

Paper Review: Consistency of Random Forests

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Introduction

Problem Setup

Main Results

Discussion and Future Work

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Background

- ▶ Random forests is an ensemble learning method for classification and regression that constructs a number of randomized decision trees during the training phase and predicts by averaging the results.
- ▶ It was first introduced by Breiman(2001).

Applications

- ▶ Random forests can be used to deal with big data and high-dimensional models (Sparsity).
- ▶ It is widely used in bioinformatics, survival analysis, quantile regression, ecology, etc.

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Decision Trees

- ▶ Decision trees can be applied to both regression and classification problems.
- ▶ Regression trees are used to predict a quantitative response and classification trees are used to predict a qualitative response.

Regression Trees

- ▶ Given a training sample $D_n = (X_1, Y_1), \dots, (X_n, Y_n)$ in $[0, 1]^p \times R$, the objective is to estimate $m_n : [0, 1]^p \rightarrow R$ of the function $m(x) = E[Y|X = x]$.
- ▶ p : dimension of predictors; n : size of the sample (training sets)
- ▶ X : input random vector used to estimate \hat{Y} , i.e. $m_n(X)$.
- ▶ In general trees, $X \in R^p$ rather than $[0, 1]^p$ stated in this paper.

Example of Regression Trees

- ▶ "Hitters" data set
- ▶ Response: log salary of a baseball player
- ▶ Predictors: number of years that he has played in the major leagues; number of hits that he made in the previous year.

Example of Regression Trees

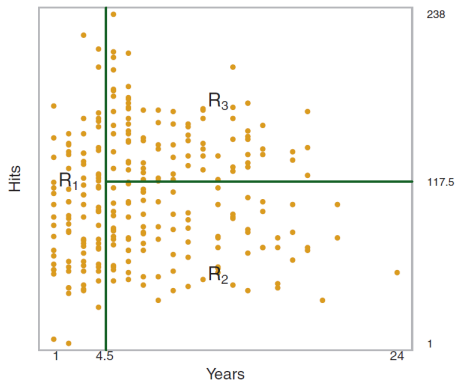


Figure : The three-region partition for "Hitters" data set from regression tree

Example of Regression Trees

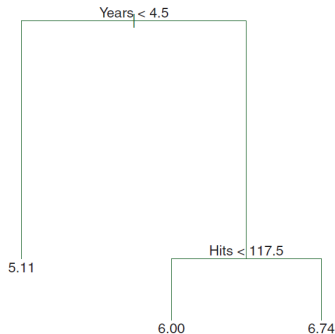


Figure : The regression tree for "Hitters" data set

Notations of Regression Trees

- ▶ $m_{try} \in \{1, \dots, p\}$: number of pre-selected directions for splitting, when $m_{try} < p$, it can be used to deal with high-dimensional data.
- ▶ $a_n \in \{1, \dots, n\}$: number of sampled data points in each tree. If $a_n < n$, it is sub-sampling, and can be used to deal with Big Data.
- ▶ $t_n \in \{1, \dots, a_n\}$: number of leaves(cells) in each tree. If $t_n < a_n$, trees are not fully developed; if $t_n = a_n$, trees are fully developed, i.e. each leaf has one number.
- ▶ A : a generic cell; $N_n(A)$: number of data points falling in A .
- ▶ j : direction of predictor of j th splitting; z : position of cut along the j th coordinate.
- ▶ $A_L = \{x \in A : x^{(j)} < z\}$, $A_R = \{x \in A : x^{(j)} \geq z\}$

CART-Split Criterion of Regression Trees

- ▶
$$L_n(j, z) = \frac{1}{N_n(A)} \sum_{i=1}^n (Y_i - \bar{Y}_A)^2 1_{X_i \in A} - \frac{1}{N_n(A)} \sum_{i=1}^n (Y_i - \bar{Y}_{A_L} 1_{X_i^{(j)} < z} - \bar{Y}_{A_R} 1_{X_i^{(j)} \geq z})^2 1_{X_i \in A}.$$
- ▶
$$(j_n^*, z_n^*) = \underbrace{\operatorname{argmax}}_{j \in M_{try}, (j, z) \in C_A} L_n(j, z).$$
- ▶ M_{try} : the set of selected predictors to build the tree.
- ▶ C_A : the set of all possible cuts in A .
- ▶ By CART-Splitting Criterion, we will build a regression tree with m_{try} predictors, a_n data points and t_n leaves.

Classification Trees

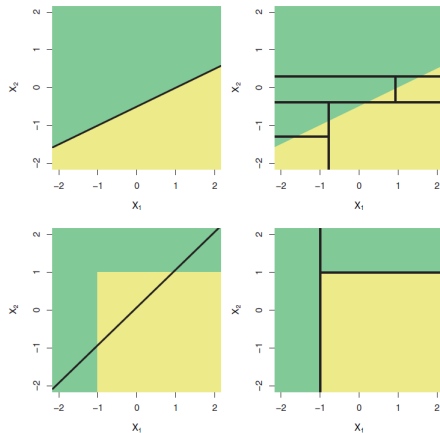


Figure : Decision Trees vs Linear Regression

Advantages and Disadvantages of Trees

► **Advantages:**

1. Trees are very easy to explain to people.
2. Decision trees are more close to human decision-making mode.
3. Trees can be displayed graphically.
4. Trees can easily handle qualitative predictors without the need to create dummy variables.

► **Disadvantages:**

1. Trees generally don't have the same level of predictive accuracy as other approaches.
 2. Trees can be very non-robust. A small change in the data may cause a large change in the final estimated tree.
- So, we need random forests method to overcome these disadvantages.

Random Forests

- ▶ Random forests contains many trees by bootstrap M trees with replacement.

- ▶ $m_{M,n}(x; \Theta_1, \dots, \Theta_M, D_n) = \frac{1}{M} \sum_{j=1}^M m_n(x; \Theta_j, D_n) \quad (1)$

- ▶ **Notations:**

- ▶ x : query point used to predict value of y .
- ▶ D_n : training sample.
- ▶ $\Theta_1, \dots, \Theta_M$: independent random variables distributed as a generic random variable Θ .

Algorithm of Random Forests

Algorithm 1: Breiman's random forest predicted value at \mathbf{x}

Input: Training set \mathcal{D}_n , number of trees $M > 0$, $m_{\text{try}} \in \{1, \dots, p\}$,
 $a_n \in \{1, \dots, n\}$, $t_n \in \{1, \dots, a_n\}$, and $\mathbf{x} \in [0, 1]^p$.

Output: Prediction of the random forest at \mathbf{x} .

```

1 for  $j = 1, \dots, M$  do
2   Select  $a_n$  points, without replacement, uniformly in  $\mathcal{D}_n$ .
3   Set  $\mathcal{P}_0 = \{[0, 1]^p\}$  the partition associated with the root of the tree.
4   For all  $1 \leq \ell \leq a_n$ , set  $\mathcal{P}_\ell = \emptyset$ .
5   Set  $n_{\text{nodes}} = 1$  and level = 0.
6   while  $n_{\text{nodes}} < t_n$  do
7     if  $\mathcal{P}_{\text{level}} = \emptyset$  then
8       level = level + 1
9     else
10      Let  $A$  be the first element in  $\mathcal{P}_{\text{level}}$ .
11      if  $A$  contains exactly one point then
12         $\mathcal{P}_{\text{level}} \leftarrow \mathcal{P}_{\text{level}} \setminus \{A\}$ 
13         $\mathcal{P}_{\text{level}+1} \leftarrow \mathcal{P}_{\text{level}+1} \cup \{A\}$ 

```

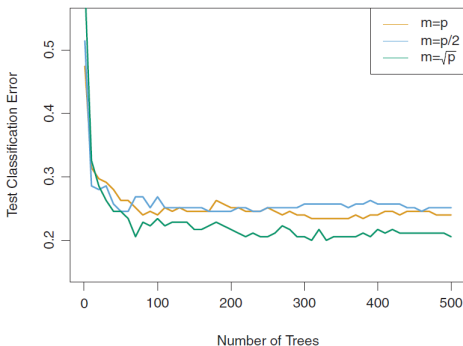
Algorithm of Random Forests

```

14 | | | else
15 | | |   Select uniformly, without replacement, a subset
    | | |    $\mathcal{M}_{\text{try}} \subset \{1, \dots, p\}$  of cardinality  $m_{\text{try}}$ .
16 | | |   Select the best split in  $A$  by optimizing the CART-split
    | | |   criterion along the coordinates in  $\mathcal{M}_{\text{try}}$  (see details
    | | |   below).
17 | | |   Cut the cell  $A$  according to the best split. Call  $A_L$  and
    | | |    $A_R$  the two resulting cell.
18 | | |    $\mathcal{P}_{\text{level}} \leftarrow \mathcal{P}_{\text{level}} \setminus \{A\}$ 
19 | | |    $\mathcal{P}_{\text{level}+1} \leftarrow \mathcal{P}_{\text{level}+1} \cup \{A_L\} \cup \{A_R\}$ 
20 | | |    $n_{\text{nodes}} = n_{\text{nodes}} + 1$ 
21 | | | end
22 | | end
23 | end
24 |   Compute the predicted value  $m_n(\mathbf{x}; \Theta_j, \mathcal{D}_n)$  at  $\mathbf{x}$  equal to the
    |   average of the  $Y_i$ 's falling in the cell of  $\mathbf{x}$  in partition
    |    $\mathcal{P}_{\text{level}} \cup \mathcal{P}_{\text{level}+1}$ .
25 | end
26 |   Compute the random forest estimate  $m_{M,n}(\mathbf{x}; \Theta_1, \dots, \Theta_M, \mathcal{D}_n)$  at the
    |   query point  $\mathbf{x}$  according to (1).
  
```

Figure : Breiman's random forest predicted value at \mathbf{x}

Example of Random Forests



- ▶ A high-dimensional data of patients.
- ▶ $n=349$; $p=500$; qualitative response: 1-15 stands for different cancers; predictors: genes.

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Assumption 0 (H0)

- ▶ **(H0)** We study in this paper the property of the infinite forest estimate obtained as limit of (1) when the number of trees M grows to infinity:

$$m_n(x; D_n) = E_{\Theta} [m_n(x; \Theta, D_n)] = \lim_{M \rightarrow \infty} m_{n,M}(x; \Theta_1, \dots, \Theta_M, D_n)$$

- ▶ We use $m_n(x)$ to denote $m_n(x; D_n)$.

Assumption 1 (H1)

- **(H1)** The response Y follows Additive Regression Model:

$$Y = \sum_{j=1}^p m_j(X^{(j)}) + \epsilon,$$

where $X = (X^{(1)}, \dots, X^{(p)})$ is uniformly distributed over $[0, 1]^p$, ϵ is an independent centered Gaussian noise with finite variance $\sigma^2 > 0$, and each component m_j is continuous.

Theorem 3.1

- ▶ **Theorem 3.1.** Assume that **(H0)** and **(H1)** are satisfied. Then, provided $a_n \rightarrow \infty$ and $t_n(\log a_n)^9/a_n \rightarrow 0$, random forests are consistent, i.e.,

$$\lim_{n \rightarrow \infty} E [m_n(X) - m(X)]^2 = 0.$$

- ▶ Interpretations:
 1. $t_n < a_n$: not fully developed trees.
 2. Theorem 3.1 holds for both sub-sampling ($a_n < n$) and full sampling ($a_n = n$).
 3. $\log a_n$ is the complexity of the tree; $(\log a_n)^9$ is used to control Gaussian error.
 4. $a_n/t_n \rightarrow 0$ is used to control the correlation between trees, eg. if $a_n = t_n = n$, all trees have the same points and splits, they are completely correlated.

The basic ideas to prove Theorem 3.1

- ▶ Step1: $H1 \Rightarrow$ Proposition 2; We get that within each cell, variation of $m(X)$ is small.
- ▶ Step2: \Rightarrow There exists as piecewise function $f(X)$: in each cell, $\lim_{n \rightarrow \infty} \inf E [f(X) - m(x)]^2 = 0$.
- ▶ Step3: With Theorem 5.1 (Gyorfi et. at. 2002), $\Rightarrow \lim_{n \rightarrow \infty} E [T_{\beta_n} m_n(X, \Theta) - m(x)]^2 = 0$ where $T_{\beta_n} u = u$ if $|u| < \beta_n$, $= \text{sign}(u)\beta_n$ if $|u| > \beta_n$ is a threshold function; $\beta_n = \|m\|_{\infty} + \sigma\sqrt{2}(\log a_n)^2$

The basic ideas to prove Theorem 3.1

► Step4:

$$\begin{aligned} \mathbb{E}[m_n(\mathbf{X}) - m(\mathbf{X})]^2 &= \mathbb{E}[\mathbb{E}_\Theta[m_n(\mathbf{X}, \Theta)] - m(\mathbf{X})]^2 \\ &\leq \mathbb{E}[m_n(\mathbf{X}, \Theta) - m(\mathbf{X})]^2 \\ &\quad (\text{by Jensen's inequality}) \\ &\leq \mathbb{E}[m_n(\mathbf{X}, \Theta) - T_{\beta_n} m_n(\mathbf{X}, \Theta)]^2 \\ &\quad + \mathbb{E}[T_{\beta_n} m_n(\mathbf{X}, \Theta) - m(\mathbf{X})]^2 \end{aligned}$$

- ▶ Step5: right $\rightarrow 0$ proved in step 3; for left, $T_\beta m_n(X, \Theta) = m_n(X, \Theta)$ if $|m_n(X, \Theta)| < \beta_n$, for outside region, we can use Markov's Inequality to prove.

Assumption 2 (H2)

- ▶ **(H2)** Let $Z_{i,j} = (Z_i, Z_j')$. Then, one of the following two conditions holds:
- ▶ **(H2.1)** One has:

$$\lim_{n \rightarrow \infty} (\log a_n)^{2p-2} (\log n)^2 E [\max_{i \neq j} |\psi_{i,j}(Y_i, Y_j) - \psi_{i,j}|]^2 = 0.$$

- ▶ **(H2.2)** There exist a constant $C > 0$ and a sequence $(\gamma_n)_n \rightarrow 0$ such that, almost surely,

$$\max_{l_1, l_2=0,1} \frac{\left| \text{Corr}(Y_i - m(X_i), 1_{Z_{i,j}=(l_1, l_2)} | X_i, X_j, Y_j) \right|}{P^{1/2} [Z_{i,j} = (l_1, l_2) | X_i, X_j, Y_j]} \leq \gamma_n,$$

and

$$\max_{l_1=0,1} \frac{\left| \text{Corr}((Y_i - m(X_i))^2, 1_{Z_i=l_1} | X_i) \right|}{P^{1/2} [Z_i = l_1 | X_i]} \leq C.$$

Notations of Assumption 2 (H2)

- ▶ $Z_i = 1_{X \overset{\Theta}{\leftrightarrow} X_i}$: the indicator that X_i falls in the same cell as X in the random tree designed with D_n and the random parameter Θ .
- ▶ $Z'_j = 1_{X \overset{\Theta'}{\leftrightarrow} X_j}$: Θ' is an independent copy of Θ .
- ▶ $\psi_{i,j}(Y_i, Y_j) = E \left[Z_i Z'_j | X, \Theta, \Theta', X_1, \dots, X_n, Y_i, Y_j \right]$.
- ▶ $\psi_{i,j} = E \left[Z_i Z'_j | X, \Theta, \Theta', X_1, \dots, X_n \right]$.

Assumption 2 (H2)

- ▶ Interpretations:
 1. **(H2.1)** means that the influence of two Y -values on the probability of connection of two couples of random points tends to be zero as $n \rightarrow \infty$.
 2. **(H2.2)** means that the correlation between the noise and the probability of connection of two couple of points vanishes fast enough as $n \rightarrow \infty$.
 3. In practice, both **(H2.1)** and **(H2.2)** may not be satisfied.

Theorem 3.2

- **Theorem 3.2.** Assume that **(H0)**, **(H1)** and **(H2)** are satisfied and let $t_n = a_n$. Then, provided $a_n \rightarrow \infty$ and $\frac{a_n \log n}{n} \rightarrow 0$, random forests are consistent, i.e.,

$$\lim_{n \rightarrow \infty} E [m_n(X) - m(X)]^2 = 0.$$

- Interpretations:
 1. $t_n = a_n$ means fully developed trees.
 2. $a_n < n$ means sub-sampling.
 3. $a_n/n \rightarrow 0$ is used to control the correlation between trees, as each observation will not show up in too many trees.

Proposition 1

- **Proposition 1.** Assume that **(H0)** and **(H1)** are satisfied. Let $k \in N^*$ and $\xi > 0$. Assume that there is no interval $[a,b]$ and no $j \in \{1, \dots, S\}$ such that m_j is constant on $[a,b]$, i.e. $Y = \sum_{j=1}^S m_j(X^{(j)}) + \epsilon$. Then, with probability $1 - \xi$, for all n large enough, we have, for all $1 \leq q \leq k$,

$$j_{q,n}(X) \in \{1, \dots, S\}.$$

- Interpretations:
 1. Proposition 1 proves the consistency of random forests in high-dimensional settings.
 2. For sparsity, when n is large enough, random forests will pick up the S informative predictors.
 3. This proposition requires $p \leq n$. It doesn't cover the case: $p > n$.

Proposition 2

- **Proposition 2.** Assume that **(H0)** and **(H1)** hold. Then, for all $\rho, \xi > 0$, there exists $N \in N^*(\text{num of cuts})$ such that, for all $n > N$,

$$P[\Delta(m, A_n(X, \Theta)) \leq \xi] \geq 1 - \rho.$$

- Interpretations:
 1. Proposition 2 states that under H1, the variation of the regression function m within a cell of a random tree is small provided n is large enough.
 2. This proposition forces the approximation error of the forests to asymptotically approach 0.

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Discussion

► Advantages:

1. Proved consistency of random forests in subsampling.
2. Proved consistency of random forests in high-dimensional settings (Sparsity).

► Disadvantages:

1. Predictors are limited in $X \in [0, 1]^p$.
2. Random forests are created without replacement which is different from Bootstrap.
3. Only the regression model is studied.
4. The high-dimensional setting doesn't include the situation when $p > n$.

Future Work

- ▶ Prove consistency of random forests with predictors $X \in R^p$.
- ▶ Prove consistency of random forests by Bootstrap with replacement .
- ▶ Prove consistency of random forests of classification.
- ▶ Prove consistency of random forests in high-dimensional settings when $p > n$.

Reference

- ▶ Breiman, L., *Random Forests*. Machine Learning, 45:5-32,2001.
- ▶ James, G., Witten, D., Hastie, T., and Tibshirani, R. *An Introduction to Statistical Learning*. First Edition. Springer, New York, 2015.
- ▶ Scornet, E., Biau, G., and Vert, J. *Consistency of Random Forests*. Annals of Statistics, 43:1716-1741, 2015.
- ▶ Györfi, M., Krzyżak, A., and Walk, H. *A Distribution-Free Theory of Nonparametric Regression*. Springer, New York, 2002.

THANK YOU!