Random Forest for Classification Problems

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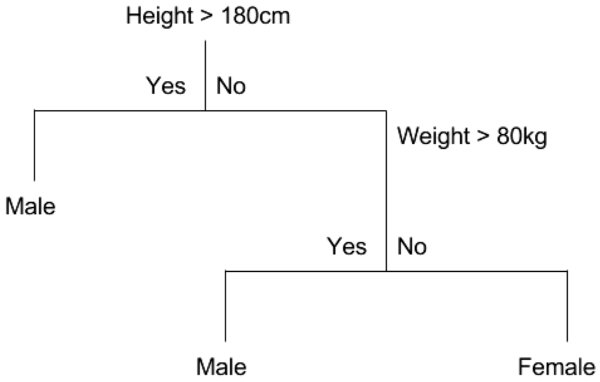
Overview

Decision Tree

Example



Decision Tree

Tree Building Process

A tree is grown starting from the root node by repeatedly using the following steps on each node (also called binary splitting):

(i) Find best split s for each feature X_m

(ii) Find the best split of the node

(iii) Repeat until stopping criterion got satisfied

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Gini Measure

$$i(t) = \sum_{c \in C} p(c|t)(1 - p(c|t))$$

Information Entropy

$$i(t) = \sum_{c \in C} p(c|t) log(p(c|t))$$

where C is the set of classes c and t a node of the tree.

Bias Variance Trade-off

The Expected Generalization Error

$y = f(x) + \epsilon$ and $\epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$

Estimate of $f(x)$: $\hat{f}(x)$

The expected generalization error: $\boldsymbol{Err}(\hat{f}(x))$

The decomposition of a model's expected generalization error is

$$\boldsymbol{Err}(\hat{f}(x)) = \sigma_\epsilon^2 + [Bias(\hat{f}(x))]^2 + Var(\hat{f}(x))$$

σ_ϵ^2 is irreducible and independent of the model.

Trade-off between bias and variance.

Aim: Decrease variance while keeping bias unincreased.

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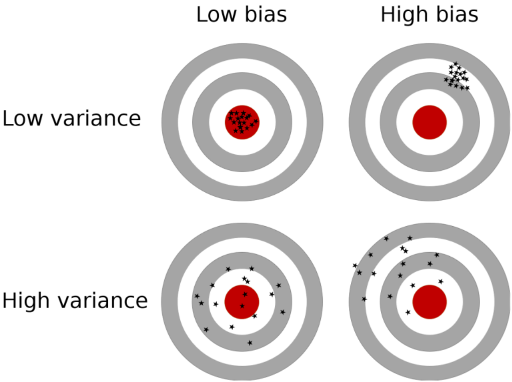
Illustration



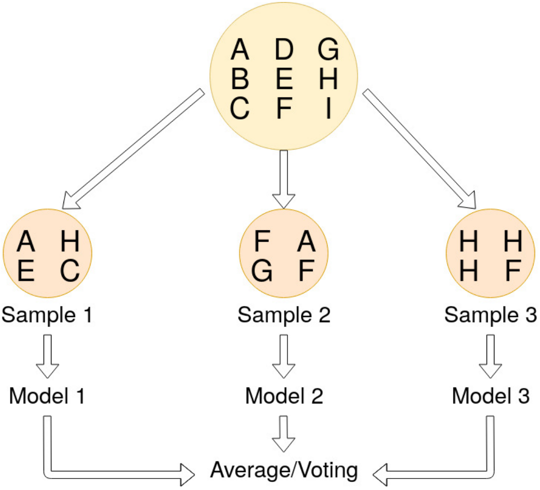
Decision trees generally have low bias and high variance.

Bagging

Bagging is:

1. created for methods with high variance
2. reduces variance and gives better predictions
3. improvement of bagging: Random Forest

Bagging
Illustration



Random Forest

Definition

Definition (by L.Breiman)

A random forest is a classifier consisting of a collection of tree-structured classifiers $\hat{T}_{\theta_b}(\mathbf{x}), b = 1, ..., B$ where the θ_b are independent identically distributed random vectors and each tree casts a unit vote for the most popular class at input $\mathbf{x}$.

Random Forest is an extension and improvement over bagging:

1. Like in bagging, multiple decision trees are built
2. Improvement: an injection of randomness is made

Two key concepts that makes decision forest "random" are:

1. Random sampling of training data points when building trees
2. Random subsets of features considered when splitting nodes. Recommended number of variables:
   a. For classification: $\lfloor \sqrt{n} \rfloor$
   b. For regression: $\lfloor \frac{n}{3} \rfloor$

Algorithm 1: Random Forest for Regression or Classification

1. For $b = 1$ to B:
   a. Draw a bootstrap sample θ_b of size N from the training data.
   b. Grow the Random Forest tree T_{θ_b} to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached:
      i. Select m variables at random from the n variables
      ii. Pick the best variable/split-point among the m
      iii. Split the node into two daughter nodes
2. Output the ensemble of trees $\{T_{\theta_b}\}_{b=1}^{B}$

Section 2

Mathematical Concept

Let $D = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$ and
$T_{D,\theta}$ is a fully grown tree trained on set D with using parameters θ.
Random Forest estimate of an observation x^* is

Majority Voting

$$\boldsymbol{RF}_{D,\theta_1,\theta_2,...,\theta_B}(x^*) = \underset{c \in Y}{argmax} \sum_{b=1}^{B} \mathbb{1}(\hat{T}_b(x^*) = c)$$

Soft Voting

$$\boldsymbol{RF}_{D,\theta_1,\theta_2,...,\theta_B}(x^*) = \underset{c \in Y}{argmax} \frac{1}{B} \sum_{b=1}^{B} \hat{p}_{D,\theta_b}(Y = c | X = x^*)$$

where $\hat{p}_{D,\theta_b}(Y = c | X = x^*)$ is the probability estimates of a tree.

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Mathematical Concept

Prediction Mechanism

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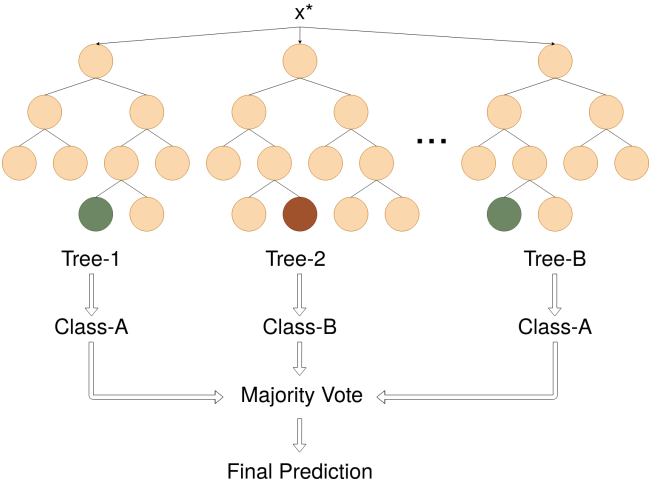
Mathematical Concept

Majority Voting Illustration



Mathematical Concept
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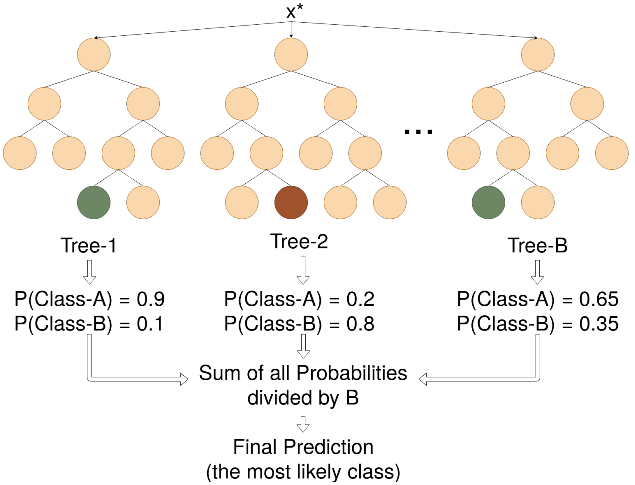

Given $D = X \cup Y$,
the expected generalization error of $T_{D,\theta}$ is

$$\boldsymbol{Err}(T_{D,\theta}(X)) = \mathbb{E}_{X,Y}\{L(Y, T_{D,\theta}(X))\}$$

where $L(Y, T_{D,\theta}(X))$ is the loss function.

The decomposition of $\boldsymbol{Err}(T_{D,\theta})$ is

$$\boldsymbol{Err}(T_{D,\theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(T_{D,\theta}(X))]^2 + Var(T_{D,\theta}(X))$$

similarly

$$\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(\boldsymbol{RF}_{D,\Theta}(X))]^2 + Var(\boldsymbol{RF}_{D,\Theta}(X))$$

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$$\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(\boldsymbol{RF}_{D,\Theta}(X))]^2 + Var(\boldsymbol{RF}_{D,\Theta}(X))$$

Theoretically, given the probability distribution of P(X,Y) Bayes Model ϕ_β i.e the best possible model can be derived and $\boldsymbol{Err}(\phi_\beta)$ can be calculated [1].

For comparison of $\boldsymbol{Err}(T_{D,\theta}(X))$ and $\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X))$ the residual error is the same.

Result: Ensembling has no effect on Bayes Error.

$$Err(RF_{D,\Theta}(X)) = Err(\phi_\beta(X)) + [Bias(RF_{D,\Theta}(X))]^2 + Var(RF_{D,\Theta}(X))$$

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With Squared Loss Function: $L(Y, T_{D,\theta}(X)) = \mathbb{E}_D\{(Y - T_{D,\theta}(X))^2\}$

$Bias^2$ of Tree

$$[Bias(T_{D,\theta}(X))]^2 = (\phi_\beta(X) - \mathbb{E}_D\{T_{D,\theta}(X)\})^2$$

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Mathematical Concept

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We can define $\mathbb{E}_D\{T_{D,\theta}(X)\} = \mu_{D,\theta}(X)$

Random Forest Estimator for regression is;

$$\boldsymbol{RF}_{D,\Theta}(X) = \frac{1}{B}\sum_{b=1}^{B} T_{D,\theta_b}(X)$$

Taking expectation gives;

$$\begin{aligned}\mathbb{E}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} &= \mathbb{E}_{D,\Theta}\{\frac{1}{B}\sum_{b=1}^{B} T_{D,\theta_b}(X)\} \\ &= \frac{1}{B}\sum_{b=1}^{B} \mathbb{E}_{D,\theta_b}\{T_{D,\theta_b}(X)\} \qquad (\theta\text{'s are i.i.d.}) \\ &= \mu_{D,\theta}(X)\end{aligned}$$

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Variance: Correlation Coefficient

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$\forall T_{D,\theta'}, T_{D,\theta''}$ such that $\theta' \neq \theta''$, the correlation coefficient can be written as follows

$$\rho(X) = \frac{\mathbb{E}_{D,\theta',\theta''}\{T_{D,\theta'}(X)T_{D,\theta''}(X)\} - \mu^2_{D,\theta}(X)}{\sigma^2_{D,\theta}(X)}$$

where $\sigma^2_{D,\theta}(X) = \mathbb{V}_{D,\theta}\{T_{D,\theta}(X)\}$.

- Highly correlated trees $\implies$ $\rho(X)$ is close to 1
- Non-correlated trees $\implies$ $\rho(X)$ is close to 0

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Variance Comparison

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Variance of Random Forest

$$\mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} = \rho(X)\sigma^2_{D,\theta}(X) + \frac{1-\rho(X)}{B}\sigma^2_{D,\theta}(X)$$

As $B \to \infty$, $\mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\}$ converges to $\rho(X)\sigma^2_{D,\theta}(X)$.

Due to randomization $\rho(X) < 1$

$$\implies \mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} = \rho(x)\sigma^2_{D,\theta}(X) < \sigma^2_{D,\theta}(X) = \mathbb{V}_{D,\theta}\{T_{D,\theta}(X)\}.$$

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As $B \to \infty$, $\mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\}$ converges to $\rho(X)\sigma^2_{D,\theta}(X)$.

Due to randomization $\rho(X) < 1$

$$\implies \mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} = \rho(x)\sigma^2_{D,\theta}(X) < \sigma^2_{D,\theta}(X) = \mathbb{V}_{D,\theta}\{T_{D,\theta}(X)\}.$$

Result: Ensembling trees decreases the variance.

Section 3

Simulation Study

The linear DGP generates the data tuples (y, x_1, x_2, x_3) as follows:

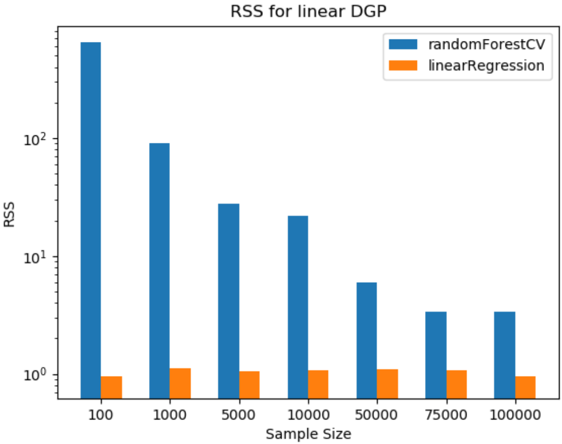
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon,$$

whereas

- $(\beta_0, \beta_1, \beta_2, \beta_3) = (0.3, 5, 10, 15)$
- $x_1, x_2, x_3 \sim \mathcal{N}(0,\ 3)$
- $\epsilon \sim \mathcal{N}(0,\ 1)$

Simulation Study

Linear DGP Results



The non-linear DGP generates the data tuples (y, x_1, x_2) as follows:

$$y = \beta_0 + \beta_1 \mathbb{1}(x_1 \geq 0, x_2 \geq 0) + \beta_2 \mathbb{1}(x_1 \geq 0, x_2 < 0) + \beta_3 \mathbb{1}(x_1 < 0) + \epsilon,$$

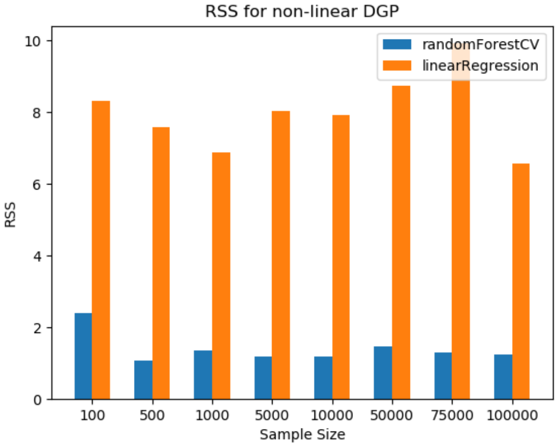
whereas

- $(\beta_0, \beta_1, \beta_2, \beta_3) = (0.3, 5, 10, 15)$
- $x_1, x_2 \sim \mathcal{N}(0,\ 3)$
- $\epsilon \sim \mathcal{N}(0,\ 1)$

are the same as in the previous DGP.

Simulation Study

Non-Linear DGP Results



Data: Titanic data

Method used:

1. Random Forest
2. Adaptive Boosting
3. Gradient Boosting

Goal: Predict which passengers survived the Titanic shipwreck given characteristics of passengers

Real Data

Results

Random Forest

Accuracy: 84.32%

	D_{pred}	S_{pred}
D_{real}	88%	12%
S_{real}	21%	79%

Adaptive Boosting

Accuracy: 82.8%

	D_{pred}	S_{pred}
D_{real}	86%	14%
S_{real}	21%	79%

Gradient Boosting

Accuracy: 82.8%

	D_{pred}	S_{pred}
D_{real}	85%	15%
S_{real}	20%	80%

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The link to presentation's repository: