

Topic 20: Random Forest

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Key points: .

Disclaimer: The note is built on Prof. *Jinchi Lv*'s lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.

20.1 Motivation

Denote by $m(\mathbf{X})$ the measurable nonparametric regression function with p -dimensional random vector \mathbf{X} taking values in $[0, 1]^p$. The Random Forest algorithm aims to learn the regression function in a non-parametric way based on the observations $\mathbf{x}_i \in [0, 1]^p$, $y_i \in \mathbb{R}$, $i = 1, \dots, n$, from the model

$$y_i = m(\mathbf{x}_i) + \epsilon_i$$

where \mathbf{X} , \mathbf{x}_i , ϵ_i , $i = 1, \dots, n$ are independent, and $\{\mathbf{x}_i\}$ and $\{\epsilon_i\}$ are two sequences of identically distributed random variables. \mathbf{x}_i is distributed identically as \mathbf{X} .

Why Random Forest (RF)? RF has gained significant popularity due to its

- **High accuracy:** RF consistently rank among the top performer, often surpassing more complex models
- **Robustness:** RF are less subject to overfitting due to the ensemble nature leveraging multiple decision trees
- **Interpretability:** RF provide rankings of feature importance

As illustrated in Figure 20.1, in a level-2 tree, each node (cell) defines the point where the current cell split and new cells are produced. The sets of features eligible for splitting cells at level $k - 1$ are denoted as $\Theta_k := \{\Theta_{k,1}, \dots, \Theta_{k,2^{k-1}}\}$, where $\Theta_{k,s} \subset \{1, \dots, p\}$.



Figure 20.1: Level-2 Tree Example

Given any T (and the associated splitting criterion) and $\Theta_{1:k}$, the tree estimate denoted as $\hat{m}_{T(\Theta_{1:k})}$ for a test

point $\mathbf{c} \in [0, 1]^p$ is defined as

$$\hat{m}_{T(\Theta_{1:k})}(\mathbf{c}, \mathcal{X}_n) := \sum_{(\mathbf{t}_1, \dots, \mathbf{t}_k) \in T(\Theta_{1:k})} \mathbf{1}_{\mathbf{c} \in \mathbf{t}_k} \left(\frac{\sum_{i \in \{i: \mathbf{x}_i \in \mathbf{t}_k\}} y_i}{\# \{i : \mathbf{x}_i \in \mathbf{t}_k\}} \right)$$

where $\mathcal{X}_n := \{\mathbf{x}_i, y_i\}_{i=1}^n$, the fraction is defined as 0 when no sample is in the cell \mathbf{t}_k , and $\mathbf{1}_{\mathbf{c} \in \mathbf{t}_k}$ is an indicator function = 1 if $\mathbf{c} \in \mathbf{t}_k$ and = 0 otherwise.

20.2 Chi et al. (2022): High Dimensional RFs

Following [Chi et al. \(2022\)](#), for a RF model where

- a sequence of distinct $\Theta_{1:k}$ results in a distinct tree
- every set of available features $\Theta_{l,s}$, $l = 1, \dots, k$; $s = 1, \dots, 2^{l-1}$

Column subsampling Define a **column subsampling** procedure: $\Theta_{l,s}, \forall l, s$ has $\lceil \gamma_0 p \rceil$ distinct integers among $1, \dots, p$, with $\lceil \cdot \rceil$ the ceiling function for some $0 < \gamma_0 \leq 1$. γ_0 is the predetermined constant parameter of column subsampling. Introduce the boldface random mappings $\Theta_{1:k}$, which are independent and uniformly distributed over all possible $\Theta_{1:k}$ for all integer k . Then random forests estimate for \mathbf{c} with observations \mathcal{X}_n is given by

$$\mathbb{E}(\hat{m}_{T(\Theta_{1:k})}(\mathbf{c}, \mathcal{X}_n) \mid \mathcal{X}_n) = \sum_{\Theta_{1:k}} \mathbb{P} \left(\bigcap_{s=1}^k \{\Theta_s = \Theta_s\} \right) \hat{m}_{T(\Theta_{1:k})}(\mathbf{c}, \mathcal{X}_n)$$

The expectation is taken over sets of available features.

Observation resampling Let $A = \{a_1, \dots, a_B\}$ be a set of subsamples with each a_i consisting of $\lceil bn \rceil$ observations (indices) drawn without replacement from $\{1, \dots, n\}$ for some positive integer B and $0 < b \leq 1$; in addition, each a_i is independent of model training. The default values of B and b are 500 and 0.632¹. Then the tree estimate using subsample a is define as

$$\hat{m}_{T(\Theta_{1:k}),a}(\mathbf{c}, \mathcal{X}_n) := \sum_{(\mathbf{t}_1, \dots, \mathbf{t}_k) \in T(\Theta_{1:k})} \mathbf{1}_{\mathbf{c} \in \mathbf{t}_k} \left(\frac{\sum_{i \in a \cap \{i: \mathbf{x}_i \in \mathbf{t}_k\}} y_i}{\#(a \cap \{i : \mathbf{x}_i \in \mathbf{t}_k\})} \right)$$

the random forests estimate given A is then

$$B^{-1} \sum_{a \in A} \mathbb{E}[\hat{m}_{T,a}(\Theta_{1:k}, \mathbf{c}, \mathcal{X}_n) \mid \mathcal{X}_n] := B^{-1} \sum_{a \in A} \mathbb{E}[\hat{m}_{T(\Theta_{1:k}),a}(\mathbf{c}, \mathcal{X}_n) \mid \mathcal{X}_n]$$

CART-split criterion Given a cell \mathbf{t} , a subset of observation indices a and a set of available features $\Theta \subset \{1, \dots, p\}$, the CART-split is defined as

$$(\hat{j}, \hat{c}) = \arg \min_{j \in \Theta, c \in \{x_{ij}: \mathbf{x}_i \in \mathbf{t}, i \in a\}} \left[\sum_{i \in a \cap P_L} (\bar{y}_L - y_i)^2 + \sum_{i \in a \cap P_R} (\bar{y}_R - y_i)^2 \right] \quad (20.1)$$

¹Or, $b = 1$ but observations are drawn with replacement.

where

$$P_L := \{i : \mathbf{x}_i \in \mathbf{t}, x_{ij} < c\} \quad P_R := \{i : \mathbf{x}_i \in \mathbf{t}, x_{ij} \geq c\}$$

$$\bar{y}_L := \sum_{i \in a \cap P_L} \frac{y_i}{\#(a \cap P_L)} \quad \bar{y}_R := \sum_{i \in a \cap P_R} \frac{y_i}{\#(a \cap P_R)}$$

The CART-split criterion conditional on the sample is a deterministic splitting criterion; conditioning on another sample leads to another deterministic splitting criterion. Define \hat{T}_a as the sample tree growing rule that is associated with a splitting criterion following Eq. (20.1), the tree estimates using \hat{T}_a can be similarly defined as

$$\hat{m}_{\hat{T}_a(\Theta_{1:k})}(\mathbf{c}, \mathcal{X}_n) := \sum_{(\mathbf{t}_1, \dots, \mathbf{t}_k) \in \hat{T}_a(\Theta_{1:k})} \mathbf{1}_{\mathbf{c} \in \mathbf{t}_k} \left(\frac{\sum_{i \in \{i: \mathbf{x}_i \in \mathbf{t}_k\}} y_i}{\#\{i : \mathbf{x}_i \in \mathbf{t}_k\}} \right)$$

the definition is the same for $\hat{m}_{\hat{T}_a, a}$. Then the random forests estimate for a test point $\mathbf{c} \in [0, 1]^p$ is given by

$$B^{-1} \sum_{a \in A} \mathbb{E} \left(\hat{m}_{\hat{T}_a, a}(\Theta_{1:k}, \mathbf{c}, \mathcal{X}_n) \mid \mathcal{X}_n \right)$$

where the average and conditional expectation correspond to the sample and column subsamplings respectively, and they are interchangeable.

Bias-variance decomposition For a tree growing rule T and $\Theta_{1:k}$, the population version is defined as

$$m_{T(\Theta_{1:k})}^*(\mathbf{c}) := \sum_{(\mathbf{t}_1, \dots, \mathbf{t}_k) \in T(\Theta_{1:k})} \mathbf{1}_{\mathbf{c} \in \mathbf{t}_k} \mathbb{E}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}_k) \quad (20.2)$$

for each test point $\mathbf{c} \in [0, 1]^p$. And the \mathbb{L}^2 prediction loss for random forests is defined as

$$\mathbb{E} \left[m(\mathbf{X}) - B^{-1} \sum_{a \in A} \mathbb{E} \left(\hat{m}_{\hat{T}_a, a}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \mid \mathbf{X}, \mathcal{X}_n \right) \right]^2 \quad (20.3)$$

if we use the full sample $a = \{1, \dots, n\}$, and denote \hat{T}_a and $\hat{m}_{\hat{T}_a, a}$ as \hat{T} and $\hat{m}_{\hat{T}}$, the sample subsampling and average $B^{-1} \sum_{a \in A} (\cdot)$ in the random forests estimate are no longer needed, then Eq.(20.3) can be simplified as

$$\mathbb{E} \left[m(\mathbf{X}) - \mathbb{E}(\hat{m}_{\hat{T}}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \mid \mathbf{X}, \mathcal{X}_n) \right]^2$$

By Jensen's inequality and Cauchy-Schwarz inequality,

$$\begin{aligned} & \frac{1}{2} \mathbb{E} \left[m(\mathbf{X}) - \mathbb{E}(\hat{m}_{\hat{T}}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \mid \mathbf{X}, \mathcal{X}_n) \right]^2 \\ & \leq \underbrace{\mathbb{E} \left[m(\mathbf{X}) - m_{\hat{T}}^*(\Theta_{1:k}, \mathbf{X}) \right]^2}_{\text{approximation error (squared bias)}} + \underbrace{\mathbb{E} \left[m_{\hat{T}}^*(\Theta_{1:k}, \mathbf{X}) - \hat{m}_{\hat{T}}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \right]^2}_{\text{estimation variance}} \end{aligned}$$

Consistency of RF Models

For a cell \mathbf{t} and its two daughter cells \mathbf{t}' and \mathbf{t}'' , define

$$\begin{aligned} \text{(I)}_{\mathbf{t}, \mathbf{t}'} &:= \mathbb{P}(\mathbf{X} \in \mathbf{t}' \mid \mathbf{X} \in \mathbf{t}) \text{Var}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}') + \mathbb{P}(\mathbf{X} \in \mathbf{t}'' \mid \mathbf{X} \in \mathbf{t}) \text{Var}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}'') \\ \text{(II)}_{\mathbf{t}, \mathbf{t}'} &:= \mathbb{P}(\mathbf{X} \in \mathbf{t}' \mid \mathbf{X} \in \mathbf{t}) [\mathbb{E}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}') - \mathbb{E}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t})]^2 \\ &+ \mathbb{P}(\mathbf{X} \in \mathbf{t}'' \mid \mathbf{X} \in \mathbf{t}) [\mathbb{E}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}'') - \mathbb{E}(m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t})]^2 \end{aligned}$$

and $(\mathbb{I})_{\mathbf{t}, \mathbf{t}'}$ and $(\mathbb{III})_{\mathbf{t}, \mathbf{t}'}$ are defined similarly.

in this context, we assume the following regularity conditions:

- **Absolutely continuous distribution**: f , the density function of \mathbf{X} , is bounded away from 0 and ∞
- **Covariates and model errors**: assume $p = O(n^{K_0})$ for $K_0 > 0$, and there is a symmetric distribution around 0 for ϵ_1 , s.t. $\mathbb{E} |\epsilon_1|^q < \infty$ for sufficiently large $q > 0$
- **Bounded regression functions**: $\sup_{\mathbf{c} \in [0,1]^p} |m(\mathbf{c})| \leq M_0$, for some $M_0 > 0$
- **Sufficient impurity decrease**: $\exists \alpha_1 \geq 1$ s.t. $\forall \mathbf{t} = t_1 \times \dots \times t_p$,

$$\text{Var} [m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}] \leq \alpha_1 \sup_{j \in \{1, \dots, p\}, c \in t_j} (\mathbb{III})_{\mathbf{t}, \mathbf{t}(j,c)}$$

where

- $(\mathbb{III})_{\mathbf{t}, \mathbf{t}'}$: conditional bias decrease (or conditional impurity decrease)
- $\text{Var} [m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}]$: conditional **total** bias, $\text{Var} [m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}] = (\mathbb{I})_{\mathbf{t}, \mathbf{t}} + (\mathbb{III})_{\mathbf{t}, \mathbf{t}}$
- **Intuition**: having large conditional bias decrease on each cell is a desired property for achieving a good control of the squared bias of random forests estimate

Sufficient impurity decrease (SID) Define the functional class

$$\text{SID}(\alpha) := \{m(\mathbf{X}) : m(\mathbf{X}) \text{ satisfies SID with } \alpha_1 \leq \alpha\}$$

the size of $\text{SID}(\alpha)$ is **non-decreasing** in $\alpha \geq 1$: if $m(\mathbf{X}) \in \text{SID}(\alpha - c)$ for some $\alpha - c \geq 1$ and $c > 0$, then $m(\mathbf{X}) \in \text{SID}(\alpha)$ ².

Under the regularity conditions mentioned above, we have the following theorem

Theorem 20.2.1: Consistency

Let $0 < b \leq 1, 0 < \gamma_0 \leq 1, \alpha_2 > 1, 0 < \eta < 1/8, 0 < c < 1/4$ and $\delta > 0, 2\eta < \delta < \frac{1}{4}$. Let $A = \{a_1, \dots, a_B\}$ with $\#a_i = \lceil bn \rceil$ for $i = 1, \dots, B$ and $a \in A$. Then $\exists C > 0$ s.t. for all large n and each $1 \leq k \leq c \log_2 \lceil bn \rceil$,

$$\begin{aligned} & \mathbb{E} \left[m(\mathbf{X}) - \mathbb{E} \left(\hat{m}_{\hat{T}_{a,a}}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \mid \mathbf{X}, \mathcal{X}_n \right) \right]^2 \\ & \leq C \left[\alpha_1 (\lceil bn \rceil)^{-\eta} + \left(1 - \gamma_0 (\alpha_1 \alpha_2)^{-1} \right)^k + (\lceil bn \rceil)^{-\delta+c} \right] \end{aligned}$$

In addition, when aggregate over row subsamples (over $a \in A$), get

$$\begin{aligned} & \mathbb{E} \left[m(\mathbf{X}) - \frac{1}{B} \mathbb{E} \left(\hat{m}_{\hat{T}_{a,a}}(\Theta_{1:k}, \mathbf{X}, \mathcal{X}_n) \mid \mathbf{X}, \mathcal{X}_n \right) \right]^2 \\ & \leq C \left[\alpha_1 (\lceil bn \rceil)^{-\eta} + \left(1 - \gamma_0 (\alpha_1 \alpha_2)^{-1} \right)^k + (\lceil bn \rceil)^{-\delta+c} \right] \end{aligned}$$

Here, the feature dimensionality p and tree height k decide the number of all possible cells when growing trees.

²Many popular regression functions belong to this functional class.

Bias-variance decomposition Under Theorem (20.2.1), both bias and variance depend implicitly on p through n in the upper bounds.

Proposition 20.2.2: Bias-Variance Decomposition

Under Thm (20.2.1), for all large n and $1 \leq k \leq c \log_2 n$, it holds that

$$\begin{aligned} \text{Squared bias} &:= \underbrace{\mathbb{E} \left[m(\mathbf{X}) - m_{\hat{T}}^* (\boldsymbol{\Theta}_{1:k}, \mathbf{X}) \right]^2}_{\text{approximation error}} \\ &\leq O \left(n^{-\eta} + \underbrace{\left(1 - \gamma_0 (\alpha_1 \alpha_2)^{-1} \right)^k}_{\text{Main term of bias}} \right) + \underbrace{O \left(n^{-\delta+c} \right)}_{\text{Uninteresting error}} \end{aligned}$$

where $n^{-\eta}$ upper-bounds the error caused by the sample CART-splits. Under theoretical CART-splits, $n^{-\eta}$ vanishes and $\alpha_2 = 1$. and

$$\begin{aligned} \text{Estimatio Variance} &:= \mathbb{E} \left[m_{\hat{T}}^* (\boldsymbol{\Theta}_{1:k}, \mathbf{X}) - \hat{m}_{\hat{T}} (\boldsymbol{\Theta}_{1:k}, \mathbf{X}, \mathcal{X}_n) \right]^2 \\ &\leq O(n^{-\eta}) + \underbrace{O(n^{-\delta+c})}_{\text{Uninteresting error}} \end{aligned}$$

where the upper bound is conservative since we establish a uniform upper bound for the variances of **individual** trees.

Relevant features Under the regularity conditions, for some cells, only the splits along the relevant feature directions can reduce a sufficient amount of bias. To be precise, introduce a variance of SID with some $S_0 \subset \{1, \dots, p\}$ below

- **Sufficient impurity decrease 2** $\exists \alpha_1 \geq 1$ s.t. for each cell $\mathbf{t} = t_1 \times \dots \times t_p$

$$\text{Var} (m(\mathbf{X}) \mid \mathbf{X} \in \mathbf{t}) \leq \alpha_1 \sup_{j \in S_0, c \in t_j} (\text{III})_{\mathbf{t}, \mathbf{t}(j,c)}$$

References

Chien-Ming Chi, Patrick Vossler, Yingying Fan, and Jinchi Lv. Asymptotic properties of high-dimensional random forests. *The Annals of Statistics*, 50(6):3415–3438, 2022.