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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 nonparametric 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 X,  $x_i$ ,  $\varepsilon_i$ ,  $i = 1, \dots, n$  are independent, and  $\{x_i\}$  and  $\{\varepsilon_i\}$  are two sequences of identically distributed random variables.  $x_i$  is distributed identically as 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  $\Theta_k := \{\Theta_{k,1}, \cdots, \Theta_{k,2^{k-1}}\}$ , where  $\Theta_{k,s} \subset \{1, \cdots, p\}$ .

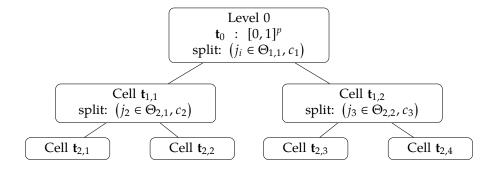


Figure 20.1: Level-2 Tree Example

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

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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  $X_n := \{x_i, y_i\}_{i=1}^n$ , 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

For a RF model where

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

**Column subsampling** Define a **column subsampling** procedure:  $\Theta_{l,s}$ ,  $\forall l,s$  has  $[\gamma_0 p]$  distinct integers among  $1, \dots, p$ , with  $[\cdot]$  the ceiling function for some  $0 < \gamma_0 \le 1$ .  $\gamma_0$  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  $X_n$  is given by

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

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  $0 < b \le 1$ ; in addition, each  $a_i$  is independent of model training. The default values of B and B are 500 and 0.632 $^1$ . Then the tree estimate using subsample B is define as

$$\hat{m}_{T(\Theta_{1:k}),a}\left(\mathbf{c},\mathcal{X}_{n}\right) \coloneqq \sum_{\left(\mathbf{t}_{1},\cdots,\mathbf{t}_{k}\right)\in T(\Theta_{1:k})} \mathbf{1}_{\mathbf{c}\in\mathbf{t}_{k}} \left(\frac{\sum_{i\in a\cap\left\{i:\mathbf{x}_{i}\in\mathbf{t}_{k}\right\}} y_{i}}{\#\left(a\cap\left\{i:\mathbf{x}_{i}\in\mathbf{t}_{k}\right\}\right)}\right)$$

the random forests estimate given A is then

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

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

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

 $<sup>{}^{1}\</sup>text{Or}$ , b = 1 but observations are drawn with replacement.

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where

$$P_{L} := \left\{ i : \mathbf{x}_{i} \in \mathbf{t}, x_{ij} < c \right\}$$

$$\overline{y}_{L} := \sum_{i \in a \cap P_{L}} \frac{y_{i}}{\#(a \cap P_{L})}$$

$$P_{R} := \left\{ i : \mathbf{x}_{i} \in \mathbf{t}, x_{ij} \geq c \right\}$$

$$\overline{y}_{R} := \sum_{i \in a \cap P_{R}} \frac{y_{i}}{\#(a \cap P_{R})}$$

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

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

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

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

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

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

By Jensen's inequality and Cauchy-Schwarz inequality,

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

$$\leq \mathbb{E}\left[m(\mathbf{X})\right]$$

Chi et al. (2022)

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## 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.