

From unbiased MDI Feature Importance to Explainable AI for Trees

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ABSTRACT

We attempt to give a unifying view of the various recent attempts to (i) improve the interpretability of tree-based models and (ii) debias the the default variable-importance measure in random Forests, Gini importance. In particular, we demonstrate a common thread among the out-of-bag based bias correction methods and their connection to local explanation for trees. In addition, we point out a bias caused by the inclusion of inbag data in the newly developed *explainable AI for trees* algorithms.

1 Variable importance in trees

Variable importance is not very well defined as a concept. Even for the case of a linear model with n observations, p variables and the standard $n \gg p$ situation, there is no theoretically defined variable importance metric in the sense of a parametric quantity that a variable importance estimator should try to estimate (Grömping, 2009). Variable importance measures for random forests have been receiving increased attention in bioinformatics, for instance to select a subset of genetic markers relevant for the prediction of a certain disease. They also have been used as screening tools (Díaz-Uriarte and De Andres, 2006, Menze et al., 2009) in important applications highlighting the need for reliable and well-understood feature importance measures.

The default choice in most software implementations (Liaw and Wiener, 2002, Pedregosa et al., 2011) of random forests (Breiman, 2001) is the *mean decrease in impurity (MDI)*. The

MDI of a feature is computed as a (weighted) mean of the individual trees' improvement in the splitting criterion produced by each variable. A substantial shortcoming of this default measure is its evaluation on the in-bag samples which can lead to severe overfitting (Kim and Loh, 2001). It was also pointed out by Strobl et al. (2007a) that *the variable importance measures of Breiman's original Random Forest method ... are not reliable in situations where potential predictor variables vary in their scale of measurement or their number of categories*. There have been multiple attempts at correcting the well understood bias of the Gini impurity measure both as a split criterion as well as a contributor to importance scores, each one coming from a different perspective.

Strobl et al. (2007b) derive the exact distribution of the maximally selected Gini gain along with their resulting p-values by means of a combinatorial approach. Shih and Tsai (2004) suggest a solution to the bias for the case of regression trees as well as binary classification trees (Shih, 2004) which is also based on p-values. Several authors (Loh and Shih, 1997, Hothorn et al., 2006) argue that the criterion for split variable and split point selection should be separated.

A different approach is to add so-called pseudo variables to a dataset, which are permuted versions of the original variables and can be used to correct for bias (Sandri and Zuccolotto, 2008). Recently, a modified version of the Gini importance called Actual Impurity Reduction (AIR) was proposed Nembrini et al. (2018) that is faster than the original method proposed by Sandri and Zuccolotto with almost no overhead over the creation of the original RFs and available in the R package *ranger* (Wright and Ziegler, 2015, Wright et al., 2017).

2 Separating inbag and out-of-bag (oob) samples

An idea that is gaining quite a bit of momentum is to include OOB samples to compute a debiased version of the Gini importance (Li et al., 2019a, Zhou and Hooker, 2019, Loecher, 2020) yielding promising results. Here, the original Gini impurity (for node m) for a cate-

gorical variable Y which can take D values c_1, c_2, \dots, c_D is defined as

$$G(m) = \sum_{d=1}^D \hat{p}_d(m) \cdot (1 - \hat{p}_d(m)), \text{ where } \hat{p}_d = \frac{1}{n_m} \sum_{i \in m} Y_i.$$

Loecher (2020) proposed a *penalized Gini impurity* which combines inbag and out-of-bag samples. The main idea is to increase the impurity $G(m)$ by a penalty that is proportional to the difference $\Delta = (\hat{p}_{OOB} - \hat{p}_{inbag})^2$:

$$PG_{oob}^{\alpha, \lambda} = \alpha \cdot G_{oob} + (1 - \alpha) \cdot G_{in} + \lambda \cdot (\hat{p}_{oob} - \hat{p}_{in})^2 \quad (1)$$

In addition, Loecher (2020) investigated replacing $G(m)$ by an unbiased estimator of the variance via the well known sample size correction.

$$\widehat{G}(m) = \frac{N}{N-1} \cdot G(m) \quad (2)$$

In this paper we focus on the following three special cases, $[\alpha = 1, \lambda = 2]$, $[\alpha = 0.5, \lambda = 1]$ as well as $[\alpha = 1, \lambda = 0]$:

$$PG_{oob}^{(1,2)} = \sum_{d=1}^D \hat{p}_{d,oob} \cdot (1 - \hat{p}_{d,oob}) + 2(\hat{p}_{d,oob} - \hat{p}_{d,in})^2 \quad (3)$$

$$PG_{oob}^{(0.5,1)} = \frac{1}{2} \cdot \sum_{d=1}^D \hat{p}_{d,oob} \cdot (1 - \hat{p}_{d,oob}) + \hat{p}_{d,in} \cdot (1 - \hat{p}_{d,in}) + (\hat{p}_{d,oob} - \hat{p}_{d,in})^2 \quad (4)$$

$$\widehat{PG}_{oob}^{(1,0)} = \frac{N}{N-1} \cdot \sum_{d=1}^D \hat{p}_{d,oob} \cdot (1 - \hat{p}_{d,oob}) \quad (5)$$

$$(6)$$

Our main contributions are to show that

- $PG_{oob}^{(1,2)}$ is equivalent to the *MDI-oob* measure defined in Li et al. (2019a).
- $PG_{oob}^{(1,2)}$ has close connections to the *conditional feature contributions* (CFCs) defined in (Saabas, 2019b),
- Similarly to MDI, both the CFCs as well as the related *SHapley Additive exPlanation* (SHAP) values defined in (Lundberg et al., 2020) are susceptible to “overfitting” to the training data.

- $PG_{oob}^{(0.5,1)}$ is equivalent to the *unbiased split-improvement* measure defined in Zhou and Hooker (2019).

We refer the reader to (Loecher, 2020) for a proof that $\widehat{PG}_{oob}^{(1,0)}$ and $PG_{oob}^{(0.5,1)}$ are unbiased estimators of feature importance in the case of non-informative variables.

3 Conditional feature contributions (CFCs)

The conventional wisdom of estimating the impact of a feature in tree based models is to measure the **node-wise reduction of a loss function**, such as the variance of the output Y , and compute a weighted average of all nodes over all trees for that feature. By its definition, such a *mean decrease in impurity* (MDI) serves only as a global measure and is typically not used to explain a *per-observation, local impact*. Saabas (2019b) proposed the novel idea of explaining a prediction by following the decision path and attributing changes in the expected output of the model to each feature along the path. Figure 1 illustrates the main idea of decomposing each prediction through the sequence of regions that correspond to each node in the tree. Each decision either adds or subtracts from the value given in the parent node and can be attributed to the feature at the node. So, each individual prediction can be defined as the global mean plus the sum of the K feature contributions:

$$f_{pred}(x_i) = \bar{Y} + \sum_{k=1}^K f_{T,k}(x_i) \quad (7)$$

where $f_{T,k}(x_i)$ is the contribution from the k -th feature (for tree T), written as a sum over all the inner nodes t such that $v(t) = k$ (Li et al., 2019a)¹:

$$f_{T,k}(x_i) = \sum_{t \in I(T): v(t)=k} [\mu_n(t^{left}) \mathbb{1}(x_i \in R_{t^{left}}) + \mu_n(t^{right}) \mathbb{1}(x_i \in R_{t^{right}}) - \mu_n(t) \mathbb{1}(x_i \in R_t)] \quad (8)$$

where $v(t)$ is the feature chosen for the split at node t .

¹ Appendix 7.1 contains expanded definitions and more thorough notation.

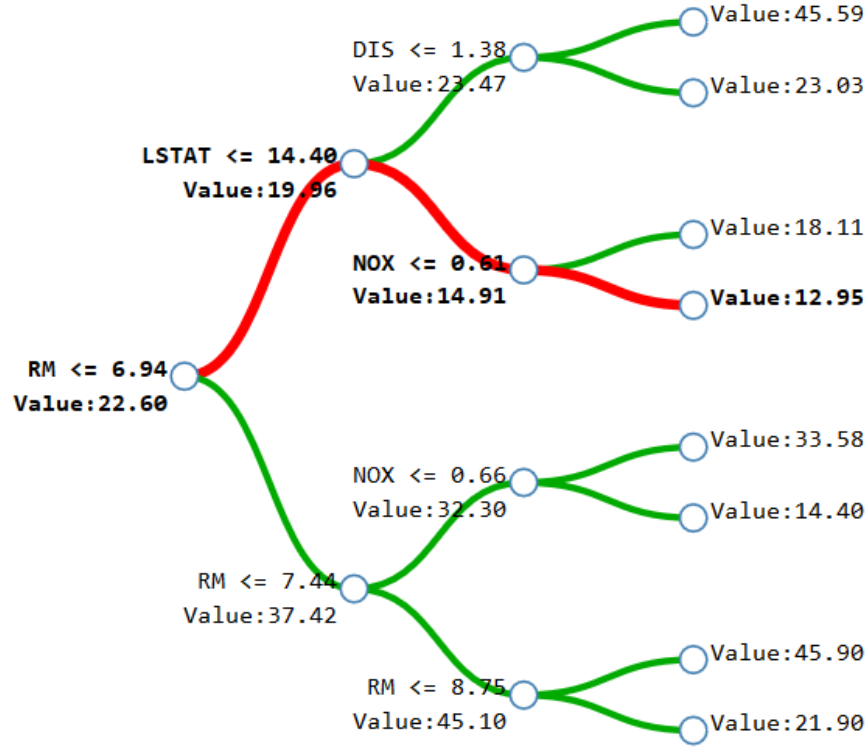


Figure 1: Taken from (Saabas, 2019a): Depicted is a regression decision tree to predict housing prices. The tree has conditions on each internal node and a value associated with each leaf (i.e. the value to be predicted). But additionally, the value at each internal node i.e. the mean of the response variables in that region, is shown. The red path depicts an example prediction $Y = 12.95$, broken down as follows:

$$12.95 \approx 22.60(\bar{Y}) - 2.64(\text{loss from RM}) - 5.04(\text{loss from LSTAT}) - 1.96(\text{loss from NOX})$$

A “local” feature importance score can be obtained by summing Eq. (8) over all trees. Adding these local explanations over all data points yields a “global” importance score:

$$Imp_{global}(k) = \sum_{i=1}^N |Imp_{local}(k, x_i)| = \sum_{i=1}^N \frac{1}{n_T} \sum_T |f_{T,k}(x_i)| \quad (9)$$

In the light of wanting to explain the predictions from tree based machine learning models, the “Saabas algorithm” is extremely appealing, because

- The positive and negative contributions from nodes convey directional information unlike the strictly positive purity gains.
- By combining many local explanations we can represent global structure while retaining local faithfulness to the original model.
- The expected value of every node in the tree can be estimated efficiently by averaging the model output over all the training samples that pass through that node.
- The algorithm has been implemented and is easily accessible in a python (Saabas, 2019b) and R (Sun, 2020) library.

However, Lundberg et al. (2020) pointed out that it is strongly biased to alter the impact of features based on their distance from the root of a tree. This causes Saabas values to be inconsistent, which means one can modify a model to make a feature clearly more important, and yet the Saabas value attributed to that feature will decrease. As a solution, the authors developed an algorithm (“TreeExplainer”) that computes local explanations based on exact Shapley values in polynomial time. This provides local explanations with theoretical guarantees of local accuracy and consistency. A python library is available at <https://github.com/slundberg/shap>. One should not forget though that the same idea of adding *conditional feature contributions* lies at the heart of *TreeExplainer*.

In this section, we call attention to another source of bias which is the result of using the same (inbag) data to (i) greedily split the nodes during the growth of the tree and (ii) computing the node-wise changes in prediction. We use the well known titanic data set to

illustrate the perils of putting too much faith into importance scores which are based entirely on training data - not on OOB samples - and make no attempt to discount node splits in deep trees that are spurious and will not survive in a validation set.

In the following model² we include *passengerID* as a feature along with the more reasonable *Age*, *Sex* and *Pclass*.

Figure 2 below depicts the distribution of the individual, “local” feature contributions, preserving their sign. The large variations for the variables with high cardinality (*Age*, *pas-*

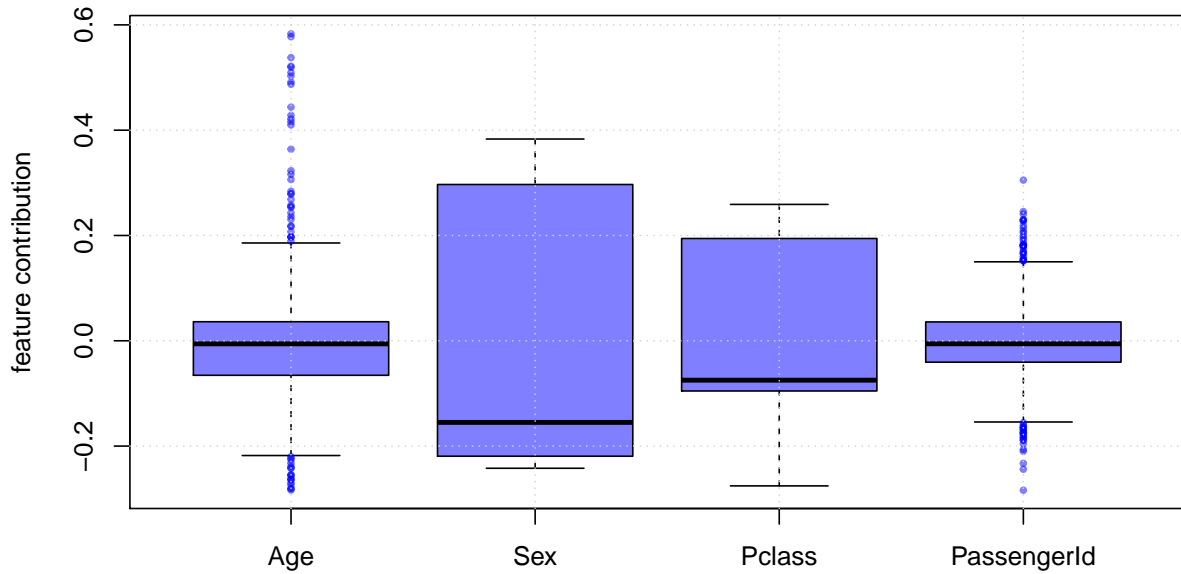


Figure 2: Conditional feature contributions (TreeInterpreter) for the Titanic data.

sengerID) are worrisome. We know that the impact of *Age* was modest and that *passengerID* has no impact on survival but when we sum the absolute values, both features receive sizable importance scores, as shown in Figure 3. This troubling result is robust to random shuffling of the ID. Similar findings hold true for the TreeExplainer (Lundberg et al., 2020)

²In all random forest simulations, we choose $mtry = 2$, $ntrees = 100$ and exclude rows with missing *Age*

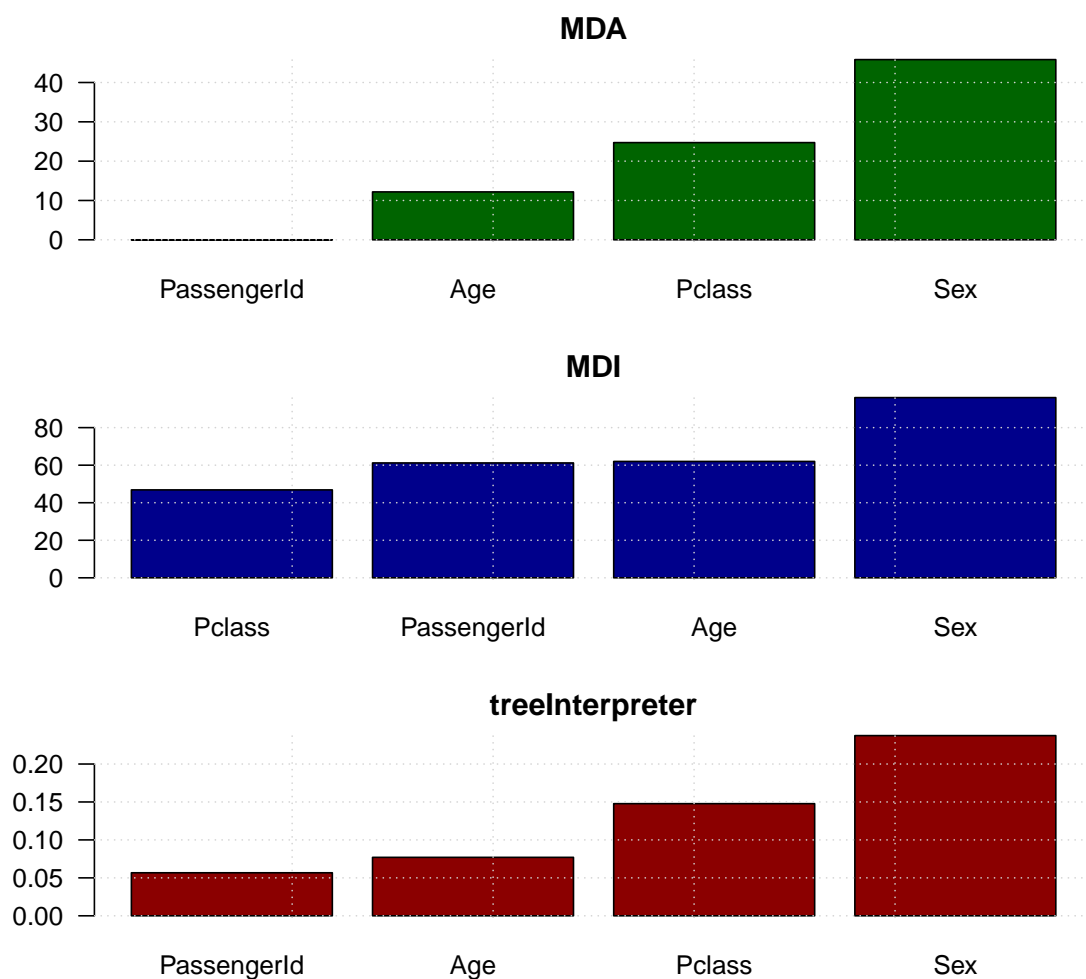


Figure 3: Permutation importance (MDA, top panel) versus Mean decrease impurity (MDI, left panel) versus conditional feature contributions (TreeInterpreter) for the Titanic data. The permutation based importance (MDA) is not fooled by the irrelevant ID feature. This is maybe not unexpected as the IDs should bear no predictive power for the out-of-bag samples.

which assigns a non zero value of feature importance to *passengerID* which is due to mixing inbag and out-of-bag data for the evaluation. The next section will point out a close analogy

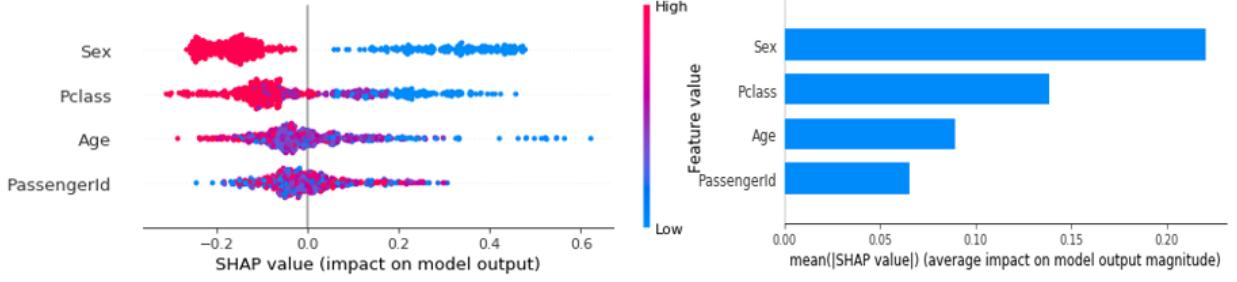


Figure 4: SHapley Additive exPlanation (SHAP) values (TreeExplainer) for the Titanic data.

between the well known MDI score and the more recent measure based on the conditional feature contributions.

4 MDI versus CFCs

As elegantly demonstrated by Li et al. (2019a), the MDI of feature k in a tree T can be written as

$$MDI = \frac{1}{|\mathcal{D}^{(T)}|} \sum_{i \in \mathcal{D}^{(T)}} f_{T,k}(x_i) \cdot y_i \quad (10)$$

where $\mathcal{D}^{(T)}$ is the bootstrapped or subsampled data set of the original data \mathcal{D} . Since $\sum_{i \in \mathcal{D}^{(T)}} f_{T,k}(x_i) = 0$, we can view MDI essentially as the sample covariance between $f_{T,k}(x_i)$ and y_i on the bootstrapped dataset $\mathcal{D}^{(T)}$. Alternatively, we can view MDI as a particular weighted average of the CFCs, which for the special case of binary classification ($y_i \in \{0, 1\}$) means that one only adds up those CFCs for which $y_i = 1$.

$$MDI = \frac{1}{|\mathcal{D}^{(T)}[y_i = 1]|} \sum_{i \in \mathcal{D}^{(T)}[y_i = 1]} f_{T,k}(x_i) \quad (11)$$

Figure 5 shows this new measure separately for the inbag and outbag components; the middle panel of Figure 3 is proportional to the left panel. The misleadingly high contribution of

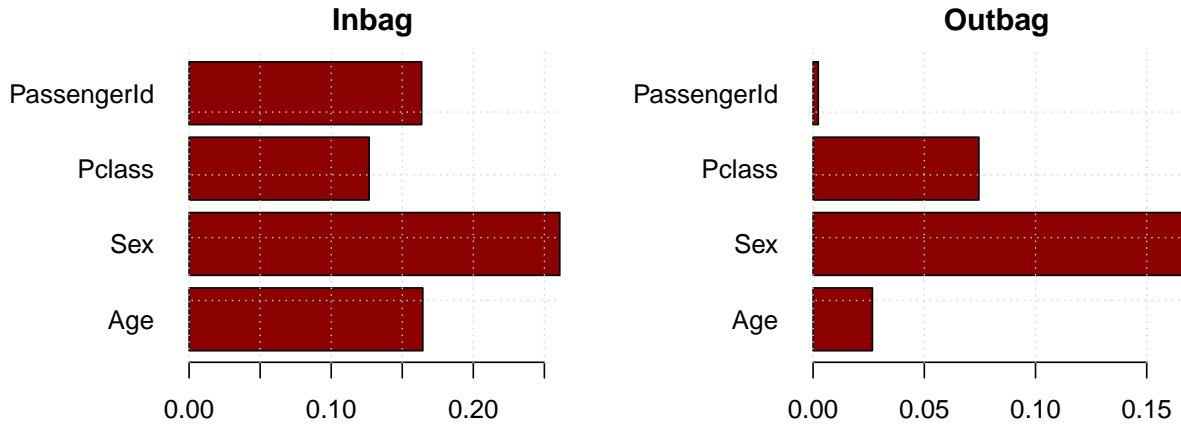


Figure 5: MDI as a restricted sum of conditional feature contributions defined by Eq. (11) for the (left panel) inbag and (right panel) outbag data, respectively.

passengerID is due to the well known shortcoming of MDI: RFs use the training data $\mathcal{D}^{(T)}$ to construct the functions $f_{T,k}()$, then MDI uses the same data to evaluate (10).

5 Debiasing MDI via oob samples

In this section we give a short version of the proof that $PG_{oob}^{(1,2)}$ is equivalent to the *MDI-oob* measure defined in Li et al. (2019a). For clarity we assume binary classification; Appendix 5 contains an expanded version of the proof including the multi-class case. *MDI-oob* is based on the usual variance reduction per node as shown in Eq. (34) (proof of Proposition (1)), but with a “variance” defined as the mean squared deviations of y_{oob} from the inbag mean μ_{in} :

$$\Delta_I(t) = \frac{1}{N_n(t)} \cdot \sum_{i \in D(T)} (y_{i,oob} - \mu_{n,in})^2 1(x_i \in R_t) - \dots$$

We can, of course, rewrite the variance as

$$\frac{1}{N_n(t)} \cdot \sum_{i \in D(T)} (y_{i,oob} - \mu_{n,in})^2 = \frac{1}{N_n(t)} \cdot \sum_{i \in D(T)} (y_{i,oob} - \mu_{n,oob})^2 + (\mu_{n,in} - \mu_{n,oob})^2 \quad (12)$$

$$= p_{oob} \cdot (1 - p_{oob}) + (p_{in} - p_{oob})^2 \quad (13)$$

where the last equality is for Bernoulli y_i , in which case the means $\mu_{in/oob}$ become proportions $p_{in/oob}$ and the first sum is equal to the binomial variance $p_{oob} \cdot (1 - p_{oob})$. The final expression is effectively equal to $PG_{oob}^{(1,2)}$.

Lastly, we now show that $PG_{oob}^{(0.5,1)}$ is equivalent to the *unbiased split-improvement* measure defined in Zhou and Hooker (2019). For the binary classification case, we can rewrite $PG_{oob}^{(0.5,1)}$ as follows:

$$\begin{aligned}
PG_{oob}^{(0.5,1)} &= \frac{1}{2} \cdot \sum_{d=1}^D \hat{p}_{d,oob} \cdot (1 - \hat{p}_{d,oob}) + \hat{p}_{d,in} \cdot (1 - \hat{p}_{d,in}) + (\hat{p}_{d,oob} - \hat{p}_{d,in})^2 \\
&= \hat{p}_{oob} \cdot (1 - \hat{p}_{oob}) + \hat{p}_{in} \cdot (1 - \hat{p}_{in}) + (\hat{p}_{oob} - \hat{p}_{in})^2 \\
&= \hat{p}_{oob} - \hat{p}_{oob}^2 + \hat{p}_{in} - \hat{p}_{in}^2 + \hat{p}_{oob}^2 - 2\hat{p}_{oob} \cdot \hat{p}_{in} + \hat{p}_{in}^2 \\
&= \hat{p}_{oob} + \hat{p}_{in} - 2\hat{p}_{oob} \cdot \hat{p}_{in}
\end{aligned}$$

□

6 Discussion

Random forests and gradient boosted trees are among the most popular and powerful (Olson et al., 2017) non-linear predictive models used in a wide variety of fields. Lundberg et al. (2020) demonstrate that tree-based models can be more accurate than neural networks and even more interpretable than linear models. In the comprehensive overview of variable importance in regression models Grömping (2015) distinguishes between methods based on (i) variance decomposition and (ii) standardized coefficient sizes, which is somewhat analogous to the difference between (i) MDI and (ii) CFCs. The latter measure the directional impact of $x_{k,i}$ on the outcome y_i , whereas MDI based scores measure a kind of *partial* R_k^2 (if one stretched the analogy to linear models). Li et al. (2019a) ingeniously illustrate the connection between these seemingly fundamentally different methods via eq. (10). And the brilliant extension of CFCs to their Shapley equivalents by Lundberg et al. (2020) bears affinity to the game-theory-based metrics LMG and PMVD (Grömping (2015) and references therein), which are based on averaging the sequential R_k^2 over all orderings of regressors.

In this paper we have (i) connected the proposals to reduce the well known bias in MDI by mixing inbag and oob data (Li et al., 2019a, Zhou and Hooker, 2019) to a common framework (Loecher, 2020), and (ii) pointed out that similar ideas would benefit/debias the *conditional feature contributions* (CFCs) (Saabas, 2019b) as well as the related *SHapley Additive exPlanation* (SHAP) values (Lundberg et al., 2020).

While the main findings are applicable to any tree based method, they are most relevant to random forests (RFs) since (i) oob data are readily available and (ii) RFs typically grow deep trees. Li et al. (2019a) showed a strong dependence of the MDI bias on the depth of the tree: splits in nodes closer to the roots are much more stable and supported by larger sample sizes and hence hardly susceptible to bias. RFs “get away” with the individual overfitting of deep trees to the training data by **averaging** many (hundreds) of separately grown deep trees and often achieve a favorable balance in the bias-variance tradeoff. One reason is certainly that the noisy predictions from individual trees “average out”, which is not the case for the summing/averaging of the strictly positive MDI leading to what could be called *interpretational overfitting*. The big advantage of conditional feature contributions is that positive and negative contributions can cancel across trees making it less prone to that type of overfitting. However, we have provided evidence that both the CFCs as well as the SHAP values are still susceptible to “overfitting” to the training data and can benefit from evaluation on oob data.

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7 Appendix

7.1 Background and notations

Definitions needed to understand Eq. (8). (The following paragraph closely follows the definitions in Li et al. (2019a).)

Random Forests (RFs) are an ensemble of classification and regression trees, where each tree T defines a mapping from the feature space to the response. Trees are constructed independently of one another on a bootstrapped or subsampled data set $\mathcal{D}^{(T)}$ of the original data \mathcal{D} . Any node t in a tree T represents a subset (usually a hyper-rectangle) R_t of the

feature space. A split of the node t is a pair (k, z) which divides the hyper-rectangle R_t into two hyper-rectangles $R_t \cap \mathbb{1}(X_k \leq z)$ and $R_t \cap \mathbb{1}(X_k > z)$ corresponding to the left child t left and right child t right of node t , respectively. For a node t in a tree T , $N_n(t) = |\{i \in \mathcal{D}^{(T)} : \mathbf{x}_i \in R_t\}|$ denotes the number of samples falling into R_t and

$$\mu_n(t) := \frac{1}{N_n(t)} \sum_{i: \mathbf{x}_i \in R_t} y_i$$

We define the set of inner nodes of a tree T as $I(T)$.

7.2 Variance Reduction View

Here, we provide a full version of the proof sketched in section 5 which leans heavily on the proof of Proposition (1) in Li et al. (2019b) .

We consider the usual variance reduction per node but with a “variance” defined as the mean squared deviations of y_{oob} from the inbag mean μ_{in} :

$$\begin{aligned} \Delta_{\mathcal{I}}(t) &= \frac{1}{N_n(t)} \sum_{i \in \mathcal{D}^{(T)}} [y_{i,oob} - \mu_{n,in}(t)]^2 \mathbb{1}(\mathbf{x}_i \in R_t) \\ &\quad - [y_{i,oob} - \mu_{n,in}(t^{\text{left}})]^2 \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{left}}}) - [y_{i,oob} - \mu_{n,in}(t^{\text{right}})]^2 \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{right}}}) \end{aligned} \tag{14}$$

$$\begin{aligned} &= \frac{1}{N_n(t)} \sum_{i \in \mathcal{D}^{(T)}} ([y_{i,oob} - \mu_{n,oob}(t)]^2 + [\mu_{n,in}(t) - \mu_{n,oob}(t)]^2) \mathbb{1}(\mathbf{x}_i \in R_t) \\ &\quad - \left([y_{i,oob} - \mu_{n,oob}(t^{\text{left}})]^2 + [\mu_{n,in}(t^{\text{left}}) - \mu_{n,oob}(t^{\text{left}})]^2 \right) \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{left}}}) \\ &\quad - \left([y_{i,oob} - \mu_{n,oob}(t^{\text{right}})]^2 + [\mu_{n,in}(t^{\text{right}}) - \mu_{n,oob}(t^{\text{right}})]^2 \right) \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{right}}}) \end{aligned} \tag{15}$$

$$\begin{aligned}
&= \frac{1}{N_n(t)} \sum_{i \in \mathcal{D}^{(T)}} \underbrace{\{[y_{i,oob} - \mu_{n,oob}(t)]^2 \mathbb{1}(\mathbf{x}_i \in R_t)\}}_{N_n(t) \cdot p_{oob}(t) \cdot (1-p_{oob}(t))} + \underbrace{[\mu_{n,in}(t) - \mu_{n,oob}(t)]^2}_{[p_{oob}(t) - p_{in}(t)]^2} \\
&- \frac{1}{N_n(t)} \sum_{i \in \mathcal{D}^{(T)}} \underbrace{\{[y_{i,oob} - \mu_{n,oob}(t^{\text{left}})]^2 \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{left}}})\}}_{N_n(t^{\text{left}}) \cdot p_{oob}(t^{\text{left}}) \cdot (1-p_{oob}(t^{\text{left}}))} + \underbrace{[\mu_{n,in}(t^{\text{left}}) - \mu_{n,oob}(t^{\text{left}})]^2}_{[p_{oob}(t^{\text{left}}) - p_{in}(t^{\text{left}})]^2} \\
&- \frac{1}{N_n(t)} \sum_{i \in \mathcal{D}^{(T)}} \underbrace{\{[y_{i,oob} - \mu_{n,oob}(t^{\text{right}})]^2 \mathbb{1}(\mathbf{x}_i \in R_{t^{\text{right}}})\}}_{N_n(t^{\text{right}}) \cdot p_{oob}(t^{\text{right}}) \cdot (1-p_{oob}(t^{\text{right}}))} + \underbrace{[\mu_{n,in}(t^{\text{right}}) - \mu_{n,oob}(t^{\text{right}})]^2}_{[p_{oob}(t^{\text{right}}) - p_{in}(t^{\text{right}})]^2}
\end{aligned}$$

where the last equality is for Bernoulli y_i , in which case the means $\mu_{in/oob}$ become proportions $p_{in/oob}$ and we replace the squared deviations with the binomial variance $p_{oob} \cdot (1 - p_{oob})$. The final expression is then

$$\begin{aligned}
\Delta_{\mathcal{I}}(t) &= p_{oob}(t) \cdot (1 - p_{oob}(t)) + [p_{oob}(t) - p_{in}(t)]^2 \\
&- \frac{N_n(t^{\text{left}})}{N_n(t)} \left(p_{oob}(t^{\text{left}}) \cdot (1 - p_{oob}(t^{\text{left}})) + [p_{oob}(t^{\text{left}}) - p_{in}(t^{\text{left}})]^2 \right) \\
&- \frac{N_n(t^{\text{right}})}{N_n(t)} \left(p_{oob}(t^{\text{right}}) \cdot (1 - p_{oob}(t^{\text{right}})) + [p_{oob}(t^{\text{right}}) - p_{in}(t^{\text{right}})]^2 \right)
\end{aligned} \tag{16}$$

which, of course, is exactly the impurity reduction due to $PG_{oob}^{(1,2)}$:

$$\Delta_{\mathcal{I}}(t) = PG_{oob}^{(1,2)}(t) - \frac{N_n(t^{\text{left}})}{N_n(t)} PG_{oob}^{(1,2)}(t^{\text{left}}) - \frac{N_n(t^{\text{right}})}{N_n(t)} PG_{oob}^{(1,2)}(t^{\text{right}}) \tag{17}$$