

# Wasserstein Random Forests at First Glance

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# 1 Overview

## 1.1 Motivation

The classical setting of supervised learning focus on the estimation of the conditional expectation  $E[Y | X = x]$  for some underlying 1-dimensional objective  $Y$  and a multidimensional covariate  $X$ . In many real-world applications, it is also important to track the additional information encoded in the conditional distribution  $\mathcal{L}(Y | X = x)$ . For example, in Heterogeneous Treatment Effect (HTE), the traditional object of interest is the *Conditional Average Treatment Effect* (CATE) function, defined by

$$\tau(x) = E[Y(1) - Y(0) | X = x],$$

where  $Y(1)$  (resp.  $Y(0)$ ) denotes the *potential outcomes* (see, e.g., [Rub74] and [IR15]) of treatment (resp. no treatment). The data is usually of form  $(Y_i(W_i), W_i, X_i; 1 \leq i \leq N)$ , where  $W_i$  denotes the treatment assignment indicators. Recently, many approaches based on modern statistical learning are investigated on the estimation of the CATE function (see, e.g., [KSBY17, AW19, NW17]).

However, the information provided by conditional expectation

$$\mu_0 := E[Y(0) | X = x] \quad \text{and} \quad \mu_1 := E[Y(1) | X = x]$$

is limited. For example, when the conditional distribution of  $Y(1)$  (resp.  $Y(0)$ ) is multimodal, the conditional expectation can not provide insights on the causal inference. A simple inference based on the CATE function may also be dangerous without any information of the conditional distribution of  $Y(0)$  and  $Y(1)$ .

In an ideal case, one is interested to estimate the joint conditional distribution

$$\mathcal{L}((Y(0), Y(1)) | X = x).$$

Unfortunately, by the essential of the problem, there is not a single sample of  $(Y_i(0), Y_i(1))$  at point  $X_i$  that can be collected in the observational study. Unlike the conditional expectation, the dependence between  $Y(0)$  and  $Y(1)$  is much more complex. It is in general difficult to design a strategy to estimate the covariance of  $Y(0)$  and  $Y(1)$  based on a similar strategy used to obtain the estimation of the conditional expectation. Therefore, it is extremely difficult to estimate the joint distribution  $\mathcal{L}((Y(0), Y(1)) | X = x)$  in practice without any further assumptions on the dependence of  $Y(0)$  and  $Y(1)$ . As a consequence, we concentrate on a subproblem: instead of estimating  $\mathcal{L}((Y(0), Y(1)) | X = x)$ , we are interested in the estimation of the conditional marginal distributions  $\mathcal{L}(Y(0) | X = x)$  and  $\mathcal{L}(Y(1) | X = x)$ . By considering the two subgroups

$$\{(X_i, Y(W_i)) | W_i = 0, 1 \leq i \leq N\} \quad \text{and} \quad \{(X_i, Y(W_i)) | W_i = 1, 1 \leq i \leq N\},$$

the subproblem thus enters in a classical supervised learning context (cf. T-learners [KSBY17]), while the objective is replaced by estimating the conditional distribution.

## 1.2 Fundamental idea

The success of Random Forests (RF) [Bre01] has been proven in many real-world applications. If we look at the final prediction at each point  $x$  provided by the RF algorithm, it can be regarded as a weighted average of some  $(Y_i; 1 \leq i \leq N)$  in the training dataset, where the weights are some random variables depending on the covariates  $(X_i; 1 \leq i \leq N)$ . A very natural idea is to use this weighted empirical measure to approximate the conditional distribution. This is also the fundamental idea in the construction of forests quantile regression [Mei06, AW19] and other literatures that combine the kernel density estimations and Random Forests [cite lot of papers]. To achieve this, the splitting criterion should be modified, in order to be compatible with conditional distribution estimation.

A natural metric to measure the distance of two measures is Wasserstein distance. More precisely, the Wasserstein distance  $\mathcal{W}_p$  between two measures  $\mu, \nu$  on  $\mathbf{R}^d$  is defined by

$$\mathcal{W}_p(\mu, \nu) := \left( \inf_{\gamma \in \Gamma(\mu, \nu)} \int |x - y|^p \gamma(dx, dy) \right)^{\frac{1}{p}},$$

where  $|\cdot|$  is the Euclidean norm in  $\mathbf{R}^d$  and  $\Gamma(\mu, \nu)$  denotes the set of all couplings of  $\mu$  and  $\nu$ , namely,

$$\int_{y \in \mathbf{R}^q} \gamma(dx, dy) = \mu(dx) \quad \text{and} \quad \int_{x \in \mathbf{R}^q} \gamma(dx, dy) = \nu(dy).$$

When  $\mu$  and  $\nu$  are the probability measures on  $\mathbf{R}$ , it is easily checked that

$$\mathcal{W}_p(\mu, \nu) := \left( \int_0^1 \left| F_\mu^{-1}(u) - F_\nu^{-1}(u) \right|^p du \right)^{\frac{1}{p}}, \quad (1)$$

where  $F_\mu^{-1}(u)$  (resp.  $F_\nu^{-1}(u)$ ) is the generalized inverse distribution function defined by

$$F_\mu^{-1}(u) := \inf \{x \in \mathbf{R} \mid F_\mu(x) \geq u\},$$

with  $F_\mu(x)$  the cumulative distribution function of  $\mu$ . Denote by  $E$  the support of  $X$  and denote by  $\pi_x(dy)$  the probability measure associated to  $\mathcal{L}(Y \mid X = x)$ . Now, let us provide some possible regularity assumptions in the following.

**Assumption 1** (Lipschitz). *For any  $(x, y) \in E \times E$ , we assume that there exists a constant  $C_\pi < +\infty$  such that*

$$\mathcal{W}_2(\pi_x, \pi_y) \leq C_\pi |x - y|.$$

**Assumption 2** (Hölder). *For any  $(x, y) \in E \times E$ , we assume that there exists  $\alpha > 0$  and a constant  $C_\pi^\alpha < +\infty$  such that*

$$\mathcal{W}_2(\pi_x, \pi_y) \leq C_\pi^\alpha |x - y|^\alpha.$$

The ultimate goal is to construct an estimator  $\pi_x^N$  of  $\pi_x$  such that for all  $x \in E$ , we have

$$\mathcal{W}_2(\pi_x^N, \pi_x) \xrightarrow[N \rightarrow \infty]{a.s. \text{ or } \mathbb{P} \text{ or } \mathbb{L}^p} 0.$$

This is inspired by the classical consistence analysis of Random Forests, where the conditional expectation is often assumed to be Lipschitz or Hölder w.r.t. covariate.

### 1.3 Splitting criterion

We present an intuitive idea on how to perform the splitting which is compatible with the Wasserstein distance. Roughly speaking, we try to maximize the  $\mathcal{W}_2$ -distance between the empirical measures w.r.t.  $Y_i$  of the newly created left node and right node, which obeys the same philosophy of the classical Random Forests: the splitting is performed greedily in order to maximize the homogeneity between the subgroups. This criterion also works when the dimension of  $Y$  is greater than 1. However, in this case, the calculation of  $\mathcal{W}_2$ -distance may become intractable (with  $\mathcal{O}(N^3)$  time complexity where  $N$  represents the sum of the number of data in the two associated empirical measures). Some regularization strategies (such as sinkhorn distance, i.e., Optimal Transport with entropic constraints) may be applied. In Breiman's original Random Forests, the splitting is performed to maximize the inter-group variance, which is compatible with the conditional expectation estimation as the conditional expectation minimizes the  $\mathbb{L}^2$ -error. The underlying philosophy is to maximize the heterogeneity between the two subgroups. Our idea is similar: we use Wasserstein distance to measure the distance between distributions, and the splitting is done by maximizing the Wasserstein distance between the associated empirical measures in the two subgroups.

**Toy example** Before proceeding further, we illustrate the splitting mechanism in a 2-dimensional toy example. Let  $X = (X^{(1)}, X^{(2)})$  be the canonical random variable of covariate, and denote by  $Y$  the associate objective. Considering a dataset  $(X_i, Y_i; 1 \leq i \leq 8)$  with  $n = 8$ , we explain the first splitting in the direction (1) (see Figure 1). Fixing a splitting point  $z$ , we denote respectively  $A_L$  and  $A_R$  the data points  $X_i$  in the left and right sides of  $z$ . We denote  $\pi_L$  and  $\pi_R$  the empirical measures associated respectively to  $A_L$  and  $A_R$ , i.e.,

$$\pi_L = \frac{1}{\#(A_L)} \sum_{i=1}^n \delta_{Y_i} \mathbf{1}_{\{X_i \in A_L\}},$$

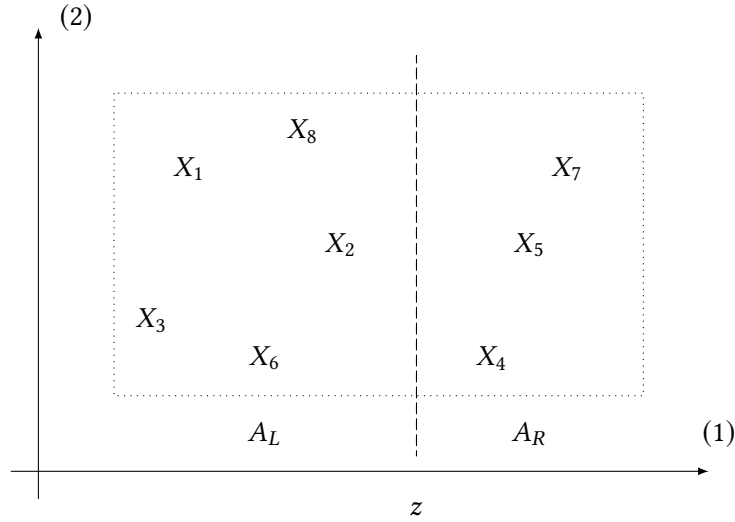
and

$$\pi_R = \frac{1}{\#(A_R)} \sum_{i=1}^n \delta_{Y_i} \mathbf{1}_{\{X_i \in A_R\}}.$$

The best splitting point  $z^*$  is determined by

$$z^* = \arg \max_z \mathcal{W}_p(\pi_L, \pi_R).$$

Note that the splitting  $z$  is always performed in the middle of two consecutive data points along the direction (1) in order to remove the possible ties in the  $\arg \max$ .



**Figure 1:** An illustration of splitting.

More concretely, in Figure 1 the Wasserstein distance to be evaluated is

$$\mathcal{W}_p \left( \frac{1}{5}(\delta_{Y_1} + \delta_{Y_2} + \delta_{Y_3} + \delta_{Y_6} + \delta_{Y_8}), \frac{1}{3}(\delta_{Y_4} + \delta_{Y_5} + \delta_{Y_7}) \right).$$

The computation can be done by the equation given in (1), with  $\mathcal{O}(N \log(N))$  time complexity, where  $N$  is the number of the data points.

## 2 Mechanism

### 2.1 Notation

We use the notation compatible with [BS15]:

- $\forall n \in \mathbb{N}^*, [n] := \{1, 2, \dots, n\};$

- $\mathcal{D}_n := ((X_1, Y_1), \dots, (X_n, Y_n))$ ;
- $\Theta$ : generic random variable to describe the randomness of tree's construction;
- $\Theta_j$ : random variable associated with  $j$ -th tree;
- $\mathcal{D}_n^*(\Theta_j)$ : dataset used to construct the  $j$ -th tree;
- $A_n(x; \Theta_j, \mathcal{D}_n)$ : the cell in the  $j$ -th tree that contains the point  $x$ ;
- $N_n(x; \Theta_j, \mathcal{D}_n)$ : the number of points in  $\mathcal{D}_n^*(\Theta_j)$  that fall into  $A_n(x; \Theta_j, \mathcal{D}_n)$ ;
- $m_n(x; \Theta_j, \mathcal{D}_n)$ : prediction of conditional expectation given by  $j$ -th tree, defined by

$$m_n(x; \Theta_j, \mathcal{D}_n) = \sum_{i \in \mathcal{D}_n^*(\Theta_j)} \frac{Y_i \mathbf{1}_{\{X_i \in A_n(x; \Theta_j, \mathcal{D}_n)\}}}{N_n(x; \Theta_j, \mathcal{D}_n)};$$

- $\mu_n(x; \Theta_j, \mathcal{D}_n)$ : prediction of conditional distribution given by  $j$ -th tree, defined by

$$\mu_n(x; \Theta_j, \mathcal{D}_n) = \sum_{i \in \mathcal{D}_n^*(\Theta_j)} \frac{\mathbf{1}_{\{X_i \in A_n(x; \Theta_j, \mathcal{D}_n)\}}}{N_n(x; \Theta_j, \mathcal{D}_n)} \delta_{Y_i};$$

- $m_{M,n}(x; \Theta_j, \mathcal{D}_n)$ : prediction of conditional expectation given by a Random Forest that contains  $M$  trees, that is

$$\begin{aligned} m_{M,n}(x; \Theta_j, \mathcal{D}_n) &= \frac{1}{M} \sum_{j=1}^M m_n(x; \Theta_j, \mathcal{D}_n) \\ &= \frac{1}{M} \sum_{j=1}^M \sum_{i \in \mathcal{D}_n^*(\Theta_j)} \frac{Y_i \mathbf{1}_{\{X_i \in A_n(x; \Theta_j, \mathcal{D}_n)\}}}{N_n(x; \Theta_j, \mathcal{D}_n)} \\ &\quad \text{(when } \bigcup_{j=1}^M \mathcal{D}_n^*(\Theta_j) = [n] \text{)} \\ &= \underbrace{\sum_{i=1}^n \sum_{j=1}^M \frac{\mathbf{1}_{\{X_i \in A_n(x; \Theta_j, \mathcal{D}_n)\}}}{M N_n(x; \Theta_j, \mathcal{D}_n)}}_{\alpha_i(x)} Y_i; \end{aligned} \tag{2}$$

- $\mu_{M,n}(x; \Theta_j, \mathcal{D}_n)$ : prediction of conditional distribution given by a Random Forest that contains  $M$  trees, that is

$$\begin{aligned} \mu_{M,n}(x; \Theta_j, \mathcal{D}_n) &= \frac{1}{M} \sum_{j=1}^M \mu_n(x; \Theta_j, \mathcal{D}_n) \\ &\quad \text{(when } \bigcup_{j=1}^M \mathcal{D}_n^*(\Theta_j) = [n] \text{)} \\ &= \sum_{i=1}^n \alpha_i(x) \delta_{Y_i}. \end{aligned} \tag{3}$$

## 2.2 Algorithm

Roughly speaking, Wasserstein Random Forests (WRF) are constructed by the same stochastic mechanism of Breiman's Random Forests. The main differences are splitting criterion and output of the prediction. As a consequence, for tuning the algorithm, we consider the following parameters that are identical to Breiman's Random Forests:

- (i)  $a_n \in [n]$ : the number of data points sampled in each tree;
- (ii)  $\mathbf{mtry} \in [p]$ : the number of possible splitting directions to be explored at each node of each tree;
- (iii)  $\mathbf{nodesize} \in [a_n]$ : the number of points below which the splitting is forced to be rejected.

Now, let us provide the mechanism of the Wasserstein Random Forests:

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**Algorithm 1:** Wasserstein Random Forests predicted distribution at  $x$ .

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**Require:** Training dataset  $\mathcal{D}_n$ , number of trees  $M > 0$ , subsample size  $a_n \in [n]$ , Wasserstein order  $p > 0$ ,  $\mathbf{mtry} \in [d]$  where  $d$  denotes the dimension of the covariate  $X$ ,  $\mathbf{nodesize} \in [a_n]$  and  $x \in \text{Supp}(X)$ .

**Result:** The sequence of weights  $(\alpha_i(x); i \in [n])$  which determines a weighted empirical measure that estimates the conditional distribution at  $x$  (see (3) for details).

```

1 for  $j \in \{1, 2, \dots, M\}$  do
2   Select  $a_n$  points with or without replacement, uniformly in  $\mathcal{D}_n$  as the sampled points.
3   Set  $\mathcal{P} = (\mathcal{D}_n^*(\Theta_j))$  the ordered list that contains the root of the tree.
4   Set  $\mathcal{P}_{final} = (\emptyset)$ .
5   while  $\mathcal{P} \neq \emptyset$  do
6     end
7     Let  $A$  be the first element of  $\mathcal{P}$ .
8     if  $A$  contains less data points than  $\mathbf{nodesize}$  or if all  $X_i \in A$  are identical then
9       Remove the cell  $A$  from the list  $\mathcal{P}$ .
10      Concatenate  $\mathcal{P}_{final}$  and  $A$ .
11    else
12      Select uniformly without replacement, a subset  $\mathcal{M}_{try} \subset [d]$  of cardinality  $\mathbf{mtry}$ .
13      Select the best split in  $A$  along the coordinates in  $\mathcal{M}_{try}$  that maximizes the  $\mathcal{W}_p$  distance
        between the empirical measures associated with the newly created two subgroup.
14      Cut  $A$  according to the best split. Denote respectively by  $A_L$  and  $A_R$  the corresponding
        cells.
15      Remove the cell  $A$  from the list  $\mathcal{P}$ .
16      Concatenate  $\mathcal{P}_{final}$ ,  $A_L$  and  $A_R$ .
17    end
18    Compute  $\alpha_{i,j}(x) := \frac{\mathbf{1}_{\{X_i \in A_n(x; \Theta_j, \mathcal{D}_n)\}}}{M N_n(x; \Theta_j, \mathcal{D}_n)} \mathbf{1}_{N_n(x; \Theta_j, \mathcal{D}_n) > 0}$  for each  $i \in \mathcal{D}_n^*(\Theta_j)$ .
19  end
20 Compute  $\alpha_i(x) = \frac{1}{M} \sum_{j=1}^M \alpha_{i,j}(x)$  for each  $i \in [n]$ .
```

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### 3 Simulations

#### 3.1 Setting

We consider the synthetic data satisfying:

- $X \sim \mathcal{X}$ ;
- $\mathcal{L}(Y | X = x) = \pi_x(dy)$ ;
- $\dim(X) = d$  and  $\dim(Y) = 1$ .

In order to illustrate the quality of estimation, we consider the following measurements:

- R-squared score ( $R^2$ ) of the conditional expectation estimation, obtained on a test dataset of size 5000 (can be compared with Breiman's Random Forests);
- Mean squared error (MSE) of the conditional expectation estimation, obtained on a test dataset of size 5000 (can be compared with Breiman's Random Forests);
- Visualization of the estimation of the conditional distribution on 9 points in the test dataset, by plotting:
  - (i) The histogram of predicted weighted empirical measure at point  $x$  (**Label = pred**);
  - (ii) The histogram of 2000 points simulated according to the real distribution  $\mathcal{L}(Y | X = x)$  (**Label = ref**);
  - (iii) The kernel density estimation of 2000 points, resampled according to the predicted weighted empirical measure (**Label = kde pred**);
  - (iv) The kernel density estimation of 2000 points of real distribution  $\mathcal{L}(Y | X = x)$ ; (**Label = kde ref**);
  - (v) The kernel density estimation of the objective in the training data ( $Y_i; 1 \leq i \leq n$ ) (**Label = kde Y**);

We expect the (**pred,kde pred**) and (**ref,kde ref**) are close, and away from **kde Y** when necessary;

- Average Wasserstein Distance (AWD) of the weighted empirical measures and empirical measure of  $1e5$  sample points of the real conditional distribution calculated on 100 points in the test dataset. This can be compared with the Wasserstein distance between  $Y$  and real conditional distribution, which corresponds to the worst case: no estimation is made and the empirical measure associated to  $(Y_i; i \in [n])$  is provided as the prediction for all points in  $\text{Supp}(X)$ . It can also be compared with the "ideal case" where we calculate the Wasserstein distance between two empirical measures of the real conditional distribution of the same size  $n$  of the training data  $\mathcal{D}_n$ .

We remark that to measure the ability of getting useful information in noisy case, we use the same **mtry** and  $M$  for both Breiman's RF and WRF.

#### 3.2 Numerical tests

We start with some "easy" low dimensional case, in order to see the convergence of WRF. It should be keep in mind that estimating the conditional distribution is a extremely difficult task since at each points, we only have one sample of the "real" conditional distribution.

### 3.3 Low dimension + big training dataset

In this section, we provide some settings in which WRF work well.

#### Model 1:

- $X \sim \text{Uniform}([0, 1]^d)$  with  $d = 4$ ;
- $\mathcal{L}(Y | X = x) = \mathcal{N}(m(x), \sigma^2(x))$ ;
- $m(x) = 10x^{(2)} + x^{(3)}$  and  $\sigma^2(x) = 9x^{(3)} \vee 0.2$ .
- $n = 50000$ ,  $p = 2$ ,  $\text{mtry} = 4$ ,  $a_n = 200$  and  $M = 500$ .

#### Results:

- $R^2 = 0.9657$  compared to 0.9673 obtained by classical RF;
- $\text{MSE} = 0.5407$  compared to 0.5277 obtained by classical RF;
- $\text{AWD} = 0.7358$  compared to 3.2012 for the worst case and 0.0384 for the ideal case.
- Visualization can be found in Figure 2.

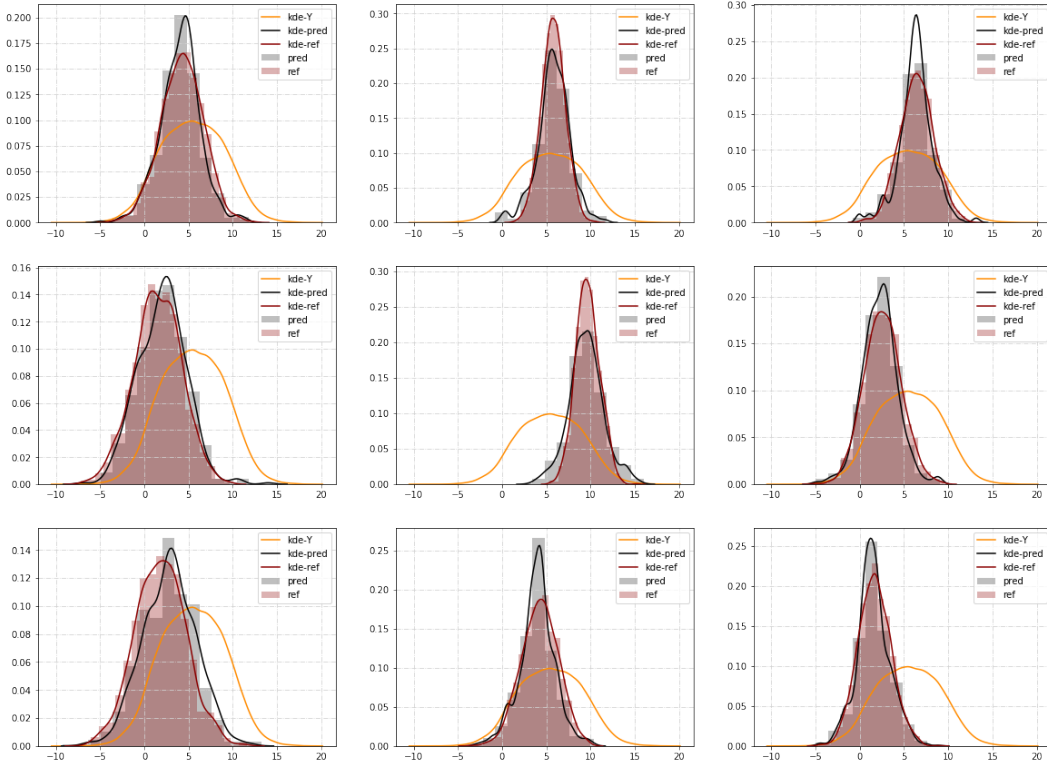


Figure 2: Visualization of Model 1 at 9 points randomly selected in test dataset.



## Model 2:

- $X \sim \text{Uniform}([0, 1]^d)$  with  $d = 4$ ;
- $\mathcal{L}(Y | X = x) = \frac{1}{2}\mathcal{N}(m(x), \sigma^2(x)) + \frac{1}{2}\mathcal{N}(-1, 1)$ ;
- $m(x) = 10x^{(2)} + x^{(3)}$  and  $\sigma^2(x) = 9x^{(3)} \vee 0.2$ .
- $n = 50000$ ,  $p = 2$ ,  $\text{mtry} = 4$ ,  $a_n = 200$  and  $M = 500$ .

## Results:

- $R^2 = -0.5788$  compared to  $-0.5071$  obtained by classical RF;
- $\text{MSE} = 3.6380$  compared to  $3.5544$  obtained by classical RF;
- $\text{AWD} = 0.9539$  compared to  $2.2100$  for the worst case and  $0.0625$  for the ideal case.
- Visualization can be found in Figure 3.

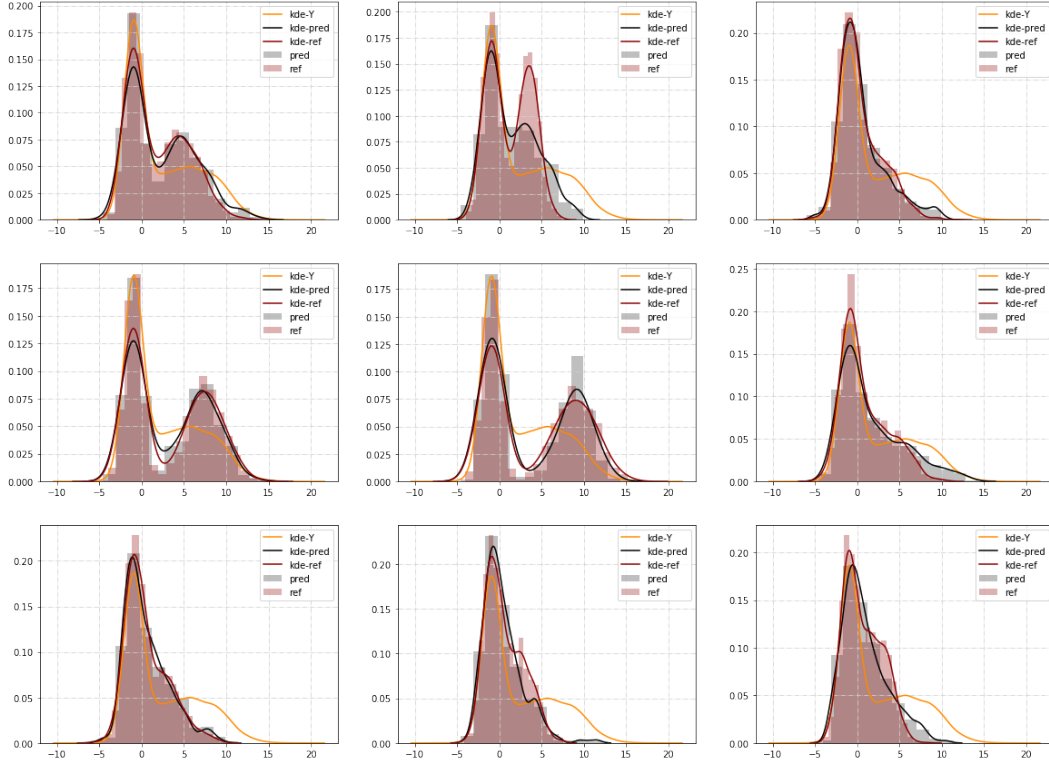


Figure 3: Visualization of Model 2 at 9 points randomly selected in test dataset.

**Comments** From these simple models, we can already see the potential of WRF for its ability to estimate the condition distribution. In the multimodal case of **Model 2**, the conditional expectation can provide very few information of the conditional distribution. In HTE, when the behavior of  $Y(1)$  is multimodal, it is then very dangerous to conduct causal inference only based on CATE function. In this scenario, WRF can provide far richer additional information, which can be used to conduct finer analysis.

### 3.4 High dimension + small training set

In this section, we provide some settings in which WRF do not work well.

#### Model 3:

- $X \sim \text{Uniform}([0, 1]^d)$  with  $d = 20$ ;
- $\mathcal{L}(Y | X = x) = \mathcal{N}(m(x), \sigma^2(x))$ ;
- $m(x) = 10x^{(2)} + x^{(3)}$  and  $\sigma^2(x) = 9x^{(3)} \vee 0.2$ .
- $n = 5000, p = 2, \text{mtry} = 20, a_n = 100$  and  $M = 500$ .

#### Results:

- $R^2 = 0.6012$  compared to 0.97424 obtained by classical RF;
- $\text{MSE} = 1.8296$  compared to 0.4650 obtained by classical RF;
- $\text{AWD} = 2.2746$  compared to 3.1731 for the worst case and 0.05113 for the ideal case.
- Visualization can be found in Figure 4.

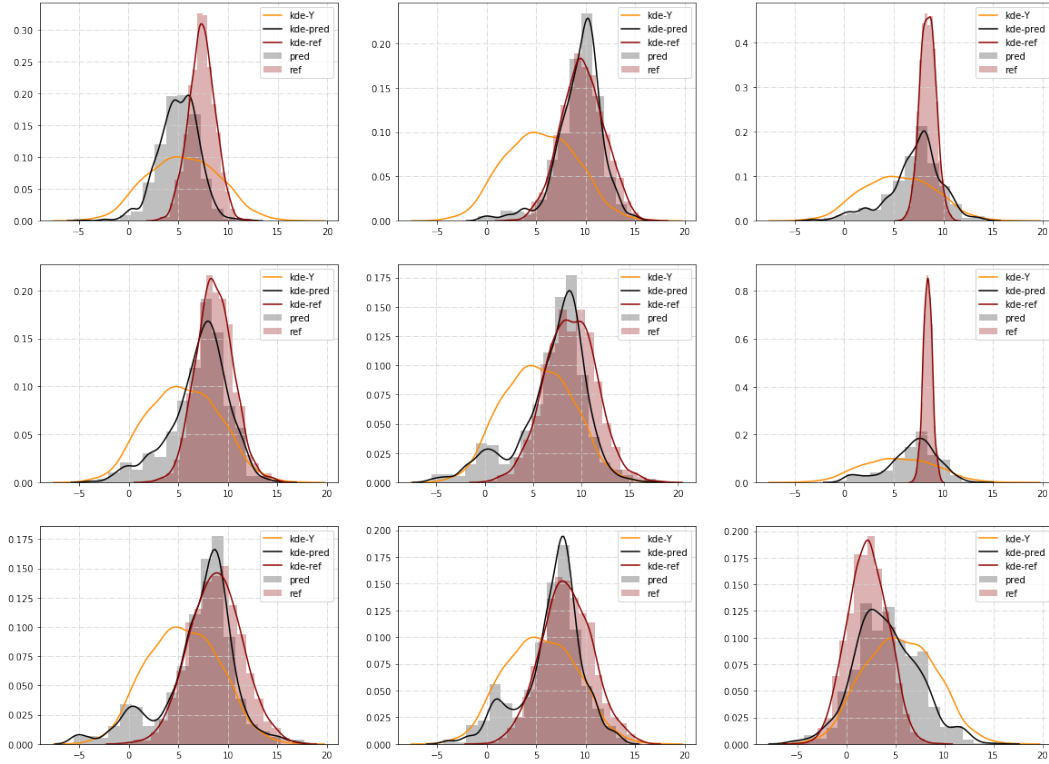


Figure 4: Visualization of Model 3 at 9 points randomly selected in test dataset.

#### Model 4:

- $X \sim \text{Uniform}([0, 1]^d)$  with  $d = 20$ ;
- $\mathcal{L}(Y | X = x) = \frac{1}{2}\mathcal{N}(m(x), \sigma^2(x)) + \frac{1}{2}\mathcal{N}(-1, 1)$ ;
- $m(x) = 10x^{(2)} + x^{(3)}$  and  $\sigma^2(x) = 9x^{(3)} \vee 0.2$ .
- $n = 5000, p = 2, \text{mtry} = 20, a_n = 100$  and  $M = 500$ .

#### Results:

- $R^2 = -1.2735$  compared to  $-0.6395$  obtained by classical RF;
- $\text{MSE} = 4.2722$  compared to  $3.6280$  obtained by classical RF;
- $\text{AWD} = 1.3489$  compared to  $2.0290$  for the worst case and  $0.1230$  for the ideal case.
- Visualization can be found in Figure 5.

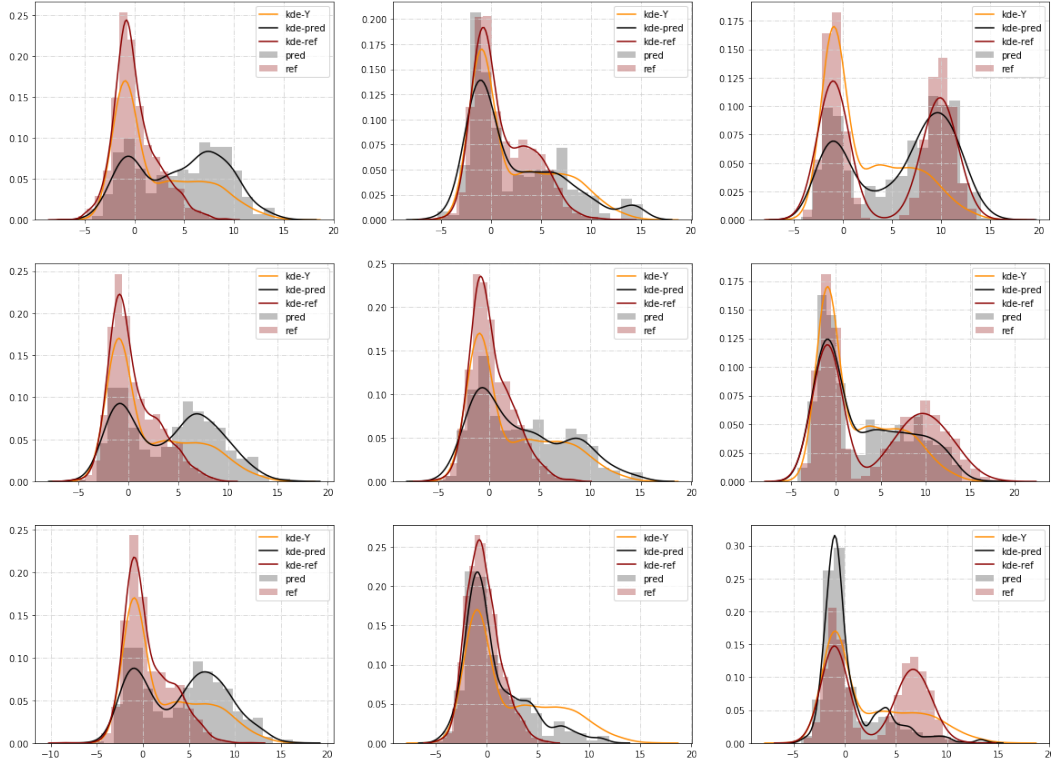


Figure 5: Visualization of Model 3 at 9 points randomly selected in test dataset.

**Comments** As we have seen in the **Model 3**, the classical RF is very robust in high dimensional case, while the quality of the estimation made by WRF is affected. At the moment, we have very few knowledge on the parameter tuning of WRF. It is still not clear that whether this can be solved by choosing the parameters more intelligently.

## 4 Applications

### 4.1 Uncertainty control of CATE function

A by-product is to provide an uncertainty control of CATE function, namely, we are interested in estimating the probability of the following form:

$$\mathbf{P}(|(Y(1) - Y(0)) - \tau(x)| > a \mid X = x). \quad (4)$$

Before proceeding further, we introduce some additional notation to simplify the writing. We denote

$$\mu_{00}(x) := \mathbf{E} [Y(0)^2 \mid X = x],$$

and

$$\mu_{11}(x) := \mathbf{E} [Y(1)^2 \mid X = x],$$

as well as

$$\mu_{01}(x) := \mathbf{E} [Y(0)Y(1) \mid X = x].$$

The conditional variances are denoted respectively by

$$\begin{aligned} \sigma_{00}(x) &:= \mathbf{E} [Y(0)^2 \mid X = x] - \mathbf{E} [Y(0) \mid X = x]^2, \\ &= \mu_{00}(x) - \mu_0(x)^2, \end{aligned}$$

and

$$\begin{aligned} \sigma_{11}(x) &:= \mathbf{E} [Y(1)^2 \mid X = x] - \mathbf{E} [Y(1) \mid X = x]^2, \\ &= \mu_{11}(x) - \mu_1(x)^2. \end{aligned}$$

Thanks to Chebyshev's inequality, we have

$$\begin{aligned} &\mathbf{P}(|(Y(1) - Y(0)) - \tau(x)| > a \mid X = x) \\ &\leq \frac{\text{Var} [Y(1) - Y(0) \mid X = x]}{a^2} \\ &= \frac{\sigma_{00}(x) + \sigma_{11}(x) - 2\mu_{01}(x) + 2\mu_0(x)\mu_1(x)}{a^2}. \end{aligned} \quad (5)$$

Moreover, Cauchy-Schwarz inequality gives

$$|\mu_{01}(x)| \leq \sqrt{\mu_{00}(x)\mu_{11}(x)},$$

whence

$$\begin{aligned} &\mathbf{P}(|(Y(1) - Y(0)) - \tau(x)| > a \mid X = x) \\ &\leq \frac{\sigma_{00}(x) + \sigma_{11}(x) + 2\mu_0(x)\mu_1(x) + 2\sqrt{\mu_{00}(x)\mu_{11}(x)}}{a^2}. \end{aligned} \quad (6)$$

The interests of the upper bound given in (6) lies in the fact that all the terms at the r.h.s. can be approximated with supervised learning algorithm, under certain regularity assumptions. In practice, this allows a finer analysis on the causal inference of the treatment. In particular, all this terms can be derived by providing an estimation of the conditional distribution.

### 4.2 Finer causal inference?

How??

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