

Machine Learning for econometrics

Flexible models for tabular data

Matthieu Doutreligne

February 18th, 2025

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, Elastic Net
- Transformation of variables: polynomial regression
-

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?

Table of contents

1. Model evaluation and selection with cross-validation
2. Flexible models: Tree, random forests and boosting
3. A word on other families of models

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

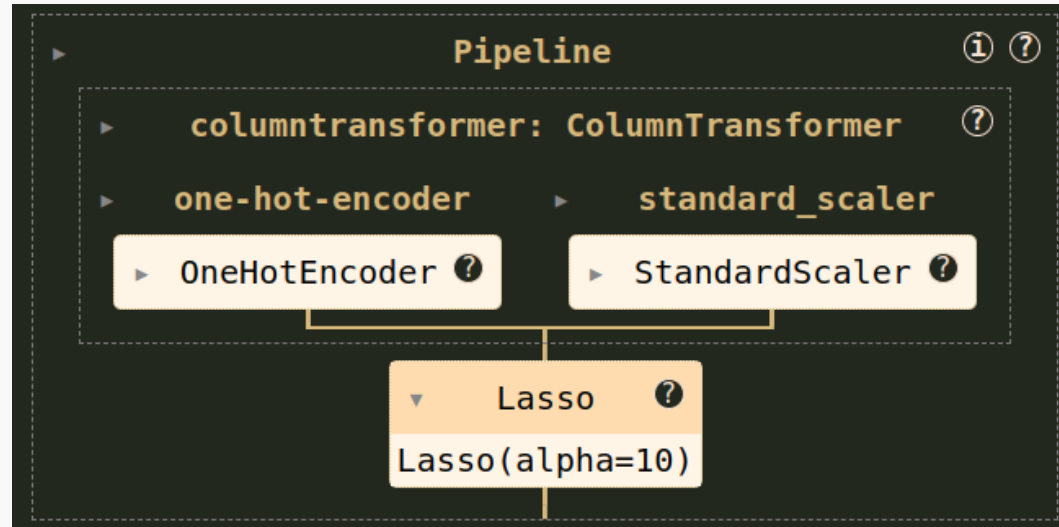
- Raw dataset: (N=534, p=11)
- Transformation: encoding categorical data, scaling numerical data: (N=534, p=23)

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	0.0
1.0	0.0	1.0	0.0	0.0	0.0
1.0	0.0	0.0	1.0	0.0	0.0
1.0	0.0	0.0	1.0	0.0	0.0
1.0	0.0	0.0	1.0	0.0	0.0

A closer look at model evaluation: Wage example

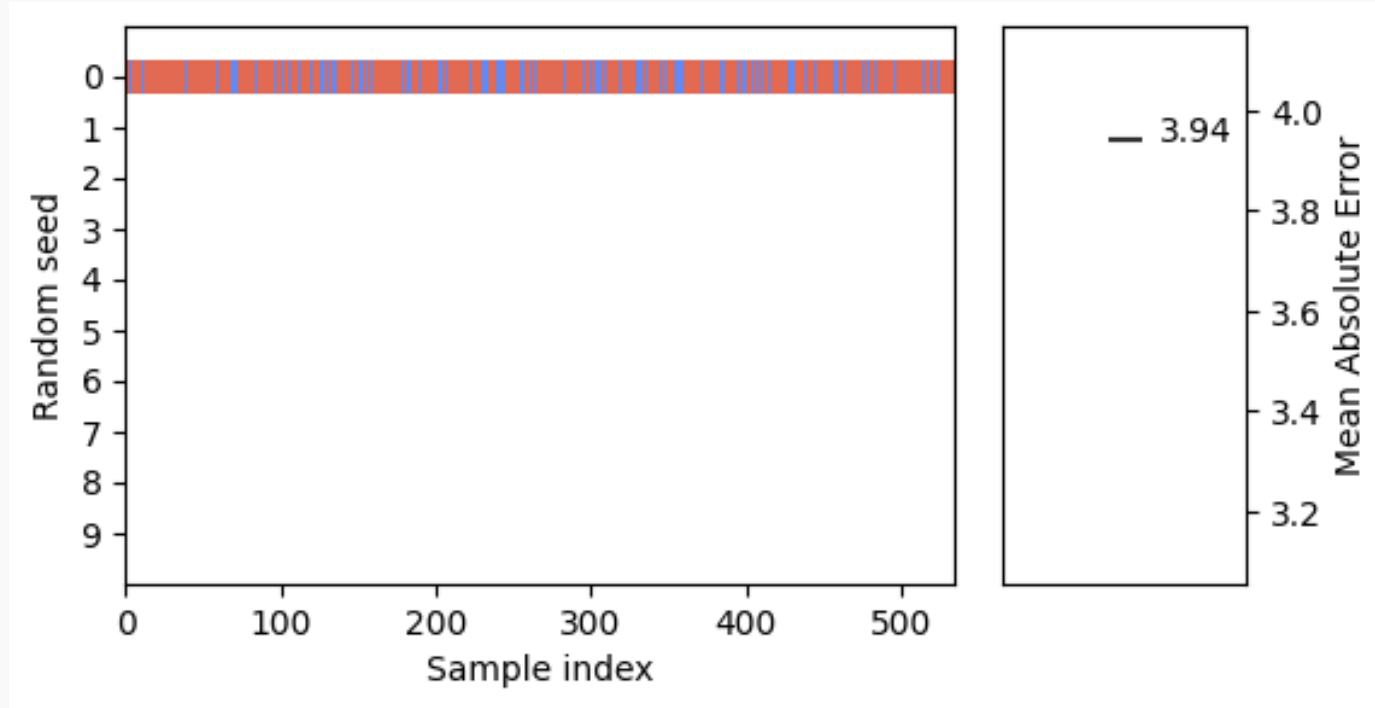
Example with the Wage dataset

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



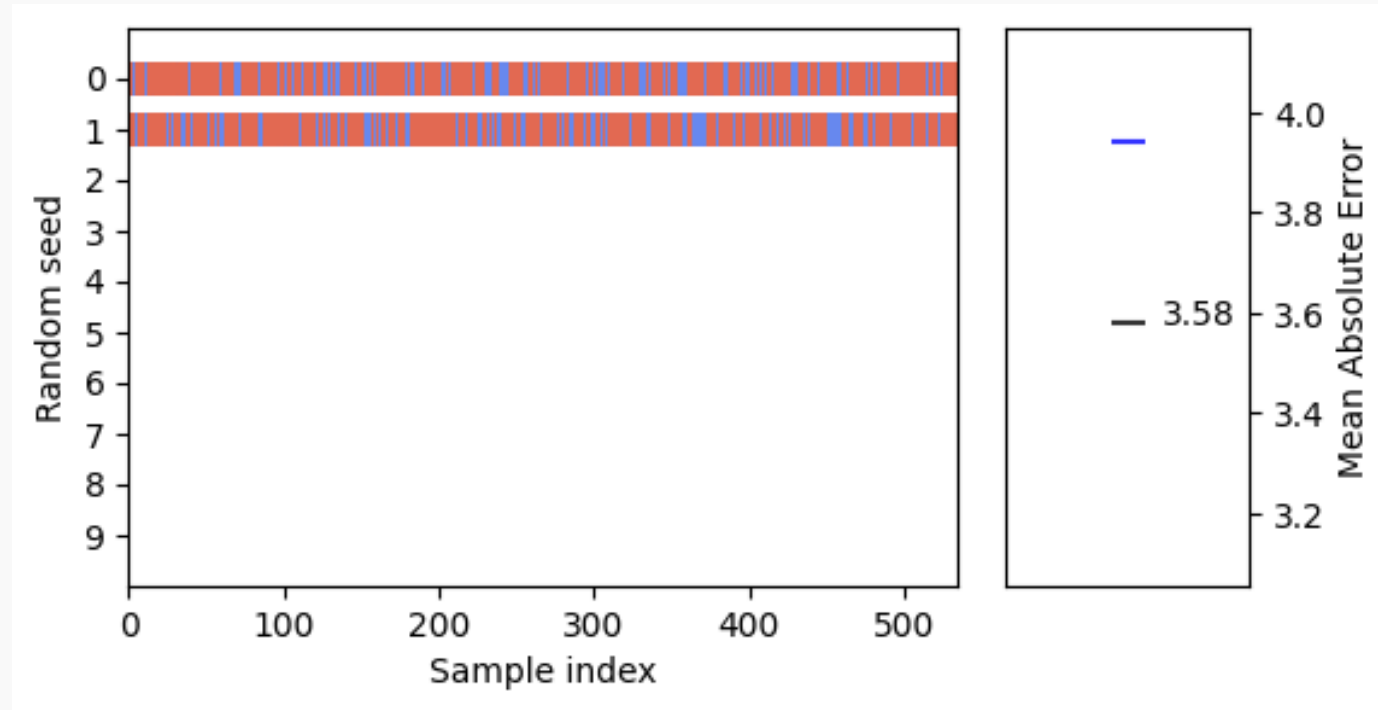
Repeated train/test splits

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



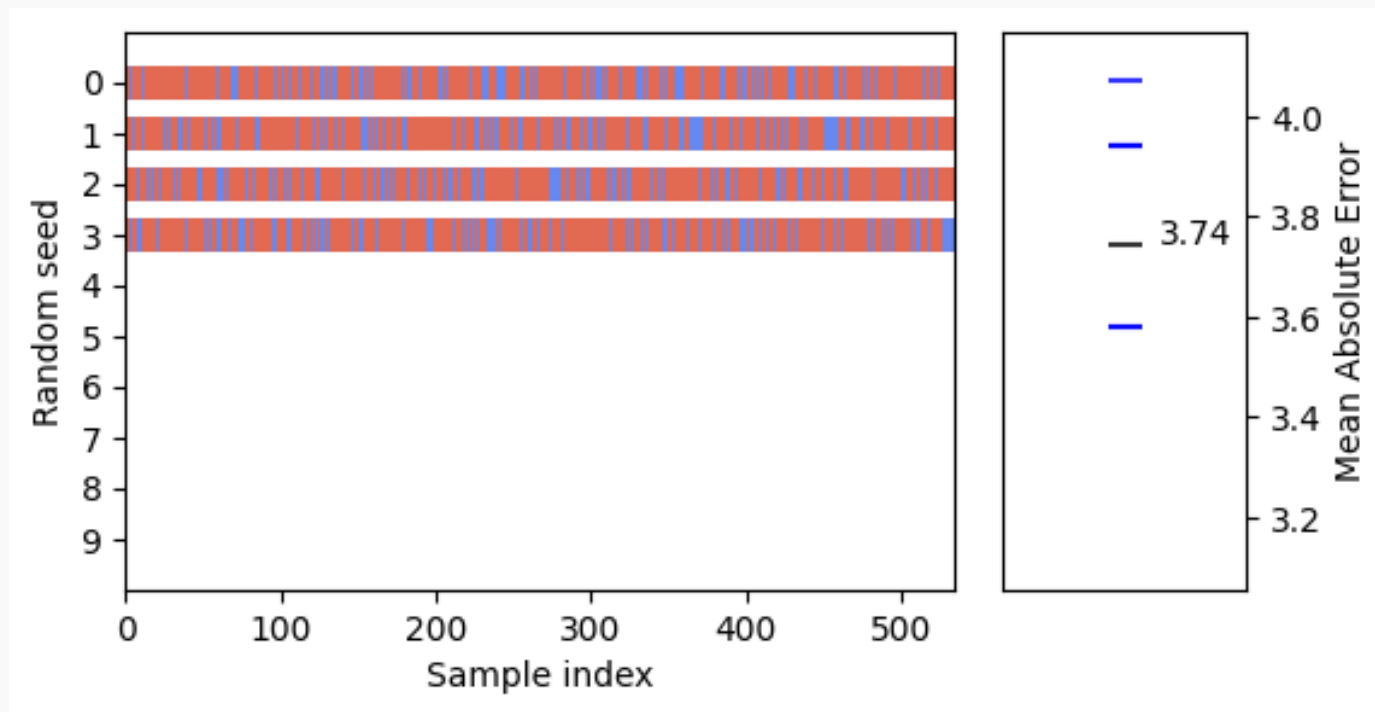
Repeated train/test splits

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



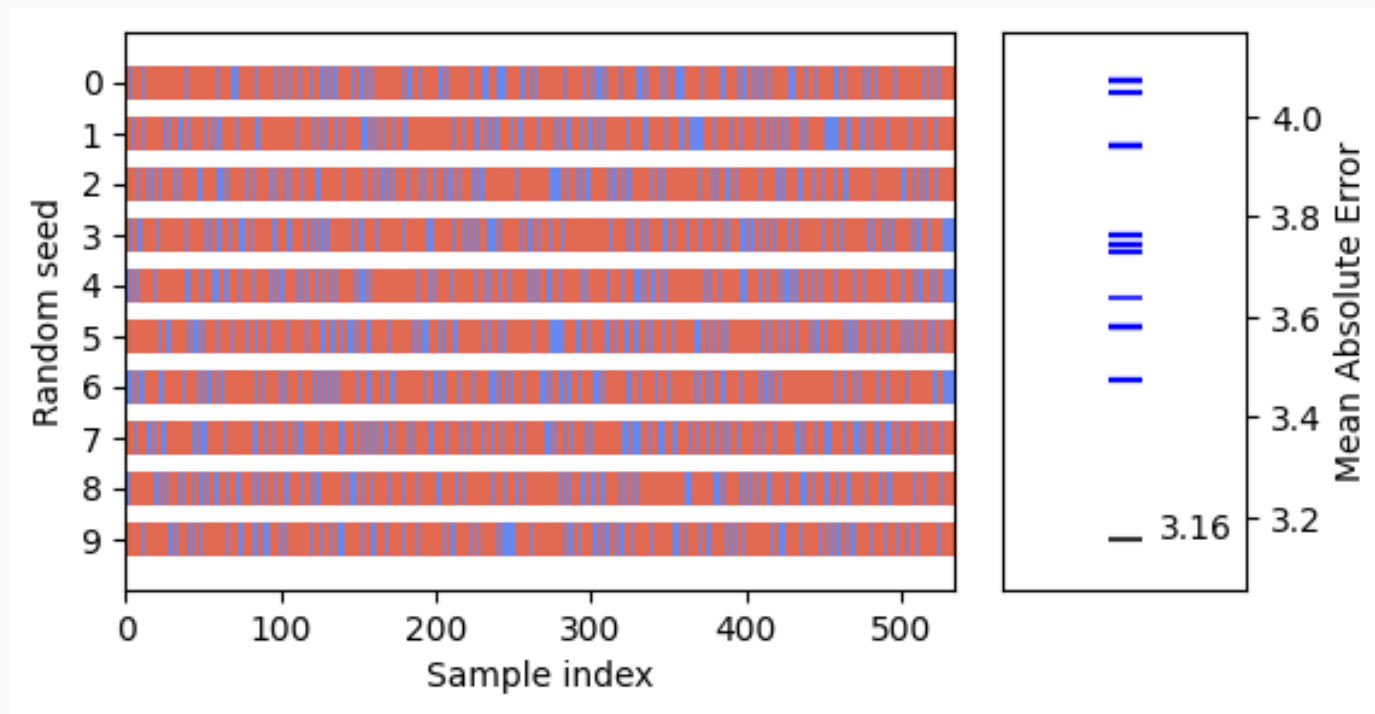
Repeated train/test splits

And another split...



Repeated train/test splits

Splitting ten times



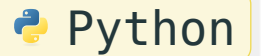
🎉 **Distribution of MAE: 3.71 ± 0.26**

Repeated train/test splits = Cross-validation

Cross-validation

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

```
1 from sklearn.model_selection import cross_validate
2 from sklearn.model_selection import ShuffleSplit
3
4 cv = ShuffleSplit(n_splits=40, test_size=0.3, random_state=0)
5 cv_results = cross_validate(
6     regressor, data, target, cv=cv, scoring="neg_mean_absolute_error"
7 )
```

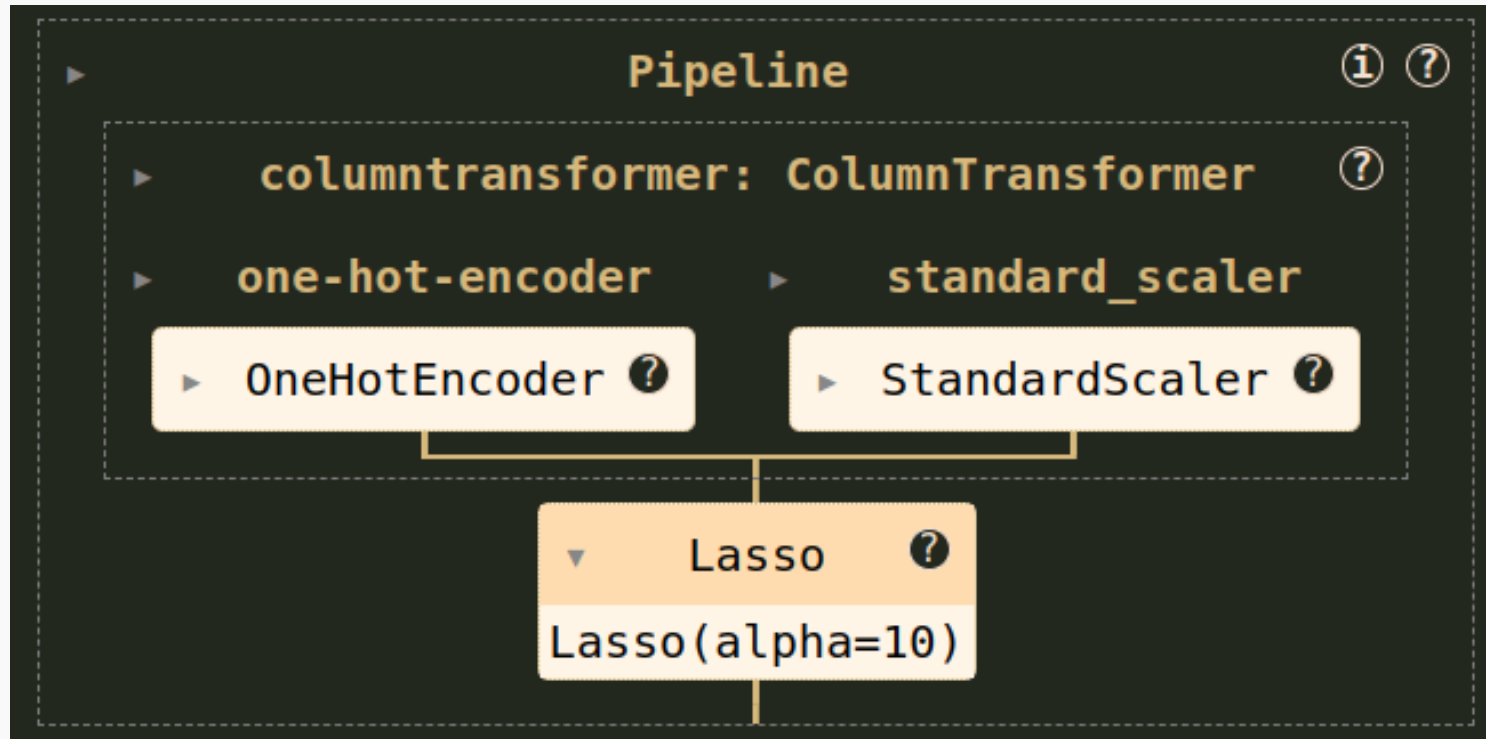


Cross-validation

- 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 candidates!

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


- Wage pipeline



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

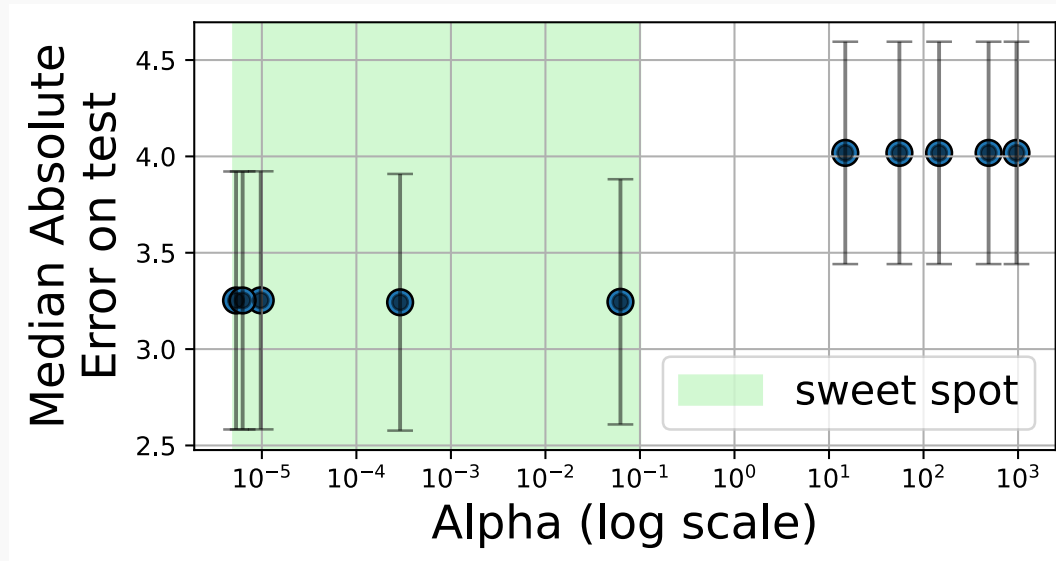
- Wage pipeline
- Random search over a distribution of α values

```
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)
```

 Python

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: often used in practice.
- 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.

- Proof that cross-validation selects the best model asymptotically among a family of models (averaging on the folds): (Lecué & Mitchell, 2012)

Naive cross-validation to select AND estimate the best performances

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
- AND to estimate the generalization performance of the selected model

 **Naive cross-validation can lead to overfitting**

Naive cross-validation to select AND estimate the best performances

Hyper-parameters selection is a kind of model fitting

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

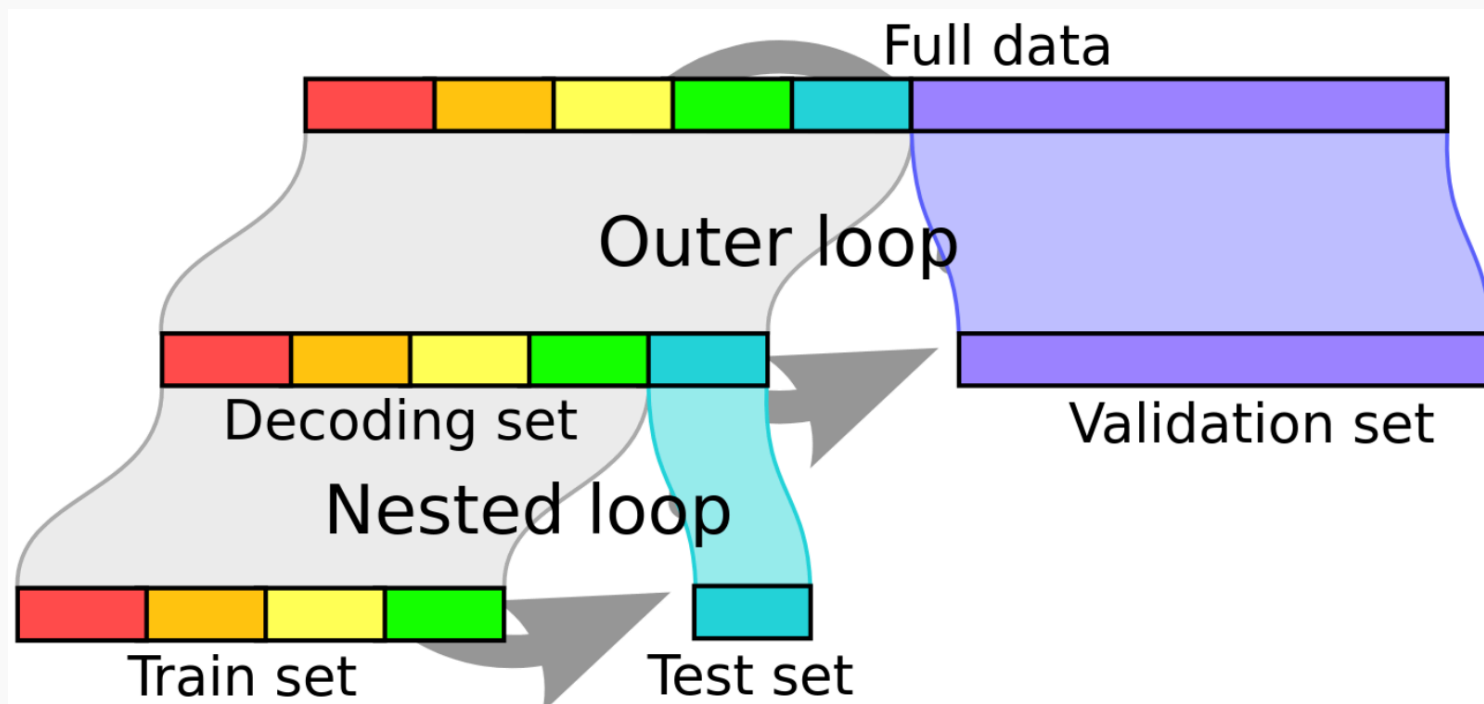
- to select the best hyper-parameters
- AND to estimate the generalization performance of the selected model

 **Naive cross-validation can lead to overfitting**

 Solution -> nested cross-validation (Varoquaux et al., 2017)

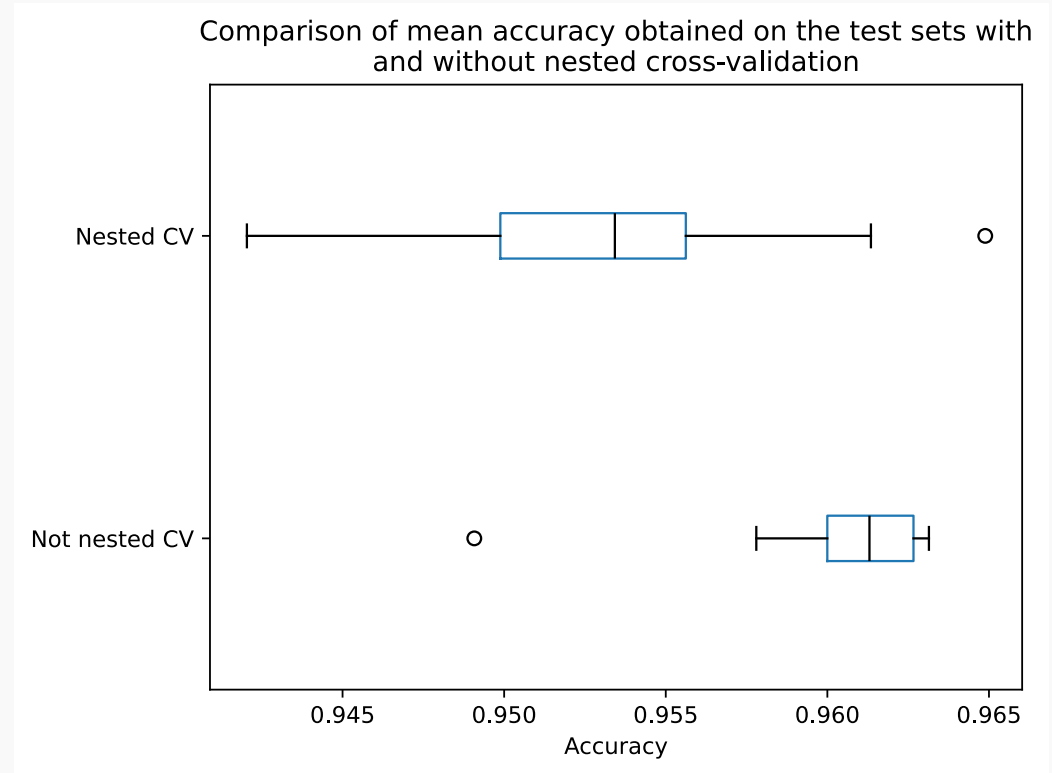
Nested cross-validation to select AND estimate the best performances

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



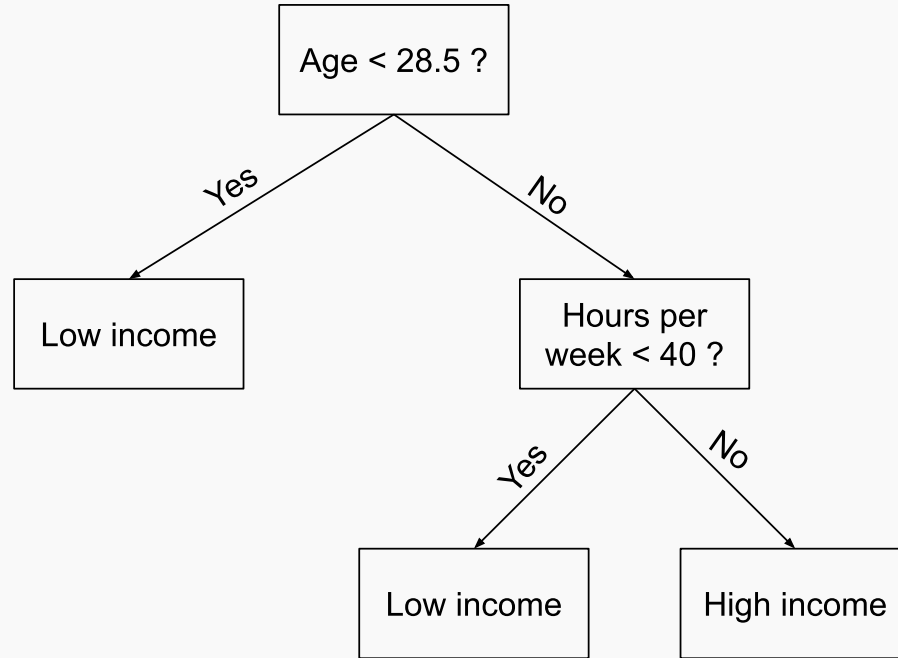
Over optimistic performance estimation: example

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

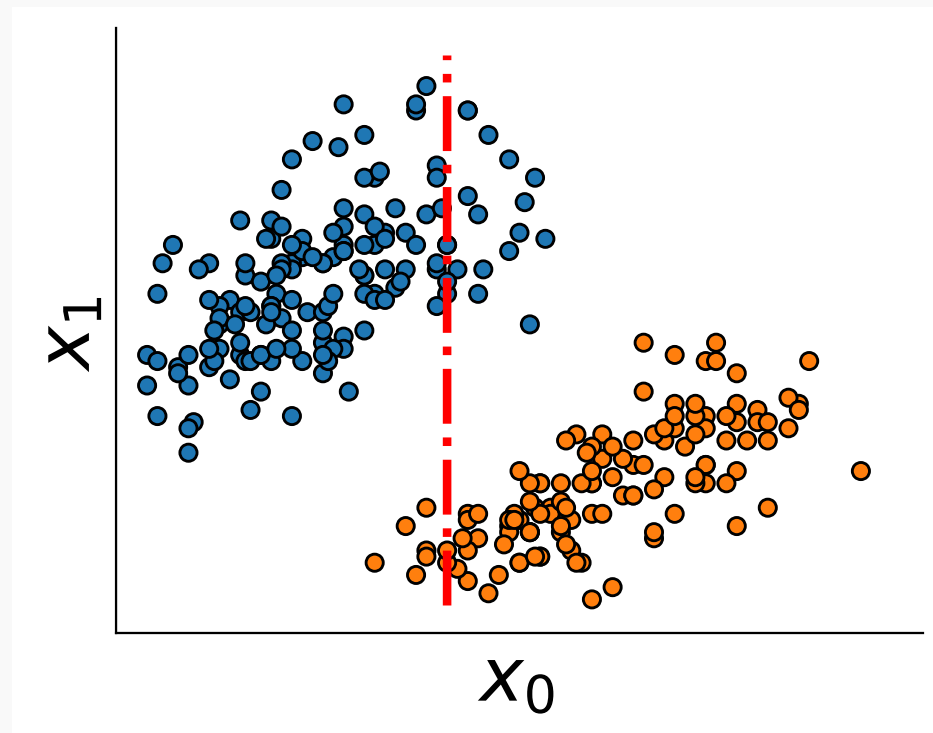
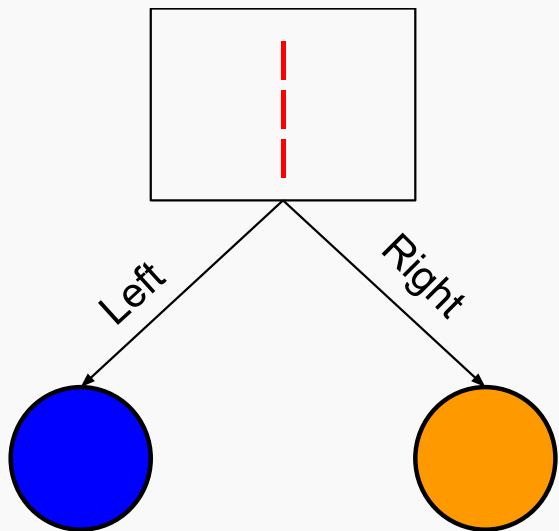


Flexible models: Tree, random forests and boosting

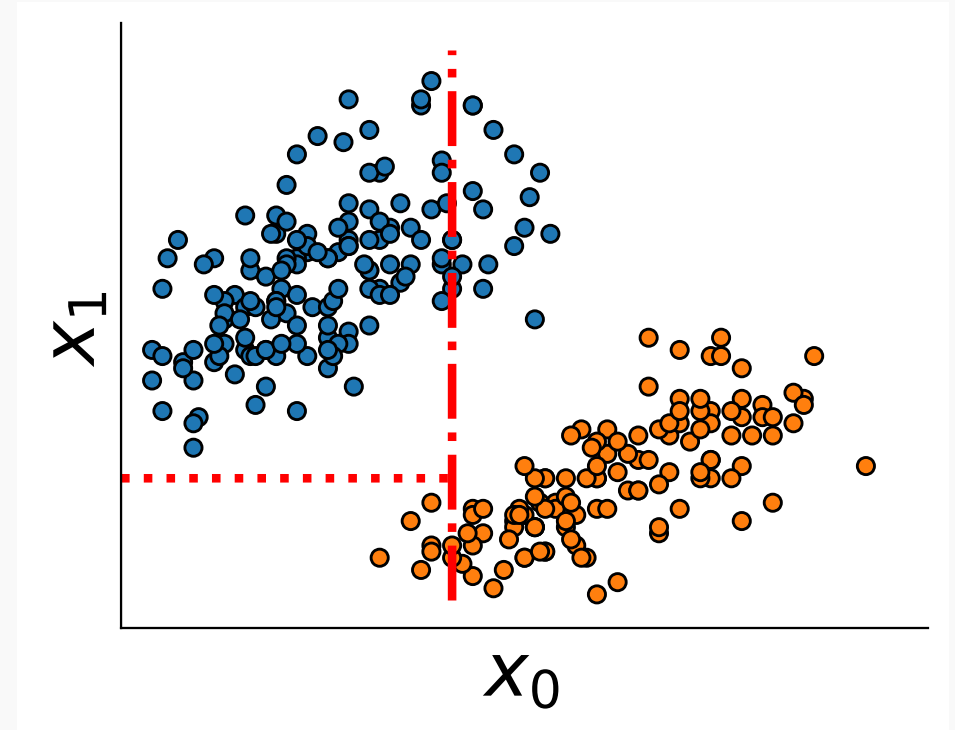
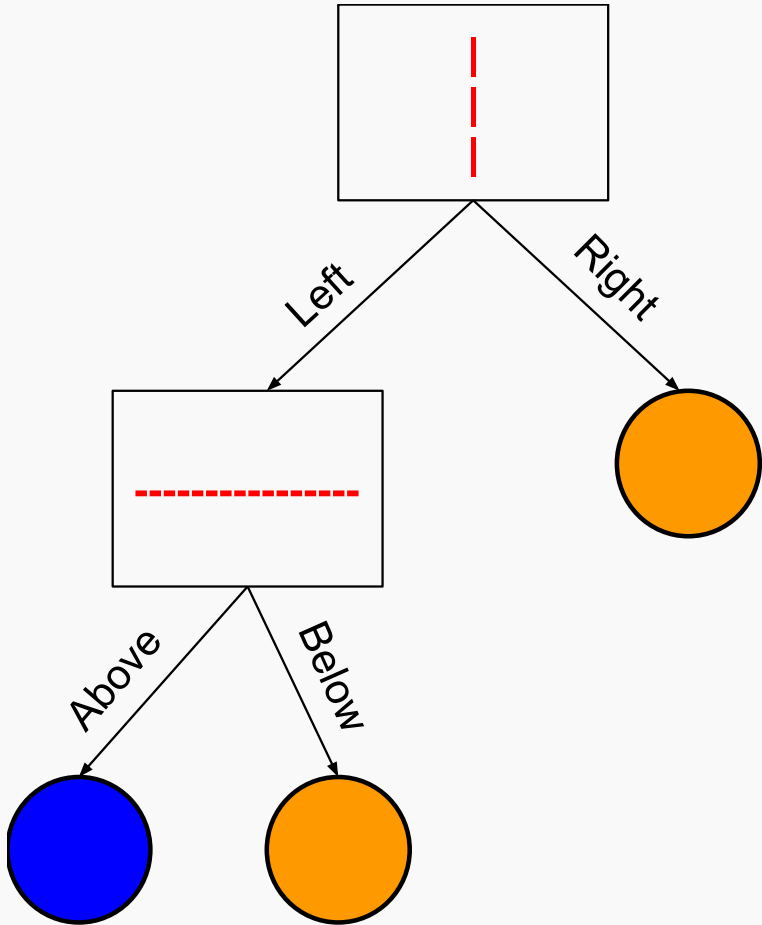
What is a decision tree? An example.



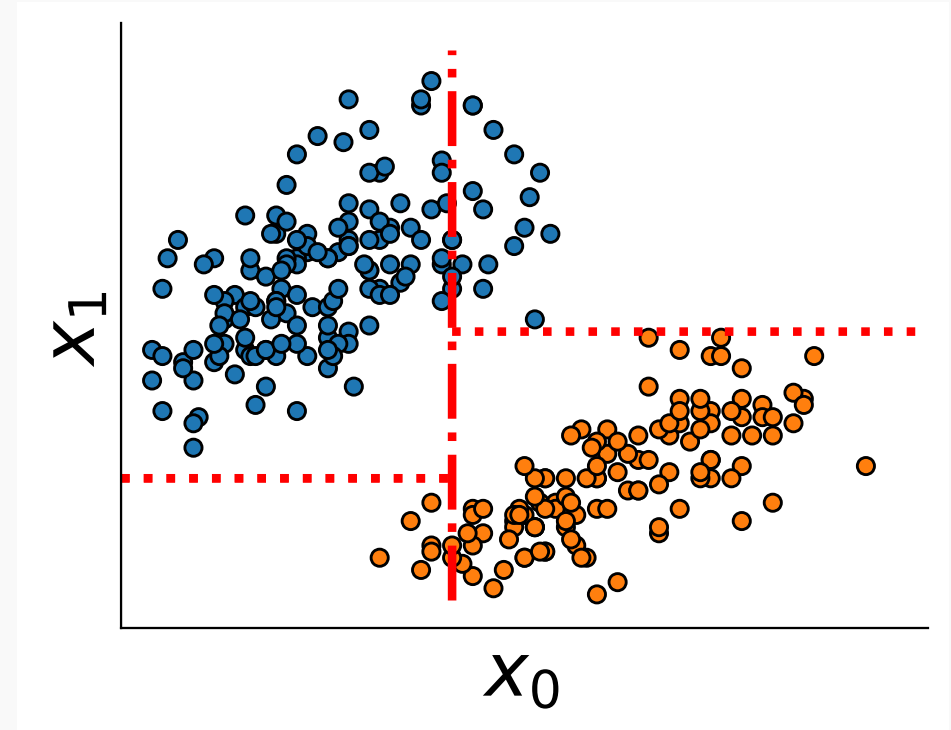
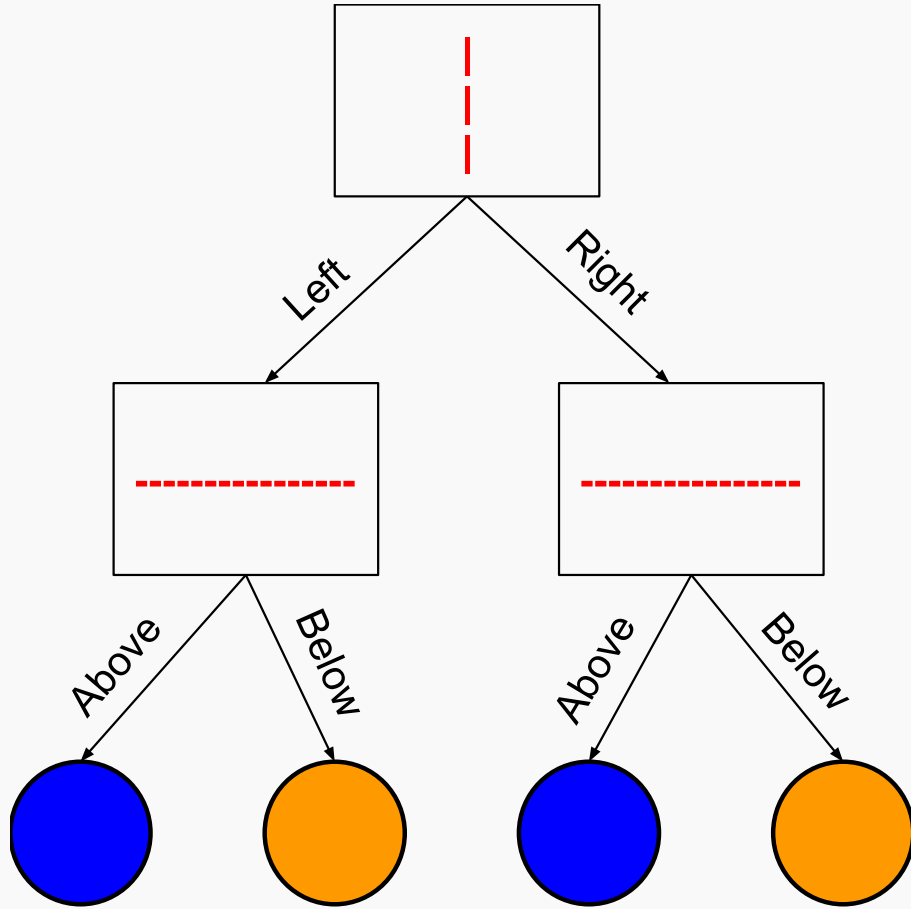
Growing a classification tree



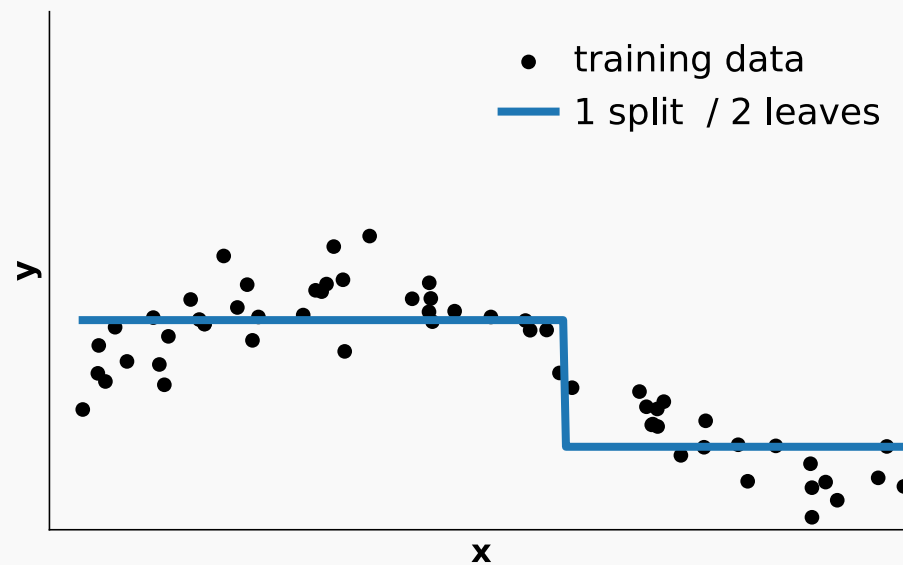
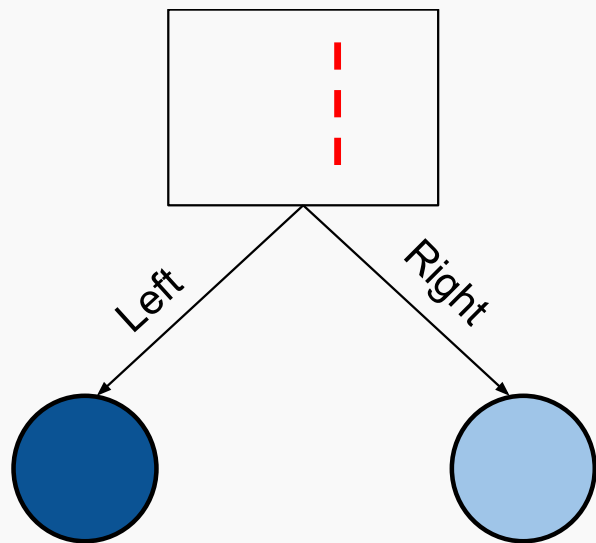
Growing a classification tree



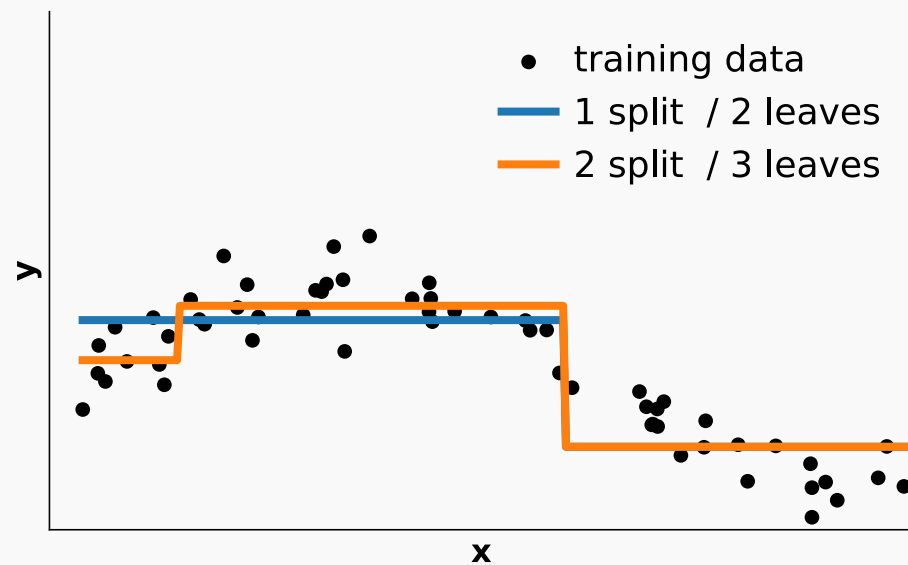
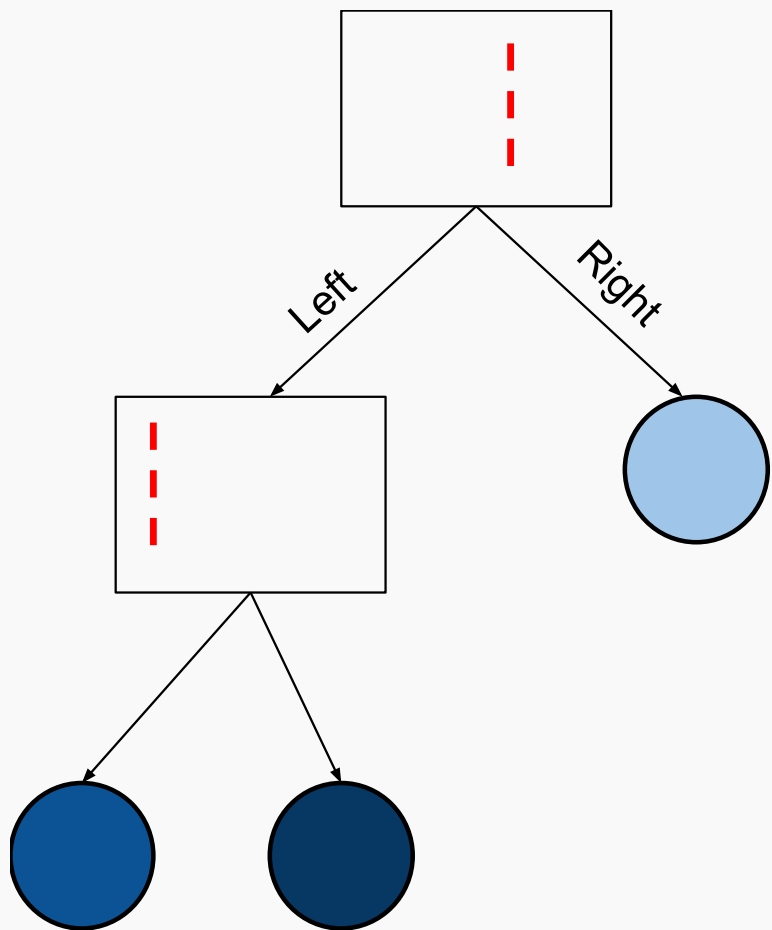
Growing a classification tree



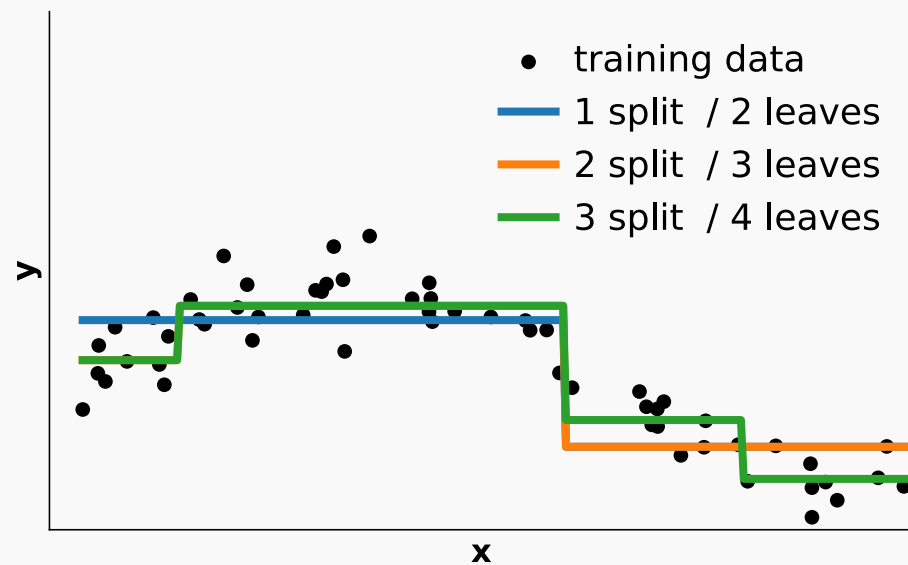
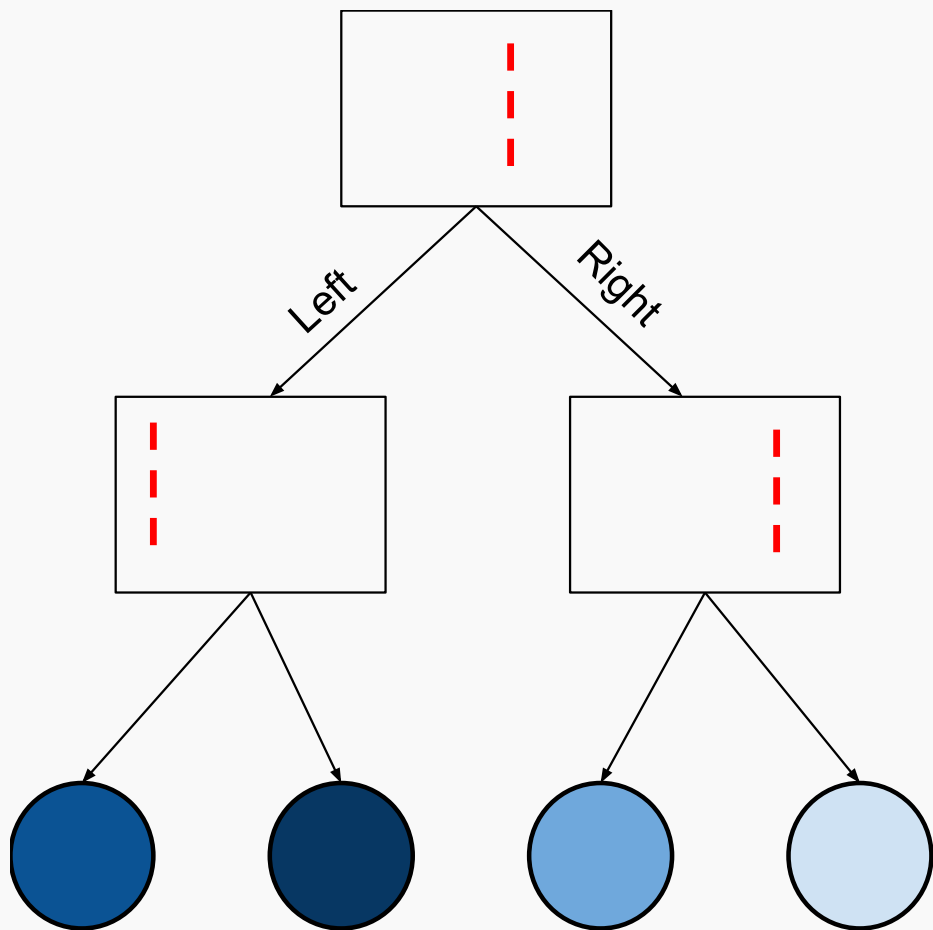
Growing a regression tree



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:

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

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

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

Impurity criteria

For classification

Gini impurity

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

Cross-entropy

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

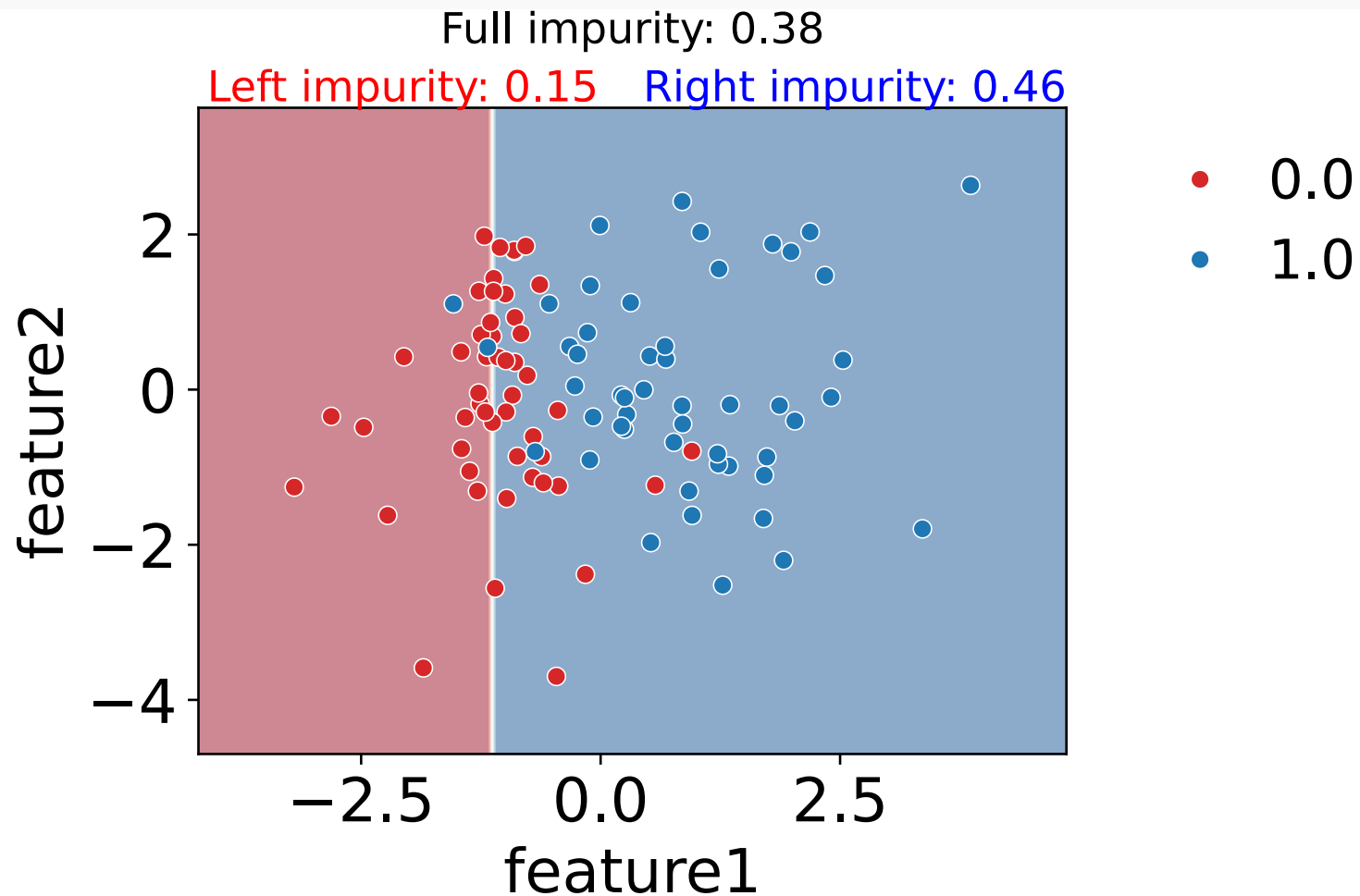
For regression

Mean squared error

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

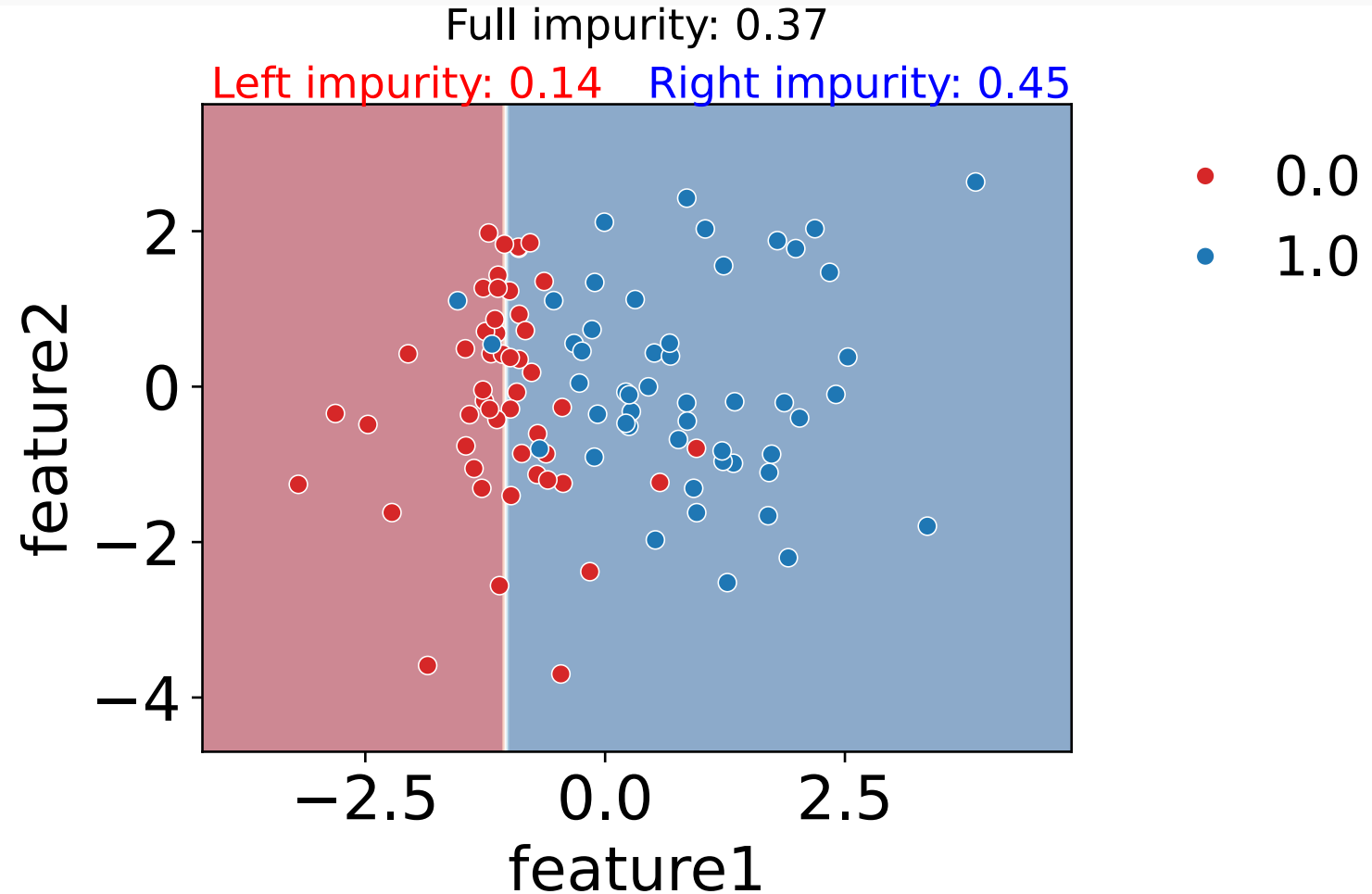
Chose the best split: example

Random split



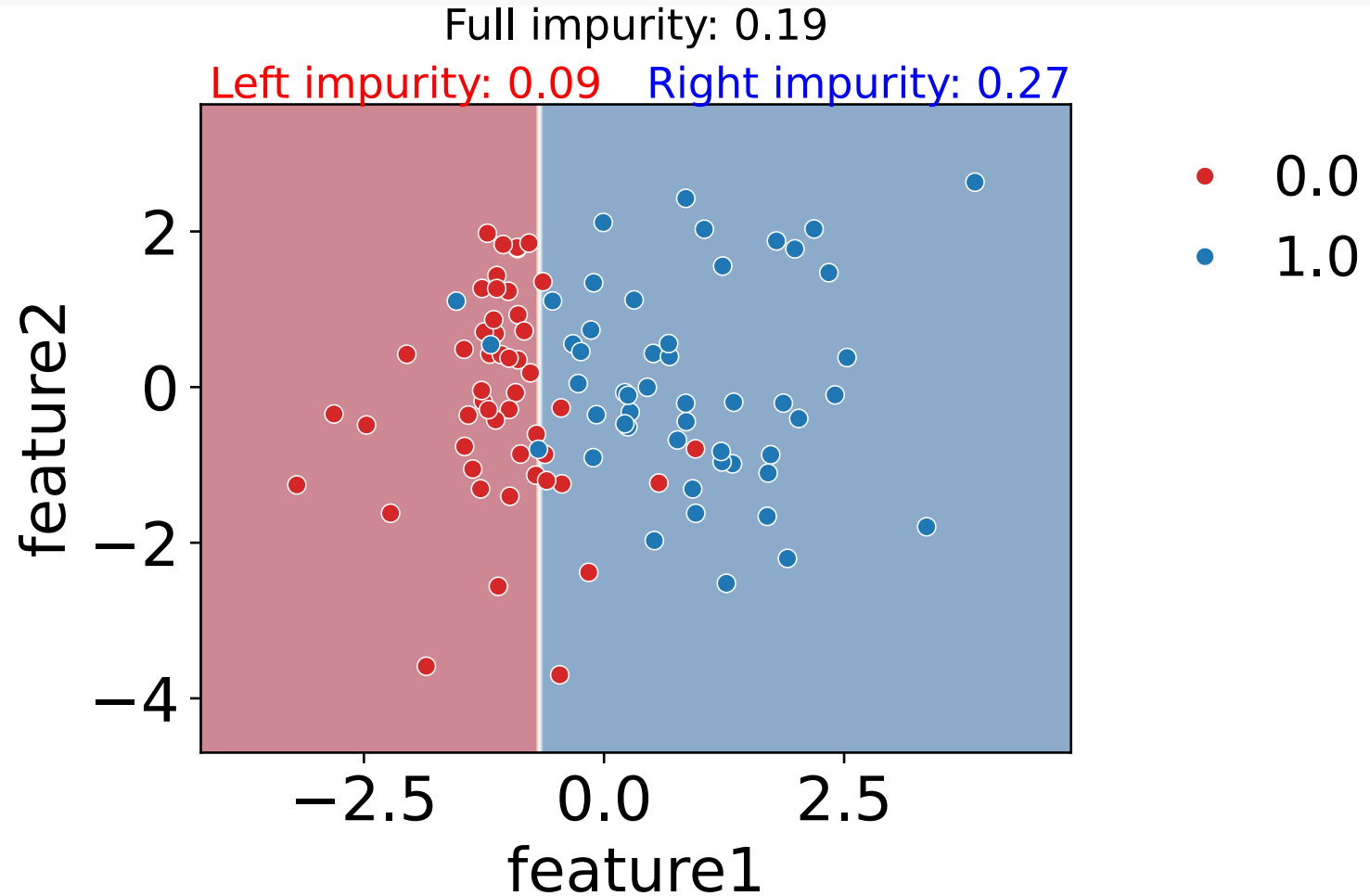
Chose the best split: example

Moving the split to the right from one point



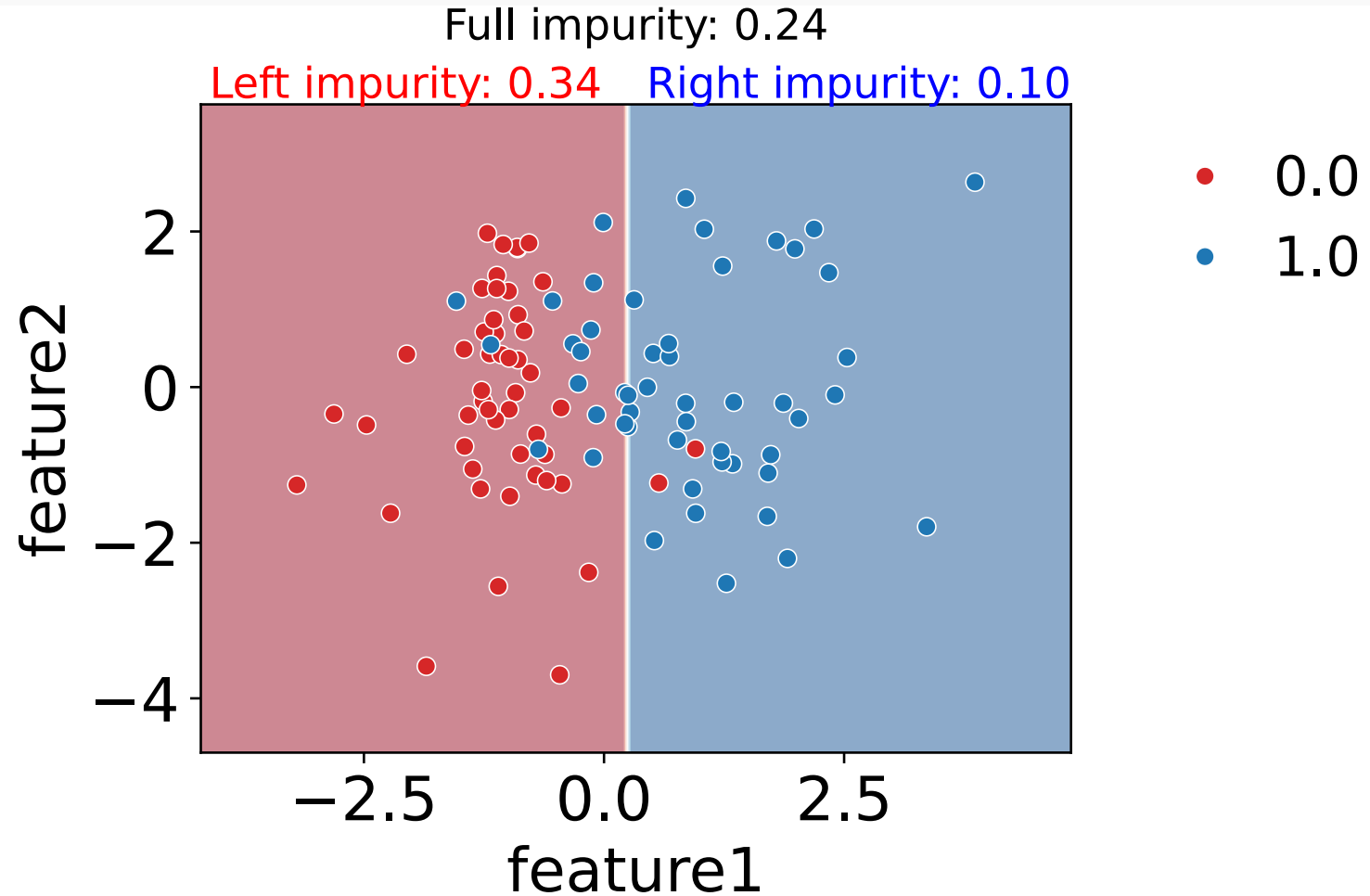
Chose the best split: example

Moving the split to the right from 10 points



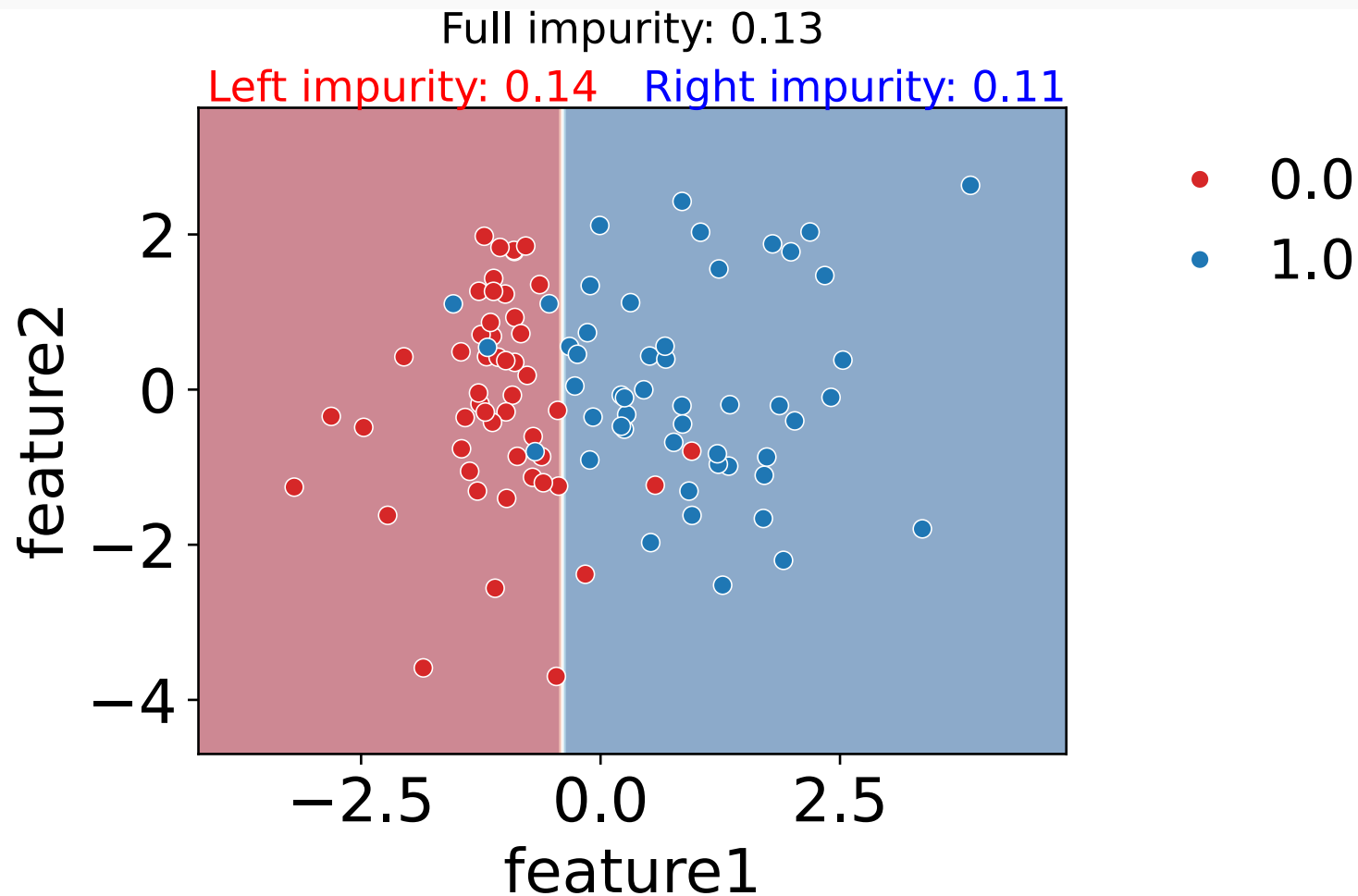
Chose the best split: example

Moving the split to
the right from 20
points

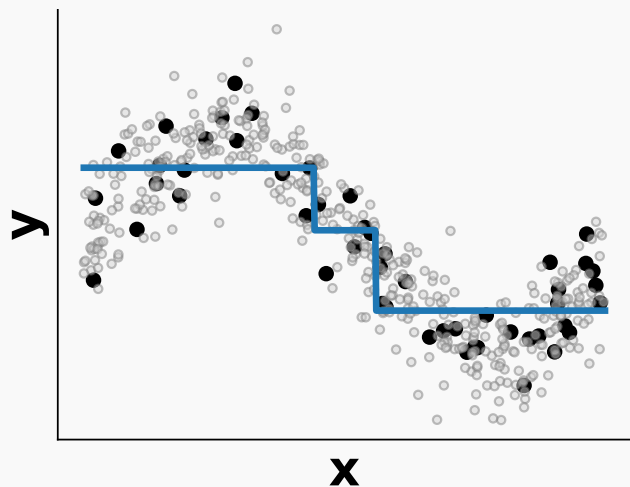


Chose the best split: example

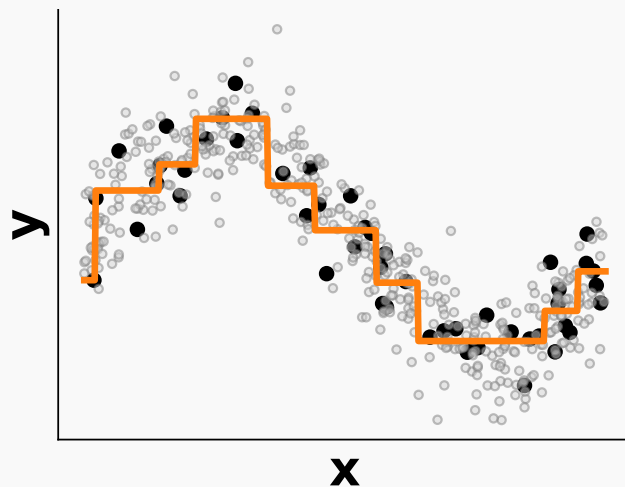
Best split



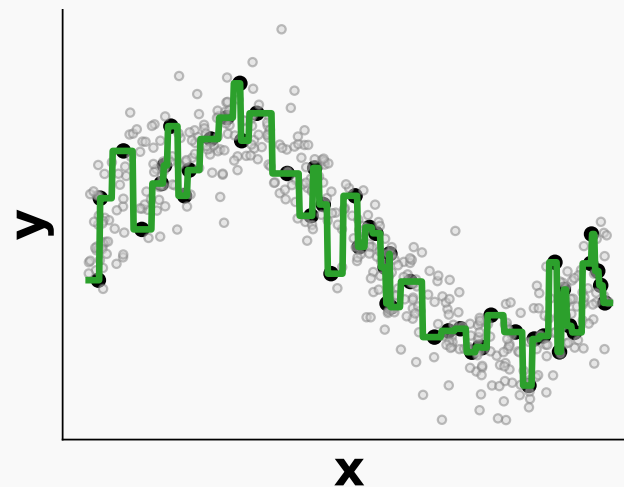
Tree depth and overfitting



Underfitting
max depth or
max_leaf_nodes
too small



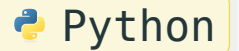
Best trade-off



Overfitting
max depth or
max_leaf_nodes
too large

Main hyper-parameters of tree models

```
1 DecisionTreeRegressor(  
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

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

Bagging: Bootstrap AGGREGatING

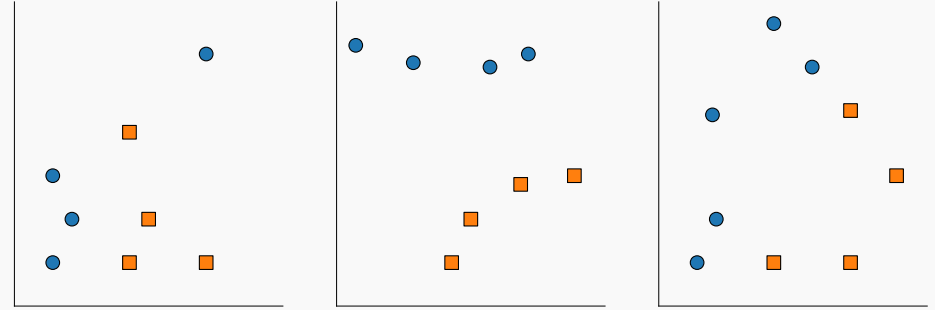
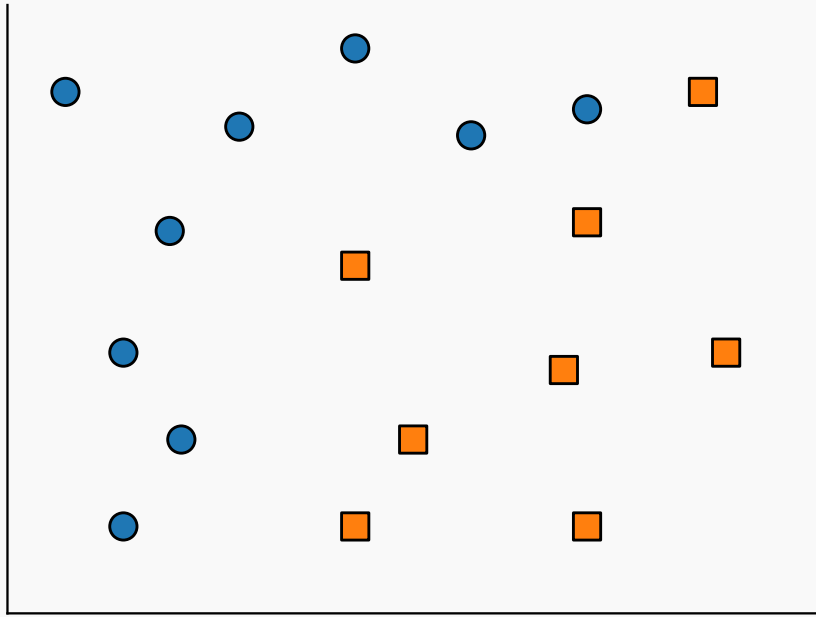
Bootstrap resampling (random sampling with replacement) proposed by (Breiman, 1996)

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

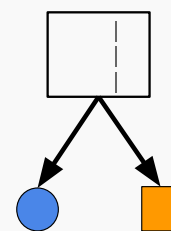
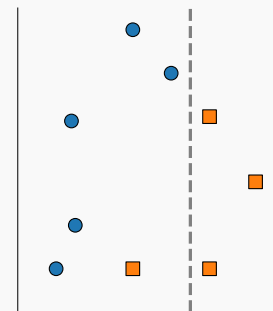
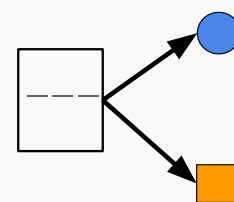
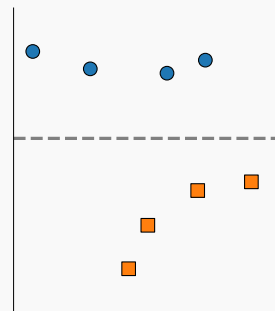
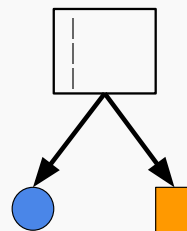
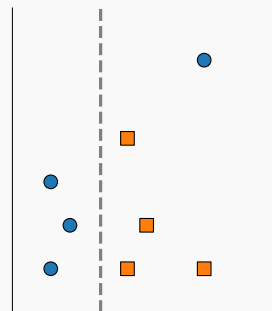
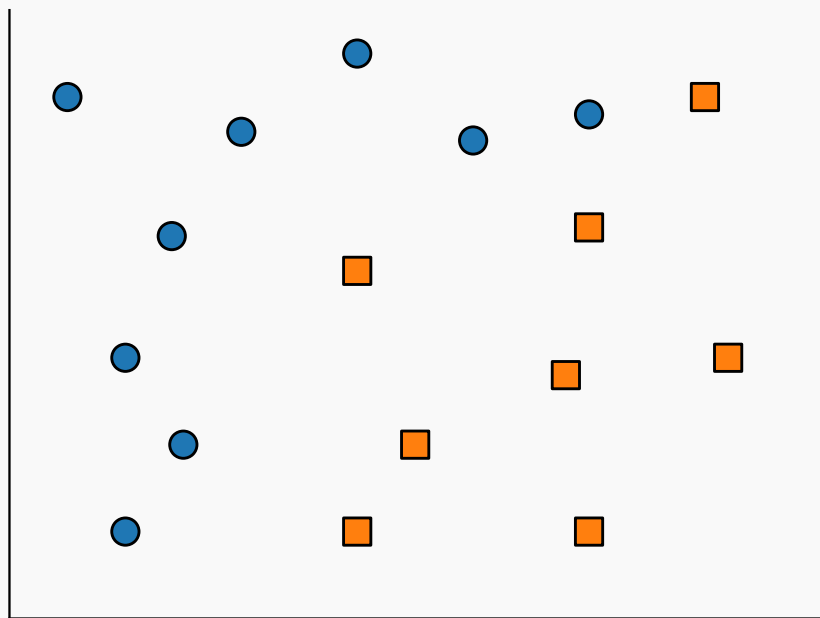
Bagging is used in machine learning to reduce the variance of a model prone to overfitting

Can be used with any model

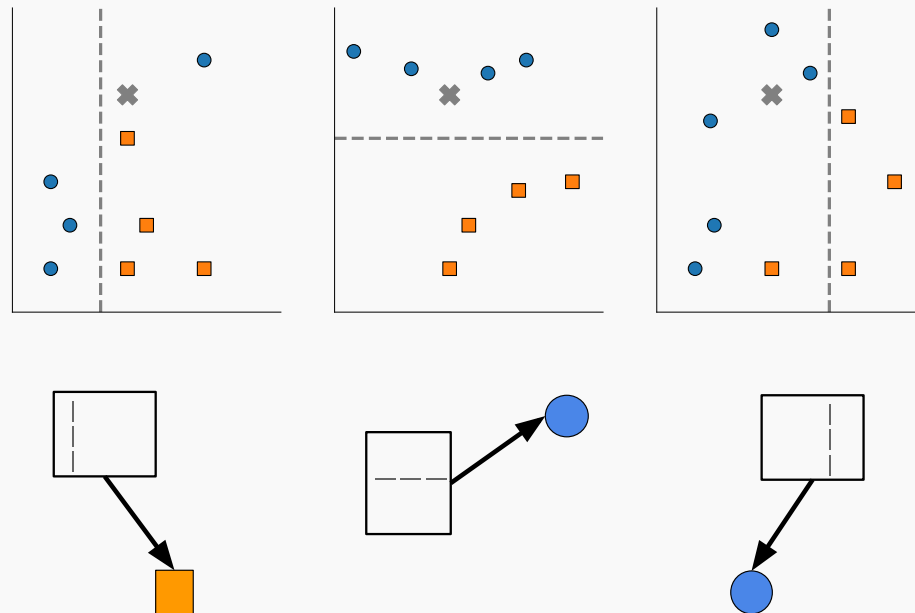
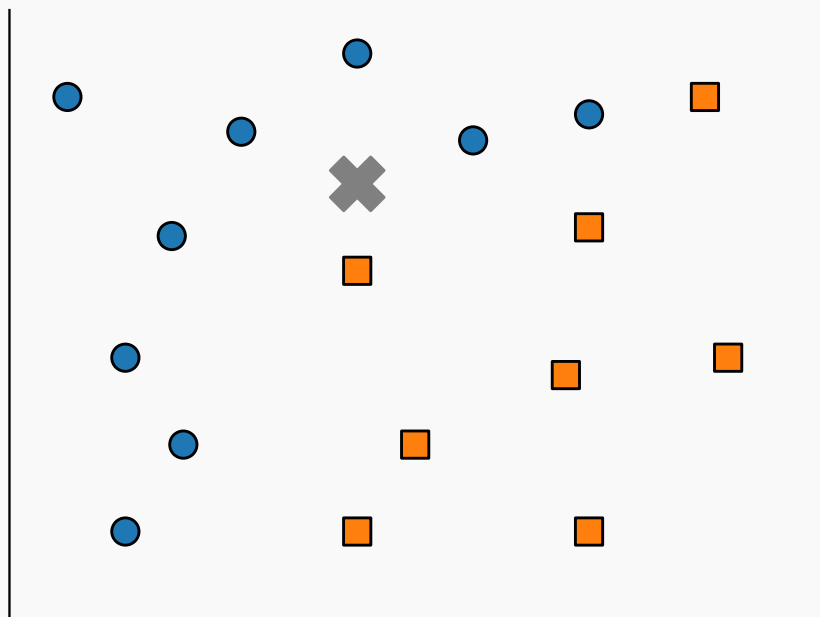
Random forests: Bagging with classification trees



Random forests: Bagging with classification trees

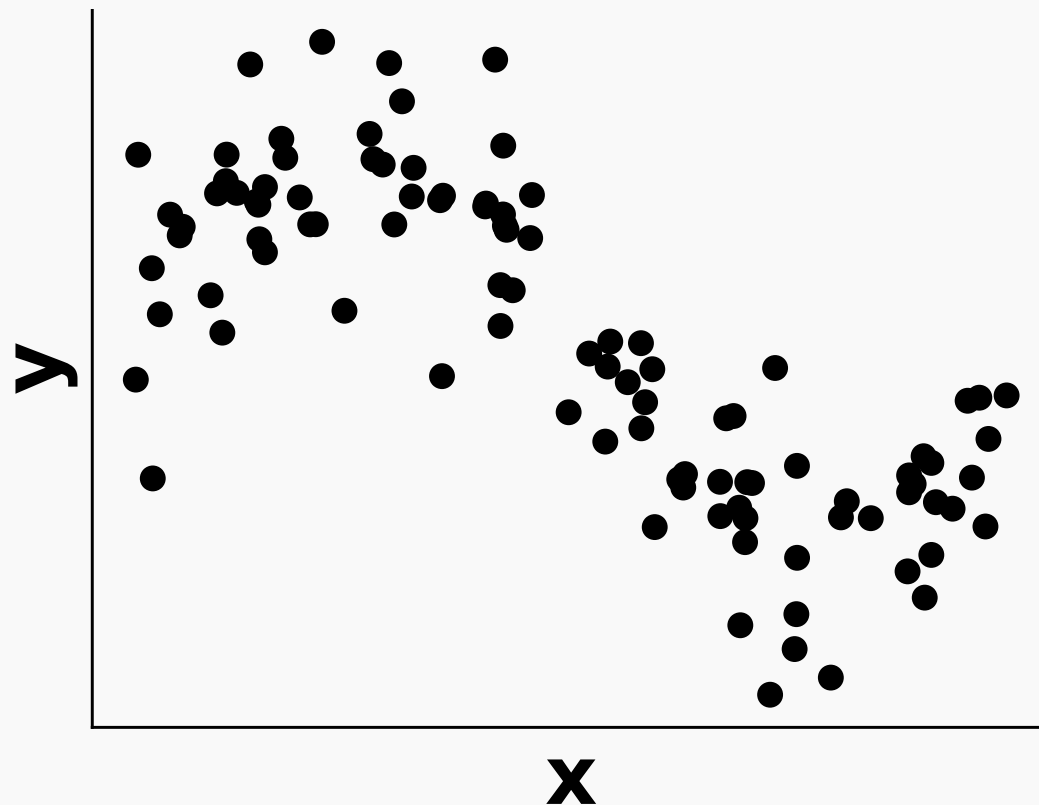


Random forests: Bagging with classification trees

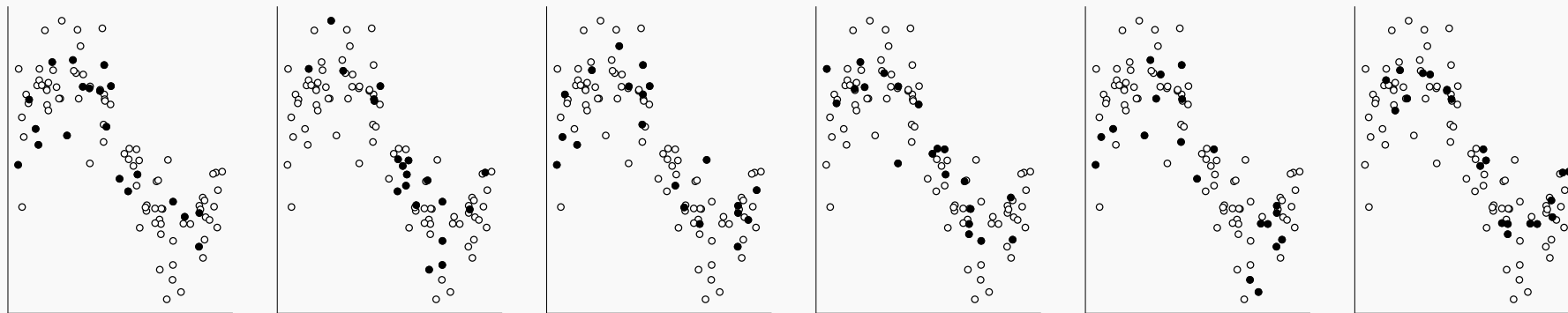


VOTE ( ,  , ) = 

Random forests: Bagging with regression trees

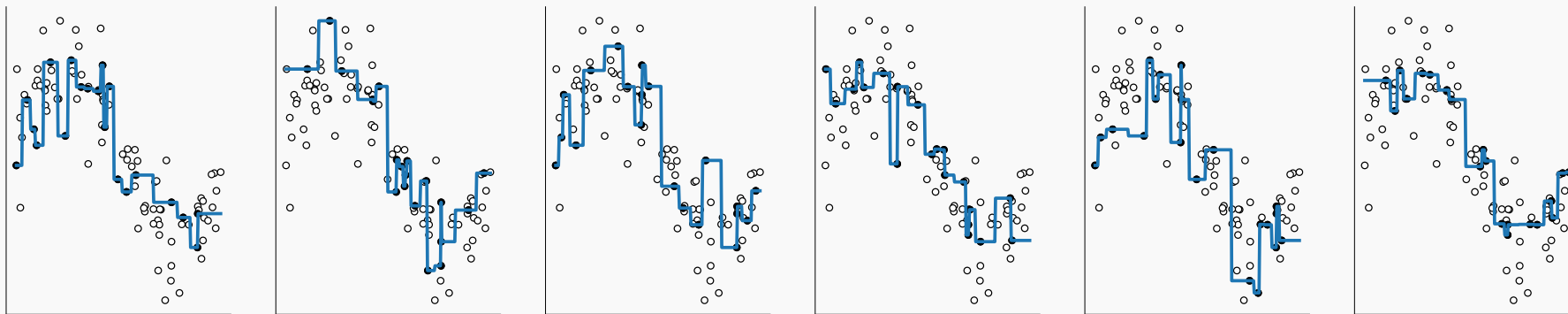


Random forests: Bagging with regression trees



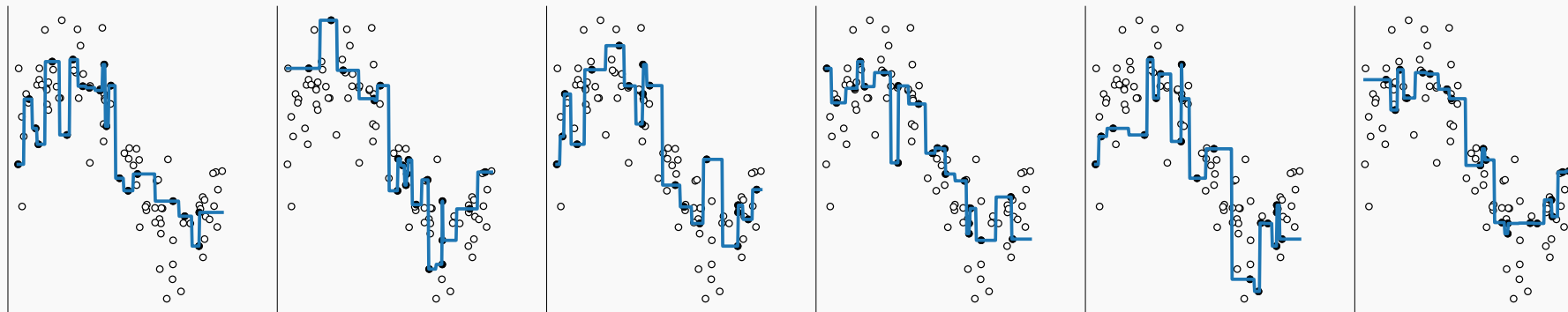
- **Select multiple subsets of the data**

Random forests: Bagging with regression trees

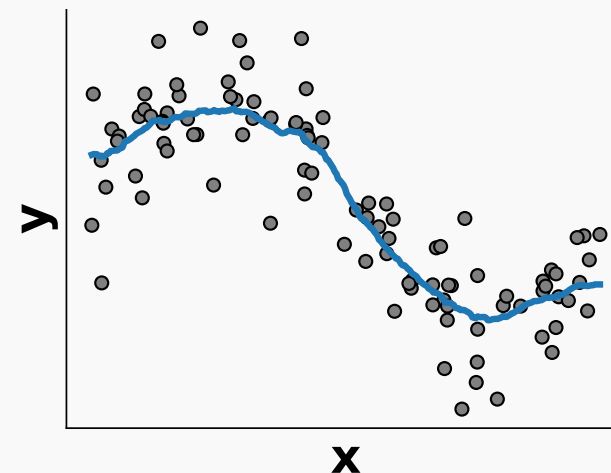


- Select multiple subsets of the data
- Fit one model on each

Random forests: Bagging with regression trees




- Select multiple subsets of the data
- Fit one model on each
- Average the predictions



Main hyper-parameters of random forests

```
1  sklearn.ensemble.RandomForestRegressor(  
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 )
```

 Python

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

Take away

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

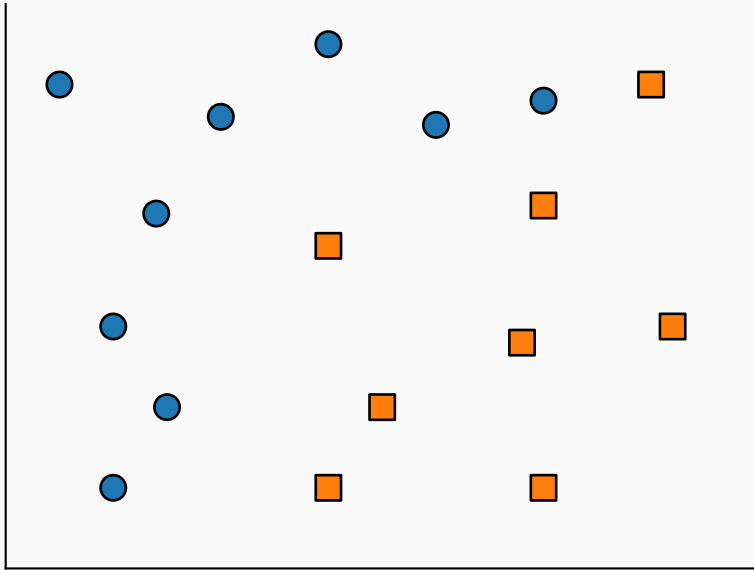
Boosting use multiple iterative models

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

Two examples of boosting

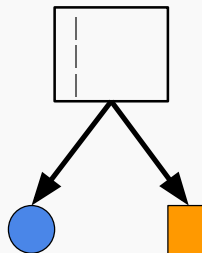
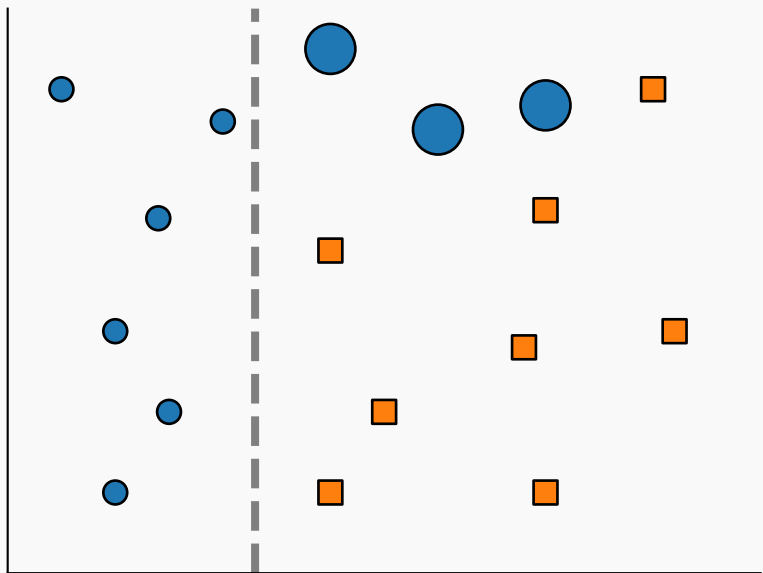
- Adaptive boosting (AdaBoost): reweight mispredicted samples at each step (Friedman et al., 2000)
- Gradient boosting: predict the negative errors of previous models at each step (Friedman, 2001)

Boosting: Adaptive boosting, classification example

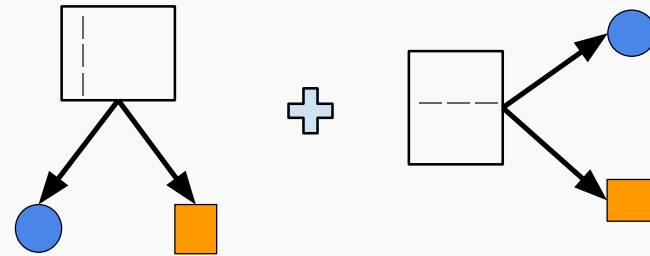
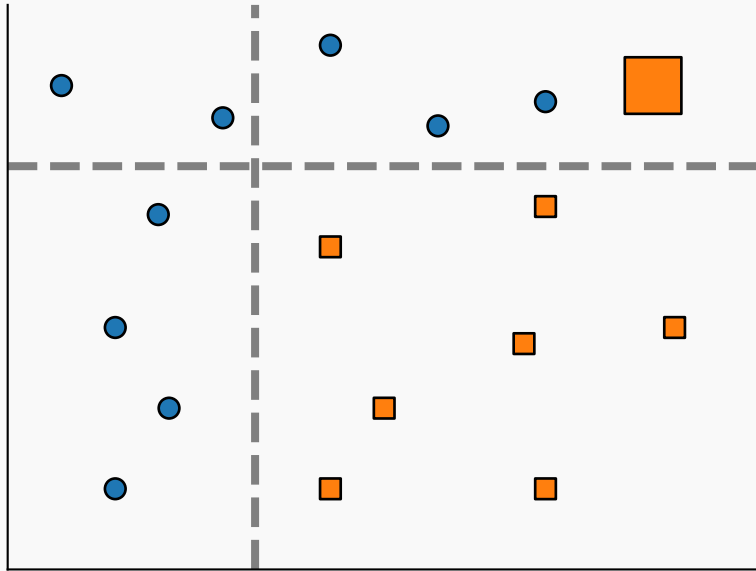


Boosting: Adaptive boosting, classification example

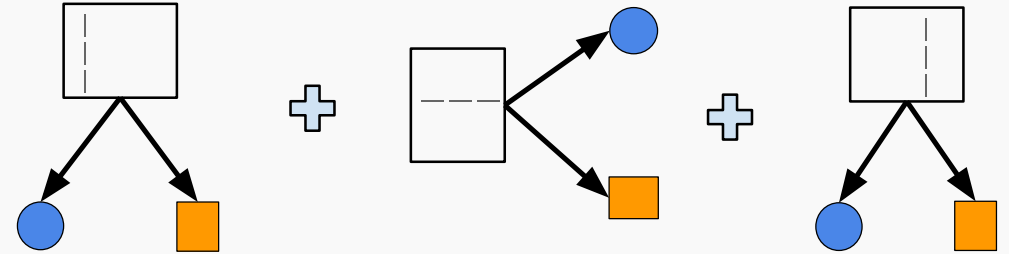
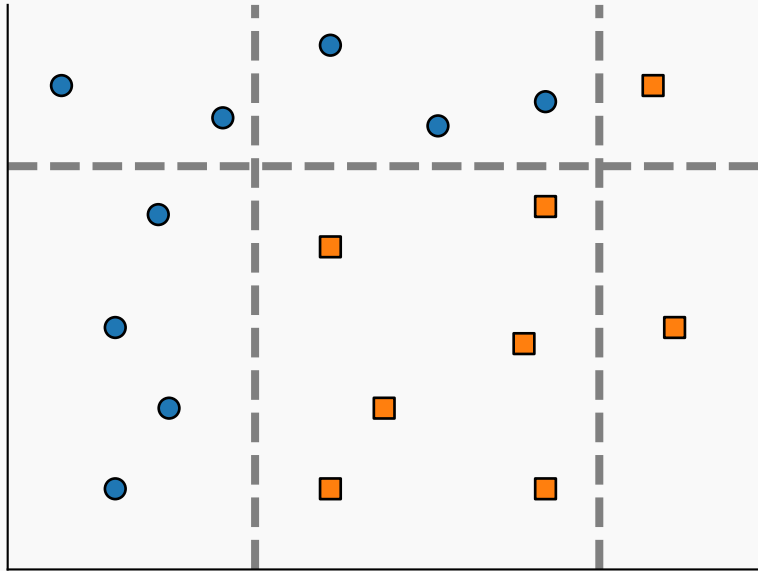
First prediction:



Boosting: Adaptive boosting, classification example



Boosting: Adaptive boosting, classification example



At each step, AdaBoost weights mispredicted samples

Adaboost for classification: choice of the weight

Algorithm for Adaboost

- Initialize the observation weights $w_i = \frac{1}{N}, i = 1..N$
- For $m = 1$ to M :
 - Fit a classifier $F_m(x)$ to the training data using weights w_i
 - Compute $\text{err}_m = \frac{\sum_{i=1}^N w_i \mathbb{1}[y_i \neq F_m(x_i)]}{\sum_{i=1}^N w_i}$
 - Compute $\alpha_m = \log\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$
 - Set $w_i \rightarrow w_i \exp[\alpha_m \mathbb{1}[y_i \neq F_m(x_i)]], i = 1..N$
- Output $F(x) = \text{sign}\left(\sum_{i=1}^M \alpha_m G_m(x)\right)$



See (Murphy, 2022) for the motivation.

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 given more importance to errors
- Any weak learner can be used

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 given more importance to errors
- Any weak learner can be used

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 week learner.

Minimization problem

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

Rewrite inside the sum:

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

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

Rewrite inside the sum:



Taylor expansion

For $l(\cdot)$ differentiable: $l(y + h) \approx l(y) + h \frac{\partial l}{\partial y}(y)$

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

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

Rewrite inside the sum:

$$l(y_i, F_{m-1}(x_i) + h(x_i)) = l(y_i, F_{m-1}(x_i)) + h(x_i) \left[\frac{\partial l(y_i, F(x_i))}{\partial F(x_i)} \right]_{F=F_{m-1}}$$



Taylor expansion

For $l(\cdot)$ differentiable: $l(y + h) \approx l(y) + h \frac{\partial l}{\partial y}(y)$

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

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

Rewrite inside the sum:

$$l(y_i, F_{m-1}(x_i) + h(x_i)) = \underbrace{l(y_i, F_{m-1}(x_i))}_{\text{constant in } h(x_i)} + \underbrace{h(x_i) \left[\frac{\partial l(y_i, F(x_i))}{\partial F(x_i)} \right]_{F=F_{m-1}}}_{\stackrel{\text{def}}{=} g_i, \text{ the gradient}}$$

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

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

Rewrite inside the sum:

$$l(y_i, F_{m-1}(x_i) + h(x_i)) = \underbrace{l(y_i, F_{m-1}(x_i))}_{\text{constant in } h(x_i)} + \underbrace{h(x_i) \left[\frac{\partial l(y_i, F(x_i))}{\partial F(x_i)} \right]_{F=F_{m-1}}}_{\stackrel{\text{def}}{=} g_i, \text{ the gradient}}$$

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

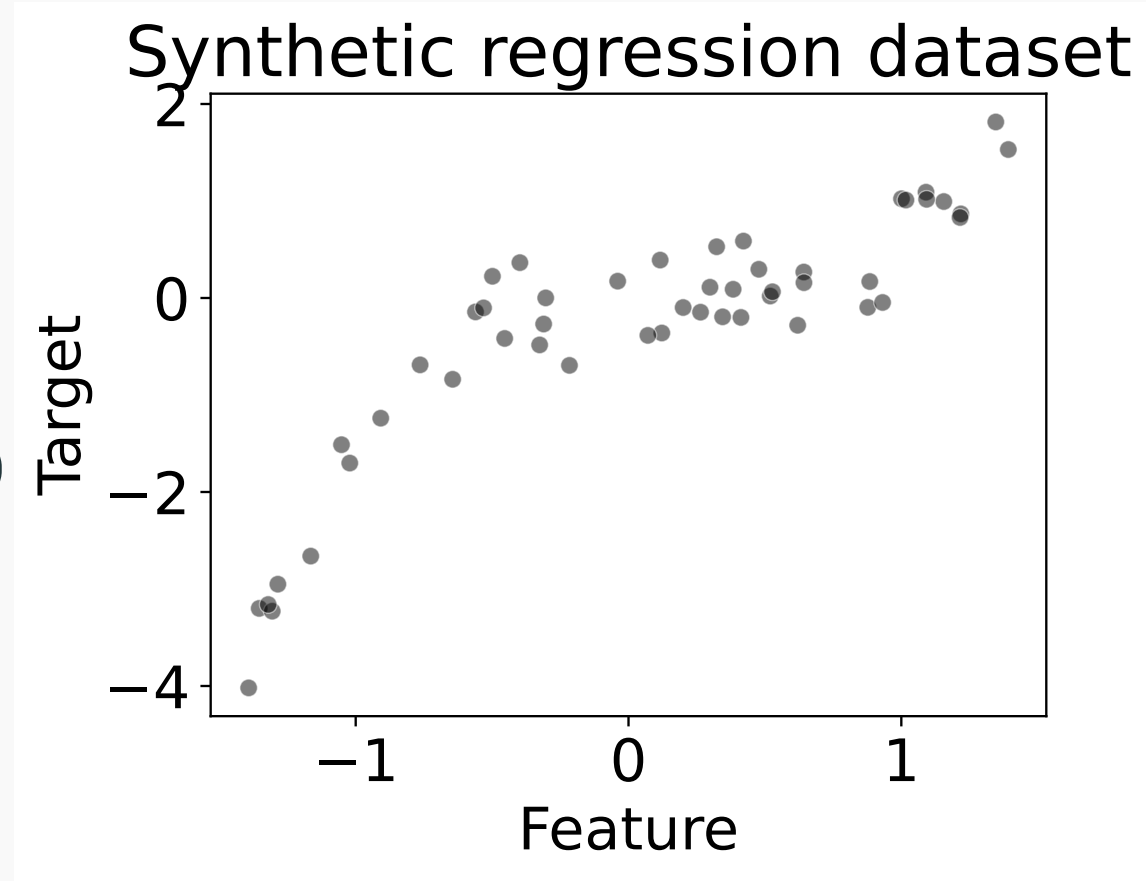
So $h_{m(x_i)}$ should be proportional to $-g_i$, so **fit h_m to the negative gradient.**

Boosting: Gradient boosting, regression example

Regression

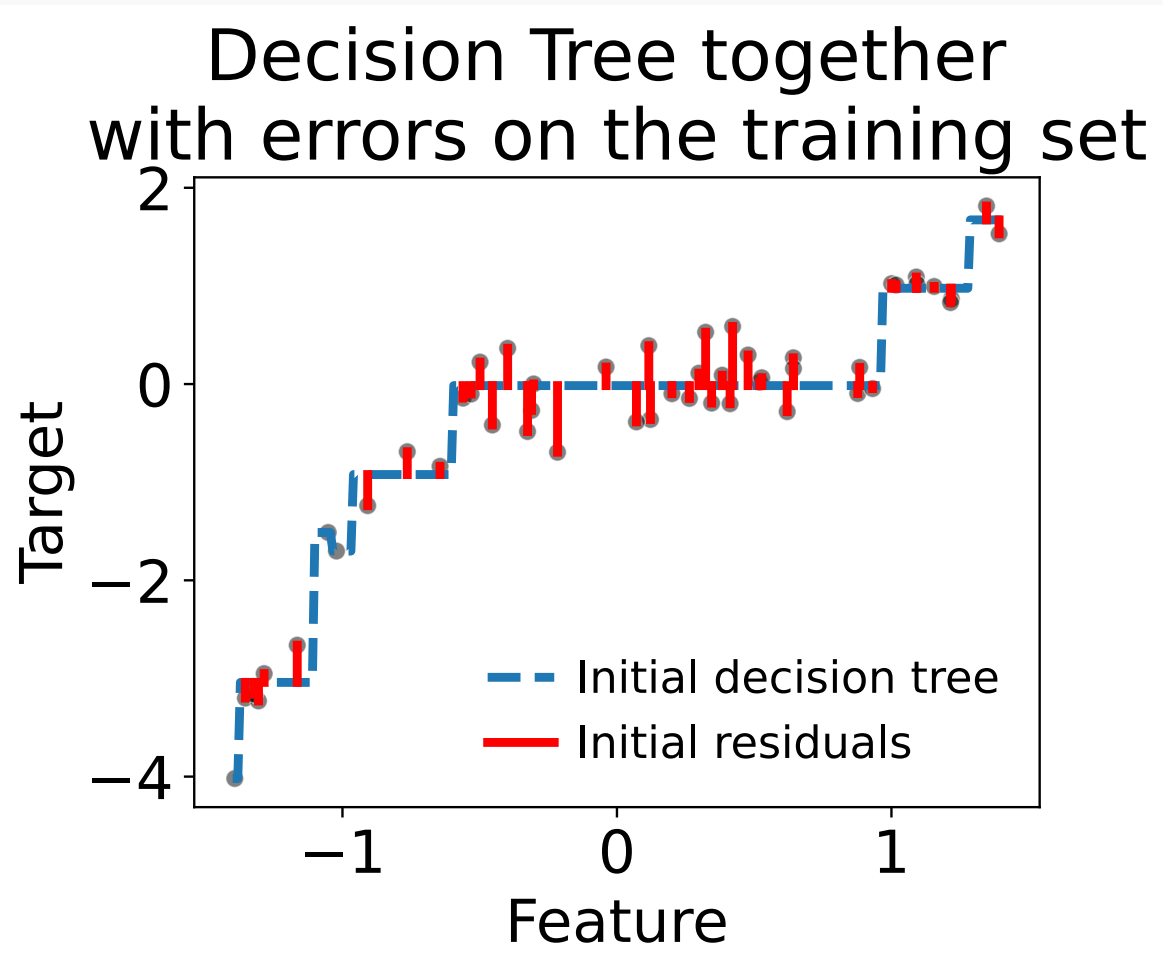
- The loss is: $l(y, F(x)) = (y - F(x))^2$
- The gradient is: $g_i = -2(y_i - F_{m-1}(x_i))$

💡 The new trees should fit the residuals



Boosting: Gradient boosting, regression example

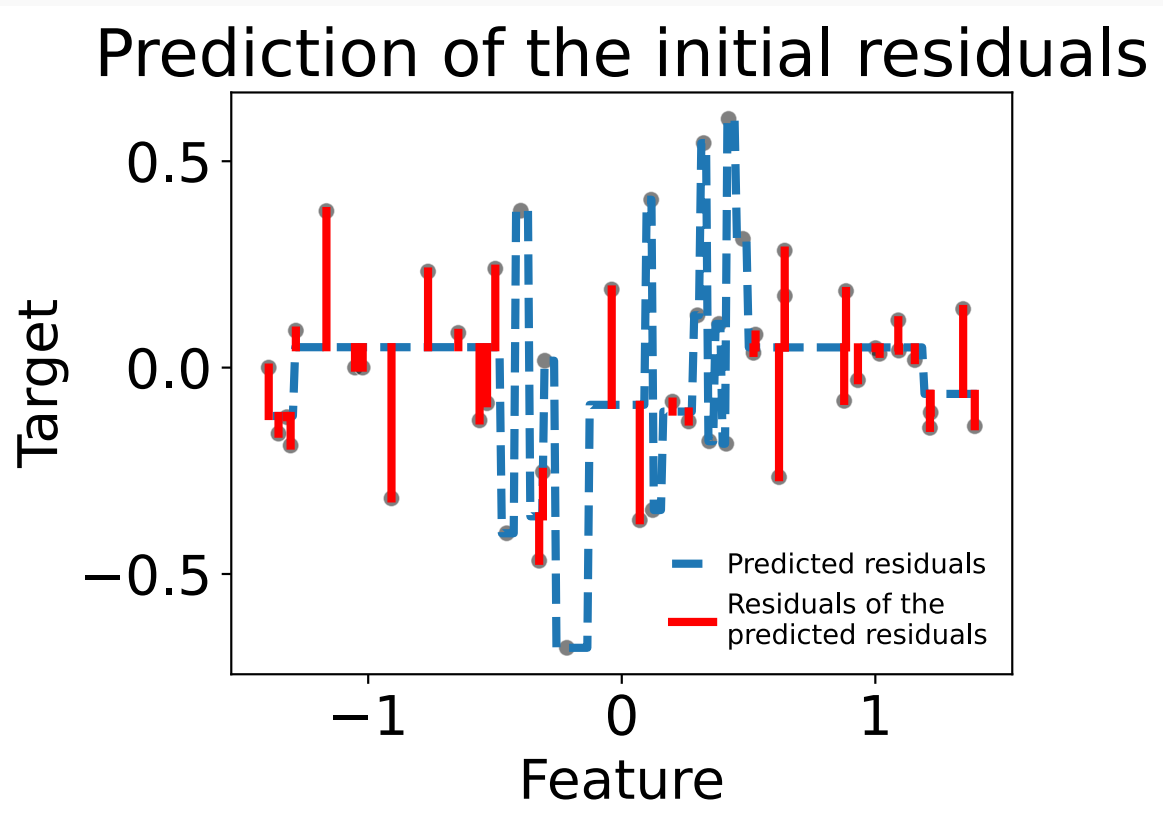
Fit a shallow tree
(depth=3)



Boosting: Gradient boosting, regression example

Fit a second tree to the residuals

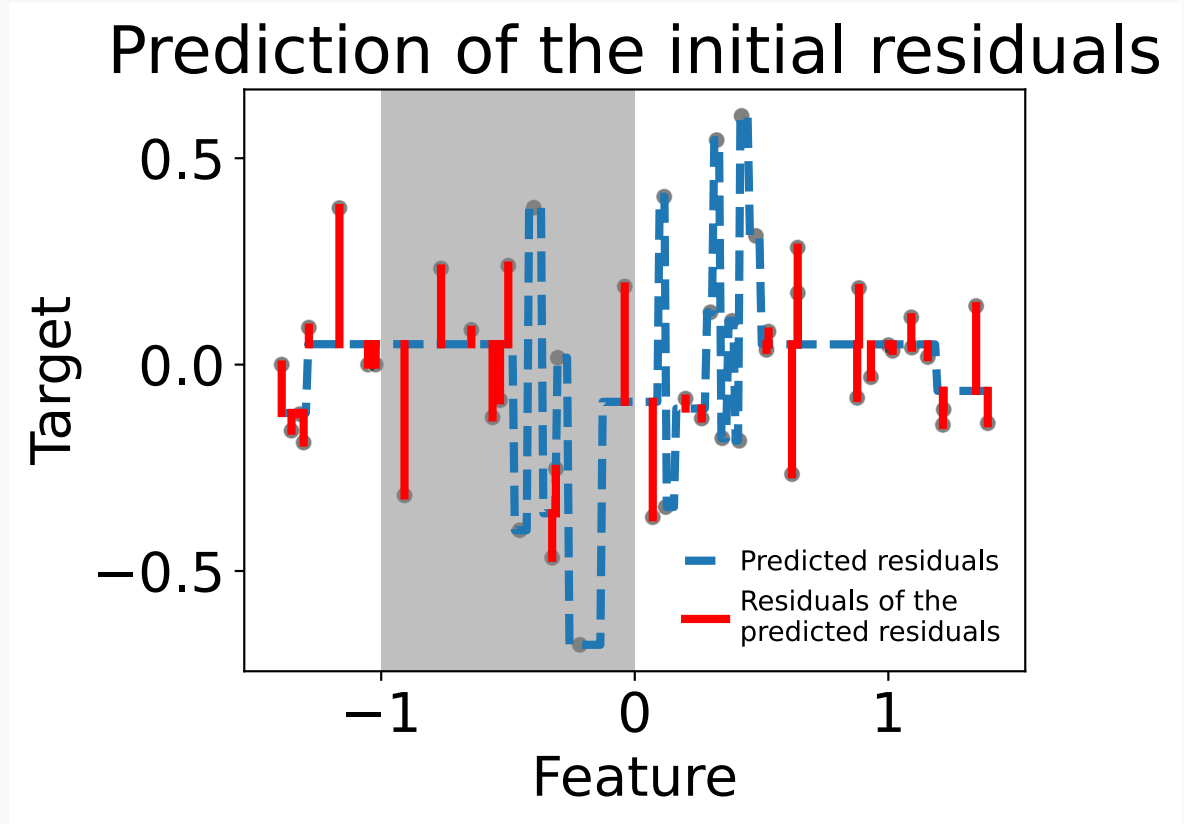
- This tree performs poorly on some samples.



Boosting: Gradient boosting, regression example

Fit a second tree to the residuals

- This tree performs well on some residuals.
- Let's zoom on one of those.



Boosting: Gradient boosting, regression example

Focus on a sample

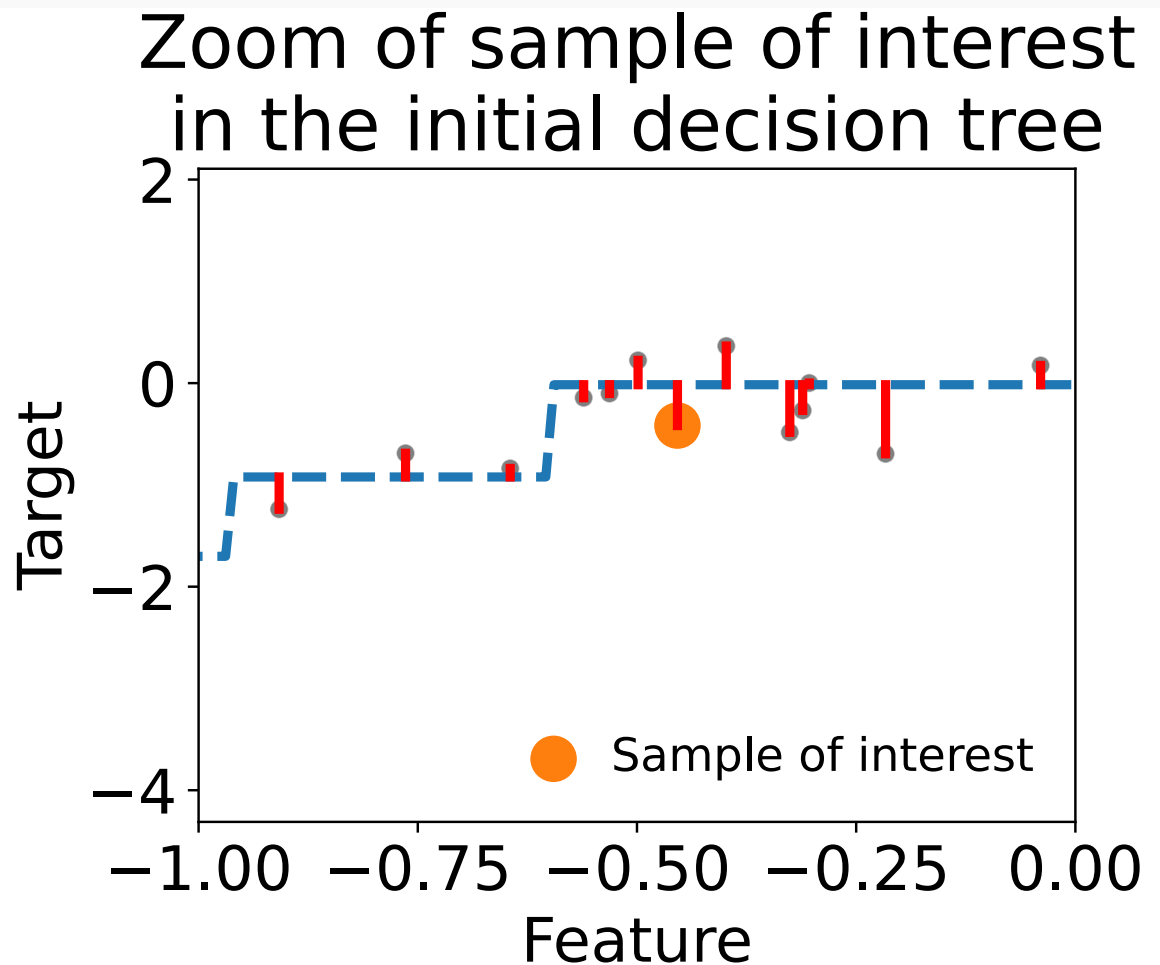
$$(x_i, y_i) = (-0.454, -0.417)$$

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

Focus on a sample

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

First tree prediction

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

Residuals:

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

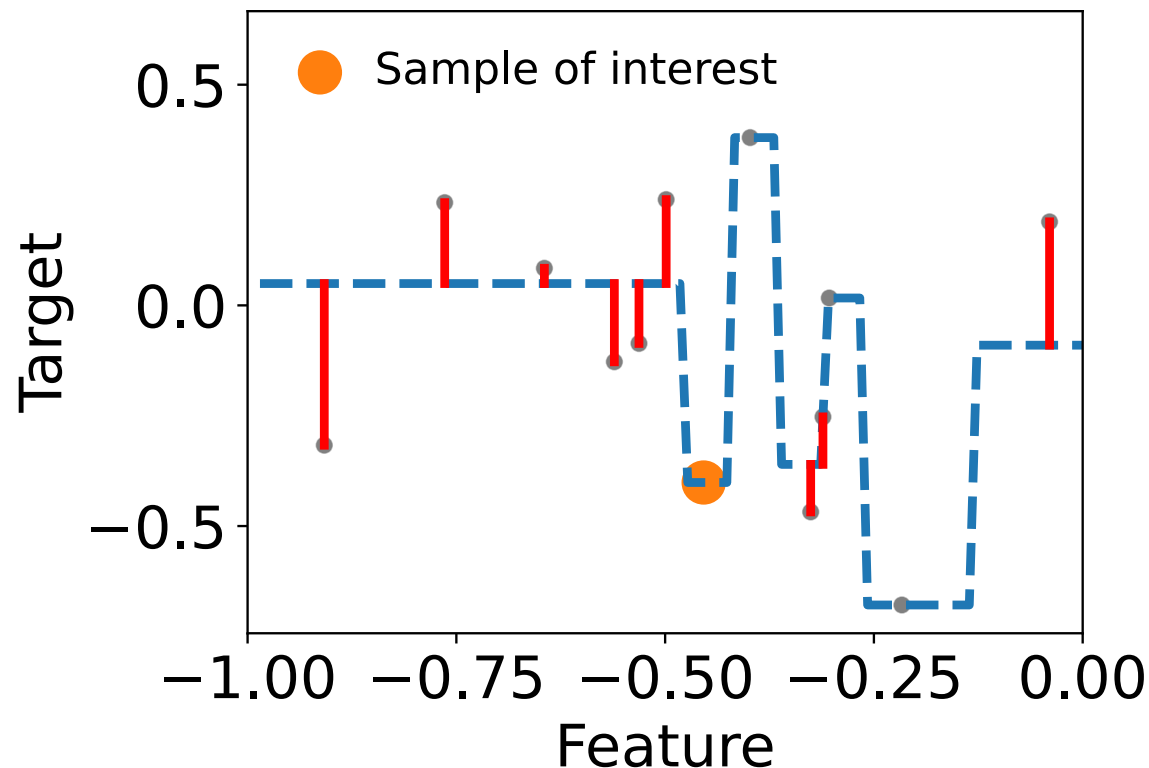
Second tree prediction

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

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

HistGradientBoosting

- Discretize numerical features into 256 bins: less costly for tree splitting
- Multi core implementation
- Much much faster

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 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?

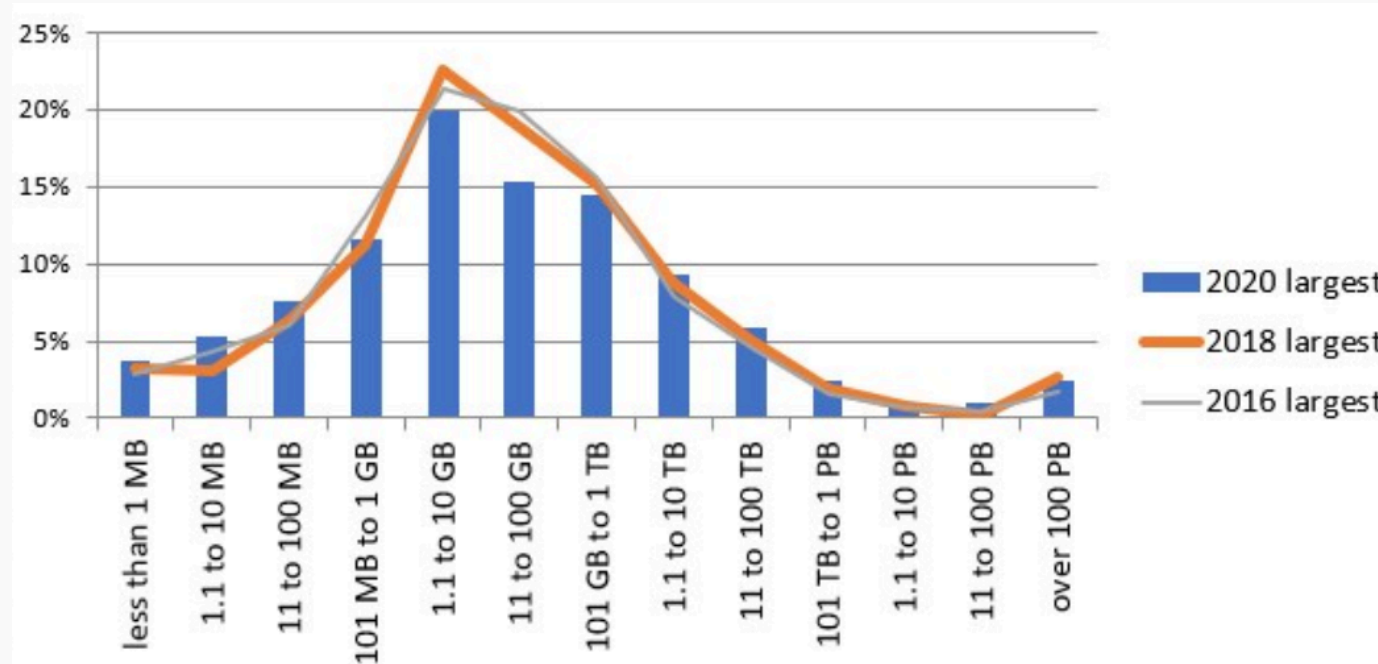
- Success of deep learning (aka deep neural networks) in image, speech recognition and text
- 🤔 Why not so used in econometrics?

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

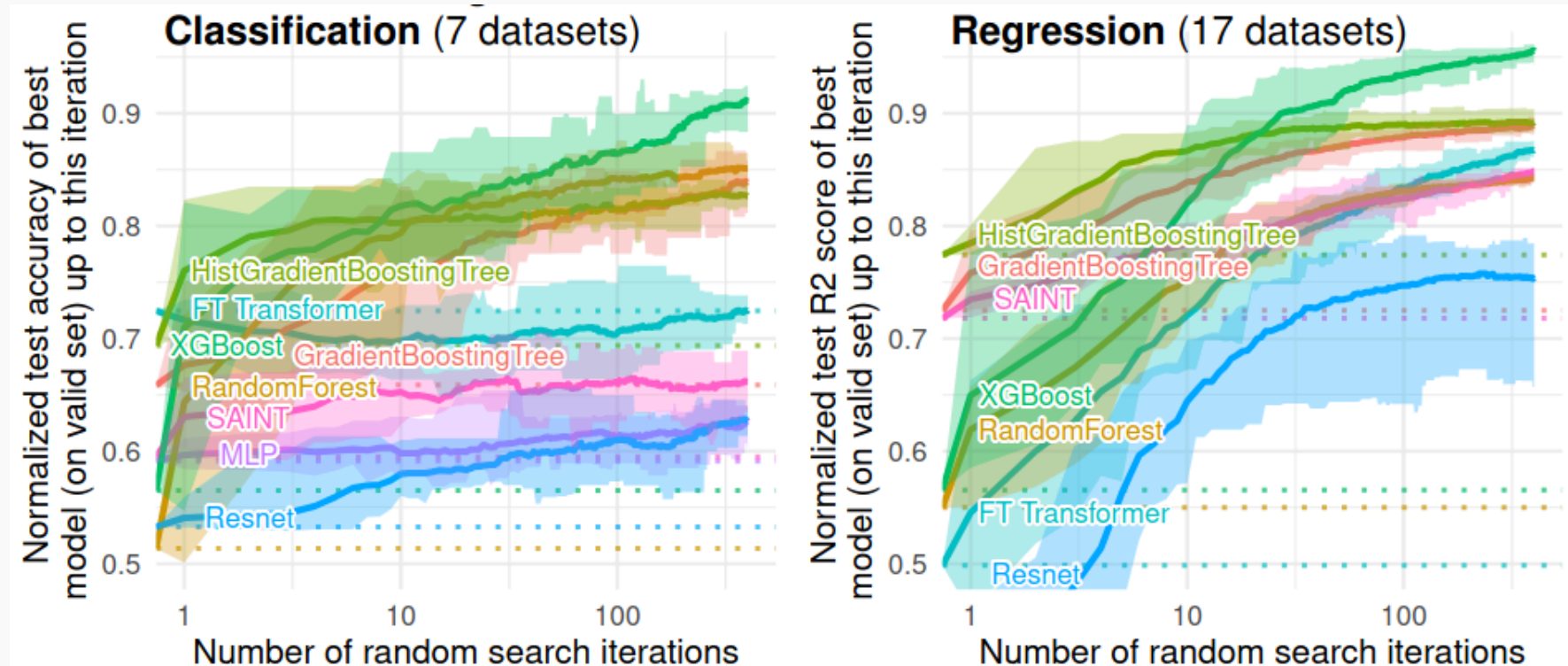


Typical dataset are mid-sized. This does not change with time.¹

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

Answer 2: Deep learning underperforms on data tables

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



Recent work showing that tree-based models can be outperformed

- 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

Breiman, L. (1996). Bagging predictors. Machine Learning, 24, 123–140.

Efron, B. (1992). Bootstrap methods: another look at the jackknife. In Breakthroughs in statistics: Methodology and distribution: Breakthroughs in statistics: Methodology and distribution (pp. 569–593). Springer.

Estève, L., Lemaitre, G., Grisel, O., Varoquaux, G., Amor, A., Lilian, Rospars, B., Schmitt, T., Liu, L., Kinoshita, B. P., hackmd-deploy, ph4ge, Steinbach, P., Boucaud, A., Muite, B., Boisberranger, J. du, Notter, M., Pierre, P, S., ... parmentelat. (2022). INRIA/scikit-learn-mooc: Third MOOC session. Zenodo. <https://doi.org/10.5281/zenodo.7220307>

Friedman, J. H. (2001). Greedy function approximation: a gradient boosting machine. Annals of Statistics, 1189–1232.

- Friedman, J., Hastie, T., & Tibshirani, R. (2000). Additive logistic regression: a statistical view of boosting (with discussion and a rejoinder by the authors). The Annals of Statistics, 28(2), 337–407.*
- 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.*
- Grinsztajn, L., Oyallon, E., Kim, M. J., & Varoquaux, G. (2023). Vectorizing string entries for data processing on tables: when are larger language models better?. Arxiv Preprint Arxiv:2312.09634.*
- Kim, M. J., Grinsztajn, L., & Varoquaux, G. (2024). CARTE: pretraining and transfer for tabular learning. Arxiv Preprint Arxiv:2402.16785.*
- Lecué, G., & Mitchell, C. (2012). Oracle inequalities for cross-validation type procedures.*
- Murphy, K. P. (2022). Probabilistic machine learning: an introduction. MIT press.*

Varoquaux, G., Raamana, P. R., Engemann, D. A., Hoyos-Idrobo, A., Schwartz, Y., & Thirion, B. (2017). Assessing and tuning brain decoders: cross-validation, caveats, and guidelines. Neuroimage, 145, 166–179.