Tree models

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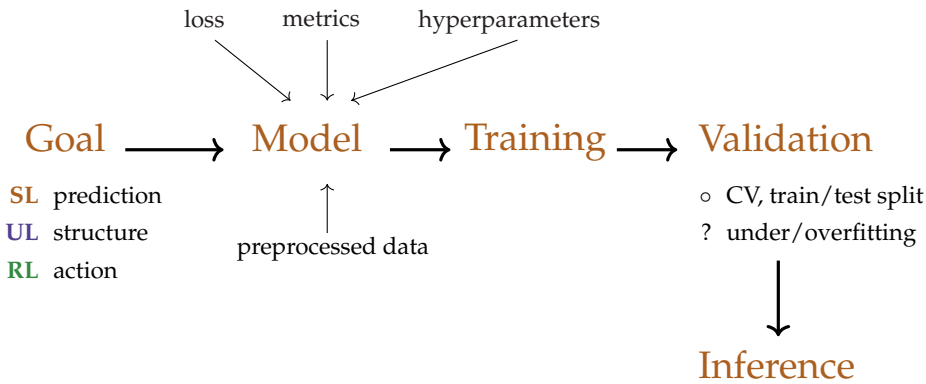
Outline

- Decision tree
  - From linear models to decision trees
  - Information entropy
  - Making a good split
  - Some insights
- Random forest
  - Random subspace method
  - Bootstrapping
  - Aggregating
- Gradient boosting
  - Some motivation
  - Gradient descent in a model space
  - BDT example

Recap

ML Problems — General pipeline



Linear models

Classification (Log. Regression)

- $Y = \{0, 1\}$
- N objects with K numeric features: $D = \mathbb{R}^K$
- $a(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{j=1}^{K} f_j(\boldsymbol{x}) \cdot \boldsymbol{\theta_j} = \langle \boldsymbol{x}, \boldsymbol{\theta} \rangle \to \sigma\big[\langle x, \theta \rangle\big]$
- $\mathcal{L}\big(a(\boldsymbol{x_i}), y_i\big) = \big[a(\boldsymbol{x}) \neq y_i\big] \to$ log. likelihood
- $Q(a, X, Y) = \sum_{i=1}^{N} \mathcal{L}\big(a(\boldsymbol{x_i}), y_i\big)$

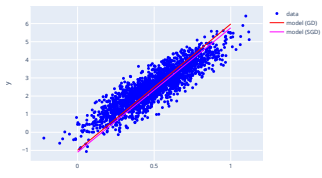
Regression

- $Y = \mathbb{R}$
- N objects with K numeric features: $D = \mathbb{R}^K$
- $a(\boldsymbol{x}, \boldsymbol{\theta}) = \langle \boldsymbol{x}, \boldsymbol{\theta} \rangle$
- $\mathcal{L}\big(a(\boldsymbol{x_i}), y_i\big) = \big(a(\boldsymbol{x}) - y_i\big)^2$
- $Q(a, X, Y) = \sum_{i=1}^{N} \mathcal{L}\big(a(\boldsymbol{x_i}), y_i\big)$

$$\hat{a} = \arg\min_{a \in A} Q(a, X, Y) \;\Leftarrow \textbf{Training}$$

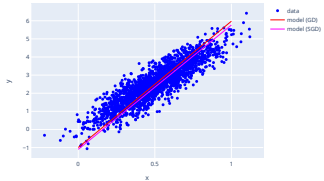
Linear models

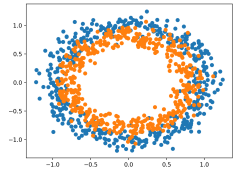
Pros & cons



- Linear models:
  - ➔ nicely describe linear correlations
  - ➔ fast and easy to train
  - ➔ performing well with large number of samples/features

Linear models — Pros & cons





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Linear models

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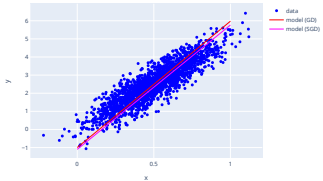

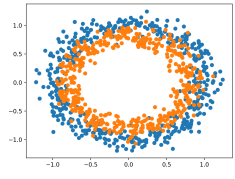

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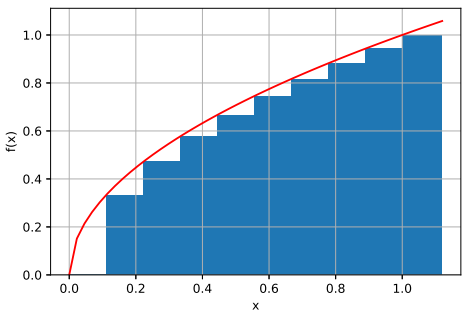
Is there a more general way to describe non-linearities?

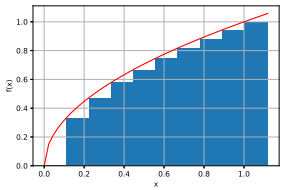
What is the simplest way to approximate a function?

Use **piecewise linear function**



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

We can define this function by introducing a set of **yes/no questions**



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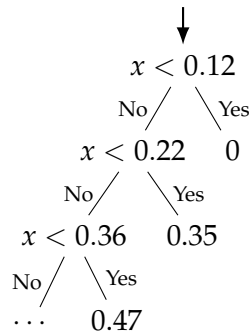
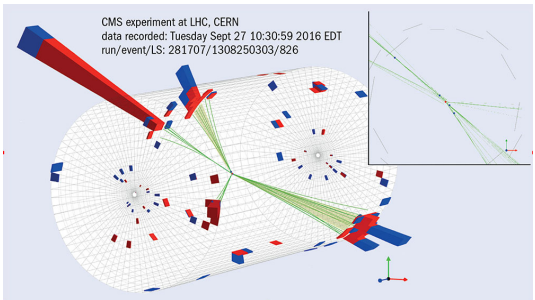


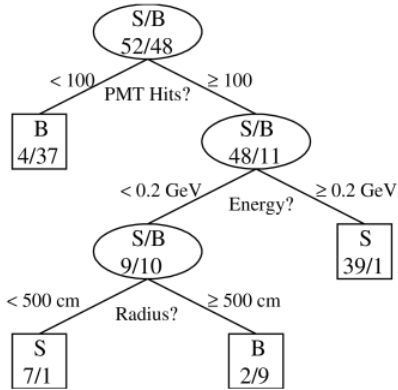
Well this looks not a tree but **decision list**

Desision tree

Intuition

This approach also works for classification problems



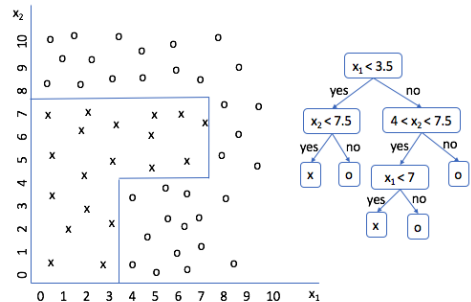


Desision tree — Algorithm

Algorithm 1: Decision tree

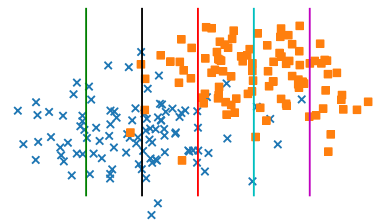
1: Initialize: hyperparameters, leaf set = $\{X_{\text{train}}\}$

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**



Desision 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?



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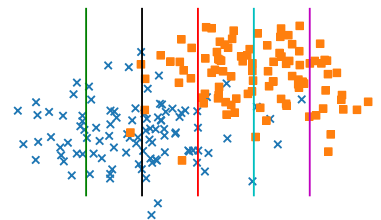
→ We need some criteria



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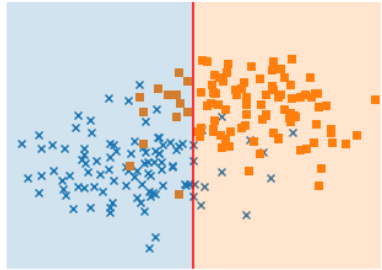
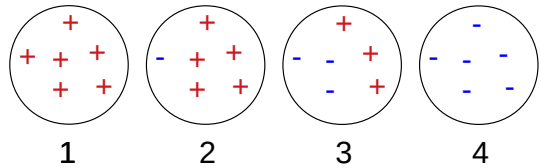


The ”best” split is a central one because it introduces **purity** in the best way. Let’s try to bring up some math to this topic.

- Consider four datasets:
  1&4 are pure
  2 is almost pure
  3 is the most impure



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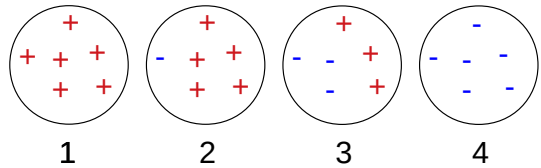

- Consider four datasets:
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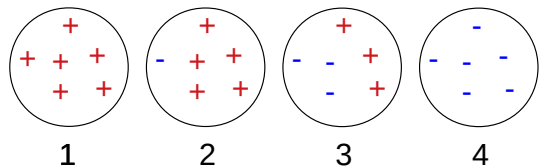
- How to numerically describe impurity?
- Introduce **information entropy:**

$$H(X) = -\sum_i p_i \log_2 p_i, \quad p_i = \frac{N_i}{X}$$



- $i = [+, -]$

1: $H(X) = -6/6 \log_2(6/6) = 0$

2: $H(X) = -5/6 \log_2(5/6) - 1/6 \log_2(5/6) \approx 0.65$

3: $H(X) = -3/6 \log_2(3/6) - 3/6 \log_2(3/6) = 1$

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Desision tree

Concept of information entropy

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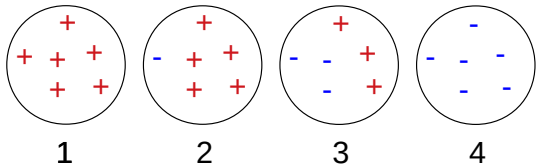

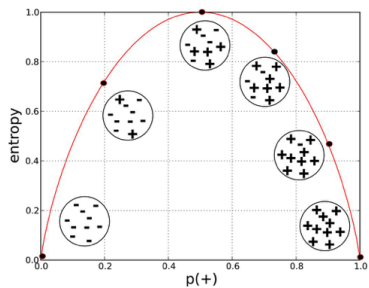

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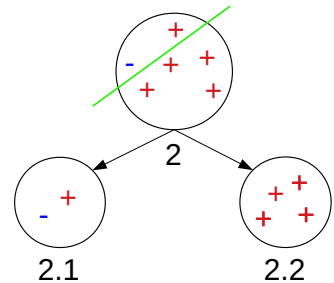

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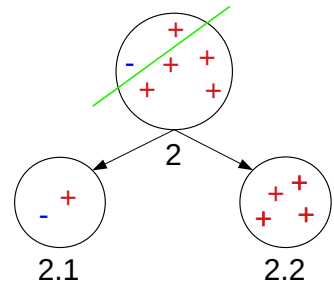
2: $H(X) \approx 0.65$
2.1: $H(L) = -2 \cdot 1/2 \log_2(1/2) = 1$
2.2: $H(R) = 0$



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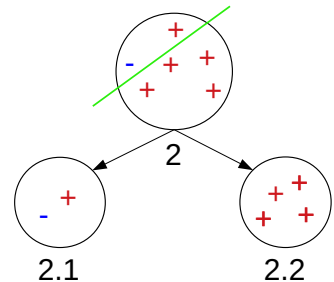
  Let's weight the results to compare with the initial case:

$$H(X|a) = \frac{L}{X}H(L) + \frac{R}{X}H(R) = \frac{2}{6} \cdot 1 + \frac{4}{6} \cdot 0 \approx 0.33$$



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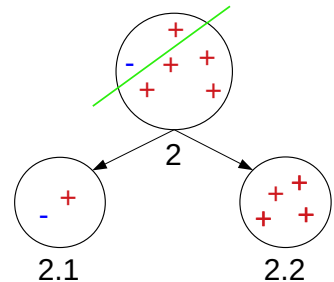

$$H(X|a) < H(X) \Rightarrow \text{profit!}$$

more about IG

- To measure the profit by a classification algorithm a we define **Information Gain** (IG):

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

- In case of binary split:

$$\mathrm{IG}(\mathrm{X}, a) = \mathrm{H}(\mathrm{X}) - \left[\frac{L}{X} H(L) + \frac{R}{X} H(R)\right]$$

- The best classifier gives maximal IG:

$$\hat{a} = \arg\min_{a \in A} \mathrm{IG}(\mathrm{X}, \mathrm{a})$$

Two questions:

1. How to find optimal split criteria?
2. How to grow a tree?

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

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

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Desision tree — Split criteria

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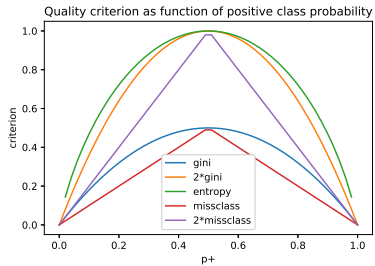
- or c_k with $\sum_k c_k = 1$, if tree predicts class probabilities
- If p_k is a fraction of class k events in a leaf
- Then one can show:
  - **Misclassification criteria**
    $\mathcal{L}(y, c) = [y \neq c] \Rightarrow \mathrm{H(R)} = 1 - \max_k \{p_k\}$
  - **Gini Impurity**
    $\mathcal{L}(y,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

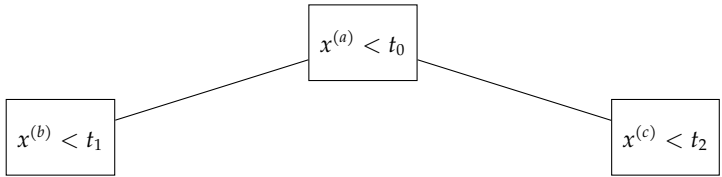


Lower diversity (higher purity)
$\Rightarrow$ **lower impurity** criterion H(R)

What about tree construction?

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

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



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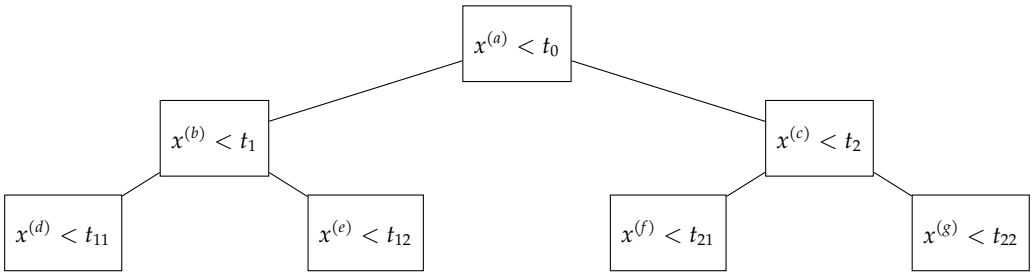

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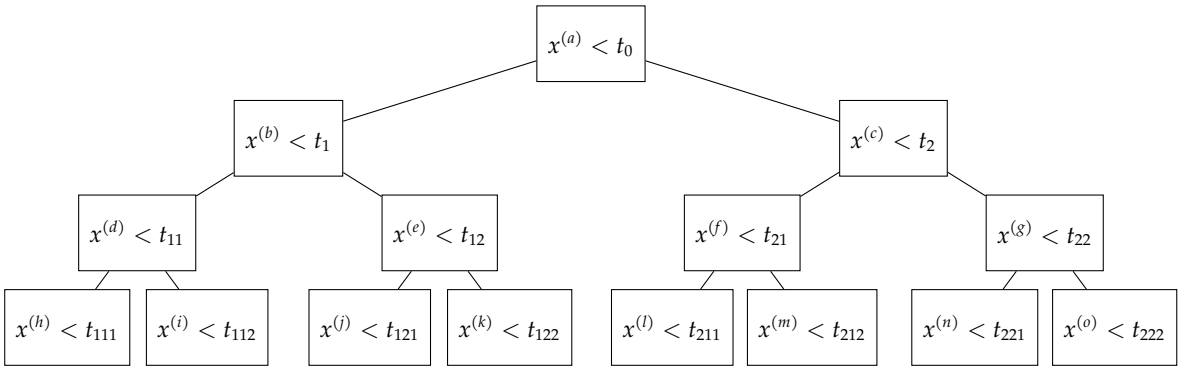
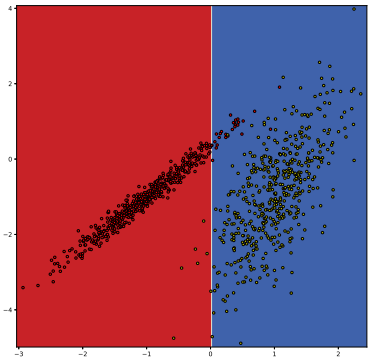
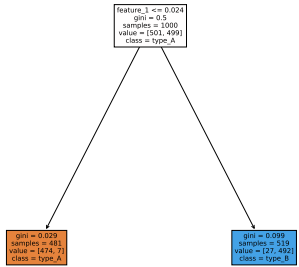


Desision tree — Growing

check out also these visuals





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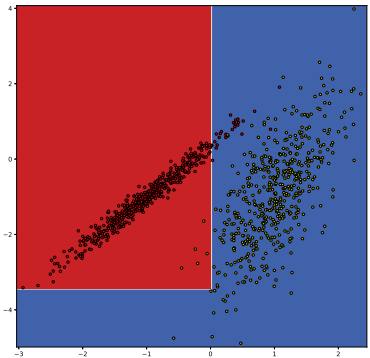

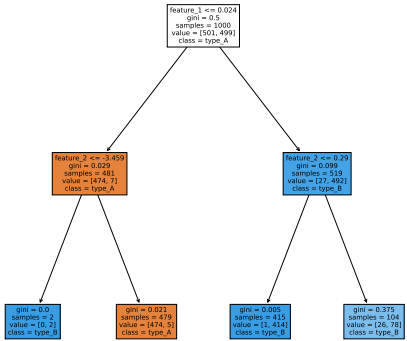

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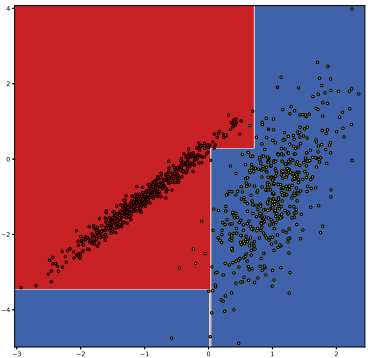
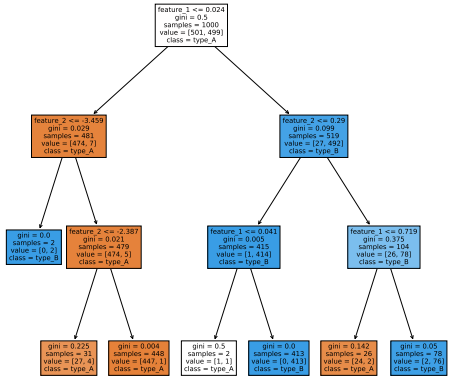
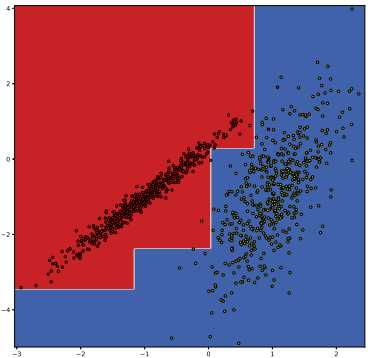
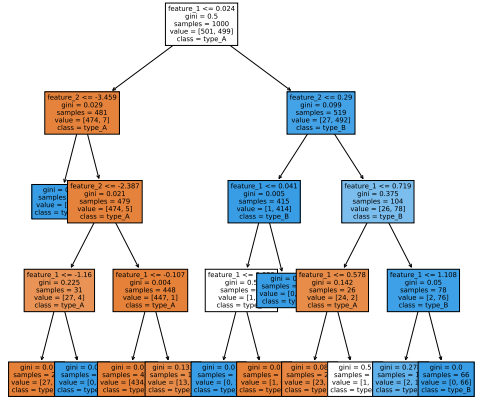




Desision tree — Growing

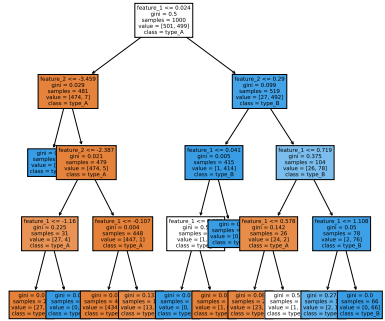
check out also these visuals





Desision 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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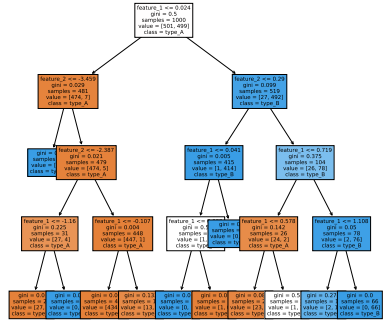
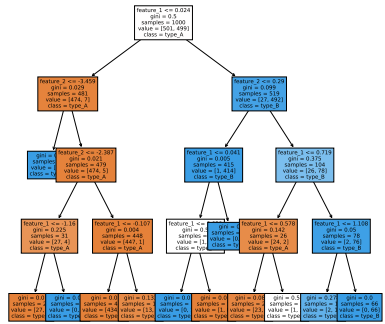
➔ The choice is up to you
(aka hyperparameter)



Desision 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



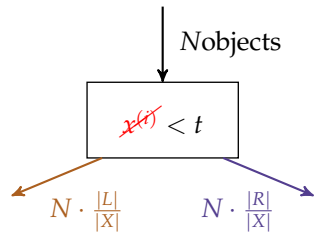
Can already trained decision tree handle **missing values** on inference step?

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

- While growing a tree, we know **split probabilities**:

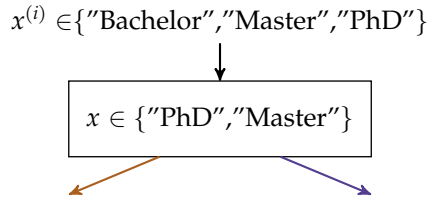
$$\hat{y} = \frac{|\mathrm{L}|}{|\mathrm{X}|}\hat{y}_{\mathrm{L}} + \frac{|\mathrm{R}|}{|\mathrm{X}|}\hat{y}_{\mathrm{R}}$$

- If at some node feature $x^{(i)}$ is missing, there still exists a way to use the tree
- Split all subset according to probabilities obtained during the training

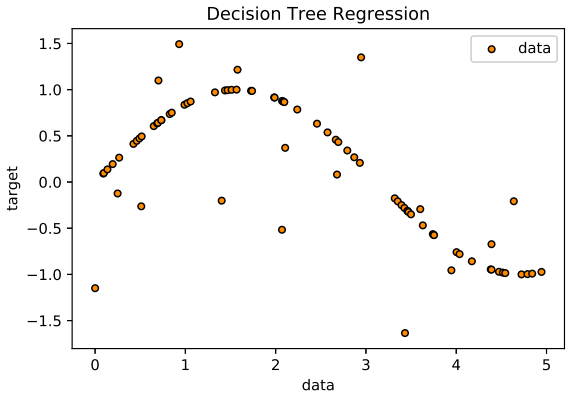


Categorical features can also easily be treated by tree:

- Loop through all combinations of its values
- Pick a set of values which result in the best IG
- Make a split using this criteria

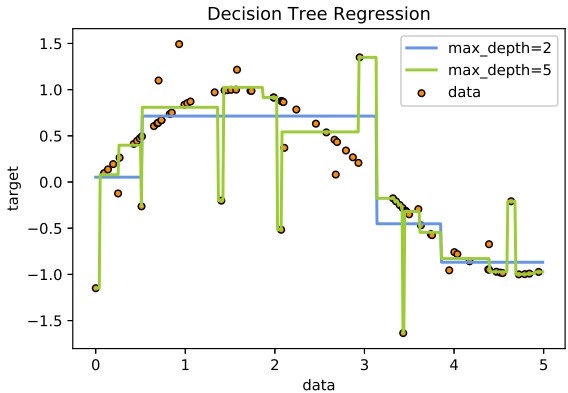


Desision tree — Regression



Can we use decision tree approach for regression problem?

Desision tree — Regression



Can we use decision tree approach for regression problem? Yes

- 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: $\mathcal{L}(y,c) = (y-c)^2 \Rightarrow \mathrm{H}(\mathrm{X}) = \min_c \frac{1}{|\mathrm{X}|}\sum_i (y_i - c)^2$

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

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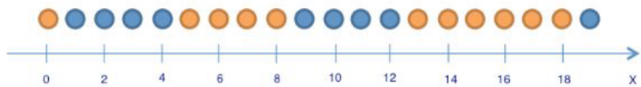
- One can further show that:

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

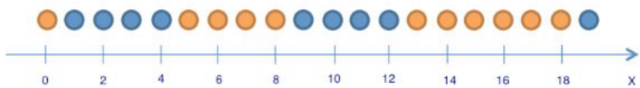
$$c^* = \mathrm{median}(y_i \in \mathrm{R})$$



- 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?
- What algorithm constructs a tree?
- Which stopping criteria can we use?

Desision 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

- Consider dataset X containing M objects $\boldsymbol{x_m}$ with targets y_m:

$$X = \{(\boldsymbol{x_m}, y_m),\ m = 1 \dots M\}$$

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$$\varepsilon_i(\boldsymbol{x}) \equiv b_i(\boldsymbol{x}) - y(\boldsymbol{x}), \quad i = 1, \dots, N$$

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more in this lecture

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$$\mathbb{E}_{\boldsymbol{x}} \left(b_i(\boldsymbol{x}) - y(\boldsymbol{x})\right)^2 = \mathbb{E}_{\boldsymbol{x}} \varepsilon_i^2(\boldsymbol{x})$$

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

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

- Assume errors to be unbiased and uncorrelated:

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

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

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

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

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**

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- Use different features *at each split* — **random subspace method** (RSM)
- Use different datasets — **bootstrapping**

Random forest

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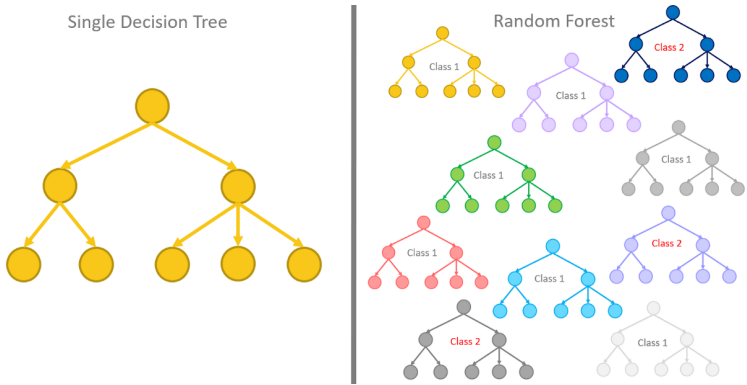
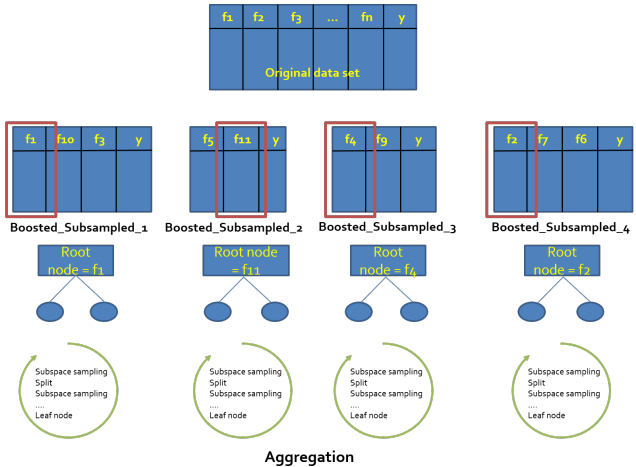
Random forest = low-biased decision trees + RSM + $\underbrace{\textbf{b}\text{ootstrap} + \textbf{agg}\text{regat}\textbf{ing}}_{\textbf{bagging}}$

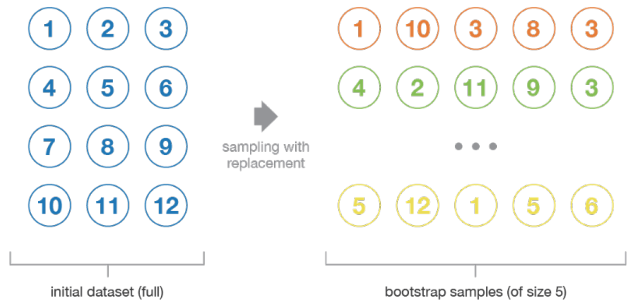
Random forest — Trees



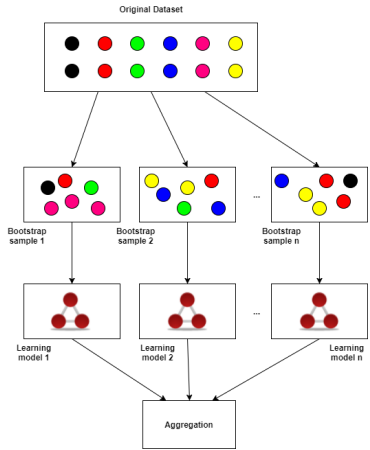
Random forest — RSM

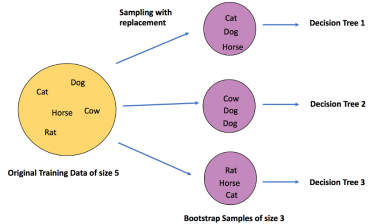


Random forest — Bootstrap



Random forest — Aggregating





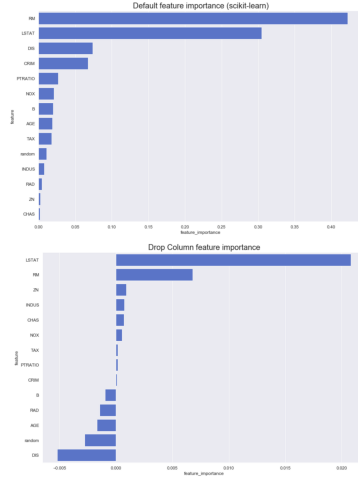
- As we use bagging, some data ($\approx 37\%$) is left unused during training
- Therefore, we can validate model on it $\Rightarrow$ **out-of-bag score**

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

Random forest — Insights

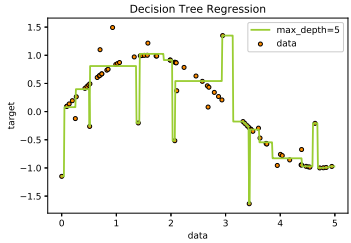
- IGs at each split can be used to calculate **feature importance**
- The higher (normalized) total reduction of IG brought by that feature – the better
- Note: this logic can be used in any tree-based model
- Caveat: might inflate the importance of numerical features and categorical features with high cardinality (many unique values)

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?

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

Gradient boosting

- 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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- However, simply training them independently sounds not quite optimal (although is easy to parallelize)
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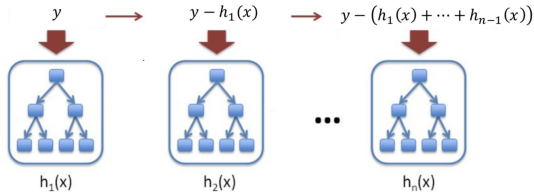
➔ e.g., iteratively by correcting upon mistakes of previous models?

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



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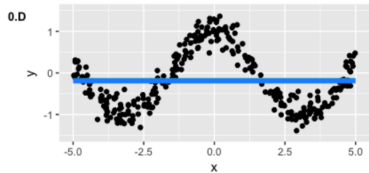
Let's look at the example and dive into theory

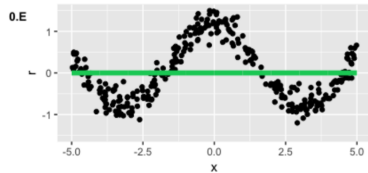
- Data: toy dataset $y = \cos(x) + \epsilon, \epsilon \sim \mathcal{N}\left(0, \frac{1}{5}\right), x \in [-5, 5]$
- Loss function: MSE
- Family of algorithms: decision trees, depth $= 2$
- Number of iterations: M $= 3$
- Initialial base algorithm: constant with mean value

playgrounds click, click

Dataset and Current ensemble



Residuals and Last model in ensemble



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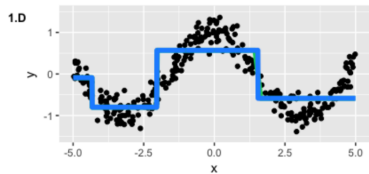
Dataset and Current ensemble



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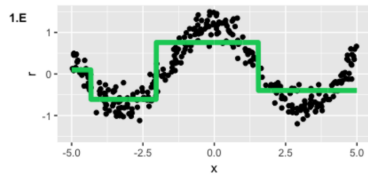

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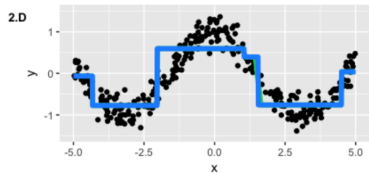

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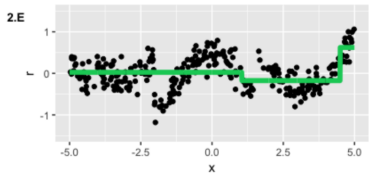

playgrounds click, click

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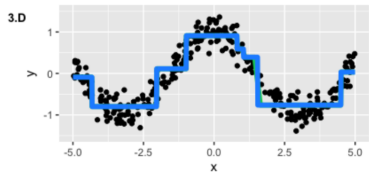

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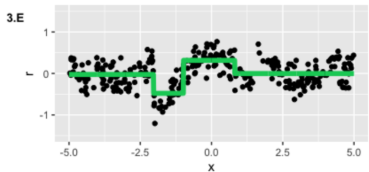

Gradient boosting

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 $L(y, a(\boldsymbol{x}))$ encodes information about the problem type:
  - classification: $\log\left(1 + e^{-y \cdot a(\boldsymbol{x})}\right)$
  - regression: $\left(y - a(\boldsymbol{x})\right)^2$ or $\left|y - a(\boldsymbol{x})\right|$

Gradient boosting

Theory

- Let's iteratively construct $\hat{a}(\boldsymbol{x})$ as a sum of base algorithms:

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

Gradient boosting

Theory

- Let's iteratively construct $\hat{a}(\boldsymbol{x})$ as a sum of base algorithms:

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

- Suppose we know how it looks like at $(t-1)$-th iteration

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$$(\hat{\rho}_t, \hat{\boldsymbol{\theta}}_t) = \arg\min_{\rho, \boldsymbol{\theta}} \mathbb{E}_{x,y}[L(y,\, \hat{a}_{t-1}(\boldsymbol{x}) + \rho \cdot h(\boldsymbol{x}, \boldsymbol{\theta}))],$$

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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:

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

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- Finally:

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

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- But people opted for trees $\rightarrow$ aka **Boosted Decision Trees** (BDT) in HEP vocabulary
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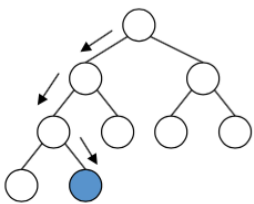

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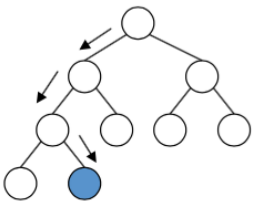

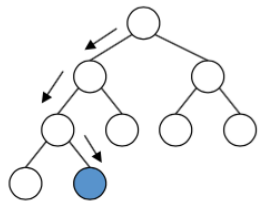

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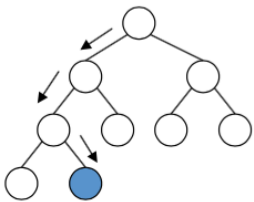

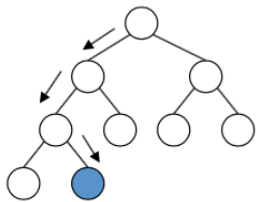

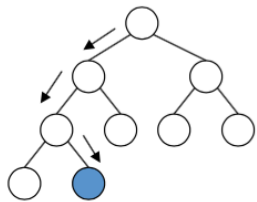

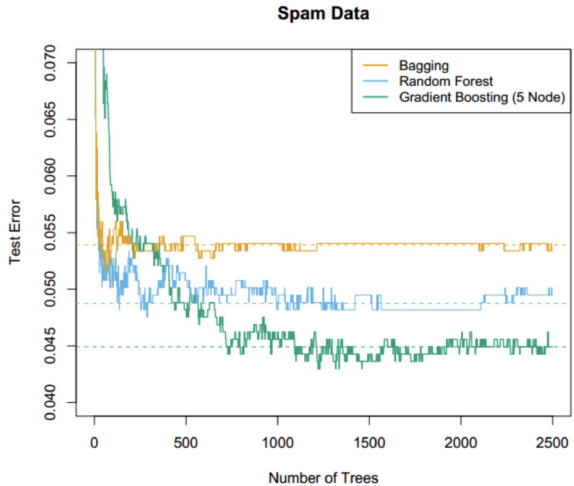
Spam Data
Bagging
Random Forest
Gradient Boosting (5 Node)
Test Error
0.040
0.045
0.050
0.055
0.060
0.065
0.070
0
500
1000
1500
2000
2500
Number of Trees

- 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?

- 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