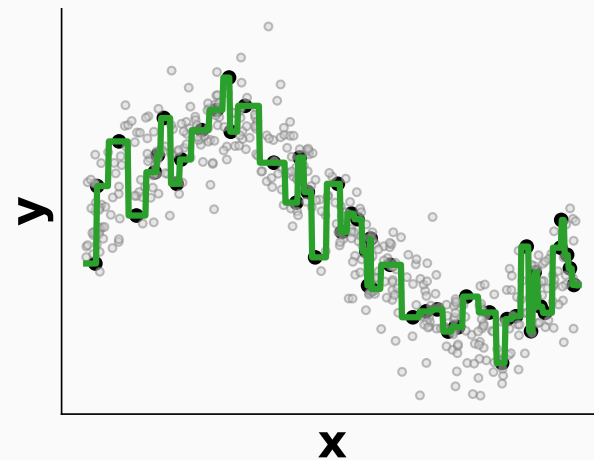
Tree depth and overfitting



Underfitting
max_depth or
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too small




Best trade-off



Overfitting
max_depth or
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Main hyper-parameters of tree models

```
1 DecisionTreeRegressor( Python  
2     criterion="squared error",  
3     max_depth=None, # Tree depth (assume symmetric trees)  
4     min_samples_split=2, # Tree depth (allowing asymmetric trees)  
5     min_samples_leaf=1, # Tree depth (allowing asymmetric trees)  
6     max_leaf_nodes=None, # Tree depth (allowing asymmetric trees)  
7     min_impurity_decrease=0.0, # Tree depth (allowing asymmetric trees)  
8 )
```

Pros

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

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

Bootstrap resampling (random sampling with replacement) proposed by (Breiman, 1996)

Built upon Bootstrap, introduced by (Efron, 1992) to estimate the variance of an estimator.

Ensemble models: Bagging ie. Bootstrap AGGREGatING

Bootstrap resampling (random sampling with replacement) proposed by (Breiman, 1996)

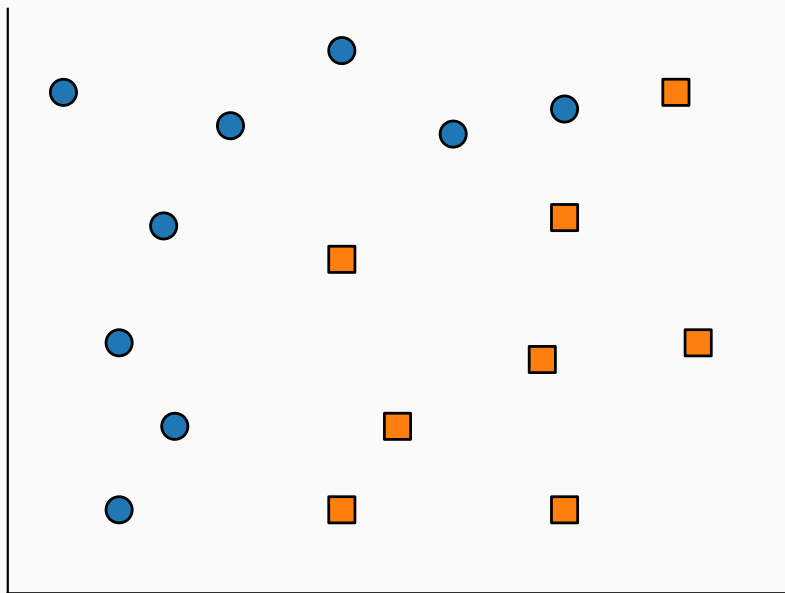
Built upon Bootstrap, introduced by (Efron, 1992) to estimate the variance of an estimator.

Bagging is used in machine learning to reduce the variance of a model prone to overfitting

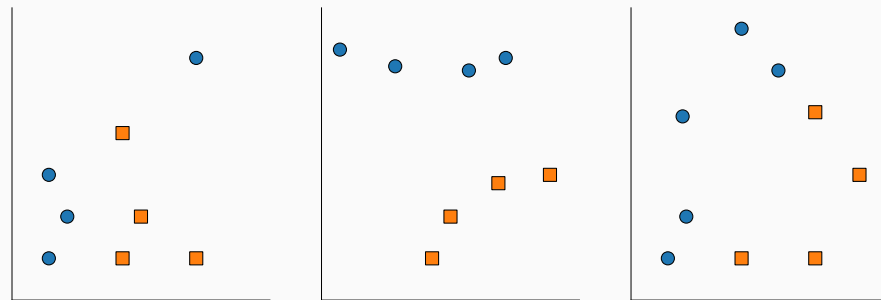
Can be used with any model!

Random forests: Bagging with classification trees

Full dataset

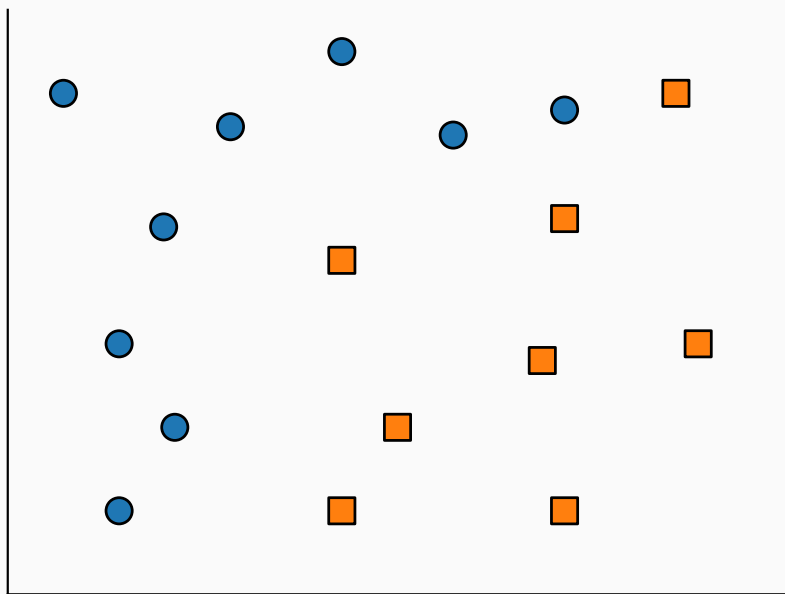


Three bootstrap samples

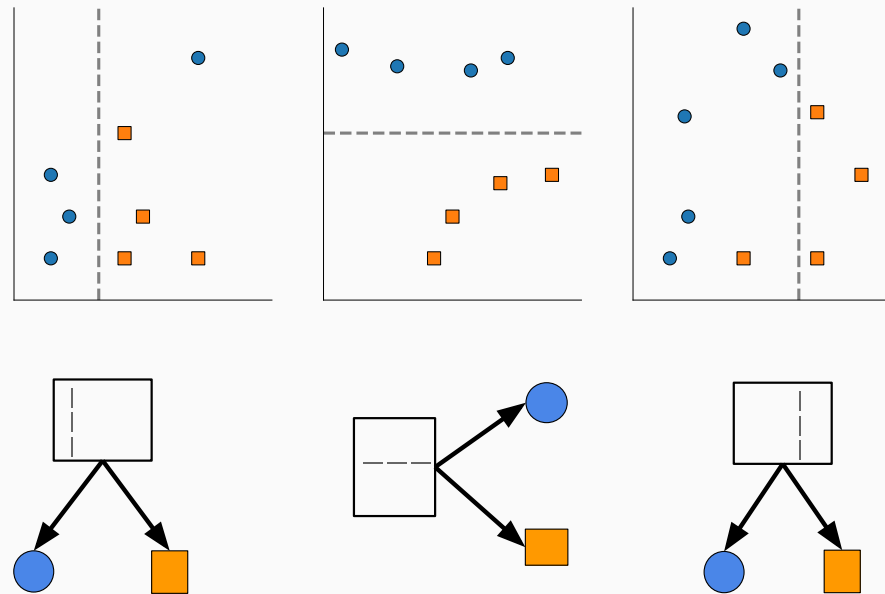


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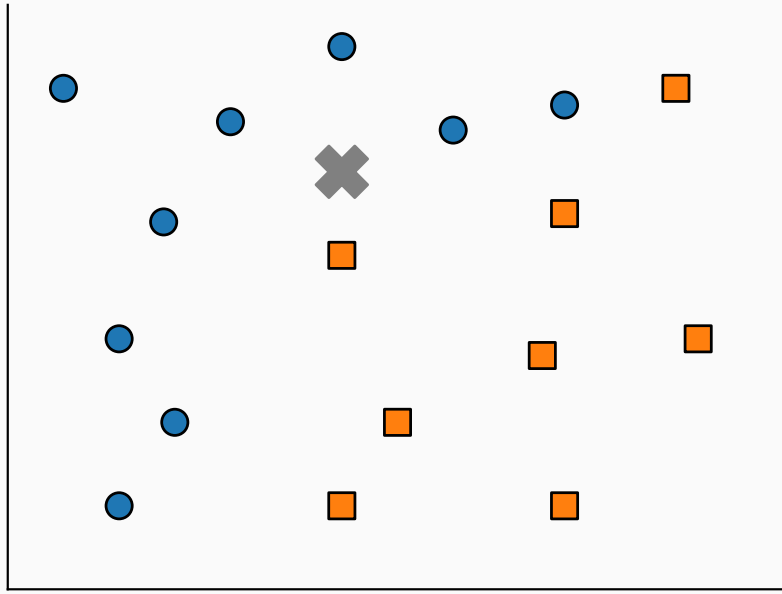


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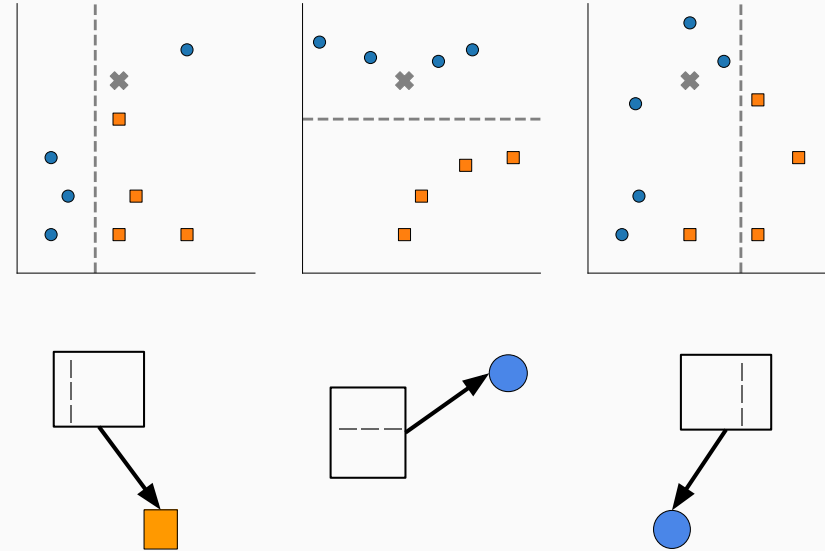


Random forests: Bagging with classification trees

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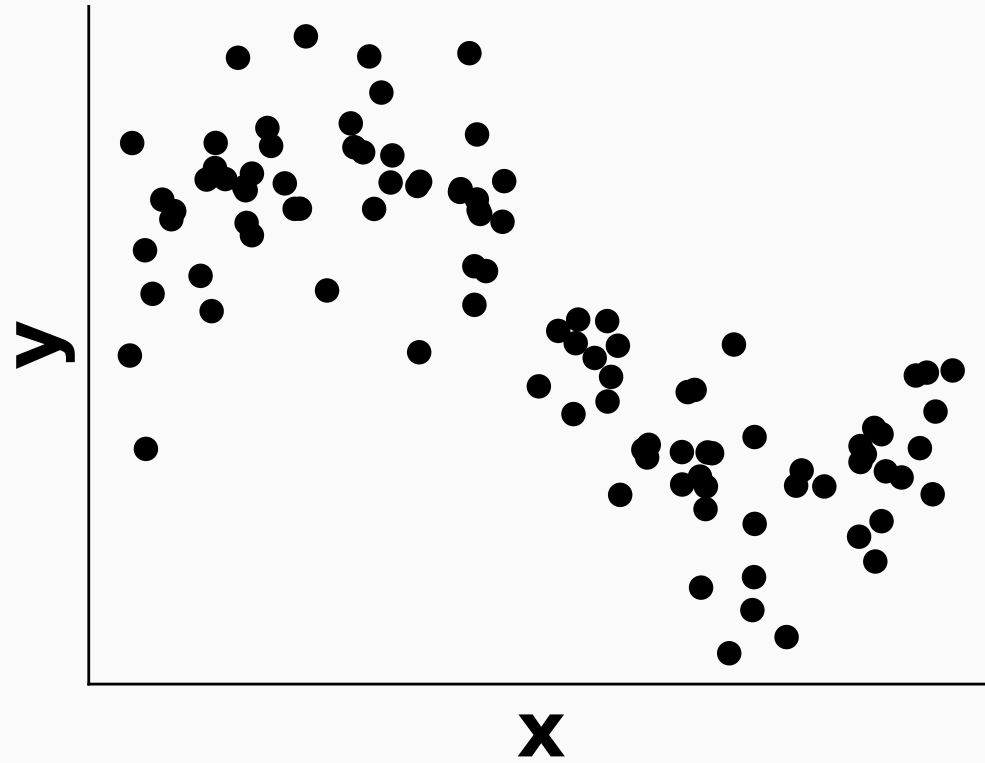
Three bootstrap samples



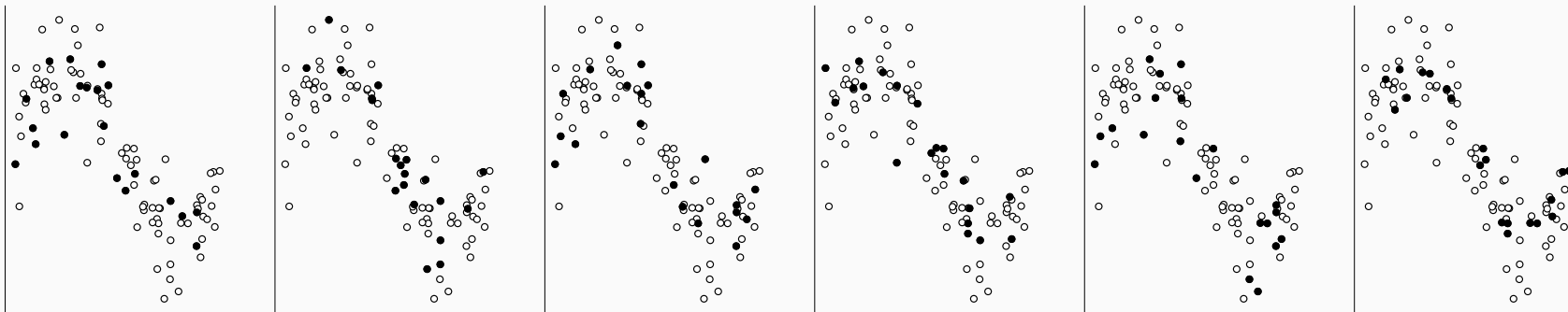
For a new observation, each tree predicts a class

$$\text{VOTE} (\blacksquare , \bullet , \bullet) = \bullet$$

Random forests: Bagging with regression trees

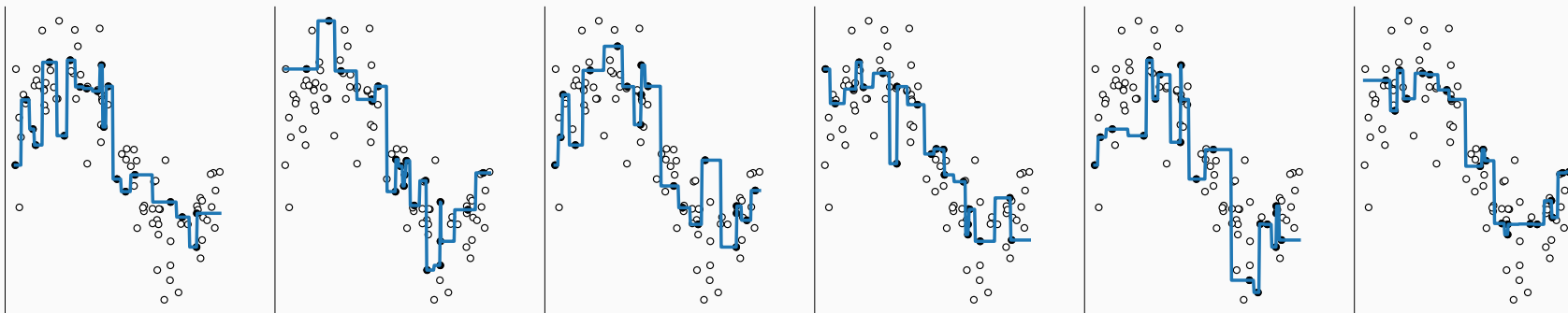


Random forests: Bagging with regression trees



Bootstrap multiple subsets

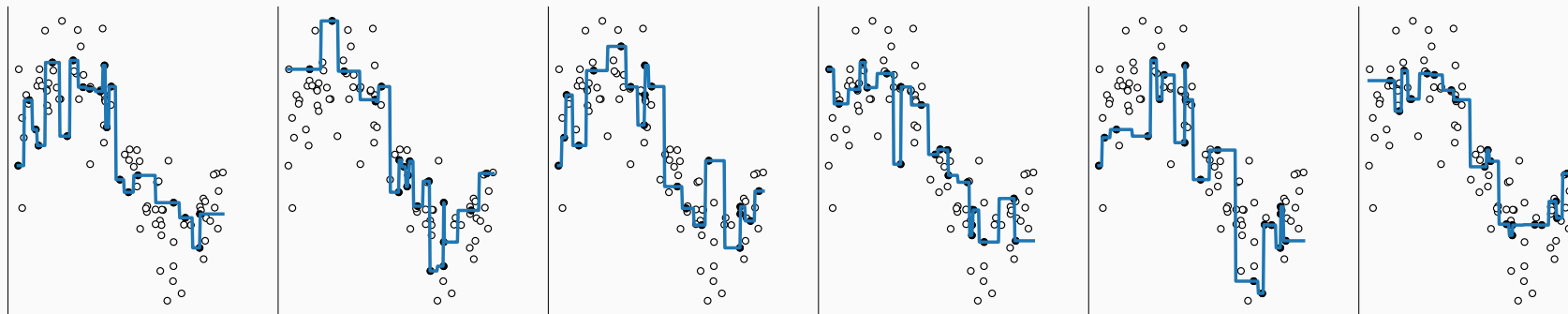
Random forests: Bagging with regression trees



Bootstrap multiple subsets

Fit one model to each subset

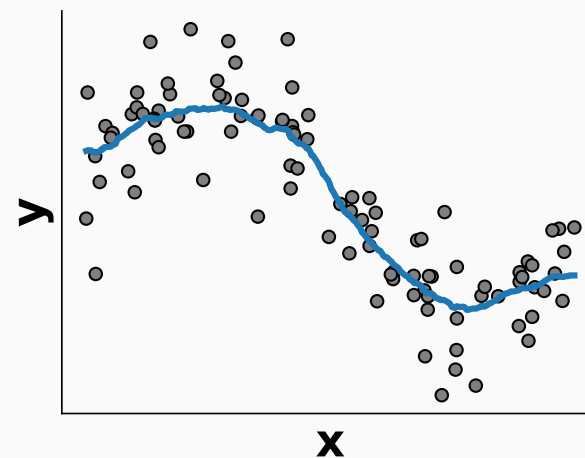
Random forests: Bagging with regression trees




Bootstrap multiple subsets

Fit one model to each subset

Average the predictions



Main hyper-parameters of random forests

```
1  sklearn.ensemble.RandomForestRegressor( Python  
2      n_estimators=100, # Number of trees to fit (sample randomization): not useful  
   to tune in practice  
3      criterion='squared_error',  
4      max_depth=None, # tree regularization  
5      min_samples_split=2, # tree regularization  
6      min_samples_leaf=1, # tree regularization  
7      min_impurity_decrease=0.0, # tree regularization  
8      n_jobs=None, # Number of jobs to run in parallel  
9      random_state=None, # Seed for randomization  
10     max_features=1.0, # Number/ratio of features at each split (feature  
   randomization)  
11     max_samples = None # Number of sample to draw (with replacement) for each tree  
12 )
```

Random Forests are bagged randomized decision trees

Random forests

- For each tree a random subset of samples are selected
- At each split a random subset of features are selected (more randomization)
- The best split is taken among the restricted subset
- Feature randomization decorrelates the prediction errors
- Uncorrelated errors make bagging work better

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Take away

- Bagging and random forests fit trees independently
- Each deep tree overfits individually
- Averaging the tree predictions reduces overfitting

Boosting use multiple iterative models

- Use of simple underfitting models: eg. shallow trees
- Each model corrects the errors of the previous one

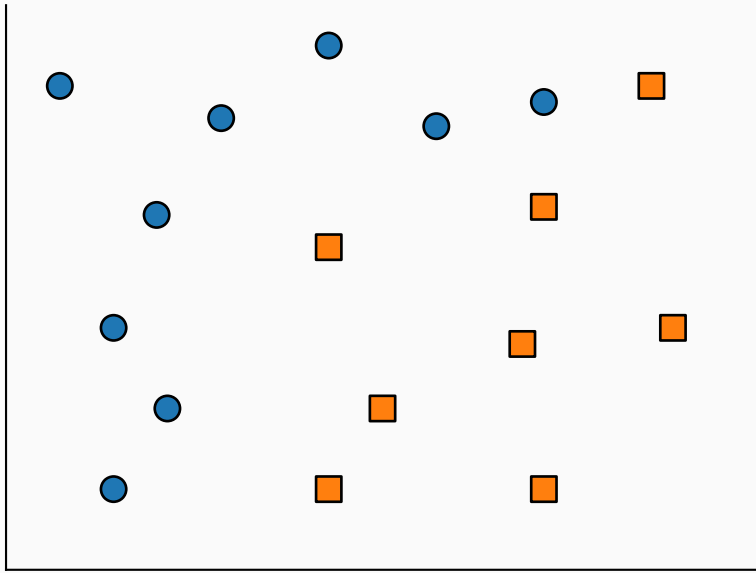
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Two examples of boosting

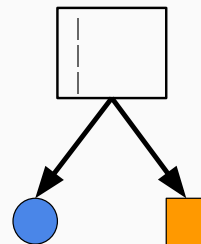
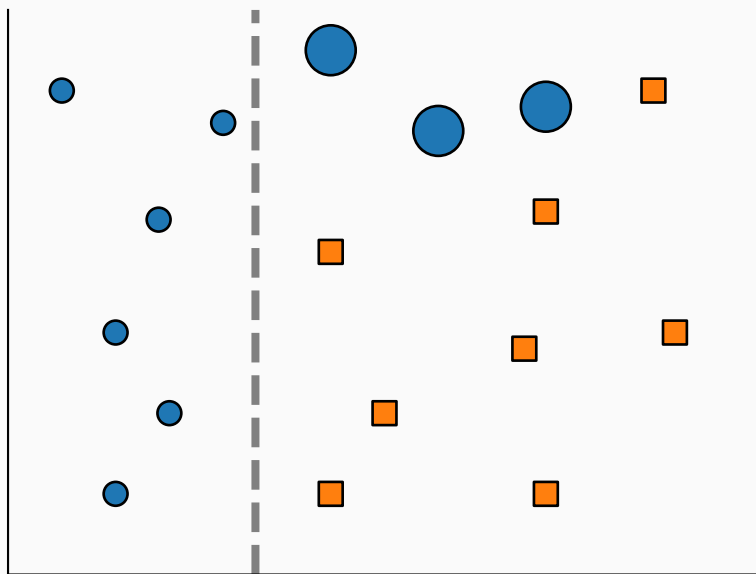
- Adaptive boosting (AdaBoost): reweight mispredicted samples at each step (Friedman et al., 2000)
- Gradient boosting: predict the negative errors of previous models at each step (Friedman, 2001)

Boosting: Adaptive boosting, classification example

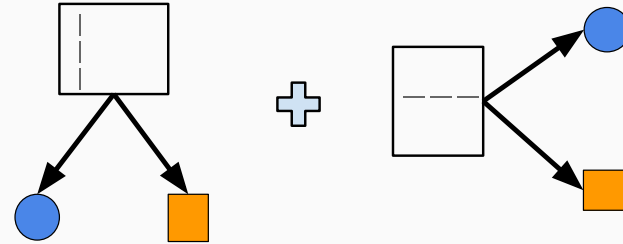
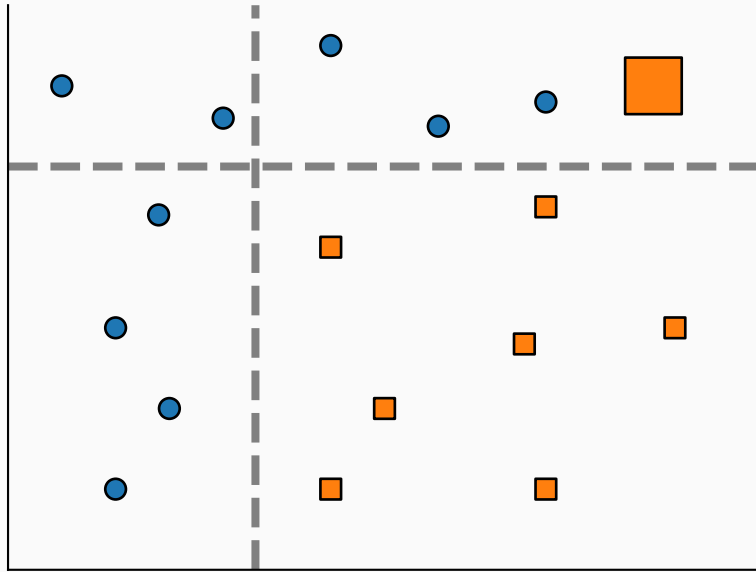


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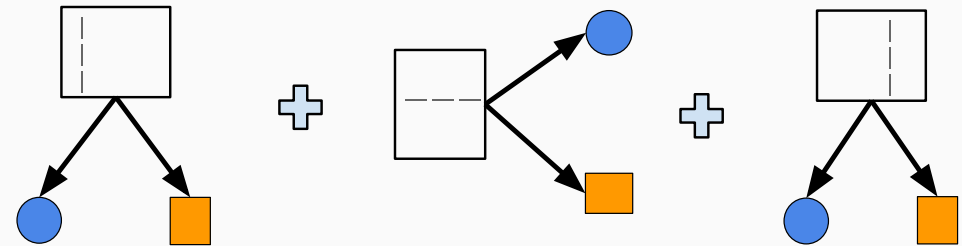
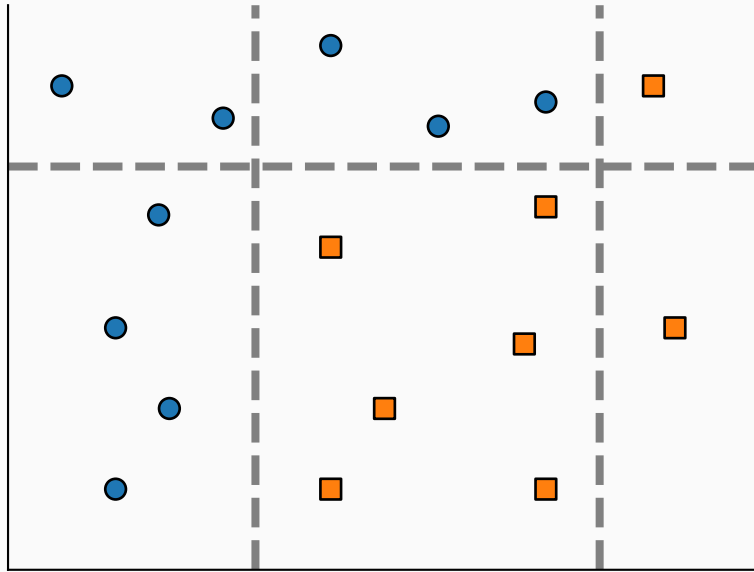
First prediction:



Boosting: Adaptive boosting, classification example



Boosting: Adaptive boosting, classification example



**At each step, reweights
mispredicted samples**

Adaboost for classification: choice of the weight

Motivation in (Murphy, 2022)

1. Initialize the observation weights $w_i = \frac{1}{N}, i = 1..N$

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Adaboost: Take-away

- Sequentially fit weak learners (eg. shallow trees)
- Each new learner corrects the errors of the previous one thanks to sample weights
- The final model is a weighted sum of the weak learners
- The weights are learned by the algorithm to give more importance to errors
- Any weak learner can be used

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Adaboost is tailored to a specific loss function (exponential loss)



Can we exploit the boosting idea for any loss function?

Gradient boosting: how to choose the iterative learners?

Boosting formulation

$F_{m(x)} = F_{m-1}(x) + h_{m(x)}$ with F_{m-1} the previous estimator, h_m , new weak learner.

Minimization problem

$$h_m = \operatorname{argmin}_h (L_m) = \operatorname{argmin}_h \sum_{i=1}^n l(y_i, F_{m-1}(x_i) + h(x_i))$$

Expand the loss inside the sum using a Taylor expansion.

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Finally: $h_m = \operatorname{argmin}_h \sum_{i=1}^n h(x_i) g_i \rightarrow$ kind of an inner product $\langle g, h \rangle$

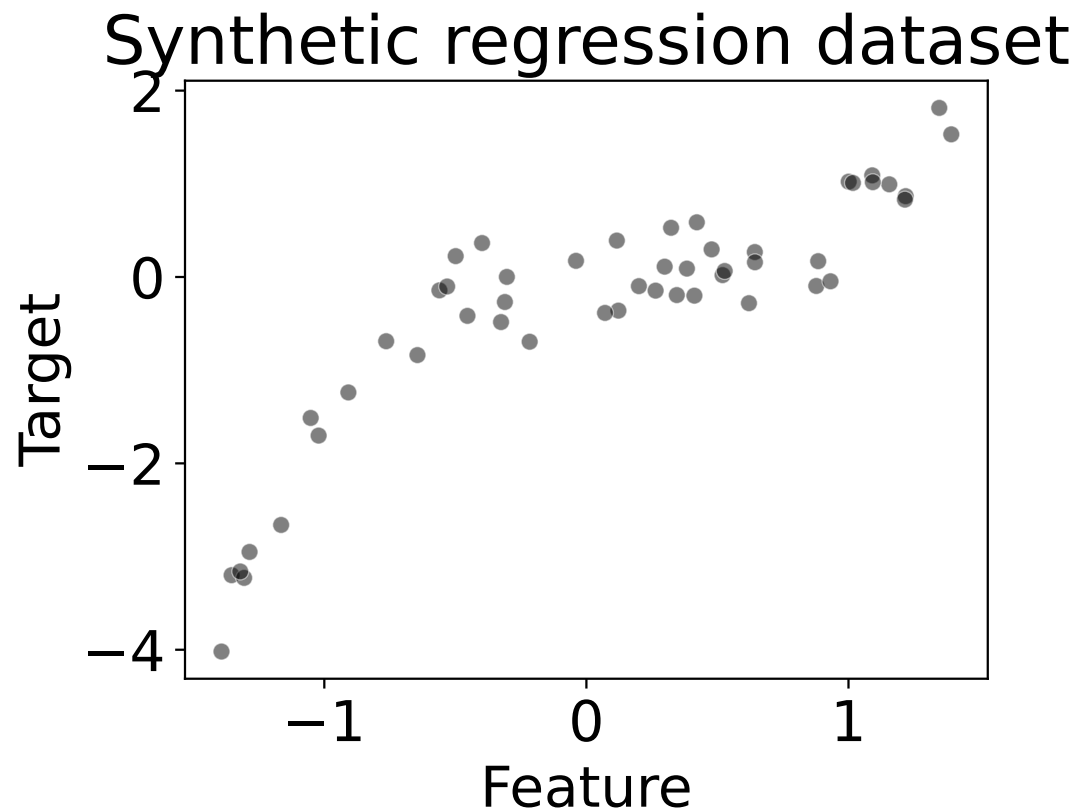
So $h_{m(x_i)}$ should be proportional to $-g_i$, so **fit h_m to the negative gradient**.

Boosting: Gradient boosting, regression example

Regression

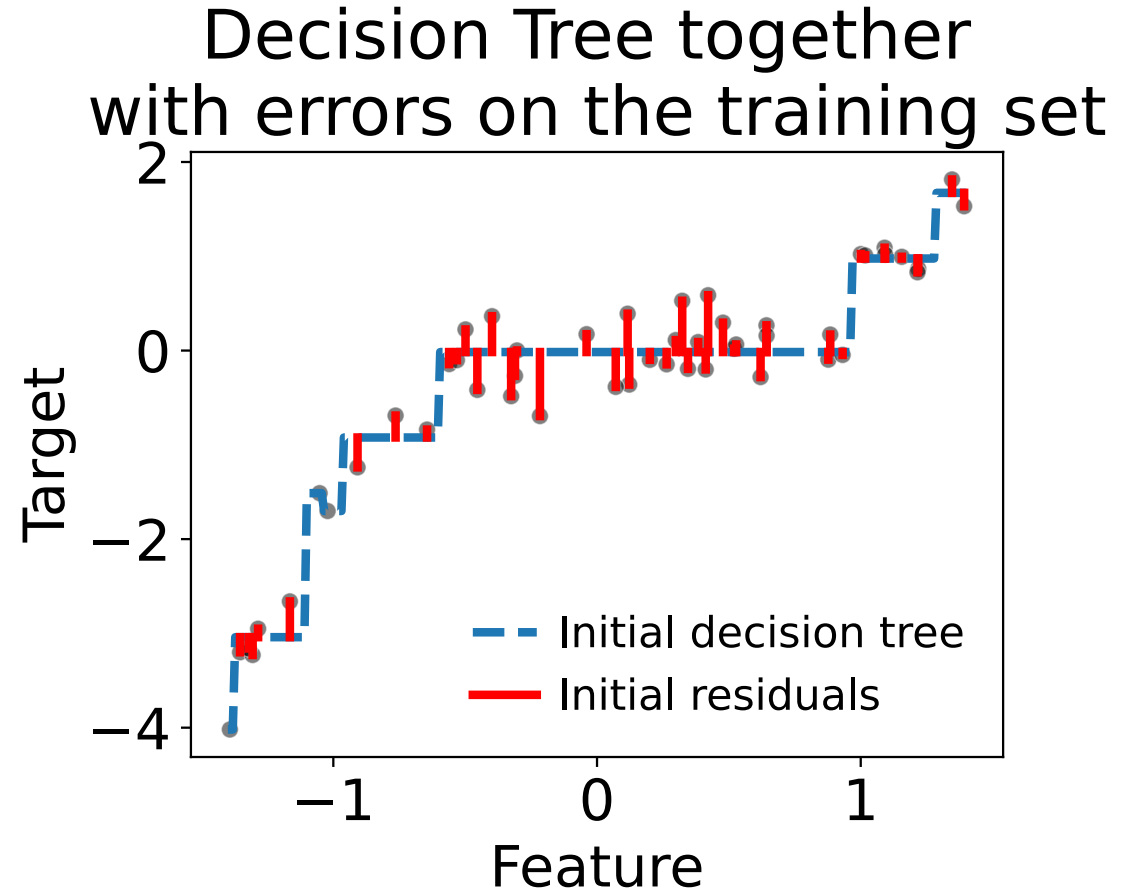
- squared loss: $l(y, F(x)) = (y - F(x))^2$
- gradient: $g_i = -2(y_i - F_{m-1}(x_i))$

💡 The new tree should fit the residuals



Boosting: Gradient boosting, regression example

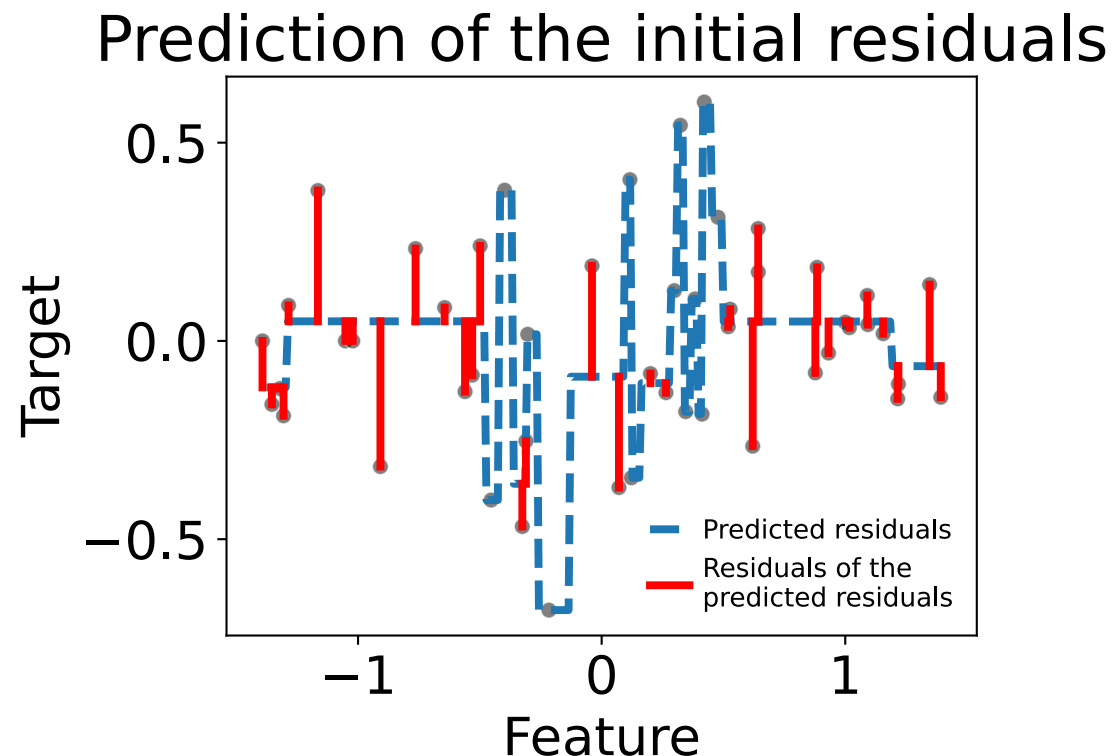
**Fit a shallow tree
(depth=3)**



Boosting: Gradient boosting, regression example

Fit a second tree to the residuals

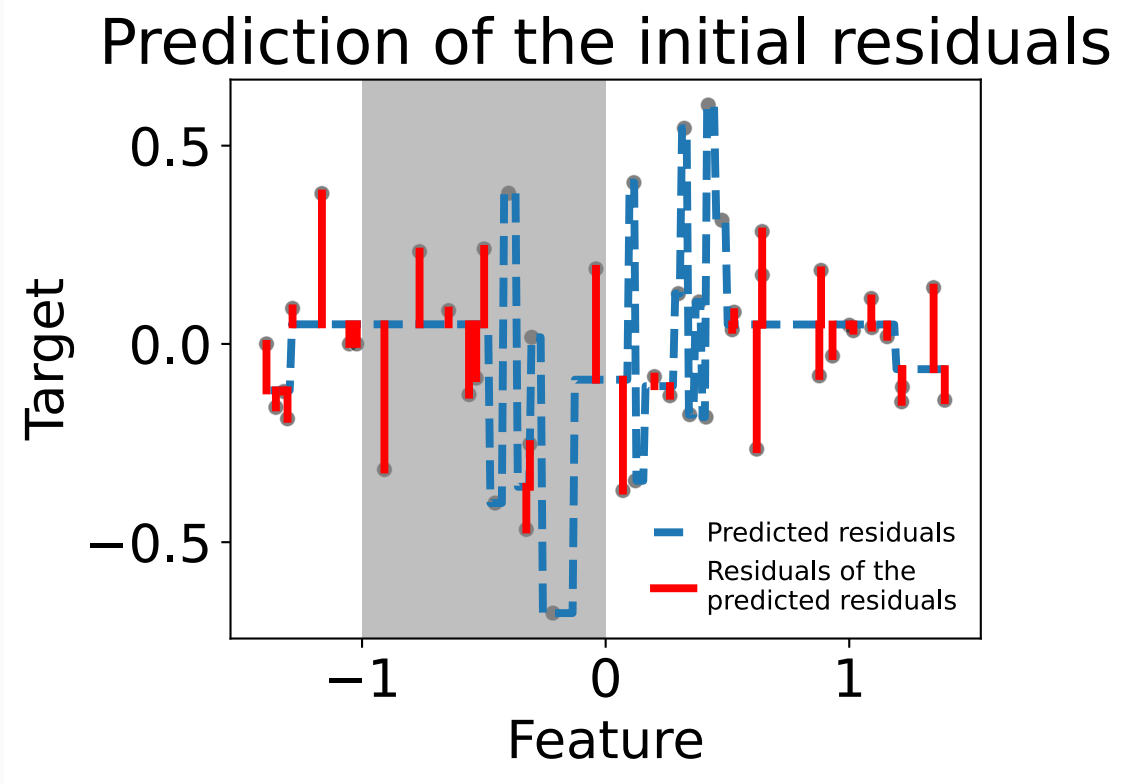
- This tree performs poorly on some samples.



Boosting: Gradient boosting, regression example

Fit a second tree to the residuals

- This tree performs well on some residuals.
- Zoom on some of these poorly fitted residuals.



Boosting: Gradient boosting, regression example

Focus on a sample

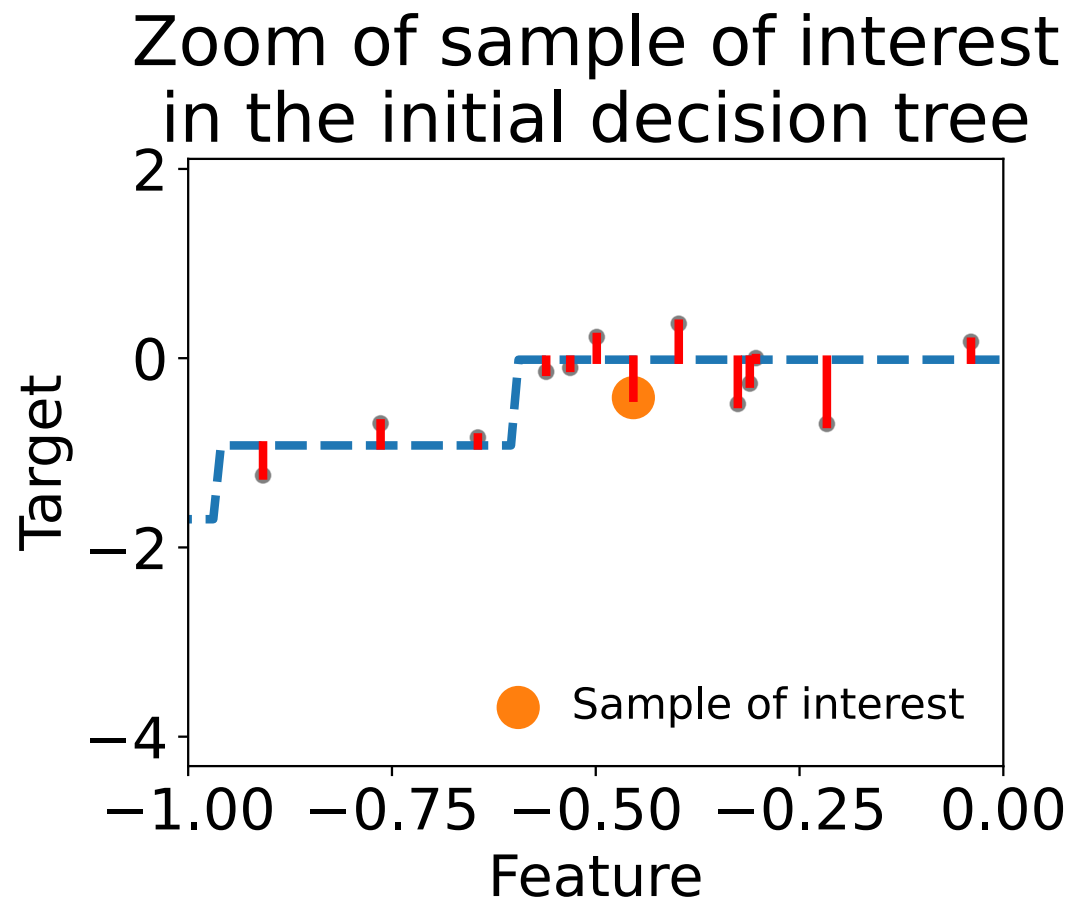
$$(x_i, y_i) = (-0.454, -0.417)$$

First tree prediction

$$\text{Prediction: } f_1(x_i) = -0.016$$

Residuals:

$$y_i - f_1(x_i) = -0.401$$



Boosting: Gradient boosting, regression example

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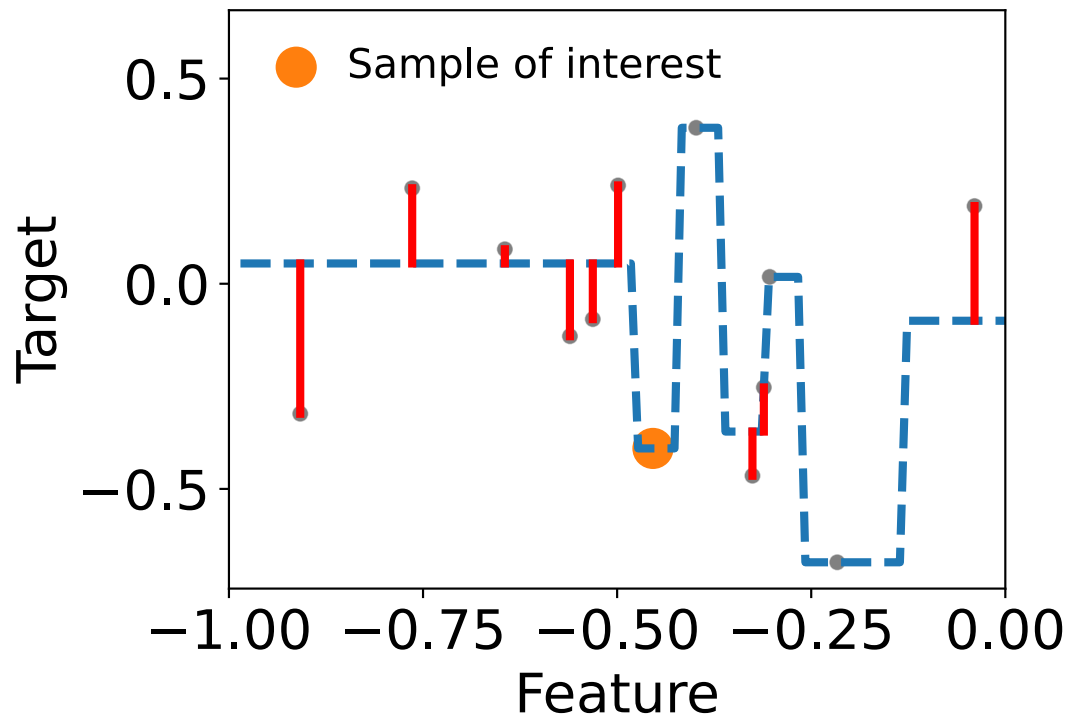
Second tree prediction

$$\text{Prediction: } f_2(x_i) = -0.401$$

Residuals:

$$y_i - f_1(x_i) - f_2(x_i) = 0$$

Zoom of sample of interest
in the initial residuals



Faster gradient boosting with binned features

 **Gradient boosting is slow when $N > 10,000$**

Fitting each tree is quite slow: $O(pN \log(N))$ operations

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 **XGBoost: eXtreme Gradient Boosting (Chen & Guestrin, 2016)**

- Missing values support
- Parallelization
- Second order Taylor expansion

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XGBoost: eXtreme Gradient Boosting (Chen & Guestrin, 2016)

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HistGradientBoosting: sklearn implementation of lightGBM (Ke et al., 2017)

- Missing values support
- Parallelization
- Discretize numerical features into 256 bins: less costly for tree splitting

Take away for ensemble models

Bagging (eg. Random forests)	Boosting
Fit trees independently	Fit trees sequentially
Each deep tree overfits	Each shallow tree underfits
Averaging the tree predictions reduces overfitting	Sequentially adding trees reduces underfitting

A quick word on other families of models

Generalized linear models

Link an OLS ($X\beta$) to the parameters of various probability distributions.

Examples: Poisson regression (for count data), logistic regression.

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Local methods with appropriate basis functions (kernels).

Kernels are often chosen with expert knowledge.

Other well known families of models

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Local methods with appropriate basis functions (kernels).

Kernels are often chosen with expert knowledge.

Deep neural networks (deep learning)

Iterative layers of parametrized basis functions: eg. $\mathbb{1}[wX + b \geq 0]$

Trainable by gradient descent: each layer should be differentiable.

Training with backpropagation ie. automatic differentiation and gradient methods.

A word on deep learning

Success of deep learning

- ◆ For images: Convolutional Neural Network (CNN) architecture (Russakovsky et al., 2015),
- ◆ For text: transformer architecture (Vaswani, 2017),
- ◆ For protein folding: transformer architecture (Jumper et al., 2021)



Imagenet challenge (Russakovsky et al., 2015)

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🤔 Why not so used in econometrics?

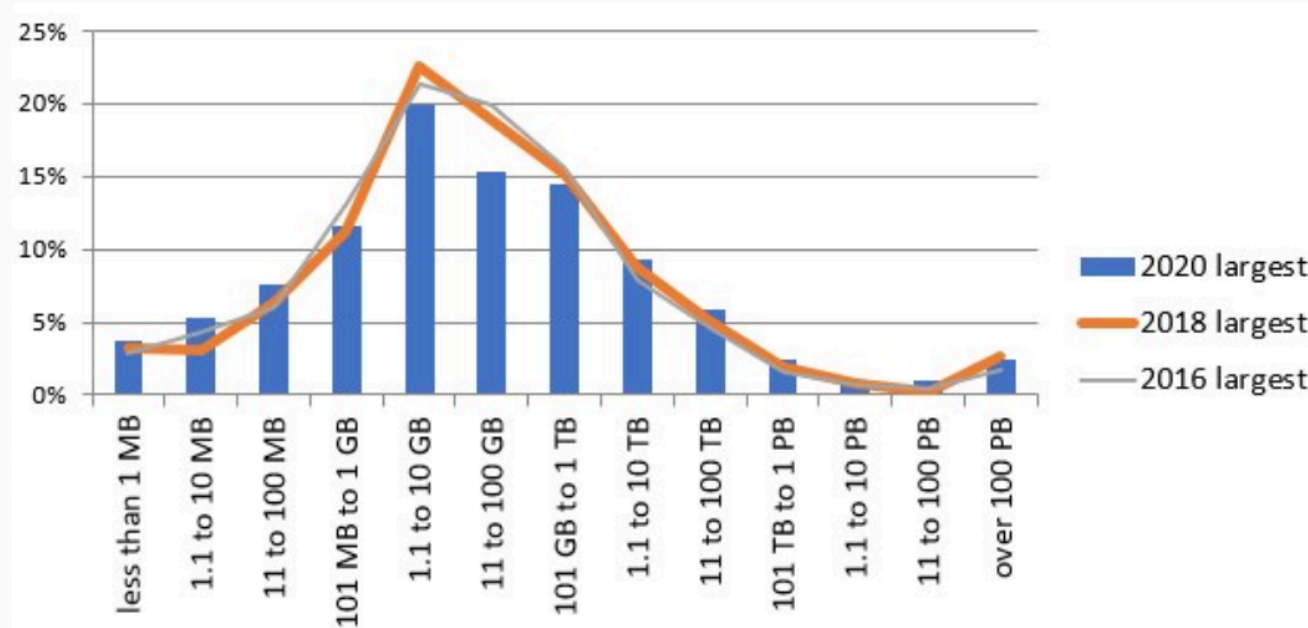


Imagenet challenge (Russakovsky et al., 2015)

Answer 1: Limited data settings (typically $N \approx 1$ million)

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

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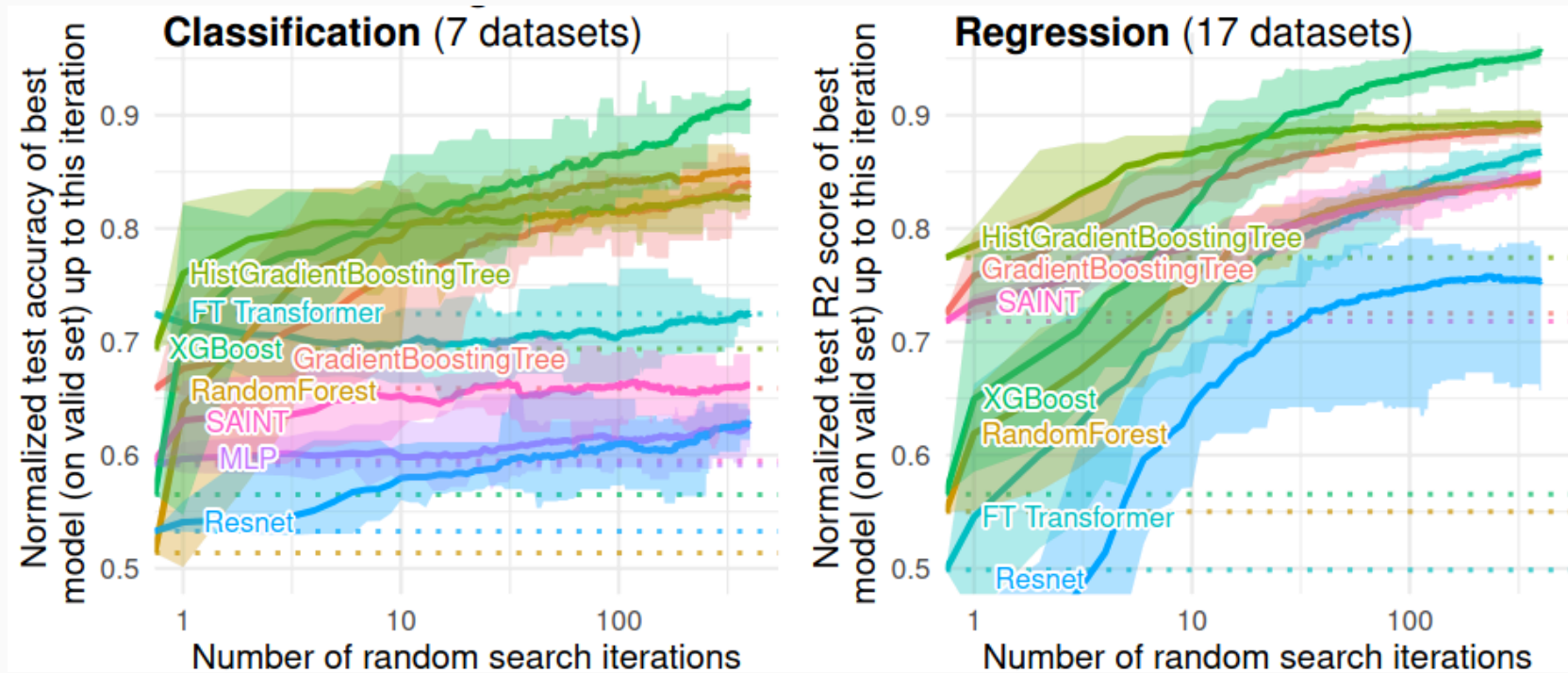


Typical dataset are mid-sized. This does not change with time.¹

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

Answer 2: Deep learning underperforms on data tables

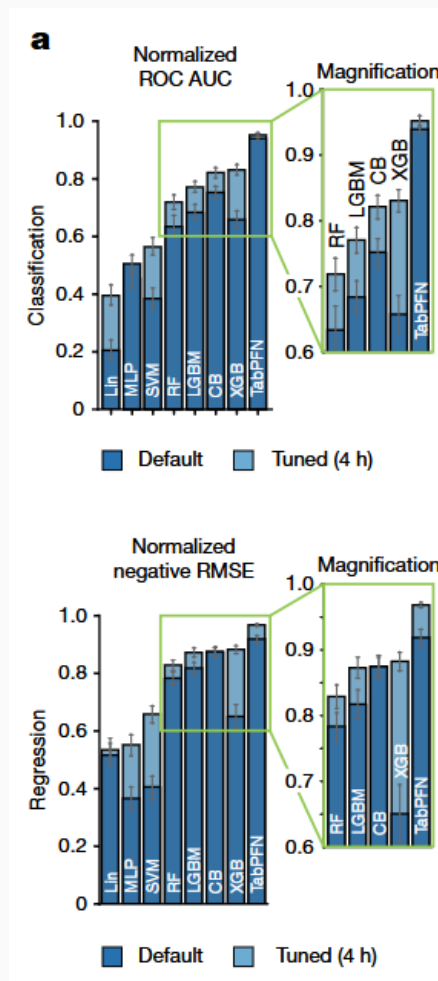
Tailored deep learning architectures lack appropriate prior of tabular data
(Grinsztajn et al., 2022)



Nuance: recent work using deep learning for tabular data

Learning appropriate representations (prior) of tabular data

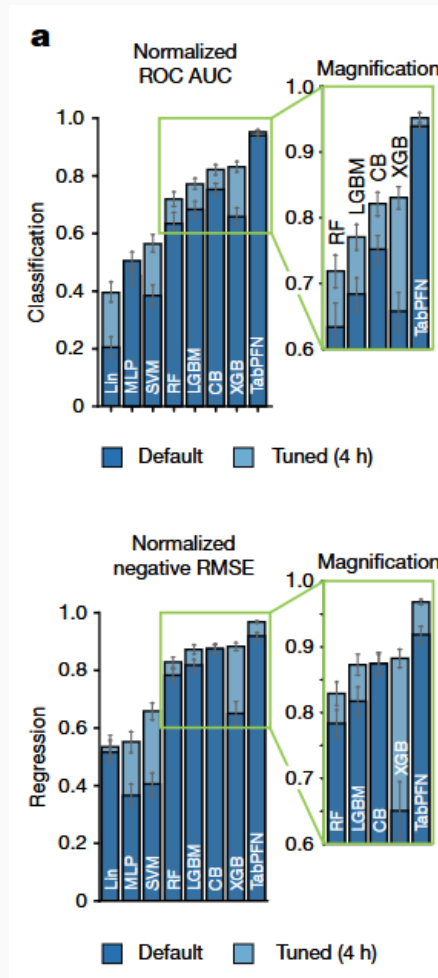
- TabPFN: large scale pretraining a transformer based model on synthetic tabular data (Hollmann et al., 2025)
- Allows In-Context Learning (ICL): learn with few examples.



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Learning appropriate representations (prior) of tabular data

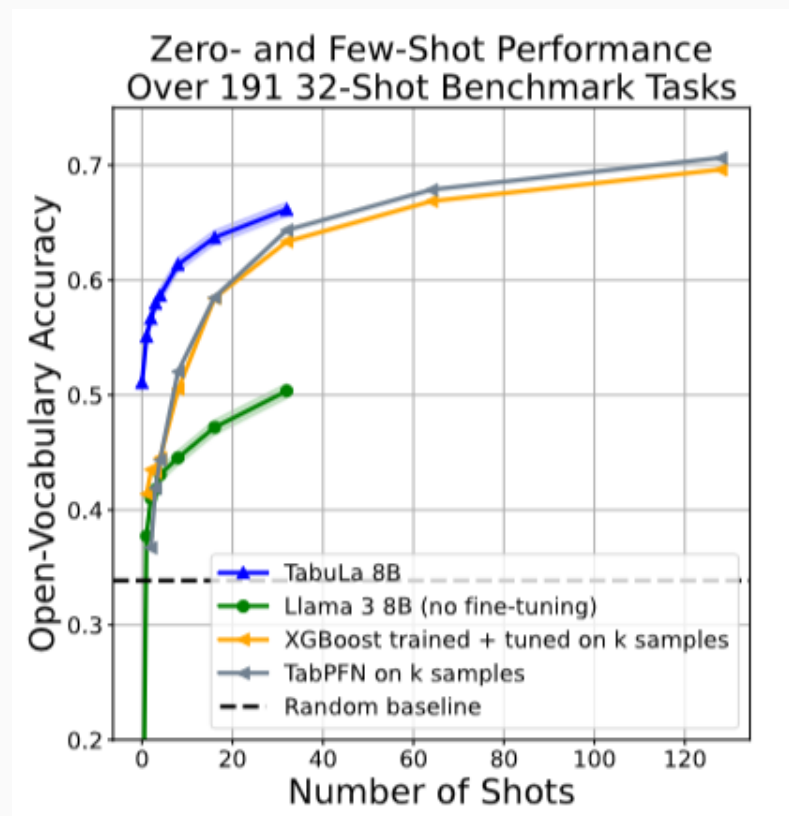
- TabPFN: large scale pretraining a transformer based model on synthetic tabular data (Hollmann et al., 2025)
- Allows In-Context Learning (ICL): learn with few examples.
- (Hollmann et al., 2025) Figure 4a: Comparison on test benchmarks, 29 classification and 28 regression datasets, containing with up to 10,000 samples and 500 features.



Nuance: recent work using deep learning for tabular data

Using Large Language Models (LLM)

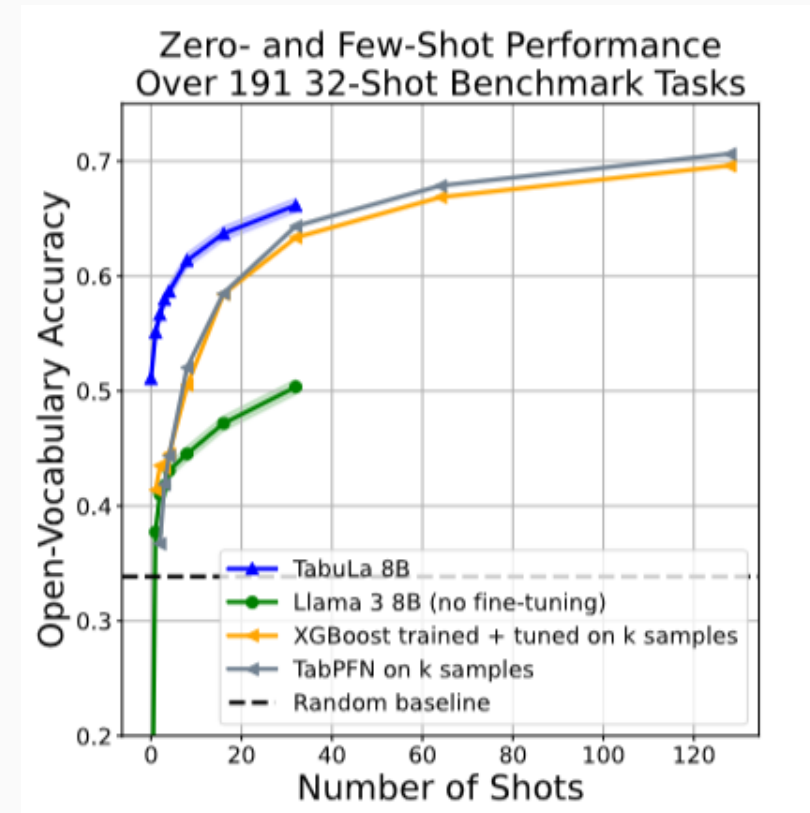
- [Tabula 8B](#) Fine-tuning existing LLM (Llama 3-8B) on tabular data (Gardner et al., 2024)



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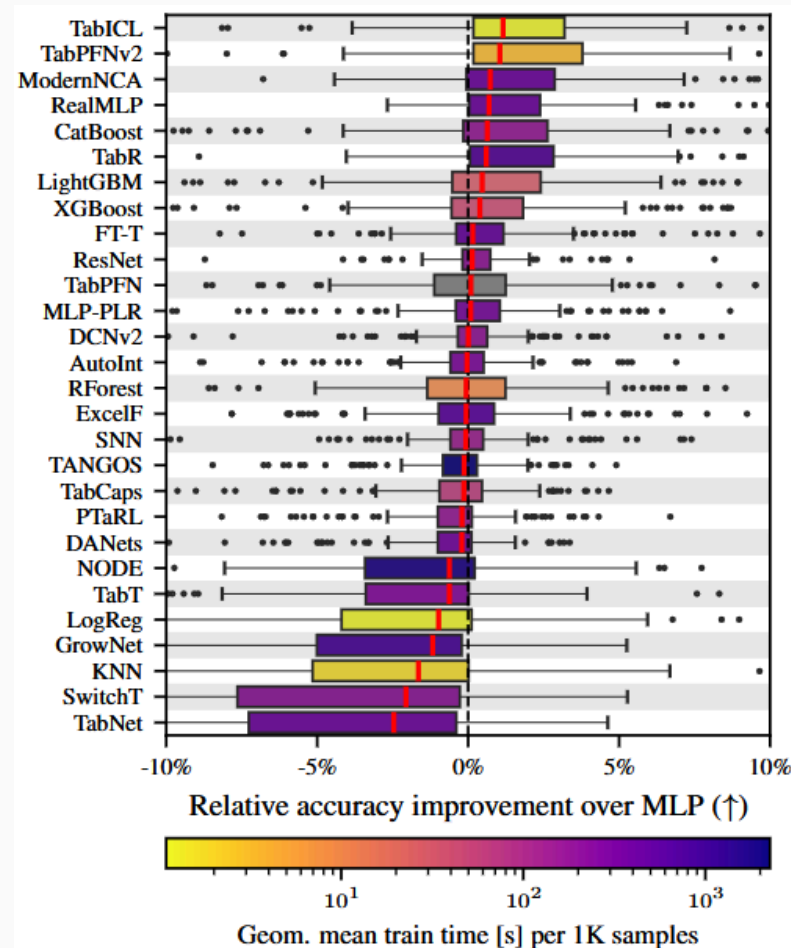
- **Tabula 8B** Fine-tuning existing LLM (Llama 3-8B) on tabular data (Gardner et al., 2024)
- Allow ICL with few examples.
- But requires large computational resources and is outperformed rapidly when number of samples grows.



Nuance: recent work using deep learning for tabular data

Transferable components tailored to tabular data

- CARTE: tailored learning components such as {key:value} representations (Kim et al., 2024)
- TABICL: Combine tailored components and pretraining on synthetic data (Qu et al., 2025)
- (Qu et al., 2025) Figure 5: Benchmark accuracy results and train times on 200 classification datasets.



Python hands-on

To your notebooks  !

2a) Hyper-parameters selection for flexible models

- url: https://straymat.github.io/causal-ml-course/practical_sessions.html

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