BOULEVARD: REGULARIZED STOCHASTIC GRADIENT BOOSTED TREES AND THEIR LIMITING DISTRIBUTION

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This paper examines a novel gradient boosting framework for regression. We regularize gradient boosted trees by introducing sub-sampling and employ a modified shrinkage algorithm so that at every boosting stage the estimate is given by an average of trees. The resulting algorithm, titled “Boulevard”, is shown to converge as the number of trees grows. We also demonstrate a central limit theorem for this limit, allowing a characterization of uncertainty for predictions. A simulation study and real world examples provide support for both the predictive accuracy of the model and its limiting behavior.

1. Introduction. This paper presents a theoretical study of gradient boosted trees (GBT: Friedman, 2001). Machine learning methods for prediction have generally been thought of as trading off both intelligibility and statistical uncertainty quantification in favor of accuracy. Recent results have started to provide a statistical understanding of methods based on ensembles of decision trees (Breiman et al., 1984). In particular, the consistency of methods related to Random Forests (RFs: Breiman, 2001) has been demonstrated in Biau (2012); Scornet et al. (2015) while Wager et al. (2014); Mentch and Hooker (2016); Wager and Athey (2017) and Athey et al. (2016) prove central limit theorems for RF predictions. These have then been used for tests of variable importance and nonparametric interactions in Mentch and Hooker (2017).

In this paper, we extend this analysis to GBT. Analyses of RFs have relied on a sub-sampling structure to express the estimator in the form of a U-statistic from which central limit theorems can be derived. By contrast, GBT produces trees sequentially with the current tree depending on the values in those built previously, requiring a different analytical approach. While the algorithm proposed in Friedman (2001) is intended to be generally applicable to any loss function, in this paper we focus specifically on nonparametric regression (Stone, 1977, 1982). Given a sample of \( n \) observations \((x_1, y_1), \ldots, (x_n, y_n) \in [0, 1]^d \times \mathbb{R},\) assume they follow the relation

\[
X \sim \mu, \quad Y = f(X) + \epsilon
\]

which satisfies the following:

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(M1) \( \mu \) the density is bounded from above and below, i.e. \( 0 < c_1 < c_2 \) s.t. \( c_1 \leq \mu \leq c_2 \).

(M2) \( f \) is bounded Lipschitz, i.e. \( |f(x)| \leq M_f < \infty \), and \( \exists \alpha > 0 \) s.t. \( |f(x_1) - f(x_2)| \leq \alpha |x_1 - x_2|, \forall x_1, x_2 \in [0, 1]^d \).

(M3) \( \epsilon \) is sub-Gaussian error with \( \mathbb{E}[\epsilon] = 0, \mathbb{E}[\epsilon^2] = \sigma^2, \mathbb{E}[\epsilon^4] < \infty \).

GBT builds correlated trees in a sequential fashion so that each tree predicts the gradient of current training error so as to perform gradient descent in functional space (Friedman et al., 2000). A typical GBT estimating \( \hat{f} = \mathbb{E}[Y|X] \), is represented as a tree ensemble version of the Robbins-Monro algorithm (Robbins and Monro, 1951), and combines standard GBT with \( L^2 \) loss leading to an iterative fitting of residuals. The procedure is given as

- start with \( \hat{f}_0 = 0 \);
- For \( b = 1, \ldots \), given \( \hat{f}_b \), calculate the gradient
  \[
  z_i \triangleq -\frac{\partial}{\partial u_i} \sum_{i=1}^{n} \frac{1}{2} (u_i - y_i)^2 \bigg|_{u_i=\hat{f}_b(x_i)} = y_i - \hat{f}_b(x_i);
  \]
- construct a tree regressor \( t_b(\cdot) \) on \( (x_1, z_1), \ldots, (x_t, z_t) \);
- update by a small learning rate \( \lambda > 0 \),
  \[
  \hat{f}_{b+1} = \hat{f}_b + \lambda t_b.
  \]

Gradient boosting developed from attempts to understand adaboost (Freund et al., 1999) in Friedman et al. (2000). Mallat and Zhang (1993) studied the Robbins-Monro algorithm and showed the convergence when the additive components are taken from a Hilbert space. As for the tree version of the Robbins-Monro algorithm, Bühlmann (2002) showed the consistency under \( L^2 \) norm. From a broad point of view, discussions on consistency and convergence of general \( L^2 \) boosting framework can be found in Bühlmann and Yu (2003), Zhang et al. (2005) and Bühlmann and Hothorn (2007).

There are a number of variations on the algorithm presented above. Friedman (2002) incorporated subsampling in each iteration and empirically showed significant improvement in predictive accuracy. Rashmi and Gilad-Bachrach (2015) argued that GBT is sensitive towards the beginning, requiring lots of later trees to make an impact. They borrowed the idea of dropout (Wager et al., 2013; Srivastava et al., 2014) which trains and weighs each new iteration with a subset of the existing ensemble to handle such imbalance which they called “over specification”. Similarly, Rogozhnikov and Likhomanenko (2017) suggested to sequentially scale down the learning rate and studied the convergence of the boosting path when the learning rate is small enough to guarantee contraction.

All methods mentioned above attempt to regularize boosting to avoid excessive dependence on the initial trees in the ensemble which may lead GBT to be trapped in local minima. We hope to unify those methods by carefully combining both subsampling and adaptive learning rate shrinkage into gradient boosted trees to study its asymptotic behavior, leading to a predictive model capable of statistical inference.
This paper is particularly inspired by the recent development of the RF inferential framework (Mentch and Hooker, 2016; Wager and Athey, 2017; Mentch and Hooker, 2017), in which the averaging structure of random forests results in an analysis based on U-statistics and Hájek projection leading to the asymptotic normality. Similarly, in classic stochastic gradient methods, Ruppert-Polyak (Polyak and Juditsky, 1992; Ruppert, 1988) averaging is used in achieving asymptotic normality for model parameter estimators by averaging the gradient descent history. The boosting framework we present results in a model that also exhibits this averaging structure which we can therefore leverage. To contrast the sequential development in GBT with RF we have named this algorithm Boulevard.

Because of the mathematical difficulties of analyzing the greedy splitting rules of trees, most current analyses of RFs have been based on variations of the procedure originally proposed in Breiman (2001). Both Mentch and Hooker (2016) and Wager and Athey (2017) replace bootstrap sampling with subsampling. Wager and Athey (2017) also imposes an honesty condition via subsample splitting to make the tree structure independent of leaf values. While these may improve performance, other simplifications such as the use of completely randomized trees are unlikely to be practically useful, but did allow the development of initial consistency results in Biau (2012) and a connection to kernel methods in Davies and Ghahramani (2014) and Scornet (2016). In a similar fashion, we believe that the use of subsampling and shrinkage are important for our results. However, we also assume a global independence between tree structures and leaf values which we term “non-adaptivity”. We think this condition can be relaxed and that doing so is important for the performance of Boulevard.

So far as we are aware, these represent the first results on a distributional limit for GBT and hence the potential for inference using this framework; we hope that they inspire further refinements. Bayesian Additive Regression Trees (BART) Chipman et al. (2010) were also motivated by GBT and allow the development of Bayesian credible intervals. However, the training procedure for BART resembles backfitting a finite number of trees, resulting in a somewhat different model class. Nonetheless, we expect that some of the stochastic contraction mapping results developed below may be useful in demonstrating frequentist properties for the resulting BART estimators.

The remainder of the paper is organized as follows: in Section 2, we illustrate the formulation of Boulevard and discuss several tree building assumptions required as regularization. In Section 3, we provide the sufficient condition to guarantee finite sample convergence. We further prove the asymptotic normality of Boulevard prediction in Section 4, implying the method applies undersmoothing to the sample. Section 5 discusses the non-adaptivity condition and ways in which it may be weakened and Section 6 presents an empirical study.

Without further specification, $\| \cdot \|_2$ is the operator norm when applied to matrices and the $L^2$ norm when applied to vectors and functions.
2. Boulevard, Honest Trees and Forests.

2.1. Boulevard. Algorithm 1 provides a formal statement of the Boulevard algorithm. This incorporates both subsampling and on-the-fly shrinkage into GBT.

\begin{algorithm}[H]
\begin{itemize}
  \item start with $\hat{f}_0 = 0$;
  \item given $\hat{f}_b$, calculate the gradient
    \begin{equation}
    z_i \triangleq -\frac{\partial}{\partial u_i} \sum_{i=1}^{n} \frac{1}{2} (u_i - y_i)^2 \bigg|_{u_i=\hat{f}_b(x_i)} = y_i - \hat{f}_b(x_i);
    \end{equation}
  \item generate a subsample $w \subset \{1, 2, \ldots, n\}$;
  \item construct a tree regressor $t_b(\cdot)$ on $\{(x_i, z_i), i \in w\}$;
  \item update by learning rate $\lambda > 0$,
    \begin{equation}
    \hat{f}_{b+1} = \frac{b-1}{b} \hat{f}_b + \frac{\lambda}{b} t_b = \frac{\lambda}{b} \sum_{i=1}^{b} t_i.
    \end{equation}
\end{itemize}
\end{algorithm}

This design transforms the ensemble to be an average over all trees instead of continually adding trees together. The benefit of this is twofold. First, shrinkage makes the ensemble less sensitive to any particular tree. It leaves part of the signal in the gradient guaranteeing that no tree is fit to entire error. Second, subsampling reduces overfitting. As a result, the final form of the predictor sits between an ordinary GBT and a random forest. The name Boulevard comes from the fact that during construction, older trees shrink but all trees are eventually of equal importance, just as if we were walking on a boulevard and looking backwards.

2.2. Honest Trees and Honest Forests. We illustrate in this section the construction of base tree leaners in the Boulevard algorithm. A decision tree (Breiman et al., 1984) predicts by iteratively segmenting the covariate space into disjoint subsets (i.e. leaves) within each of which the average (or the majority vote) of observations serves as the leaf value. Therefore we can represent a regression tree as a linear combination of observations.

Suppose a regression tree $t_n(\cdot)$ segments certain covariate space $\Omega$ into a disjoint union $\Omega = \bigcup_{j=1}^{m} A_j$. We also refer to $\{A_j\}_{j=1}^{m}$ as the leaves or the tree structure. In our case, $\Omega = [0, 1]^d$ and $\{A_j\}_{j=1}^{m}$ hyper-rectangles. We explicitly express $t_n(\cdot)$ as

\begin{equation}
    t_n(x) = \sum_{i=1}^{n} s_{n,i}(x) y_i,
\end{equation}

where, given $x \in A_j$,

\begin{equation}
    s_{n,k}(x) = \frac{I(x_k \in A_j)}{\sum_{i=1}^{n} I(x_i \in A_j)}.
\end{equation}
Slight changes should be made to this expression when a subsample is used instead of the full sample to calculate the leaf value. For given subsample \( w \subset \{1, \ldots, n\} \), we write

\[
t_n(x; w) = \sum_{i=1}^{n} s_{n,i}(x; w)y_i.
\]

In this case, for any \( x \in A_j \),

\[
s_{n,k}(x) = s_{n,k}(x; w) = \frac{I(x_k \in A_j)}{\sum_{i=1}^{n} I(x_i \in A_j)I(i \in w)} = \frac{I(x_k \in A_j)I(k \in w)}{\sum_{i=1}^{n} I(i \in w)}.
\]

In both cases, we call \( s_n(x) = (s_{n,1}(x), \ldots, s_{n,n}(x))^T \) the (column) structure vector of \( x \), and

\[
S_n = \begin{bmatrix}
  s_{n,1}(x_1) & \ldots & s_{n,n}(x_1) \\
  \vdots & \ddots & \vdots \\
  s_{n,1}(x_n) & \ldots & s_{n,n}(x_n)
\end{bmatrix} = \begin{bmatrix}
  s_{n}(x_1)^T \\
  \vdots \\
  s_{n}(x_n)^T
\end{bmatrix}
\]

the structure matrix as the stacked structure vectors of the sample.

The greedy algorithms typically used to build decision trees have proved particularly challenging for mathematical analysis. It is difficult to provide guarantees that it will not isolate sample points with large observation errors, i.e. outliers, thereby de-stabilizing the resulting predicted values. We describe this behavior as “chasing order statistics”. As a result, most results on trees and tree ensembles rely on randomization, for example, using completely randomized splits or retaining a small chance of making randomized split covariates (Bühlmann et al., 2002; Biau, 2012; Scornet, 2016; Wager and Athey, 2017).

In particular, Wager and Athey (2017) introduced concept of honesty through double-sample trees which apply two different subsamples: one to decide tree structure and another to calculate leaf values. While this strategy allows the sample to determine the tree structure, it creates conditional independence between the tree structure and the leaf values to prevent trees from being doubly influenced by clustered outliers. In a similar manner, our analysis requires stringent isolation between these two steps. One way to achieve so is by not looking at the training responses while deciding the tree structure, as shown in the second step of the clarification of our honest tree strategy with subsampling given in Algorithm 2.

Algorithm 2 (Honest Trees).

- **Start with a sample of size** \( n, (x_1, y_1), \ldots, (x_n, y_n) \).
- **Obtain the tree structure** \( q = \{A_j\}_{j=1}^{m} \) independently of \( y_1, \ldots, y_n \).
- **Uniformly subsample an index set** \( w \in \{1, \ldots, n\} \) of size \( \theta n \).
- Decide the leaf values, hence \( t_n(\cdot) \), merely w.r.t \( w \) as for \( x \in A_j \),

\[
t_n(x) = \sum_{x_i \in A_j} \frac{I(i \in w)}{\sum_{x_l \in A_j} I(l \in w)} \cdot y_i,
\]

with 0/0 defined to be 0.

However, a disadvantage of honest trees is the possibility that there could be no subsample points in a terminal leaf when deciding the leaf values by the second subsample. We choose to predict 0 for expediency, in which case the corresponding tree structure vector for points in such leaf will be zeroes. We refer to this issue as **missing terminal subsample** and will later show that it can be avoided asymptotically by selecting a sufficiently large subsample rate.

The following theorem shows the properties we obtain by applying the honest tree strategy. One major contribution of honesty is the symmetry of the expected structure matrix, which connects it to the kernel form of a subsample decision tree.

**Theorem 2.1.** Denote \( \mathbb{E}_w \) as the expectation over all possible subsample index sets. For a fixed segmentation (tree structure) \( q = \{A_j\}_{j=1}^{m} \),

(i) \( \mathbb{E}_w[S_n] \) is element-wisely nonnegative, symmetric.

(ii) \( \mathbb{E}_w[S_n] \) is positive semi-definite.

(iii) \( \|\mathbb{E}_w[S_n]\| \leq 1 \).

We now move from a single tree to a tree ensemble, starting from random forests (Breiman, 2001). The concept of subsampling and bagging has been intensely used in the construction of random forests whose component trees have distinct structures due to the random set of sample points and splitting covariates. Denote by \( (Q_n, Q_n) \) the probability space of all possible tree structures given sample \( (x_1, y_1), \ldots, (x_n, y_n) \) of size \( n \) and an approach of deciding tree structures with randomness, where \( q = \{A_i\}_{i=1}^{m_q} \in Q_n \) is the structure of a single possible tree. On one hand, if each tree in the forest is honest, we could write the expected random forest prediction on the sample as

\[
\hat{Y} = \mathbb{E}_q \mathbb{E}_w[S_n] \cdot Y = \mathbb{E}_{q,w}[S_n] \cdot Y,
\]

where \( Y = (y_1, \ldots, y_n)^T \) and \( \mathbb{E}_q \) the expectation w.r.t. probability measure \( Q_n \). On the other hand, supposing we build a single honest tree deciding tree structure from the structural space \( Q_n \) with probability measure \( Q_n \), \( \mathbb{E}_{q,w}[S_n] \) is also the expected structure matrix which carries most properties of \( \mathbb{E}_w[S_n] \).

**Corollary 2.1.1.** Denote \( \mathbb{E}_{q,w} \) as the expectation over all possible tree structures and subsample index sets, then
(i) $E_{q,w}[S_n]$ is symmetric, element-wisely nonnegative.
(ii) $E_{q,w}[S_n]$ is positive semi-definite.
(iii) $\|E_{q,w}[S_n]\| \leq 1$.

Here $E_{q,w}[S_n]$ is similar to the random forest kernel defined by the corresponding tree structure space, subsampling strategy and tree structure randomization approach.

2.3. Adaptivity of Boosted Trees. As mentioned above, when building a random forest, the current ensemble has no influence on either the structure or the leaf values of the following trees. We could also imagine an ideal boosting scenario that has reached stationarity, after which all subsequent trees should behave identically regardless of the current ensemble. One common property is that the distribution of tree structures should be identical across trees. We refer to this property as the (non)-adaptivity of tree ensembles, which is defined formally as follows.

**Definition 2.1.** Denote $(Q_{n,b}, Q_{n,b})$ the probability space of all possible tree structures given sample $(x_1,y_1),\ldots,(x_n,y_n)$ of size $n$ after $b$ trees have been built. A tree ensemble is **non-adaptive** if $(Q_{n,b}, Q_{n,b})$ is identical across $b$. A tree ensemble is **eventually non-adaptive** if $(Q_{n,b}, Q_{n,b})$ is identical for sufficiently large $b$.

The non-adaptivity of random forests contributes to the convenience of taking expectation of the ensemble since all trees are independent and identically distributed. In contrast, conventional gradient boosted trees are adaptive. For each new tree, both the structure and the leaf values use the latest gradient that changes along with the growing ensemble. As a result, any analysis has to condition on the current ensemble state. Honesty and non-adaptivity resolve this issue on different levels. In terms of a single decision tree, building a honest tree helps to reduce the dependence by untying the tree structure from the gradient. In terms of the entire tree ensemble, non-adaptivity further simplifies the analysis that we use a shared tree structure space and distribution.

In contrast, eventual non-adaptivity is a necessary condition should boosting predictions become stationary after enough iterations. We will discuss the details in Section 5.

In practice, there are a few possible means to enforce non-adaptivity by deciding all tree structures independently of the gradient. One is through completely randomized trees for which the gradient only influences the leaf values. An alternative strategy is to acquire another independent sample $(x'_1,y'_1),\ldots,(x'_n,y'_n)$ solely for determining tree structures. We will refer to the Boulevard algorithm equipped with this mechanism as **non-adaptive Boulevard** for the rest of the paper.

3. Boulevard Convergence. Following from Zhang et al. (2005), a first “theoretical issue” of analyzing boosting method is the difficulty of attaining convergence. As a starting point we will show that Boulevard guarantees point-wise convergence under finite sample settings.
3.1. **Stochastic Contraction and Boulevard Convergence.** To prove convergence of the Boulevard algorithm, we introduce the following definition, lemmas and theorem inspired by the unpublished manuscript by Almudevar (Almudevar) regarding a special class of stochastic processes. We refer the readers to the original manuscript, but key points of the proof are briefly reproduced and extended here for the study of Boulevard asymptotics.

**Theorem 3.1 (Multidimensional Stochastic Contraction).** Given $\mathbb{R}^d$ stochastic process $\{Z_t\}_{t \in \mathbb{N}}$, a sequence of $0 < \lambda_t \leq 1$, define

$$F_0 = \emptyset, F_t = \sigma(Z_1, \ldots, Z_t), \quad \epsilon_t = Z_t - \mathbb{E}[Z_t | F_{t-1}].$$

We call $Z_t$ a (multidimensional) stochastic contraction if the following properties hold

(C1) Vanishing coefficients

$$\sum_{t=1}^{\infty} (1 - \lambda_t) = \infty, \quad i.e. \quad \prod_{t=1}^{\infty} \lambda_t = 0.$$

(C2) Mean contraction

$$||\mathbb{E}[Z_t | F_{t-1}]|| \leq \lambda_t ||Z_{t-1}||, \text{ a.s..}$$

(C3) Bounded deviation

$$\sup ||\epsilon_t|| \to 0, \quad \sum_{t=1}^{\infty} \mathbb{E}[||\epsilon_t||^2] \leq \infty.$$

In particular, a multidimensional stochastic contraction exhibits the following behavior

(i) **Contraction**

$$Z_t \xrightarrow{a.s.} 0.$$

(ii) **Kolmogorov inequality**

$$P \left( \sup_{t \geq T} ||Z_t|| \leq ||Z_T|| + \delta \right) \geq 1 - \frac{4\sqrt{d} \sum_{t=T+1}^{\infty} \mathbb{E}[\epsilon_t^2]}{\min\{\delta^2, \beta^2\}},$$

where $\beta = ||Z_T|| + \delta - \sqrt{d} \sup_{t>T} ||\epsilon_t|| > 0$.

The proof is provided in Appendix A.2. The Kolmogorov inequality, which is novel from the original manuscript, is a direct corollary from the original proof in Almudevar (Almudevar).

Working with non-adaptive Boulevard, adaptive shrinkage grants it the structure of a stochastic contraction. We now apply Theorem 3.1 to show the convergence.
THEOREM 3.2. Given sample \((x_1, y_1), \ldots, (x_n, y_n)\). If we construct gradient boosted trees non-adaptively with identical tree structure space \((Q_n, Q_n)\) and honest regression trees, by choosing \(M \gg \max\{M_f, y_1, \ldots, y_n\}\) and defining \(\Gamma_{M}(x) = \text{sign}(x)(|x| \wedge M)\) as a truncation function, let Boulevard iteration take form of

\[
\hat{f}_b(x) = \frac{b - 1}{b} \hat{f}_{b-1}(x) + \frac{\lambda}{b} s_b(x)(Y - \Gamma_{M}(\hat{Y}_{b-1})),
\]

where \(Y = (y_1, \ldots, y_n)^T\) the observed response vector, \(\hat{Y}_b = (\hat{f}_b(x_1), \ldots, \hat{f}_b(x_n))^T\) the predicted response vector by the first \(b\) trees, \(s_b\) the random tree structure vector. Hence

\[
\hat{Y}_b \to \left[ \frac{1}{\lambda} I + \mathbb{E}[S_n] \right]^{-1} \mathbb{E}[S_n]Y,
\]

where \(\mathbb{E}[] = \mathbb{E}_{q, u}[]\), \(S_n\) the random tree structure matrix defined above.

PROOF. Due to non-adaptivity \(S_n\) is independent of \(\hat{Y}_b\) for any \(b\). Notice that \(Y^* = \lambda \mathbb{E}[S_n](Y - Y^*)\) for \(Y^* = [\frac{1}{\lambda} I + \mathbb{E}[S_n]]^{-1} \mathbb{E}[S_n]Y\). Define the filtration \(\mathcal{F}_b = \sigma(\hat{Y}_0, \ldots, \hat{Y}_b)\) and consider the sequence \(Z_b = \hat{Y}_b - Y^*\). This sequence satisfies the stochastic contraction condition. First, \(\|Z_0\| = \|Y^*\| \leq \infty\). Notice

\[
\|\mathbb{E}[Z_b|\mathcal{F}_{b-1}]\| = \left\| \mathbb{E} \left[ \frac{b - 1}{b} \hat{Y}_{b-1} + \frac{\lambda}{b} S_b(Y - \Gamma_{M}(\hat{Y}_{b-1})) - Y^* \bigg| \mathcal{F}_{b-1} \right] \right\|
\]

\[
\leq \frac{b - 1}{b} \left\| \hat{Y}_{b-1} - Y^* \right\| + \left\| \frac{\lambda}{b} S_b(Y - \Gamma_{M}(\hat{Y}_{b-1})) - \frac{\lambda}{b} \mathbb{E}[S_n](Y - Y^*) \right\|
\]

\[
\leq \frac{b - 1 + \lambda}{b} \left\| \hat{Y}_{b-1} - Y^* \right\| \triangleq k_b \|Z_{b-1}\|,
\]

where \(\sum_{b=1}^{\infty} (1 - k_b) = \infty\). Since entries and row sums of are both \(\leq 1\),

\[
\|S_n\| \leq \sqrt{\|S_n\|_\infty^1} \leq \sqrt{1 \times n} = \sqrt{n}.
\]

Therefore

\[
\|e_b\| = \|Z_b - \mathbb{E}[Z_b|\mathcal{F}_{b-1}]\| = \left\| \frac{\lambda}{b} (\mathbb{E}[S_n] - S_n)(Y - \Gamma_{M}(\hat{Y}_{b-1})) \right\| \leq \frac{\lambda}{b} (1 + \sqrt{n}) 2\sqrt{n}M.
\]

Hence

\[
\sum_{b=1}^{\infty} \mathbb{E}[\|e_b\|^2] \leq \left( \sum_{b=1}^{\infty} \frac{1}{b^2} \right) \cdot \lambda^2(1 + \sqrt{n})^2 4nM < \infty.
\]

We conclude that \(Z_b \overset{a.s.}{\to} 0\), i.e. \(\hat{Y}_b \overset{a.s.}{\to} Y^*\). \(\square\)
This theorem guarantees the convergence of Boulevard path under finite sample setting once we threshold it by a large $M$. Non-adaptivity serves here to decompose every tree model into the multiplication of an independent structure matrix and a predictable response vector.

As a corollary we obtain the expression of the prediction at any point of interest $x$. The result takes the form of a kernel ridge regression with the random forest kernel (Scornet, 2016).

**Corollary 3.2.1.** By defining $f = \lim_{b \to \infty} \hat{f}_b$,

$$
\hat{f}(x) = \mathbb{E}[s_n(x)] \left[ \frac{1}{\lambda} I + \mathbb{E}[S_n] \right]^{-1} Y.
$$

Ridge regression tends to shrink the predictions towards 0 and so does (3). The iterative averaging of Boulevard algorithm along with $\lambda$ results in Boulevard predictions covering $\frac{\lambda}{1+\lambda}$ of the signal instead of the full signal. We will prove and discuss in details this behavior in Section 4.5.

**3.2. Beyond $L^2$ Loss.** Besides regression, other tasks may require alternative loss functions for boosting, for instance, the exponential loss $L(w, y) = \exp(-wy)$ in adaboost (Freund and Schapire, 1995). Analogous to the proof for $L^2$ loss, we can write the counterparts for any general loss $L(u) = \sum_i L(u_i, y_i)$ whose non-adaptive Boulevard iteration takes the form of

$$
\hat{Y}_b = \frac{b-1}{b} \hat{Y}_{b-1} - \frac{\lambda}{b} S_n \nabla_w L(w)\bigg|_{w=\hat{Y}_{b-1}}.
$$

Suppose the existence of the fix point $\hat{Y}^* = -\lambda \mathbb{E}[S_n] \nabla_w L(w)\bigg|_{w=\hat{Y}^*}$, then

$$
\mathbb{E}[\hat{Y}_b - \hat{Y}^* | F_{b-1}] = \frac{b-1}{b} (\hat{Y}_{b-1} - \hat{Y}^*) - \frac{\lambda}{b} \mathbb{E}[S_n] \left( \nabla_w L(w)\bigg|_{w=\hat{Y}_{b-1}} - \nabla_w L(w)\bigg|_{w=\hat{Y}^*} \right).
$$

If the gradient term is bounded and Lipschitz (which could be enforced by truncation), i.e.

$$
\left\| \nabla_w L(w)\bigg|_{w=w_1} - \nabla_w L(w)\bigg|_{w=w_2} \right\| \leq M \|w_1 - w_2\|,
$$

we can similarly show such Boulevard iteration converges by choosing $\lambda \leq M^{-1}$. However, the closed form of $\hat{Y}^*$ can be intractable to obtain and potentially non-unique. For example for AdaBoost, $\hat{Y}^*$ is the solution to $\hat{Y}^* = -\lambda \mathbb{E}[S_n] (\exp(-\hat{Y}^*_1 y_1), \ldots, \exp(-\hat{Y}^*_n y_n))^T$.

**4. Limiting Distribution.** Inspired by recent results demonstrating the asymptotic normality of random forest predictions, in this section we prove the asymptotic normality of predictions from Boulevard. Before detailing these results, we need some prerequisite
discussion on the rates used for decision tree construction in order to ensure asymptotic local behavior. In general, the variability of model predictions comes from two sources: the variability of the random sample we use to train the model, and the variability of the response errors. The strategy for our proof is as follows: we first consider the fixed design case where the sequence of increasing samples are supposedly determined and have the properties we require, so only the response errors contribute to the variability. We then establish the uniformity over almost all random sample sequences to extend the limiting distribution to random design cases, showing that it is still the response errors that dominate the prediction variability.

4.1. Building Deeper Trees. Decision trees can be thought as k-nearest-neighbor (k-NN: Altman, 1992) models where $k$ is the leaf size and the distance metric is given by whether two points are in the same leaf. This adapts the metric to the local geometry of the response function. As the conclusions on k-NN predictions require growing-in-size and shrinking-in-radius neighborhoods (Gordon and Olshen, 1984), so are the counterparts of building deeper trees. Assuming non-adaptivity, the following assumptions are sufficient for our analysis below. Recall the notation that $A \in q \in Q_n$ means any leaf $A$ of a tree structure $q$ in the structure space $Q_n$. We make the following assumptions of the tree building process:

(L1) Asymptotic locality. Writing $diam(A) = \sup_{x,y \in A} |x - y|$, we require

$$\sup_{A \in q \in Q_n} diam(A) = O(d_n), \quad d_n \to 0.$$ 

(L2) Minimal leaf size. If we write $V(\cdot)$ as the volume function in terms of Lebesgue measure, we require that

$$\inf_{A \in q \in Q_n} V(A) \geq O(v_n) > 0.$$ 

These assumptions together bound the space occupied by any leaf of any possible tree from being either too extensive or too small. It indicates that any leaf is a geometrically shrinking neighborhood of the points it contains, while the the number of neighborhood points increases. We will later specify the rates we require in Boulevard.

4.2. Fixed Design. We first consider a fixed sequence of samples with increasing sizes, i.e. for each $n$, the sample $(x_{n,1}, y_{n,1}), \ldots, (x_{n,n}, y_{n,n})$ is given. The first subscript $n$ will be dropped when there is no ambiguity. We specify the rates for the size of leaf nodes as:

(R1) For some $\epsilon_1 > 0$,

$$d_n = O\left(n^{-\frac{1}{d_1^2} - \epsilon_1}\right).$$

(R2) For some $\epsilon_2 > \epsilon_1 > 0$,

$$\inf_{A \in q \in Q_n} \sum_{i=1}^{n} I(x_i \in A) \geq O\left(n^{\frac{2}{d_2^2} - d_2}\right).$$
One compatible realization is
\[ d_n = O \left(n^{-\frac{1}{d+1}}\right), \inf_{A \in q \in Q_n} \sum_{i=1}^n I(x_i \in A) \geq O \left(n^{\frac{1}{d+2}}\right). \]

For simplicity all our proofs are under this setting. However, any other rates satisfying these conditions are also sufficient.

### 4.3. Missing Terminal Subsample

Starting here we use the abbreviations that
\[ k_n^T = \mathbb{E}[s_n(x)], \quad K_n = \mathbb{E}[S_n], \quad r_n^T = k_n^T \left[\frac{1}{\lambda} I + K_n\right]^{-1}. \]

We take a close look at the missing terminal subsample issue due to which we can only guarantee \( \|k_n\|_1 \leq 1 \). Working with the tree construction rate as above, the subsample rate \( \theta \) effectively determines how far \( \|k_n\|_1 \) is from 1.

Without loss of generality, let each terminal leaf contains no fewer than \( n^{-\frac{1}{d+2}} \) sample points before subsampling according to our assumed rates. If the subsample size is \( \theta n = n^{-\frac{1}{d+2}} \log n \), i.e. \( \theta = n^{-\frac{1}{d+2}} \log n \), the chance of missing terminal subsample in a given leaf is
\[
p(n, \theta) = \left(\frac{n - \theta n}{n - n^{-\frac{1}{d+2}}}\right)^{n^{\frac{1}{d+2}}} = \left(1 - n^{-\frac{1}{d+2}} \log n\right)^{n^{\frac{1}{d+2}}} \leq e \cdot \left(1 - n^{-\frac{1}{d+2}} \log n\right)^{n^{\frac{1}{d+2}}} \leq O \left(\frac{1}{n}\right).
\]

Therefore, for any \( x \), \( 1 - \|k_n\|_1 \leq O \left(\frac{1}{n}\right) \) if we use subsample size at least of \( n^{-\frac{1}{d+2}} \log n \).

This requires the subsample to be relatively large, which is compatible with, practically, both constant subsample rate i.e. \( \theta \) is constant, or \( \log n \) subsample rate i.e. \( \theta = (\log n)^{-1} \). We will refer to \( p(n, \theta) \) as the **missing weight** in subsequent proofs.

To reach a similar statement for \( r_n \), we first examine \( K_n \) since every row and column of \( K_n \) suffers from missing terminal subsample. The conclusion is summarized in the following lemma, whereas the detail calculations are in Appendix A.5.

**Lemma 4.1.** Using above settings and notations,
\[
\left|\sum_{i=1}^n r_{n,i} - \frac{\lambda}{1 + \lambda}\right| \leq O \left(\frac{1}{n}\right).
\]
4.4. Exponential Decay of Influence and Asymptotic Normality. The prediction that Boulevard makes at a point is a linear combination of responses $y_1, \ldots, y_n$ whose coefficients are given by $r_n$. Distant points ideally are less influential on the prediction, and such decay of influence in our case is exponential. To show this, we first introduce the notation of vector component selection. Given any $n$-vector $v$ and an index set $D$, denote

$$v|_D = \begin{bmatrix} v_1 \cdot I(1 \in D) \\ \vdots \\ v_n \cdot I(n \in D) \end{bmatrix}.$$

Easy to verify that $v = v|_D + v|_{D^c}$.

**Lemma 4.2.** Given sample $(x_1, y_1), \ldots, (x_n, y_n)$, a point of interest $x$, set $l_n = \log n - \log \lambda = c_1 \log n$, and define index set $D_n = \{ i : |x_i - x| \leq l_n \cdot d_n \}$, then

$$\|r_n|_{D_n}\|_1 \leq O \left( \frac{1}{n} \right).$$

Lemma 4.2 indicates that Boulevard trees will asymptotically rely on a log $n$ shrinking neighborhood around the point of interest. Given sample size $n$ and a point of interest $x$, we can therefore define $B_n = \{ i : |x_i - x| \leq d_n \}$ and $D_n = \{ i : |x_i - x| \leq l_n \cdot d_n \}$. $B_n$ contains all points that have direct influence on $x$ in a single tree, and $D_n$ contains the points that dominate the prediction at $x$. $|B_n|$ and $|D_n|$ follow Binomial distributions with parameters depending on the local covariate density. These two quantities will appear in later proofs through the following lemma, whose proof results from simply verifying the Lindeberg-Feller condition for sums of Bernoulli random variables.

**Lemma 4.3.** Assume $X_1, \ldots, X_n, \ldots$, independent binomial random variables s.t. $X_i \sim Binom(n, p_n)$ and $np_n \to \infty$.

$$\frac{X_n - np_n}{\sqrt{np_n(1 - p_n)}} \xrightarrow{d} N(0, 1).$$

We are now ready to show the limiting distribution of fixed design cases. We check the Lindeberg-Feller condition for the sequence of predictions $\hat{f}_n(x)$. The following lemma is used to bound $\|k_n\|$ and $\|r_n\|$.

**Lemma 4.4.** With increasing $n$ and sample $(x_{n,1}, y_{n,1}), \ldots, (x_{n,n}, y_{n,n})$ at size $n$, assume $|B_n| \geq O \left( n \cdot d_n^d \right)$ and

$$\inf_{A \in \mathcal{Q}_n} \sum_{i=1}^{n} I(x_{n,i} \in A) \geq O \left( n^{\frac{1}{d+2}} \right),$$

then

$$O \left( n^{-\frac{1}{2} \cdot \frac{1}{d+1}} \right) \leq \|k_n\|, \|r_n\| \leq O \left( n^{-\frac{1}{2} \cdot \frac{1}{d+2}} \right).$$
**Theorem 4.1.** For given $x \in [0,1]^d$, suppose we have fixed sample $(x_{1,1}, y_{1,1}), \ldots, (x_{n,n}, y_{n,n})$ for each $n$ s.t. $\|k_n^T\|_\infty \leq O \left( n^{-\frac{1}{d+2}} \right)$. Write $f(X_n) = (f(x_1), \ldots, f(x_n))^T$, then

$$\frac{\hat{f}_n(x) - r_n^T f(X_n)}{\|r_n\|} \xrightarrow{d} N(0, \sigma^2).$$

**Proof.** Notice that

$$\hat{f}_n(x) - r_n^T f(X_n) = r_n^T \epsilon_n.$$

To obtain a CLT we check the Lindeberg-Feller condition of $r_n^T \epsilon_n$, i.e. for any $\delta > 0$,

$$\lim_{n \to \infty} \frac{1}{\|r_n\|^2} \sigma^2 \sum_{i=1}^n \mathbb{E} \left[ (r_{ni} \epsilon_i)^2 I(|r_{ni} \epsilon_i| > \delta \|r_n\| \sigma) \right] = 0.$$

Since $\|k_n\|_\infty \leq O \left( n^{-\frac{1}{d+2}} \right)$ and $\left[ \frac{1}{\lambda} I + K_n \right]^{-1}$ having row sums of $\frac{1}{1+\lambda} + O \left( n^{-1} \right)$, we have

$$\|r_n\|_\infty \leq \|k_n\|_\infty \cdot \left\| \left[ \frac{1}{\lambda} I + K_n \right]^{-1} \right\|_1 \leq O \left( n^{-\frac{1}{d+2}} \right).$$

Furthermore, since $\|r_n\| \geq O \left( n^{-\frac{1}{2d+1}} \right)$, we get

$$\frac{\|r_n\|_\infty}{\|r_n\|} \leq O \left( n^{-\frac{1}{2d+1}} + \frac{1}{2d+1} \right),$$

which justifies the Lindeberg-Feller condition when $\epsilon$ is sub-Gaussian by

$$\sum_{i=1}^n \mathbb{E} \left[ (r_{ni} \epsilon_i)^2 I(|r_{ni} \epsilon_i| > \delta \|r_n\| \sigma) \right] \leq \sum_{i=1}^n r_{ni}^2 \sqrt{\mathbb{E} \epsilon_i^4} \cdot \mathbb{E} [I(|r_{ni} \epsilon_i| > \delta \|r_n\| \sigma)]^2 \leq \sum_{i=1}^n r_{ni}^2 \sqrt{\mathbb{E} \epsilon_i^4} \cdot \sqrt{P \left( |\epsilon_i| \geq \delta \|r_n\| \sigma / r_{ni} \right)} \leq \sum_{i=1}^n r_{ni}^2 \sqrt{\mathbb{E} \epsilon_i^4} \cdot \sqrt{2 \exp \left( -\frac{1}{2\sigma^2 \epsilon} \cdot (\delta \|r_n\| \sigma / r_{ni})^2 \right)} \leq \|r_n\|^2 \exp \left( -O \left( n^{\frac{2}{d+2}} - \frac{1}{d+1} \right) \right) \to 0,$$

since

$$P(\epsilon > t) \leq \exp \left( -\frac{t^2}{2\sigma^2} \right)$$

for sub-Gaussian $\epsilon$. \qed
4.5. Random Design. In this section we analyze the random design case where the covariates $x_1, \ldots, x_n$ are considered randomly drawn from the underlying distribution. To extend the scope of the fixed design limiting distribution to the random design, we start from the following lemma.

**Lemma 4.5.** Assume $X : \Omega_1 \to S$, independent of $\epsilon : \Omega_2 \to S$, $\{f_n : S \times S \to \mathbb{R}\}$ sequence of measurable functions. Assuming for a.s. $x \in \Omega_1$, $f_n(x, \epsilon) \overset{d}{\to} N(0, 1)$.

Then

$$f_n(X, \epsilon) \overset{d}{\to} N(0, 1).$$

The idea behind the lemma is to incorporate the sample randomness by showing an almost sure point-wise convergence conclusion in a well-defined probability space. To translate the lemma into our context, we extend the original covariate and error space by Kolmogorov’s extension theorem. Define $(x_1, \ldots) = X \in [0, 1]^d \times \mathbb{N}$ and $\epsilon = (\epsilon_1, \ldots) \in \mathbb{R}^\mathbb{N}$, where the probability measures on $[0, 1]^d \times \mathbb{N}$ and $\mathbb{R}^\mathbb{N}$ are uniquely decided by the product measures on the cylinder spaces reflecting i.i.d. sampling i.e. $y_i = f(x_i) + \epsilon_i$ for $i \in \mathbb{N}$.

Write $\pi_i$ the cumulative coordinate projection, i.e. $\pi_i(a_1, \ldots, a_n, \ldots) = (a_1, \ldots, a_i)$. We can calculate $k_n$ and $K_n$ w.r.t. $\Pi_n = (\pi_n(X), \pi_n(\epsilon))$. Thus

$$\rho_n(X, \epsilon) = \frac{\hat{f}_n(x; \Pi_n) - k^T_n(x; \Pi_n)[\frac{1}{2}I + K_n(\Pi_n)]^{-1}f(\Pi_n)}{\|k_n(x; \Pi_n)[\frac{1}{2}I + K_n(\Pi_n)]^{-1}\|}$$

reflects the prediction after using a random sample of size $n$. Using Lemma 4.5, CLT of $\rho_n$ requests an almost surely claim of Theorem 4.1 where the sequence of $(x_1, y_1), \ldots, (x_n, y_n)$ comes from $(\pi_n(X), \pi_n(\epsilon))$.

To help develop our analysis, we further increase the leaf size by a small amount assuming that the minimal terminal leaf geometric volume $v_n$ follows

$$v_n = n^{\frac{d+1}{d+2}} = n^{-\frac{d}{d+2}} \leq n^{-\frac{d}{d+1}} = O\left(d^{\frac{d}{n}}\right),$$

for small $\nu > 0$. The following lemma shows the asymptotic normality where the mean depends on the random sample, whose proof is in Appendix A.9.

**Lemma 4.6.** For given $x \in [0, 1]^d$, suppose we have random sample $(x_1, y_1), \ldots, (x_n, y_n)$ for each $n$. If we restrict the cardinality of tree space $Q_n$ by

$$|Q_n| \leq O\left(\frac{1}{n} \exp\left(\frac{1}{2n^{\frac{1}{d+2}}}\right)\right),$$

then

$$\frac{\hat{f}_n(x) - r^T_n f(X_n)}{\|r_n^T\|} \overset{d}{\to} N(0, \sigma^2).$$
The proof of Lemma 4.6 also allows us to substitute all $O(\cdot)$ by $O_p(\cdot)$ in the analyses of random design. Further, we can replace the data driven mean $r_n^T f(X_n)$ by its population version $\frac{\lambda}{1+\lambda} f(x)$. Combining all above we obtain the main theorem of this paper that the limiting distribution of the random design in our case is normal.

**Theorem 4.2.** For given $x \in [0, 1]^d$,

$$\frac{\hat{f}_n(x) - \frac{\lambda}{1+\lambda} f(x)}{\|r_n^T\|} \overset{d}{\rightarrow} N(0, \sigma^2).$$

**Proof.** We first show that for given $x \in [0, 1]^d$,

$$\frac{r_n^T f(X_n) - \frac{\lambda}{1+\lambda} f(x)}{\|r_n^T\|} \overset{p}{\rightarrow} 0.$$  

Recall the index set $D_n = \{i : |x_i - x| \leq l_n \cdot d_n\}$. Denote $\Delta = \frac{\lambda}{1+\lambda} - \sum_{i=1}^n r_{n,i} = O(n^{-1})$ and $\tilde{f}(x) = (f(x), \ldots, f(x))^T$ an $n$-vector. We split

$$\frac{r_n^T f(X_n) - \frac{\lambda}{1+\lambda} f(x)}{\|r_n^T\|} = \frac{r_n^T [f(X_n) - \tilde{f}(x)]}{\|r_n^T\|} - \frac{\Delta \cdot f(x)}{\|r_n^T\|} = - \frac{\Delta \cdot f(x)}{\|r_n^T\|} + \frac{r_n|_{D_n} \cdot [f(X_n) - \tilde{f}(x)]|_{D_n}}{\|r_n\|} + \frac{r_n|_{D_n^c} \cdot [f(X_n) - \tilde{f}(x)]|_{D_n^c}}{\|r_n\|}.$$  

By replacing $O(\cdot)$ in the fixed case by $O_p(\cdot)$ in the random design case, recall that

$$O_p \left( n^{-\frac{1}{2+1}} \right) \leq \|k_n\|, \|r_n\| \leq O_p \left( n^{-\frac{1}{2+2}} \right).$$

On one hand, we notice that

$$|r_n|_{D_n^c} \cdot |[f(X_n) - \tilde{f}(x)]|_{D_n^c} \leq \left| r_n|_{D_n^c} \right|_{1} \cdot \left| [f(X_n) - \tilde{f}(x)]|_{D_n^c} \right| \leq O_p \left( \frac{1}{n} \cdot 2M_f \right) = O_p \left( n^{-1} \right).$$

Therefore

$$\frac{r_n|_{D_n^c} \cdot [f(X_n) - \tilde{f}(x)]|_{D_n^c}}{\|r_n\|} \overset{p}{\rightarrow} 0.$$  

And similarly since $|\Delta| \leq O(n^{-1})$,

$$\frac{\Delta \cdot f(x)}{\|r_n\|} \overset{p}{\rightarrow} 0.$$
On the other hand, we can show similarly as $|B_n|$ that $|D_n| = O\left(n \cdot (l_n \cdot d_n)^d\right)$ a.s. and therefore

$$\left| r_n |D_n| \cdot [f(X_n) - \tilde{f}(x)] |D_n| \right| \leq \left| r_n |D_n| \right| \left| [f(X_n) - \tilde{f}(x)] |D_n| \right| \leq \left| [f(X_n) - \tilde{f}(x)] |D_n| \right| \leq O_p\left(\sqrt{n \cdot (l_n d_n)^d \cdot (l_n d_n \cdot \alpha)^2}\right) = O_p\left(\sqrt{n \cdot \log n d_n^d \cdot (d_n^d + \alpha^d)}\right) = O_p\left(\sqrt{n \cdot \log n d_n^d \cdot n^{-\frac{d+2}{2}}}\right) = O_p\left(\sqrt{n \cdot \log n d_n^d \cdot \frac{1}{2 n^{-\frac{d+1}{2}}}}\right).$$

Therefore

$$\frac{r_n |D_n| \cdot [f(X_n) - \tilde{f}(x)] |D_n|}{\| r_n \|} \rightarrow 0.$$

Combining the above calculations gives the result that

$$\frac{r_n^T f(X_n) - \lambda f(x)}{\| r_n^T \|} \rightarrow 0.$$

Therefore by Slutsky’s Theorem,

$$\frac{\hat{f}_n(x) - \frac{\lambda}{1+\lambda} f(x)}{\| r_n^T \|} = \frac{\hat{f}_n(x) - r_n^T f(X_n)}{\| r_n^T \|} + \frac{r_n^T f(X_n) - \frac{\lambda}{1+\lambda} f(x)}{\| r_n^T \|} \rightarrow N(0, \sigma^2).$$

Instead of the whole signal, Boulevard converges to $\frac{\lambda}{1+\lambda}$ of it. In standard boosting, we expect to converge to the whole signal. Boosting after this point will result in a random forest regressing on pure noise, which is redundant. In comparison, Boulevard down-weighs the boosting history to regularize that each tree in the finite ensemble reflects partial signal. It thus avoids being dominated by the first few trees then repeatedly fitting on noise. In practice, as we showed that the prediction from Boulevard is consistent w.r.t $\frac{\lambda}{1+\lambda} f(x)$, we simply rescale it by $\frac{1+\lambda}{\lambda}$ to retrieve the whole signal.

4.6. Undersmoothing, Tree Space Capacity and Subsampling. In the expression in Theorem 4.2, the mean is deterministic, but the variance is random. From results on kernel ridge regression, we would expect that this stochastic variance converges in probability if
the random forest kernel behaves as generic kernel with a shrinking bandwidth. From a theoretical perspective, the optimal rate of \( \|r_{nT}\| \) is bounded from below by \( O \left( n^{-\frac{1}{2} d + \frac{1}{2}} \right) \), which corresponds to the optimal nonparametric regression rate using \( \frac{1}{2} \)-Hölder continuous functions as base learners (Stone, 1982). In practice, \( \|r_{nT}\| \) relies on the specific method of growing the boosted trees, therefore may vary from case to case.

Furthermore, this demonstrates that with carefully structured trees the prediction is consistent while the variance involves no signal but the error. It acts like an undersmoothed local smoother whose bias term shrinks faster than the variance term.

We have a strict requirement that the tree terminal node size grows at a rate between \( O \left( n^{\frac{1}{d + 1}} \right) \) and \( O \left( n^{\frac{1}{d + 2}} \right) \) to guarantee undersmoothing. Any log term is allowed to be added to the existing polynomial result without changing the behavior. We notice that different subsample rates (i.e. \( \log n \) in Wager et al. (2014), \( \sqrt{n} \) in Mentch and Hooker (2016)) have been applied for measuring uncertainty. In comparison, Boulevard algorithm requires a relatively restricted rate between these. In addition, though Boulevard training implements subsampling at each iteration, this does not influence the asymptotic distribution. The impact of subsampling is on the possible deviation from the mean process therefore the convergence speed if we assume non-adaptivity.

In the proof we have required the size of tree space to scale at a rate of \( \frac{1}{n} \exp \left( \frac{1}{2 n^{\frac{1}{d + 2}}} \right) \). In comparison, Wager and Walther (2015) have shown that, in fixed dimension, any tree can be well approximated by a collection of \( O(\exp(\log n)^2) \) hyper rectangles. Therefore the capacity of our designated tree space is decently large from a practical perspective.

5. Eventual Non-adaptivity. All the results mentioned above have assumed the non-adaptivity of the boosting procedure of Boulevard in order to separate the tree structure from the leaf values. In standard boosting however, it is conventional and reasonable to decide tree structures on the current gradients in order to better exploit the gap between the prediction and the signal. Such procedures are known for their tendency to overfit which can be relieved by subsampling. However, when seeking to extend our results to this case we lose the easy identifiability of a Boulevard convergence point since the tree structure distribution changes at each iteration. We therefore need more assumptions and further theoretical development to extend the asymptotic normality to a more practical Boulevard algorithm that allows the current gradient to determine tree structure.

A first approach to this is to relax non-adaptivity to eventual non-adaptivity. We postulate a convergent sequence of predictions, indicating that underlying the tree spaces will be stabilized after boosting for sufficiently long time. Here we introduce the notation \( E[S_n(Y, \hat{Y})] \) where \( Y = (y_1, \ldots, y_n)^T \) and \( \hat{Y} = (f(x_1), \ldots, f(x_n))^T \) indicating the expected tree structure given the gradient of the loss between observed responses and current predictions. In regression this is \( Y - \hat{Y} \), and we will take this form into the following discussion instead of a generic gradient expression.
5.1. Local Homogeneity and Contraction Regions. We start with trees whose splits are based on the optimal Gini gain (Breiman et al., 1984). For \((x_1, z_1), \ldots, (x_n, z_n)\), the chosen split minimizes the impurity in the form of

\[
\inf_{L,R} \sum_{i \in L} (z_i - \bar{z}_L)^2 + \sum_{i \in R} (z_i - \bar{z}_R)^2,
\]

where \(L \subset \{1, \ldots, n\}, R = L^C\). Once the optimal split is unique, i.e. the optimum has a positive margin over the rest, we could allow a small change of all \(y\)'s values without changing the split decision. This also holds true if the split is decided by a subsample instead. In terms of adaptive boosting, this observation demonstrates local homogeneity that, except a set \(\Omega_0 \subset \mathbb{R}^n\) with Lebesgue measure 0 where \((z_1, \ldots, z_n)^T = Y - \hat{Y} \in \Omega_0\) has multiple optima for (4), we can segment \(\mathbb{R}^n\), the space of possible \(Y - \hat{Y}\), into subsets \(\bigcup_{i=1}^n C_i = \mathbb{R}^n \setminus \Omega_0\) s.t. \(E[S_n(Y, \hat{Y})] = E[S_n(Y, \hat{Y}')]\) for \(Y - \hat{Y}, Y - \hat{Y}' \in C_i\) the same subset.

Notice that Gini gain is insensitive to scaling, i.e. multiplying \((y_1, \ldots, y_n)\) by a nonzero factor. Therefore all \(C_i\)'s are open double cones in \(\mathbb{R}^n\).

**Definition 5.1 (Contraction Region).** Given the sample \((x_1, y_1), \ldots, (x_n, y_n)\). Write \(Y = (y_1, \ldots, y_n)\) and current prediction \(\hat{Y} = (\hat{y}_1, \ldots, \hat{y}_n)\). Following the above segmentation \(\bigcup_{i=1}^n C_i = \mathbb{R}^n \setminus \Omega_0\). We call \(C_i\) a contraction region if \(Y^* \in C_i\) for the following \(Y^*\)

\[
Y^* = \lambda E[S_n(Y, \hat{Y})](Y - Y^*), \text{ i.e. } Y^* = \left[ \frac{1}{\lambda}I + E[S_n(Y, \hat{Y})] \right]^{-1} E[S_n(Y, \hat{Y})]Y,
\]

for any \(Y - \hat{Y} \in C_i\), where \(E[S_n(Y, \hat{Y})]\) is the unique structural matrix in this region.

The intuition behind this definition is that, as long as a Boulevard process stays inside a contraction region, the subsequent tree structures will be conditionally independent of the predicted values. Therefore the path becomes non-adaptive, collapsing to \(Y^*\). To achieve this eventual non-adaptivity, we would like to know when a Boulevard path is permanently contained in a contraction region.

We should point out here that we have not shown the existence and the uniqueness of such contraction regions. Such an analysis would rely on the split proposing methods, the sample and the choice of \(\lambda\).

5.2. Escaping the Contraction Region. In this section we explore possible approaches to restrict a Boulevard process inside a contraction region. Assuming the existence of contraction regions, we recall Theorem 3.1 which indicates that the Boulevard process has positive probability of not moving far from the fixed point. We formally state this as follows.

**Theorem 5.1.** Denote \(B(x, r)\) the open ball of radius \(r\) centered at \(x\) in \(\mathbb{R}^n\). Suppose \(C \subset \mathbb{R}\) a contraction region, \(Y^* \in C\) the contraction point and \(B(Y, 2r) \subset C\) for some \(r > 0\). Write \(\hat{Y}_b\) the Boulevard process. For sufficiently large \(t\),

\[
P \left( \hat{Y}_b \in C, \forall b \geq t | \hat{Y}_t \in B(Y^*, r) \right) \rightarrow 1, t \rightarrow \infty.
\]
**Proof.** We refer to Theorem 3.1. Choose $\delta = r$, and choose $T$ s.t. $\forall t > T$,
\[
\frac{\lambda}{t}(1 + \sqrt{n})2\sqrt{n}M \leq \frac{r}{\sqrt{d}}, \text{ i.e. } \sup \| \epsilon_t \| \leq \frac{r}{\sqrt{d}},
\]
In this case, $\beta = \| \hat{Y}_t \| + \delta - \sqrt{d} \sup_{t \geq T} \| \epsilon_t \| \geq \delta = r$. By the conditional independence of $\hat{Y}_t$ and $\epsilon_b, b > t$ in the contraction region,
\[
P \left( \hat{Y}_b \in C, \forall b \geq t | \hat{Y}_t \in B(Y^*, r) \right) \geq P \left( \sup_{b > t} \| \hat{Y}_b - Y^* \| \leq \| \hat{Y}_t - Y^* \| + \delta | \hat{Y}_t \in B(Y^*, r) \right)
\]
\[
= P \left( \sup_{b > t} \| \hat{Y}_b - Y^* \| \leq \| \hat{Y}_t - Y^* \| + \delta \right)
\]
\[
\geq 1 - \frac{4\sqrt{d} \sum_{b=t+1}^{\infty} E[\epsilon_b^2]}{r^2} \to 1.
\]
\[
\square
\]

Theorem 5.1 guarantees neither the existence or the uniqueness of the contraction region. A possible *ad hoc* solution to the existence is to apply a tail snapshot which uses the tree space that applies to some iteration $b^*$ for the rest of the boosting steps when the Boulevard path begins to become stationary. This manually enforces the conditional independence between tree structures and boosting gradients, leading to non-adaptivity after $b^*$. A example of Boulevard regression implementing the tail snapshot is detailed in Algorithm 3.

**Algorithm 3 (Tail Snapshot Boulevard).**

- **Start with** $\hat{f}_0 = 0$.
- For $b = 1, \ldots$, given $\hat{f}_b$, calculate the gradient
  \[
  z_i \triangleq -\frac{\partial}{\partial u_i} \sum_{i=1}^{n} \frac{1}{2} (u_i - y_i)^2 \bigg|_{u_i = \Gamma_M(f_b(x_i))} = y_i - \Gamma_M(\hat{f}_b(x_i));
  \]
- If $b^*$ is not found, update by $1 > \lambda > 0$ and the tree structure space $Q_b$ decided by all subsamples of current gradient,
  \[
  \hat{f}_{b+1}(x) = \frac{b}{b+1} \hat{f}_b(x) + \frac{\lambda}{b+1} s_b(x; Q_b)(z_1, \ldots, z_n)^T,
  \]
where $s_b(x; Q)$ denotes the random tree structure vector based on tree space $Q$. If $b^*$ is found, update by $Q_{b^*}$ instead, i.e.
  \[
  \hat{f}_{b+1}(x) = \frac{b}{b+1} \hat{f}_b(x) + \frac{\lambda}{b+1} s_b(x; Q_{b^*})(z_1, \ldots, z_n)^T.
  \]
• When \( b^* \) is not found, check the empirical training loss as a measure of the distance to the fixed point.

\[
L_{b+1} = \frac{1}{2n} \sum_{i=1}^{n} \left( \frac{\lambda y_i - \hat{f}_{b+1}(x_i)}{1 + \lambda} \right)^2.
\]

If \( L_{b+1} < L^* \) a preset threshold, we claim Boulevard is close enough to a fixed point and choose the current \( b + 1 \) to be \( b^* \).

6. Empirical Study. We have conducted a minimalist empirical study to demonstrate the performance of Boulevard. Despite the fact that our purpose in developing Boulevard lies in statistical inference, we require its accuracy to be on par with other predominant tree ensembles, which is assessed on both simulated and real world data. In addition, we inspect the empirical limiting behavior of non-adaptive Boulevard to show its agreement with our theory. We summarize the result of the empirical study in this section, while additional details can be found in the appendix.

6.1. Predictive Accuracy. We first compare Boulevard predictive accuracy with the following tree ensembles: Random Forest (RF), gradient boosted trees without subsampling (GBT), stochastic gradient boosted trees (SGBT), non-adaptive Boulevard achieved by completely randomized trees (rBLV), adaptive Boulevard whose tree structures are influenced by gradient values (BLV). All the tree ensembles build same depth of trees (see Appendix B for details) throughout the experiment.

Results on simulated data are shown in Figure 1. We choose sample size of 5000 and use the following two settings as underlying response functions: (1) \( y = x_1 + 3x_2 + x_3 x_4 \) (top), and (2) \( y = x_1 + 3x_2 + (1 - x_3)^2 + x_4 x_5 + (1 - x_6)^6 + x_7 \) (bottom). Error terms are Unif[-1,1] (left) and equal point mass on \{−1, 1\} (right). Training errors are evaluated on the training set with noisy responses, while testing errors are evaluated by error from the underlying signal on a separate test set. BLV and rBLV are comparable with RF, while all the three equal-weight tree ensembles are slightly inferior to GBM and SGBM.

Results on four real world data sets selected from UCI Machine Learning Repository (Dheeru and Karra Taniskidou, 2017; Tüfekci, 2014; Kaya et al., 2012) are shown in Figure 2. All curves are averages after 5-fold cross validation. Different parameters are used for different data sets. Rankings of the five methods in comparison are quite volatile here, nevertheless rBLV and BLV manage to achieve decent performance on test sets despite the fact that BLV has the lowest training error which is a common indicator for overfitting.

6.2. Limiting Distribution. To examine the limiting behavior of non-adaptive Boulevard, we start with the model

\[
y = x_1 + 3x_2 + x_3^2 + 2x_4 x_5.
\]
A set of 10 fixed test points (see Appendix B) are used along the experiments. We set a sample size of 1000, add different sub-Gaussian error terms to this signal and built non-adaptive Boulevard until ensemble size reaches 2000. This is repeated 1000 times with a new sample each time and we plot the distribution of the predictions in Figure 3. All these curves are undistinguishable from normal distribution by Kolmogorov-Smirnov test.

In addition, Table 1 shows the experiment in which we apply symmetric uniform errors and observe the scaling of prediction standard deviation along with the increase of error standard deviation.

6.3. Reproduction Interval. Similar to prediction intervals which quantify the uncertainty of future predictions, we introduce the reproduction interval as the uncertainty measure for where the prediction would be if it were made on another independent sample.
Theorem 4.2 is used to create reproduction intervals for Boulevard. \( k_n \) in the stochastic variance is empirically estimated directly using the ensemble, while \( \left[ \frac{1}{\lambda} I + K_n \right]^{-1} \) is conservatively simplified to its largest possible norm \( \lambda \). We then scale the variance estimate by 2 to account for having separate independent samples. We use the training sample to create reproduction intervals for the test points, then repeatedly train and predict each test point for another 100 times with a different sample each time. Figure 4 shows the 95% reproduction intervals we capture under different settings. We anticipate more accurate results with larger sample size.

Furthermore, we notice the uniform pattern of biases in those plots. This bias comes from two known causes. One is that we are using small samples which are far from guaranteeing the consistency. The other is because of the edge effects; the distance of the ten chosen test points to the center of the hypercube is respectively 0.000, 0.671, 0.894, 0.894, 0.894,
Fig 3. Distributions of predictions of test points with different error terms. The errors are \( N(0,1) \), \( \text{Unif}[-1,1] \), equal point mass at \( \{-1,1\} \), and half chance -1 half chance \( \text{Unif}[0,2] \), respectively.

0.693, 0.520, 0.436, 0.510 and 0.469. We in general expect biased prediction when the point is near the boundary.

7. Discussion. This work is so far the first we know to have established a limiting distribution for gradient boosted trees. The roadmap consists of the following key components. We implemented the honest tree construction to reduce the chance of chasing order statistics, applied downweighting towards averaging to achieve convergence, and carefully selected tree construction rate to obtain asymptotic normality. With the uncertainty measure of Boulevard predictions, we are looking forward to exploring the use of regularized gradient boosting with inference, making the model more interpretable and analyzable.

The sequential correlation induced by GBT is the major issue complicating our analysis, while the resistance of decision trees to mathematical quantification adds more complication. Much of our effort is spent on seeking rational conditions to compromise these features.
Honest trees, non-adaptivity and down-weighing all contribute to making sequential trees less correlated.

As briefly discussed above, there are two remaining questions in our paper. The first question regards the stochastic variance. To allow a richer collection of decision tree construction strategies, it is essential to discover the weakest tree condition under which the variance term converges in probability. The second question is the convergence of adaptive Boulevard which appears to hold in practice. In spite of the ad hoc tail snapshot we proposed, the existence and uniqueness of the contraction region of generic Boulevard requires more mathematical formulation of decision trees or some variation of decision trees.

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Fig 4. Reproduction intervals. Boxplots show distributions of predictions; red intervals are reproduction intervals; blue dots are truths. Sample sizes are 1000 (top row) and 5000 (bottom row), error terms Unif[-1,1] (left column) and Unif[-2,2] (right column). Coverage is shown by numbers next to interval centers.

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APPENDIX A: PROOFS

A.1. Proof to Theorem 2.1.

Proof. To prove (1), element-wise non-negativity is trivial. To show symmetry, consider any given $i \neq j$ and assume $x_i \in A$ and $x_j \in A'$ under the assumption of subsample uniformity,

$$\mathbb{E}_w[S_n]_{i,j} = \mathbb{E}_w[s_{n,j}(x_i)] = \frac{1}{n \theta_n} \sum_{w} I(x_j \in A) I(j \in w) \sum_{x_l \in A} I(l \in w)$$

$$\mathbb{E}_w[S_n]_{j,i} = \mathbb{E}_w[s_{n,i}(x_j)] = \frac{1}{n \theta_n} \sum_{w} I(x_i \in A') I(i \in w) \sum_{x_l \in A'} I(l \in w)$$
Therefore $E_w[S_n]_{i,j} = E_w[S_n]_{j,i} = 0$ if $A \neq A'$.
In the cases of $A = A'$, $I(x_j \in A) = I(x_i \in A') = 1$. We consider the following possibilities of $w$.
(a) For $i \notin w, j \notin w$,
$$\frac{I(j \in w)}{\sum_{x_l \in A} I(l \in w)} = \frac{I(i \in w)}{\sum_{x_l \in A} I(l \in w)} = 0.$$
(b) For $i \in w, j \in w$,
$$\frac{I(j \in w)}{\sum_{x_l \in A} I(l \in w)} = \frac{I(i \in w)}{\sum_{x_l \in A} I(l \in w)} = \frac{1}{\sum_{x_l \in A} I(l \in w)}.$$
(c) For $i \in w, j \notin w$, consider $w' = w \setminus \{i\} \cup \{j\}$ s.t. $\sum_{x_l \in A} I(l \in w) = \sum_{x_l \in A} I(l \in w')$,
$$\frac{I(j \in w')}{\sum_{x_l \in A} I(l \in w')} = \frac{I(i \in w)}{\sum_{x_l \in A} I(l \in w')} = \frac{1}{\sum_{x_l \in A} I(l \in w')}.$$
(d) Similarly, for $i \notin w, j \in w$, consider $w' = w \setminus \{j\} \cup \{i\}$,
$$\frac{I(j \in w)}{\sum_{x_l \in A} I(l \in w)} = \frac{I(i \in w')}{\sum_{x_l \in A} I(l \in w')} = \frac{1}{\sum_{x_l \in A} I(l \in w')}.$$
Since all $w$’s are equally likely, we conclude by symmetry that $E_w[S_n]_{i,j} = E_w[S_n]_{j,i}$, hence $E_w[S_n]$ is symmetric.
To prove (2), notice $\forall x_i, x_j, x_k \in A$,
$$E_w[S_n]_{k,i} = \frac{1}{\binom{n}{3}} \sum_w \frac{I(i \in w)}{\sum_{x_l \in A} I(l \in w)} = E_w[S_n]_{j,i}.$$
Therefore $E_w[S_n]$, after proper permutation to gather points in same leaves together, is diagonally blocked with equal entries in each diagonal block and 0 elsewhere, thus positive semi-definite.

To show (3), notice that $S_n$ has row sums of $\leq 1$ (not exactly 1 due to cases of missing subsample points in the leaf), so does $E_w[S_n]$. Thus $\|E_w[S_n]\|_1 \leq 1$. Similarly, $E_w[S_n]$ has column sums of $\leq 1$ due to symmetry and $\|E_w[S_n]\|_\infty \leq 1$. By the Hlder inequality,
$$\rho(E_w[S_n]) = \|E_w[S_n]\|_1 \leq \sqrt{\|E_w[S_n]\|_1 \|E_w[S_n]\|_\infty} \leq 1.$$
A.2. Stochastic Contraction.

**Definition A.1 (Stochastic Contraction).** Given real-valued stochastic process \( \{X_t\}_{t \in \mathbb{N}} \), a sequence of \( 0 < \lambda_t \leq 1 \), define

\[
\mathcal{F}_0 = \emptyset, \mathcal{F}_t = \sigma(X_1, \ldots, X_t),
\]

\[
\epsilon_t = X_t - \mathbb{E}[X_t|\mathcal{F}_{t-1}].
\]

We call \( X_t \) a stochastic contraction if the following is satisfied

- **Vanishing coefficients**
  \[
  \sum_{t=1}^{\infty} (1 - \lambda_t) = \infty, \text{ i.e. } \prod_{t=1}^{\infty} \lambda_t = 0.
  \]

- **Mean contraction**
  \[
  \lambda_t X_{t-1} I(X_{t-1} \leq 0) \leq \mathbb{E}[X_t|\mathcal{F}_{t-1}] \leq \lambda_t X_{t-1} I(X_{t-1} \geq 0), \text{ a.s.}.
  \]

- **Bounded deviation**
  \[
  \sup |\epsilon_t| \to 0, \quad \sum_{t=1}^{\infty} \mathbb{E}[\epsilon_t^2] \leq \infty.
  \]

**Lemma A.1.** If \( \{X_t\}_{t \in \mathbb{N}} \) is a stochastic contraction,

- **Almost sure convergence**
  \( X_t \overset{a.s.}{\to} 0 \).

- **Kolmogorov maximal inequality.** For any \( T, \delta \) s.t. \( \beta = |X_T| + \delta - \sup_{t > T} |\epsilon_t| > 0 \),

  \[
  P\left( \sup_{t \geq T} |X_t| \leq |X_T| + \delta \right) \geq 1 - \frac{4\sum_{t=T+1}^{\infty} \mathbb{E}[\epsilon_t^2]}{\min\{\delta^2, \beta^2\}}.
  \]

**Proof.** Define the stopping time of sign changes

\( T_0 = 0, T_k = \inf\{t > T_{k-1}|X_{t-1} \leq 0, X_t > 0 \text{ or } X_{t-1} \geq 0, X_t < 0 \}. \)

We now look at every realized path and examine the segment of the process holding the same sign. W.o.l.g., suppose \( X_t \geq 0 \) for \( T_k < t < T_{k+1} \). Easy to check

\[
X_t = \mathbb{E}[X_t|\mathcal{F}_{t-1}] + \epsilon_t \leq \lambda_t X_{t-1} + \epsilon_t \leq X_{t-1} + \epsilon_t \leq X_{T_k} + \sum_{s=T_k+1}^{t} \epsilon_s.
\]
Therefore $|X_t| \leq |X_{T_k}| + \left| \sum_{s=T_k+1}^{t} \epsilon_s \right|$, same for the negative case. Since $\epsilon_t$’s are independent and $\sum_{t=1}^{\infty} \mathbb{E}[\epsilon_t^2] \leq \infty$, $\sum_{t=1}^{\infty} \epsilon_t$ exists a.s.. Write $N = \sup_k \{T_k \leq \infty\}$ the number of sign changes.

If there are infinite sign changes, i.e. $N = \infty$, by sending $k \to \infty$, $|X_{T_k}| \xrightarrow{a.s.} 0$ and $\left| \sum_{s=T_k+1}^{T_k+n} \epsilon_s \right| \xrightarrow{a.s.} 0, \forall n > 0$. Hence $X_t \xrightarrow{a.s.} 0$.

If there are finite sign changes, we assume w.l.o.g. that for some $k$, $X_t \geq 0, \forall t \geq T_k$. (6) can be written as $X_t - \epsilon_t \leq X_{t-1}$ which indicates $X_t - \sum_{s=T_k+1}^{t} \epsilon_s$ is decreasing, therefore has a limit $(-\infty)$. Since $\sum_{s=T_k+1}^{\infty} \epsilon_s$ exists a.s., $X_t \xrightarrow{a.s.} c \geq 0$. Assume $c > 0$,

$$\sum_{s=T_k+1}^{\infty} \epsilon_s \geq \sum_{s=T_k+1}^{\infty} X_s - \lambda_s X_{s-1} = -\lambda_{T_k+1} X_{T_k} + \sum_{s=T_k+2}^{\infty} (1 - \lambda_s) X_{s-1} = \infty,$$

which is a contradiction. Therefore $X_t \xrightarrow{a.s.} 0$.

To show the maximum inequality, we take the same notations above, and also look at segmentations by sign changes. For any $t$ in the same segment as $T$,

$$|X_t| \leq |X_T| + \left| \sum_{s=T+1}^{t} \epsilon_t \right| \leq |X_T| + \sup_{T' > T} \left| \sum_{s=T+1}^{T'} \epsilon_s \right| .$$

For any $t$ in a different segment starting at $T'$,

$$|X_t| \leq |X_T'| + \left| \sum_{s=T'+1}^{t} \epsilon_t \right| \leq |X_T'| + \sup_{S > T'} \left| \sum_{s=T'+1}^{S} \epsilon_s \right| \leq \sup_{S > T} |\epsilon_s| + \left| \sum_{s=T'+1}^{S} \epsilon_s \right| .$$

Now we consider any possible sequence of $\{\epsilon_t, t > T\}$ and allow $T', S$ to change. Kolmogorov maximal inequality implies

$$P \left( \sup_{i > T} \left| \sum_{s=i}^{j} \epsilon_{s} \right| \leq x \right) \geq P \left( \sup_{i > T} \left| \sum_{s=T}^{i} \epsilon_{s} \right| \leq \frac{x}{2} \right) \geq 1 - \frac{4 \sum_{s=T}^{\infty} \mathbb{E}[\epsilon_s^2]}{x^2} .$$

The conclusion is obtained by noticing that $|X_t| \leq |X_T| + \delta$ for any $\{\epsilon_t\}_{t > T}$ satisfying

$$\sup_{i,j > T} \left| \sum_{s=i}^{j} \epsilon_{s} \right| \leq \min\{\delta, \beta\}.$$
A.3. Proof to Theorem 3.1.

Proof. The idea is to define a sequence of adaptive orthonormal rotations $R_t \in F_{t-1}$ to align the expected update with the previous step so that we can apply the $\mathbb{R}$ result component-wisely. Define $R_t \mathbb{E}[Z_t|F_{t-1}] = \gamma_{t-1} Z_{t-1}$, for some $\gamma_{t-1} > 0, \gamma_{t-1} \in F_{t-1}$. The contraction assumption also implies that $\gamma_{t-1} \leq \lambda_{t-1}$. Define a new process $Z_t^*$ satisfying

1. $Z_1^* = Z_1, R_1 = I$,
2. writing $R_t^* = \prod_{i=1}^{n} R_i \in F_{t-1}$ s.t. $Z_t^* = R_t^* Z_t = R_t^* \epsilon_t + R_t^* \mathbb{E}[Z_t|F_{t-1}]$.

Above implies $\|Z_t\| = \|Z_t^*\|$, thus we need to prove the equivalence that $Z_t^* \xrightarrow{a.s.} 0$. Notice that $\sum_{i=1}^{n} R_t^* \epsilon_i$ is component-wisely a martingale with

$$\sum_{i=1}^{\infty} E[|R_t^* \epsilon_i|^2] = \sum_{i=1}^{\infty} E[|\epsilon_i|^2] < \infty,$$

hence $\sum_{i=1}^{n} R_t^* \epsilon_i$ exists a.s.. Since the construction aligns $Z_t^*$ with $\mathbb{E}[Z_t^*|F_{t-1}]$ we apply Lemma A.1 to obtain almost sure convergence to 0 component-wisely, thus $\|Z_t^*\| \xrightarrow{a.s.} 0$. 

A.4. Proof to Corollary 3.2.1.

Proof. Expanding $\hat{f}(x)$ gives

$$\hat{f}(x) = \lim_{B \to \infty} \frac{1}{B} \sum_{b=1}^{B} s_b(x)(Y - \hat{Y}_b)$$

$$= \lim_{B \to \infty} \frac{1}{B} \sum_{b=1}^{B} s_b(x)(Y - Y^* + Y^* - \hat{Y}_b)$$

$$= \lim_{B \to \infty} \frac{1}{B} \sum_{b=1}^{B} s_b(x)(Y - Y^*) + \lim_{B \to \infty} \frac{1}{B} \sum_{b=1}^{B} s_b(x)(Y^* - \hat{Y}_b)$$

$$= \mathbb{E}[s_b(x)](Y - Y^*) + 0$$

$$= \mathbb{E}[s_n(x)] \left[ \frac{1}{\lambda} I + \mathbb{E}[S_n] \right]^{-1} Y.$$

A.5. Proof to Lemma 4.1.

Proof. Consider the expansion

$$\left[ \frac{1}{\lambda} I + K_n \right]^{-1} = \lambda \sum_{i=0}^{\infty} \left( (\lambda)^{2i} K_n^{2i} - (\lambda)^{2i+1} K_n^{2i+1} \right).$$
We examine the column sums of each of the matrix powers. Start with $K_n^2$:

$$\sum_{i=1}^n (K_n^2)_{i,1} = \sum_{i=1}^n \sum_{j=1}^n (K_n)_{i,j}(K_n)_{j,1} = \sum_{j=1}^n (K_n)_{j,1} \sum_{i=1}^n (K_n)_{i,j}.$$ 

Since $K_n$ consists of structure vectors of sample points, for some $c > 0$,

$$1 - \frac{c}{n} \leq \sum_{j=1}^n (K_n)_{i,j} = \sum_{j=1}^n (K_n)_{i,j} \leq 1, \quad i = 1, \ldots, n.$$

Given $K_n$ is nonnegative,

$$\left(1 - \frac{c}{n}\right)^2 \leq \sum_{i=1}^n (K_n^2)_{i,1} = \sum_{j=1}^n (K_n)_{j,1} \sum_{i=1}^n (K_n)_{i,j} \leq 1.$$

Repeating the same discussion yields

$$\left(1 - \frac{c}{n}\right)^m \leq \sum_{i=1}^n (K_n^m)_{i,1} \leq 1.$$

Therefore,

$$\lambda \left(1 - \frac{1}{1 - \lambda^2(1 - \frac{c}{n})^2} - \frac{\lambda}{1 - \lambda^2}\right) \leq \sum_{j=1}^n \left[\frac{1}{\lambda} I + K_n\right]^{-1}_{j,1} = \lambda \left(\sum_{i=0}^{\infty} (\lambda)^{2i}(K_n^{2i})_{j,1} - (\lambda)^{2i+1}(K_n^{2i+1})_{j,1}\right) \leq \lambda \left(\frac{1}{1 - \lambda^2} - \frac{\lambda}{1 - \lambda^2(1 - \frac{c}{n})^2}\right),$$

where both the LHS and RHS reduce to $\frac{\lambda}{1 + \lambda} + O \left(\frac{1}{n}\right)$. So is true for any column sum of $\left[\frac{1}{\lambda} I + K_n\right]^{-1}$. Now given $k_n$ is nonnegative and $1 - \|k_n\|_1 \leq O \left(\frac{1}{n}\right)$ we reach the assertion.

\[\Box\]

**A.6. Proof to Lemma 4.2.**

**Proof.** Under locality, $k_{nj} = 0$ if $|x_i - x_j| > d_n$, while $[K_n]_{i,j} = 0$ if $|x_i - x_j| > d_n$. Recursively, if $|x_i - x_j| > l_n \cdot d_n$ then $[K_n^l]_{i,j} = 0$ for $l \leq l_n$. As $k_n$ and $K_n$ are element-wisely
nonnegative, we again expand the matrix inverse

\[ \left\| r_n \right\|_{D_n} = \sum_{|x-x_i|>l_n \cdot d_n} \left| r_{ni} \right| = \sum_{|x-x_i|>l_n \cdot d_n} \left| \sum_j k_{nj} \left[ \frac{1}{\lambda} I + K_n \right]^{-1} \right| \]

\[ \leq \sum_{|x-x_j| \leq d_n} k_{nj} \sum_{|x-x_j|>l_n \cdot d_n} \left| \frac{1}{\lambda} I + K_n \right|^{-1} \]

\[ \leq \sum_{|x-x_j| \leq d_n} k_{nj} \sum_{|x-x_j|>l_n \cdot d_n} \lambda \sum_{l=l_n}^{\infty} \lambda^l [K_n]^{l,j,i} \]

\[ \leq \sum_{|x-x_j| \leq d_n} k_{nj} \sum_{|x-x_j|>l_n \cdot d_n} \lambda^{l+1} \]

\[ \leq \sum_{l=l_n}^{\infty} \lambda^{l+1} = \frac{\lambda}{1 - \lambda} \frac{1}{n}. \]

\[ \]

**A.7. Proof to Lemma 4.4.**

**Proof.** The idea is to bound \( k_{nj} \) from both above and below. The condition

\[ \inf_{A \in Q_n} \sum_{i=1}^{n} I(x_i \in A) \geq O \left( n^{\frac{1}{d+2}} \right) \]

implies that \( k_{nj} \leq O \left( n^{-\frac{1}{d+2}} \right) \). Given \( \left\| k_n \right\|_1 \leq 1 \),

\[ \left\| k_n \right\| \leq \sqrt{\left\| k_n \right\|_1 \left\| k_n \right\|_\infty} \leq O \left( n^{-\frac{1}{2}} \frac{1}{d+2} \right) \]

On the other hand, given \( |B_n| \geq O \left( n \cdot d_n^d \right) \), there are at most

\[ O \left( n \cdot d_n^d \right) = O \left( n^{\frac{1}{d+1}} \right) \]
$k_{nj}$’s that are positive. Since $\|k_n\|_1 \geq 1 - O(n^{-1})$,

$$\|k_n\| \geq O\left(\sqrt{\frac{1}{n^{d+1}}} \cdot n^{\frac{1}{d+1}}\right) = O\left(n^{-\frac{1}{d+1}}\right).$$

Those bounds also work for $\|r_n\|$ given

$$\lambda \leq \text{eigen} \left(\left[\frac{1}{\lambda} I + K_n\right]^{-1}\right) \leq \lambda.$$

\[\square\]

**A.8. Proof to Lemma 4.5.**

**Proof.** Probabilistic DCT guarantees that

$$\lim_n P(f_n(X, \epsilon) \leq t) = \lim_n \int \int 1_{\{f_n(x, \epsilon) \leq t\}} \mu_x \mu_\epsilon$$

$$= \lim_n \int P(f_n(x, \epsilon) \leq t) \mu_x$$

$$= \int \lim_n P(f_n(x, \epsilon) \leq t) \mu_x$$

$$= \int \Phi(t) \mu_x = \Phi(t).$$

\[\square\]

**A.9. Proof to Lemma 4.6.**

**Proof.** In order to prove the lemma, we combine Lemma 4.4, Theorem 4.1 and Lemma 4.5 and show that all assumptions are met from a point-wise perspective on $[0, 1]^{d \times N}$, i.e. fixed sample sequence are given by $\theta_n X, n \geq 1$.

i) We show for a.s. $X$, $|B_n^*| = |B_n(\theta_n X)| \geq O(n \cdot d_n)$. Consider random $X$. Noticing $E[|B_n|] = na_n = O(\sqrt{d_n})$ and referring to CLT for binomials as $nd_n \to \infty$,

$$\frac{|B_n| - na_n}{\sqrt{na_n(1-a_n)}} \sim N(0, 1).$$

Take fixed $0 < c < 1$,

$$P(|B_n| \leq c \cdot na_n) \to \Phi\left(\frac{(c-1)na_n}{\sqrt{na_n(1-a_n)}}\right)$$

$$\leq \Phi((c-1)\sqrt{na_n})$$

$$\leq O\left(\frac{1}{\sqrt{na_n}} \exp\left(-\frac{(c-1)^2na_n}{2}\right)\right).$$
Further, since \( na_n = O \left( n^{d+\frac{1}{2}} \right) = O \left( n^{\frac{1}{\pi + 2}} \right) \),

\[
\sum_{n=1}^{\infty} \frac{1}{\sqrt{na_n}} \exp \left( -\frac{(c-1)^2na_n}{2} \right) \leq \infty.
\]

As per Borel-Contelli, since

\[
\sum_{n=1}^{\infty} P(\{B_n(\theta_nX) \leq c \cdot na_n\}) \leq \infty,
\]

then for a.s. \( X \), events of \( |B_n(\theta_nX)| \leq c \cdot na_n \) happens finite times. Since \( a_n \) is uniformly bounded away from 0 due to \( \mu(x) \) is bounded, we reach our conclusion.

ii) To show

\[
\inf_{A \in q \in Q_n} \sum_{i=1}^{n} I(x_i \in A) \geq O \left( n^{\frac{1}{\pi + 2}} \right)
\]

for a.s. \( X \), evaluate the CLT of binomial again

\[
P \left( \exists A \in q \in Q_n \text{ s.t.} \sum_{i=1}^{n} I(x_i \in A) \leq n^{\frac{1}{\pi + 2}} \right)
\leq O \left( |Q_n| \cdot |q| \cdot P \left( \sum_{i=1}^{n} I(x_i \in A) \leq n^{\frac{1}{\pi + 2}} \right) \right)
\leq O \left( \frac{d+1}{n^{\frac{d+2}{\pi + 2}}} \cdot \Phi \left( \frac{n^{\frac{1}{\pi + 2}} - n^{\frac{1}{\pi + 2} + \nu}}{\sqrt{n^{\frac{1}{\pi + 2} + \nu} \left(1 - n^{-\frac{d+1}{\pi + 2} + \nu}\right)}} \right) \right)
\leq O \left( \frac{d+1}{n^{\frac{d+2}{\pi + 2}}} \cdot \Phi \left( -\frac{1}{2} \left( 1 + \frac{1}{\pi + 2} \right) \right) \right)
\leq O \left( \frac{d+1}{n^{\frac{d+2}{\pi + 2}}} \cdot \frac{1}{2} \left( 1 + \frac{1}{\pi + 2} \right) \exp \left( -\frac{1}{2} \frac{n^{\frac{1}{\pi + 2} + \nu}}{n} \right) \right)
\leq O \left( \exp \left( -\frac{1}{2} n^{\frac{1}{\pi + 2} + \nu} \right) \right) \rightarrow 0.
\]

Therefore, noticing that

\[
\sum_{n=1}^{\infty} \exp \left( -\frac{1}{2} n^{\frac{1}{\pi + 2} + \nu} \right) = \sum_{n=1}^{\infty} n^{-\frac{\pi + 2 + \nu}{2}} < \infty,
\]

the Borel-Cantelli theorem indicates our assertion. Hence, for a.s. \( X^* \), \( \theta_nX^* \) satisfies the assumptions in Theorem 4.1. \( \square \)
APPENDIX B: EMPIRICAL STUDY SETTINGS

Figure 5 shows the distribution of true responses for our simulated training set. The 10 test points we used in the simulation study are: (0.5, 0.5, 0.5, 0.5, 0.5), (0.2, 0.2, 0.2, 0.2, 0.2), (0.1, 0.9, 0.1, 0.9, 0.1), (0.1, 0.1, 0.9, 0.9, 0.9), (0.9, 0.1, 0.1, 0.1, 0.9), (0.5, 0.1, 0.9, 0.1, 0.5), (0.3, 0.2, 0.7, 0.8, 0.6), (0.4, 0.2, 0.3, 0.6, 0.7), (0.2, 0.7, 0.8, 0.3, 0.5), (0.3, 0.6, 0.4, 0.9, 0.5). Table 2 shows the settings we use across all empirical study. The labels are: MSE for Figure 1, MSE-DatasetName for Figure 2, Limiting for Figure 3, Variance for Table 1 and RI for Figure 4. Abbreviations: n for sample size, θ for subsample rate, ntree for ensemble size, k for terminal leave size after subsample (which has to be corrected when no subsample is involved, i.e. GBT), λ as in Boulevard iterations.

Fig 5. Distribution of truth used when assessing limiting distribution and reproduction interval.

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| label        | n   | $\theta$ | ntree | k | $\lambda$ |
|--------------|-----|----------|-------|---|-----------|
| MSE-(1-4)    | 5000| 0.3      | 1000  | 20| 0.8       |
| MSE-Boston   | 506 | 0.8      | 1000  | 5 | 0.8       |
| MSE-CCPP     | 9568| 0.5      | 1000  | 50| 0.8       |
| MSE-CASP     | 20000| 0.5     | 1000  | 50| 0.8       |
| MSE-Airfoil  | 1503| 0.8      | 1000  | 40| 0.8       |
| Limiting-(1-4) | 1000| 0.8     | 2000  | 10| 0.5       |
| Variance-(1-4) | 5000| 0.8    | 3000  | 20| 0.5       |
| RI-(1-2)     | 1000| 0.8      | 2000  | 10| 0.5       |
| RI-(3-4)     | 5000| 0.8      | 2000  | 10| 0.5       |

Table 2
Parameters we use in empirical study.