Tree models

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[1]MIPT [2]DESY

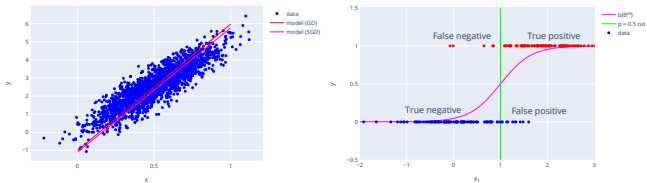
Outline

- Decision tree
- Random forest
- Gradient boosting

Decision tree

Decision tree

motivation



- In the previous lecture we explored a family of linear models:
  - → nicely describe linear correlations
  - → fast and easy to train
  - → performing well with large number of samples/features

Decision tree

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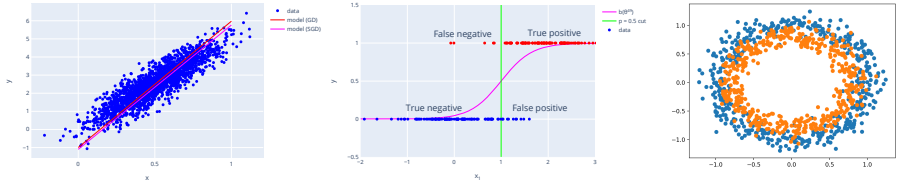

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- Additional heuristics might be applied (e.g. polynomial features) but are ad-hoc

Decision tree

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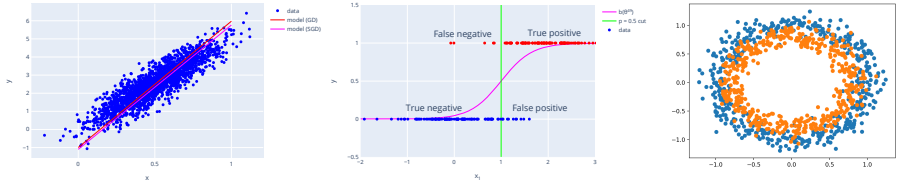

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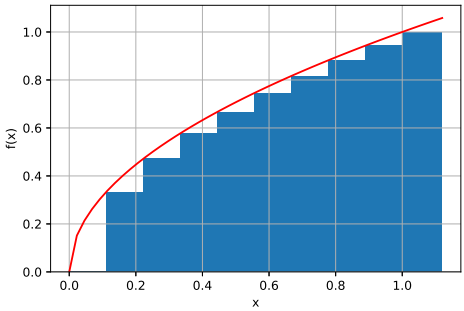
Is there a more general way to describe non-linearities?

Decision tree

motivation

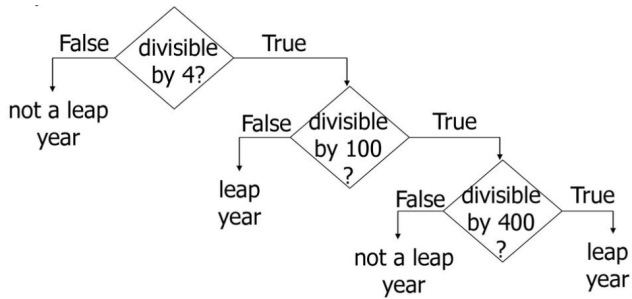
- What is the simplest way to approximate a function?
- Using **piecewise linear function**



$$f(x) = \begin{cases} 0, & x < 0.12 \\ 0.35, & 0.12 \le x < 0.22 \\ 0.47, & 0.22 \le x < 0.36 \\ \dots \end{cases}$$

Decision tree — intuition

- What is the simplest way to categorize things?
- Ask **yes/no questions**



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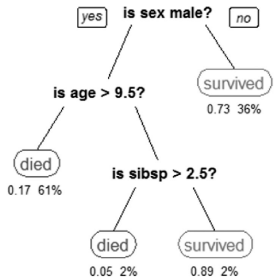

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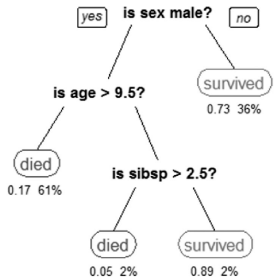


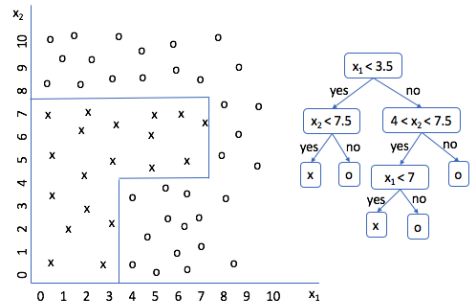
Can we mathematically formulate this?

Decision tree — algorithm

Algorithm 1: Decision tree

1: Initialize: hyperparameters, leaf set = $\{X_{\text{train}}\}$

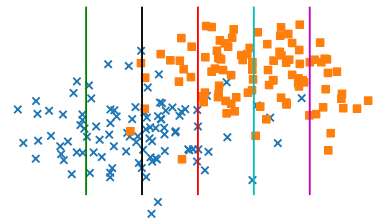
2: **while** not stopping criteria **do**
3: leaf to split = Choose(leaf set)
4: left leaf, right leaf = Split(leaf to split)
5: Add left leaf, right leaf to leaf set
6: Remove leaf to split from leaf set
7: **end while**



Decision tree

split criteria

- Suppose there is a classification problem
- So we want to separate one class from the other by constructing **decision boundary**
- And using decision tree algorithm described earlier
- To do that we need to start splitting on features
- Which **split** is the best?



Decision tree — split criteria

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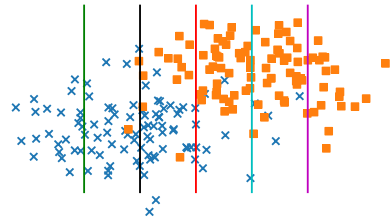
→ We need some criteria



Decision tree — split criteria

more about IG

- Suppose we have n features $x^{(1)}, x^{(2)}, ..., x^{(n)}$ in our dataset X
- If we want to split on some feature $x^{(j)}$ at threshold t then we propose to maximize **Information Gain** (IG):

$$\mathrm{IG}(\mathrm{X}, \mathrm{a}) = \mathrm{H}(\mathrm{X}) - \mathrm{H}(\mathrm{X} \mid \mathrm{a}) \to \max_{\mathrm{a}}$$

$$\mathrm{H}(\mathrm{X} \mid \mathrm{a}) = \sum_{v \in vals(\mathrm{a})} \frac{|S_{\mathrm{a}}(v)|}{|\mathrm{X}|} \cdot \mathrm{H}\left(S_{\mathrm{a}}(v)\right)$$

- In case of a binary tree with L(R) elements in the left (right) split we've got:

$$\mathrm{IG}(j, t) = \frac{|\mathrm{L}|}{|\mathrm{X}|}\mathrm{H}(\mathrm{L}) + \frac{|\mathrm{R}|}{|\mathrm{X}|}\mathrm{H}(\mathrm{R}) \to \min_{j,t}$$

Decision tree — split criteria

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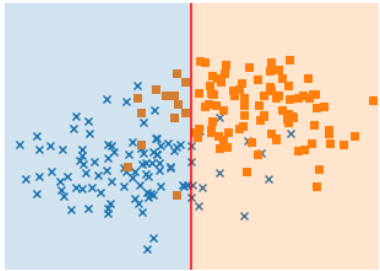
How to choose H(X)?

Decision tree — split criteria



The ”best” split is a central one because it introduces **purity** in the best way. And we have some functions to measure the purity!

Decision tree — split criteria

- Define H(R) in a leaf as a goodness of approximation with the ″best″ constant c

$$\mathrm{H}(\mathrm{R}) = \min_{c \in \mathbb{Y}} \frac{1}{|N|} \sum_{(x_i, y_i) \in \mathrm{R}} \mathcal{L}(y_i, c)$$

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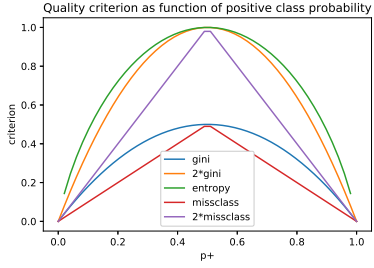
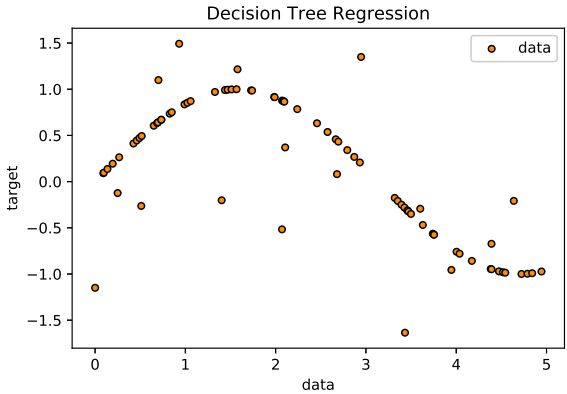
- or c_k with $\sum_k c_k = 1$, if tree predicts class probabilities
- Define a fraction of class k in a leaf as p_k
- Then one can show:
  - **Misclassification criteria**
    $\mathcal{L}(y, c) = [y \neq c] \Rightarrow \mathrm{H(R)} = 1 - \max_k \{p_k\}$
  - **Gini Impurity**
    $\mathcal{L}(y, c) = \sum_k (c_k - [y = k])^2 \Rightarrow \mathrm{H(R)} = 1 - \sum_k (p_k)^2$
  - **Entropy criteria**
    $\mathcal{L}(y, c) = -\sum_k [y = k] \log c_k \Rightarrow \mathrm{H(R)} = -\sum_k p_k \log_2 p_k$



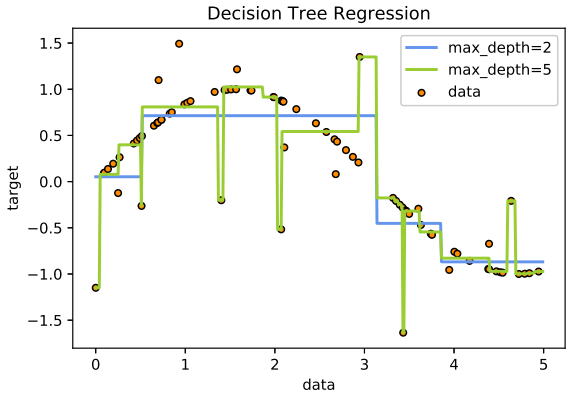
Lower diversity (higher purity)
$\Rightarrow$ **lower impurity** criterion H(R)

Decision tree — regression



Can we use decision tree approach for regression problem?

Decision tree — regression



Can we use decision tree approach for regression problem? Yes

Decision tree — regression

- How should we modify decision criteria?

$$\mathrm{IG}(j,t) = \frac{|\mathrm{L}|}{|\mathrm{Q}|}\mathrm{H}(\mathrm{L}) + \frac{|\mathrm{R}|}{|\mathrm{Q}|}\mathrm{H}(\mathrm{R})$$

→ Mean squared error: $\mathcal{L}(y,c) = (y-c)^2 \Rightarrow \mathrm{H}(\mathrm{R}) = \min_c \frac{1}{|\mathrm{R}|}\sum_{(x_i,y_i)\in \mathrm{R}} (y_i - c)^2$

→ Mean absolute error: $\mathcal{L}(y,c) = |y-c| \Rightarrow \mathrm{H}(\mathrm{R}) = \min_c \frac{1}{|\mathrm{R}|}\sum_{(x_i,y_i)\in \mathrm{R}} |y_i - c|$

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- One can further show that:

$$c^* = \frac{1}{|\mathrm{R}|}\sum_{y_i \in \mathrm{R}} y_i$$

$$c^* = \mathrm{median}(y_i \in \mathrm{R})$$

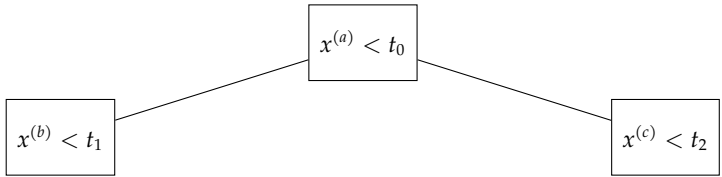
Decision tree — growing

What about tree construction?

$$x^{(a)} < t_0$$

Decision tree — growing

What about tree construction? Do it recursively by **greedy** algorithm



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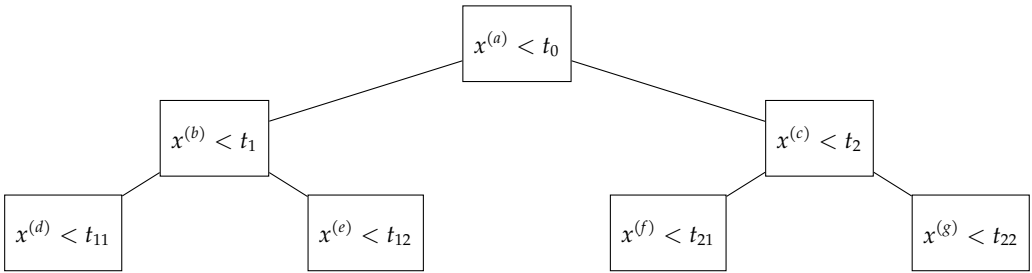

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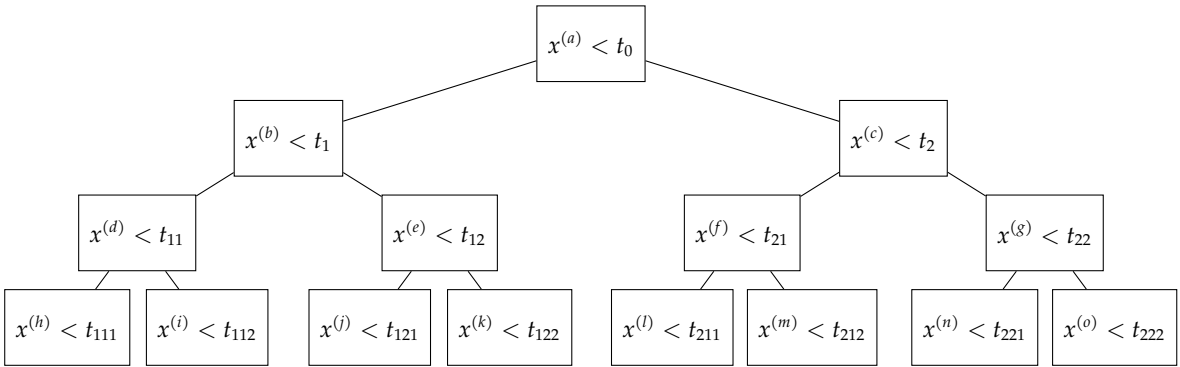
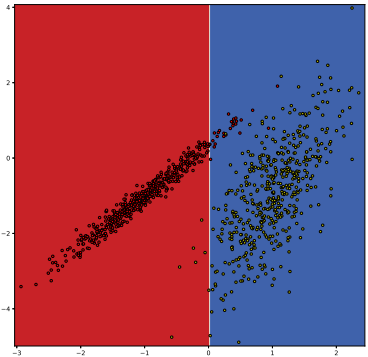
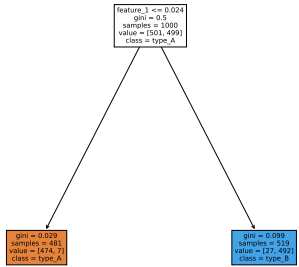


Decision tree — growing

check out also these visuals





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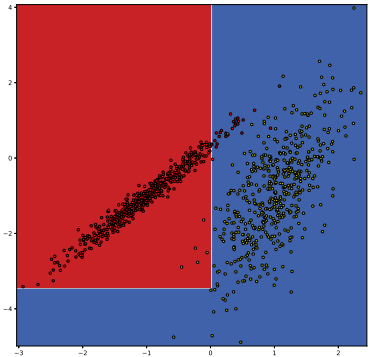

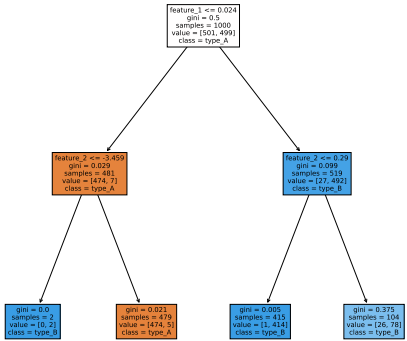

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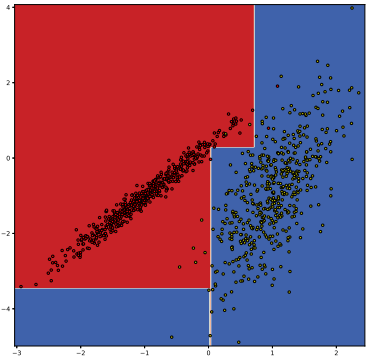

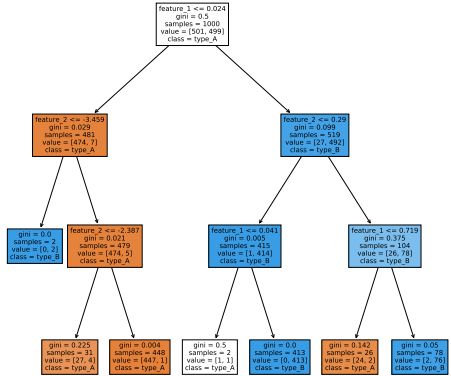

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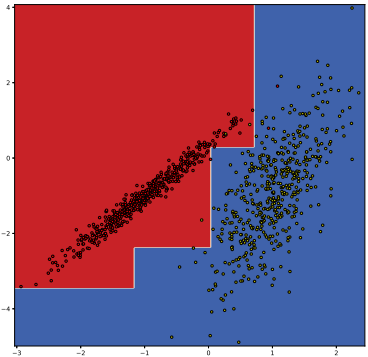
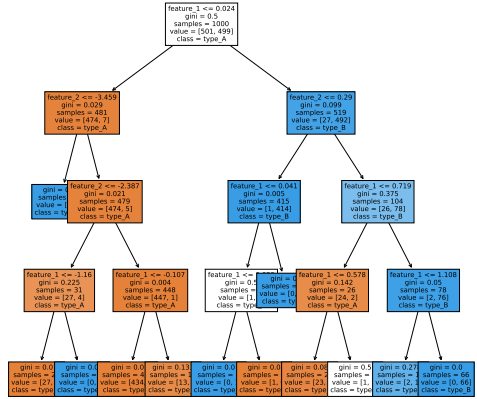
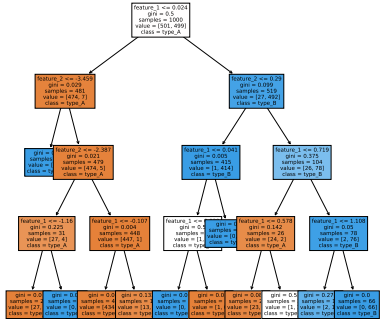




Decision tree — stopping criteria

- What about stopping criteria?
  1. Split until one element in leaf
     (which problems can we meet?)
  2. Limit max depth/max number of leaves
  3. Limit amount of elements in leaf/split
  4. All elements in a leaf belong to a single class
  5. IG(j, t) isn't improving by x%
  6. Combination of limitations



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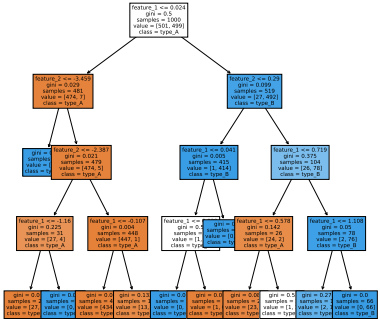
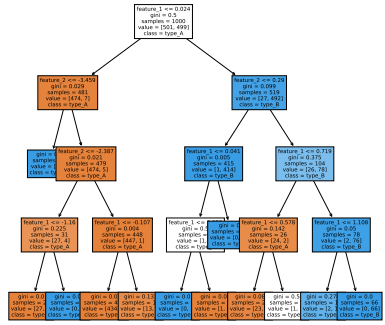
→ The choice is up to you
(aka hyperparameter)



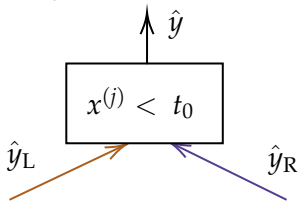
Decision tree ⟶ prediction

1. Once tree is built, look at the training samples in each leaf
2. Assign to every leaf a value according to:
   - Classification: majority vote
     ➔ assign the most frequent class
   - Classification: class probabilities
     ➔ approximate with class fractions
   - Regression: mean, median over the values in a leaf
3. During inference step, propagate every sample through the tree
4. Assign a value of the leaf where the sample ended up



Can already trained decision tree handle **missing values** on inference step?

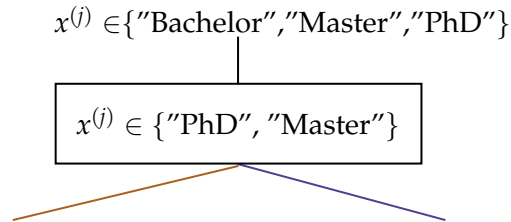
Can already trained decision tree handle **missing values** on inference step? Yes!



$$\hat{y} = \frac{|L|}{|X|}\hat{y}_L + \frac{|R|}{|X|}\hat{y}_R$$

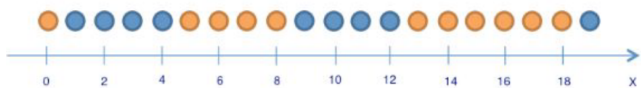
Categorical features can also easily be treated by tree:

- If categorical feature is selected at particular node
- Loop through all combination of its values
- Pick those set of values which result in best IG
- Split the leaf as before



Decision tree

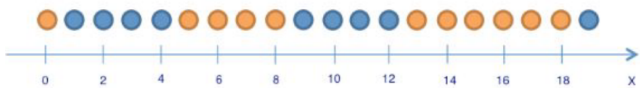
check your understanding



- What is the entropy of the distribution on the figure?
- What task do we solve to make a split?
- How many hyperparameters of decision tree do we know?
- How is the tree construsted?
- Which stopping criteria can we use?

Decision tree

check your understanding



- $\frac{11}{20} \log \frac{11}{20} + \frac{9}{20} \log \frac{9}{20}$
- Maximization of Information Gain
- Stopping criteria hyperparameters, Splitting criteria
- Recursively by greedy algorithm
- Max depth, Min elements in leaf, Min elements to make split, Combination

Random forest

Random forest — theoretical insight

more in this lecture

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Random forest

theoretical insight

more in this lecture

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- Average error of base algorithms $b_i(\boldsymbol{x})$:

$$\mathcal{E} \equiv \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{\boldsymbol{x}} \varepsilon_i^2(\boldsymbol{x})$$

Random forest — theoretical insight

- Assume errors to be unbiased and uncorrelated:

$$\mathbb{E}_x \varepsilon_i(\boldsymbol{x}) = 0, \quad \forall i$$

$$\mathbb{E}_{\boldsymbol{x}}[\varepsilon_i(\boldsymbol{x})\varepsilon_j(\boldsymbol{x})] = 0, \quad i \neq j$$

- Let's construct an algorithm so that it averages predictions of base algorithms:

$$a(\boldsymbol{x}) = \frac{1}{N}\sum_{i=1}^{N} b_i(\boldsymbol{x})$$

Random forest — theoretical insight

but there's also bias-variance trade-off

- Then the error of this algorithm:

$$\mathcal{E}_N \equiv \mathbb{E}_{\boldsymbol{x}} \left(a(\boldsymbol{x}) - y(\boldsymbol{x})\right)^2 = \mathbb{E}_{\boldsymbol{x}} \left(\frac{1}{N}\sum_{i=1}^{N} b_i(\boldsymbol{x}) - y(\boldsymbol{x})\right)^2 =$$

$$= \mathbb{E}_{\boldsymbol{x}} \left(\frac{1}{N}\sum_{i=1}^{N} \varepsilon_i(\boldsymbol{x})\right)^2 =$$

$$= \frac{1}{N^2}\mathbb{E}_{\boldsymbol{x}} \left(\sum_{i=1}^{N} \varepsilon_i^2(\boldsymbol{x}) + \underbrace{\sum_{i\neq j} \varepsilon_i(\boldsymbol{x})\varepsilon_j(\boldsymbol{x})}_{=0}\right) = \frac{1}{N}\frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{\boldsymbol{x}}\varepsilon_i^2(\boldsymbol{x}) = \frac{\mathcal{E}}{N}$$

→ Composition of N algorithms has N times smaller error!

Random forest

how to achieve these assumptions?

$\mathbb{E}_x \varepsilon_i(\boldsymbol{x}) = 0$

➔ Strong models provide low bias $\Rightarrow$ train *overfitted* models $\Rightarrow$ **decision trees**

Random forest

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Random forest

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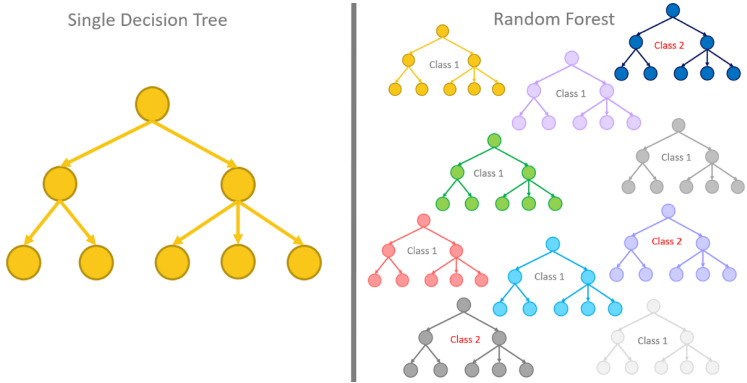
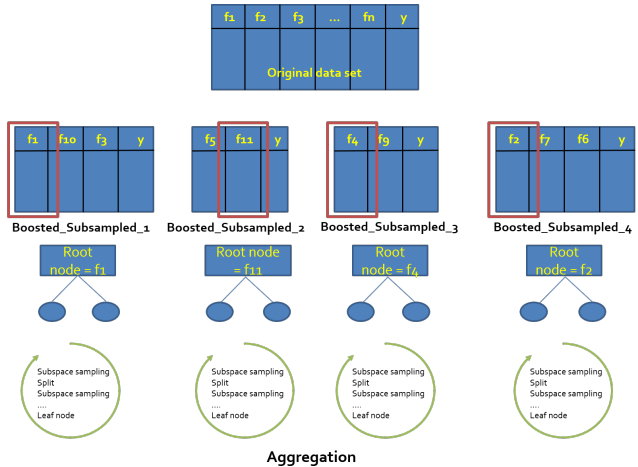
Random forest = low-biased decision trees + RSM + $\underbrace{\textbf{b}\text{ootstrap} + \textbf{agg}\text{regat}\textbf{ing}}_{\textbf{bagging}}$

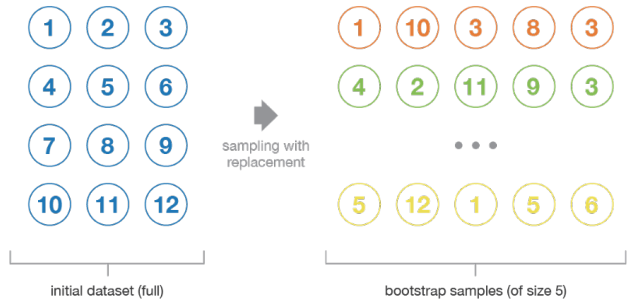
Random forest — trees



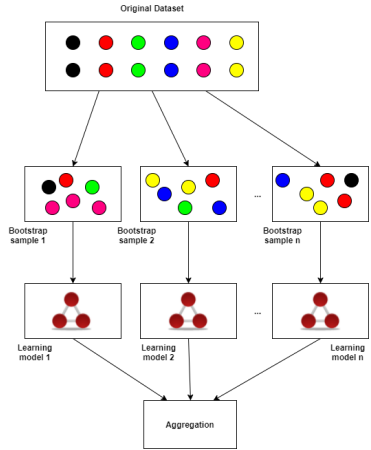
Random forest — RSM



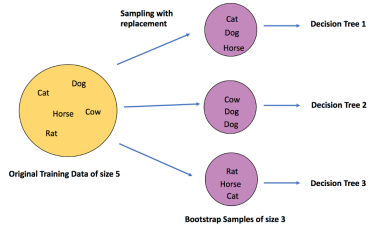
Random forest — bootstrap



Random forest — aggregating



Random forest — insights



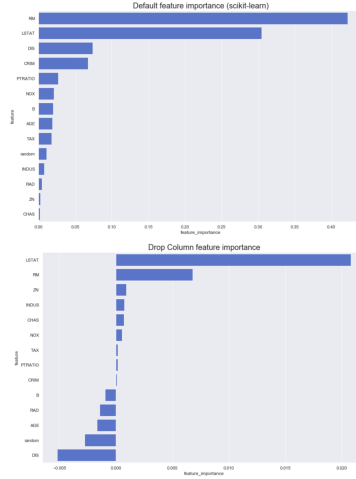
- As we use bagging, some data ($\approx 37\%$) is left unused during training
- Therefore, we can validate model on it $\Rightarrow$ **out-of-bag score**

$$\text{OOB} = \sum_{i=1}^{\ell} L\left(y_i, \frac{1}{\sum_{n=1}^{N}[x_i \notin X_n]} \sum_{n=1}^{N} [x_i \notin X_n]\, b_n(x_i)\right)$$

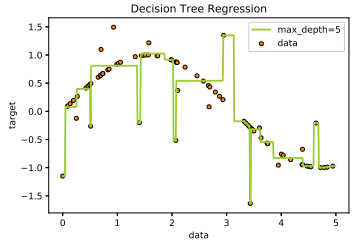
Random forest — insights

- IGs at each split can be used to calculate **feature importance**
- The higher (normalized) total reduction of IG brought by that feature – the better
- Note: this logic can be used in any tree-based model
- Caveat: inflates the importance of features features with high cardinality (many unique values)
- Other methods such as permutation importance exist
- And you might want to look at SHAP values too

more here



Random forest — check your understanding



- Can Random Forest be applied to regression task?
- What's the motivation for using Random Forest: decrease bias or variance?
- Given 1000 observations, minimum observation required to split a node: 200, minimum leaf size: 300 – what's the possible maximum depth of a Decision Tree?
- How would you propose to make the model on the figure better? Does it correspond to RF or Decision Tree?

- Yes
- Decrease variance
- 2
- Weaken the model by changing stopping criteria: low max depth, increase min elements in leaf, etc.

Gradient boosting

Gradient boosting

motivation

- Ensembling models improves performance comparing to a single model
- However, simply training them independently sounds not quite optimal (although is easy to parallelize)
- Maybe, we can add models to ensemble in a cleverer way?

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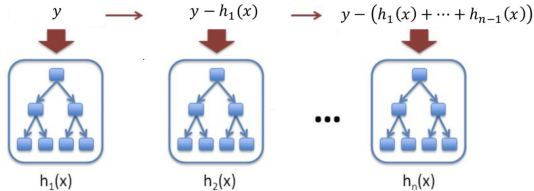
➔ e.g., iteratively by correcting upon mistakes of previous models?

$$a_n(x) = h_1(x) + \cdots + h_n(x)$$



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Let's dive into theory

Gradient boosting — theory

- Suppose we have dataset $\{(\boldsymbol{x}_i, y_i)\,,\ i = 1, \ldots, N\}$, model $a(\boldsymbol{x})$ to be found and loss function $L(y, a(\boldsymbol{x}))$
- Optimal model:
$$\hat{a}(\boldsymbol{x}) = \arg\min_{a(\boldsymbol{x})} \mathbb{E}_{x,y}[L(y, a(\boldsymbol{x}))]$$
- Let it be from parametric family:
$$\hat{a}(\boldsymbol{x}) = a(\boldsymbol{x}, \hat{\boldsymbol{\theta}})$$
$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \mathbb{E}_{x,y}[L(y, a(\boldsymbol{x}, \boldsymbol{\theta}))]$$
- Here $L(y, z)$ encodes information about the problem type:
  - classification: $\log\left(1 + e^{-yz}\right)$
  - regression: $(y - z)^2$ or $|y - z|$

Gradient boosting

theory

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$$\hat{a}(\boldsymbol{x}) = \sum_i \hat{\rho}_i \cdot h(\boldsymbol{x}, \hat{\theta}_i)$$

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- At t-th iteration we want to improve the current model by adding a new base algorithm:

$$\hat{a}_t(\boldsymbol{x}) = \hat{a}_{t-1}(\boldsymbol{x}) + \hat{\rho}_t \cdot h(\boldsymbol{x}, \hat{\theta}_t)$$

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- In fact, it looks pretty much like a gradient descent in a model space $\Rightarrow$

- So let's train each base learner to predict this gradient:

$$\boldsymbol{r}_{it} = -\left[\frac{\partial L\left(y_i,\, a\left(\boldsymbol{x}_i\right)\right)}{\partial a\left(\boldsymbol{x}_i\right)}\right]_{a(\boldsymbol{x}_i)=\hat{a}(\boldsymbol{x}_i)}, \quad \text{for } i = 1, \ldots, N$$

$$\hat{\theta}_t = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \left(\boldsymbol{r}_{it} - h\left(\boldsymbol{x}_i, \boldsymbol{\theta}\right)\right)^2,$$

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- And learning the optimal learning rate (but can be skipped and set to constant):

$$\hat{\rho}_t = \arg\min_{\rho} \sum_{i=1}^{N} L\left(y_i,\, \hat{a}_{t-1}\left(\boldsymbol{x}_i\right) + \rho \cdot h\left(\boldsymbol{x}_i, \hat{\theta}_t\right)\right)$$

Gradient boosting — theory

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- Finally:

$$\hat{a}_t(\boldsymbol{x}) = \hat{a}_{t-1}(\boldsymbol{x}) + \hat{\rho}_t \cdot h(\boldsymbol{x}, \hat{\theta}_t)$$

Gradient boosting

theory

- In theory, you can boost whatever algorithm you want
- But people opted for trees $\rightarrow$ aka **Boosted Decision Trees** (BDT) in HEP vocabulary
- What type of models we should use: weak or strong?

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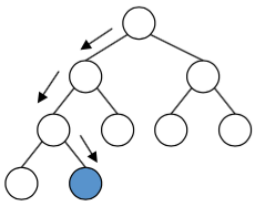

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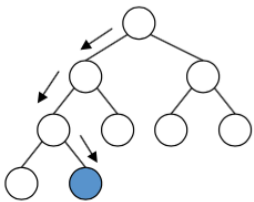

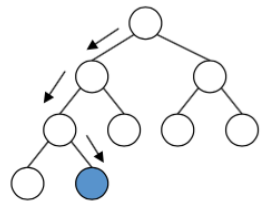

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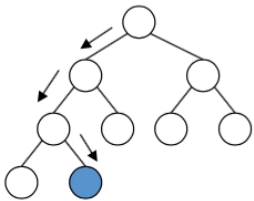
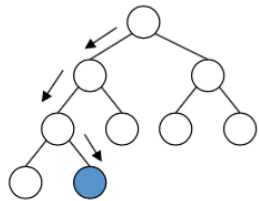
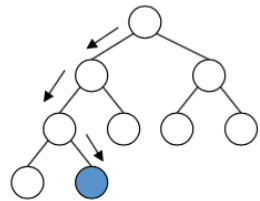






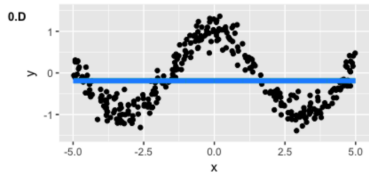
- Data: toy dataset $y = \cos(x) + \epsilon, \epsilon \sim \mathcal{N}\left(0, \frac{1}{5}\right), x \in [-5, 5]$
- Loss function: MSE
- Family of algorithms: decision trees, depth $= 2$
- Number of iterations: M $= 3$
- Initialial base algorithm: constant with mean value

Gradient boosting

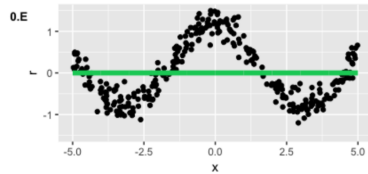
examples

playgrounds click, click

Dataset and Current ensemble



Residuals and Last model in ensemble



Gradient boosting

examples

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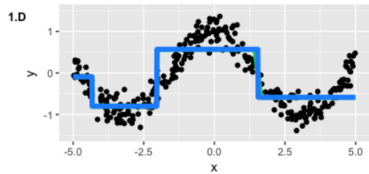

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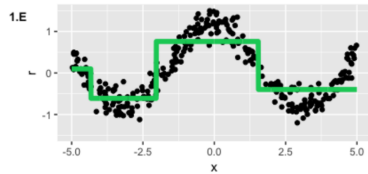

Gradient boosting

examples

playgrounds click, click

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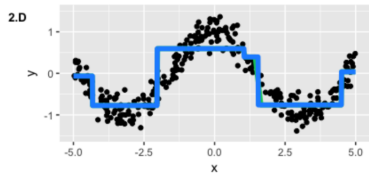

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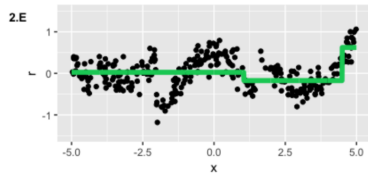

Gradient boosting

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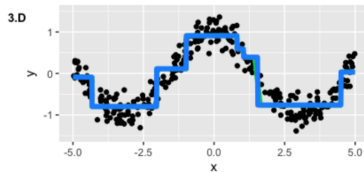
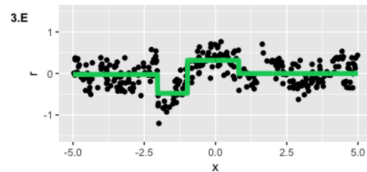
playgrounds click, click

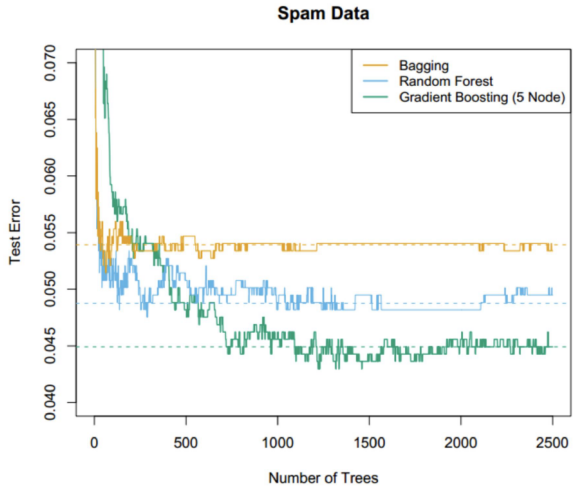
Dataset and Current ensemble



Residuals and Last model in ensemble



Gradient boosting — examples



Gradient boosting

check your understanding

- Are base models in boosted desicion trees independent of each other?
- Does boosting method improve performance because of aggregation of weak learners predictions?
- Can we use Random forests as base models in Gradient Boosting?
- What will happen if we remove first tree from Boosting?
- What will happen if we remove first tree from Random Forest?

Gradient boosting

check your understanding

- No
- Yes
- You shouldn't do that
- Model will break
- Almost nothing

Summary

- **Decision tree**
  - binary decisions to model non-linearities
  - grow greedily leaf by leaf
  - split leaves to improve Information Gain
  - until stopping criteria is reached
  - predict with constant in a leaf after propagating through
- **Random forest**
  - combine trees into ensemble for smaller error
  - each tree is independent of others
  - low-biased trees + RSM + bagging
- **Gradient boosting**
  - combine algorithms into ensemble for even smaller error
  - each next algorithm improves predictions of previous ones