Fast Interpretable Greedy-Tree Sums (FIGS)

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Abstract
Modern machine learning has achieved impressive prediction performance, but often sacrifices interpretability, a critical consideration in many problems. Here, we propose Fast Interpretable Greedy-Tree Sums (FIGS), an algorithm for fitting concise rule-based models. Specifically, FIGS generalizes the CART algorithm to simultaneously grow a flexible number of trees in a summation. The total number of splits across all the trees can be restricted by a pre-specified threshold, thereby keeping both the size and number of its trees under control. When both are small, the fitted tree-sum can be easily visualized and written out by hand, making it highly interpretable. A partially oracle theoretical result hints at the potential for FIGS to overcome a key weakness of single-tree models by disentangling additive components of generative additive models, thereby reducing redundancy from repeated splits on the same feature. Furthermore, given oracle access to optimal tree structures, we obtain $\ell_2$ generalization bounds for such generative models in the case of $C^1$ component functions, matching known minimax rates in some cases. Extensive experiments across a wide array of real-world datasets show that FIGS achieves state-of-the-art prediction performance (among all popular rule-based methods) when restricted to just a few splits (e.g. less than 20). We find empirically that FIGS is able to avoid repeated splits, and often provides more concise decision rules than fitted decision trees, without sacrificing predictive performance. All code and models are released in a full-fledged package on Github.

1. Introduction
Modern machine-learning methods such as random forests [2], gradient boosting [3,4], and deep learning [5] display impressive predictive performance, but are complex and opaque, leading many to call them “black-box” models. This is unfortunate, as model interpretability is critical in many applications [6,7], particularly in high-stakes settings such as medicine, biology, and policy-making. Interpretability allows models to be audited for general validation, errors, biases, and therefore also more amenable to improvement by domain experts. It facilitates counterfactual reasoning, which is the bedrock of scientific insight, and it instills trust/distrust in a model when warranted. As an added benefit, interpretable models tend to be faster and more computationally efficient than black-box models.

Decision trees are a prime example of interpretable models [1,3,8,10]. They can be easily visualized and simulated even by non-experts, and thus fit naturally into the operating human-in-the-loop AI workflow of many organizations. While they are flexible, and thus have the potential to adapt to complex data, they often tend to be outperformed by black-box models in terms of prediction accuracy. However, this performance gap is not intrinsic to interpretable models, e.g. see examples in [11,10–12]. Indeed, in this paper, we will show how this gap can be partially bridged by carefully examining how and why decision trees fall short, and then directly targeting these weaknesses.

Our starting point is the observation that decision trees can be statistically inefficient at fitting regression functions with additive components [13]. To illustrate this, consider the following toy example: $y = \mathbb{1}_{X_1 > 0} + \mathbb{1}_{X_2 > 0} \cdot \mathbb{1}_{X_3 > 0}$. The two components of this function can be individually implemented by trees with 1 split and 2 splits respectively. However, implementing their sum with a single tree requires at least 5 splits, as we are forced to combine their tree structures in a fractal manner: a copy of the second tree has to be grown out of every leaf node of the first tree (see Fig 1). Indeed, it is easy to see that a single tree $f$ implementing...
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Figure 1. FIGS algorithm overview for learning the toy function \( y = \mathbb{1}_{X_1 > 0} + \mathbb{1}_{X_2 > 0} \cdot \mathbb{1}_{X_3 > 0} \). FIGS greedily adds one node at a time, considering splits not just in an individual tree but within an ensemble of trees. This can lead to much more compact models, as it avoids repeated splits (e.g. in the final CART model shown in the top-right).

The sum of independent tree functions \( f_1, \ldots, f_k \) satisfies

\[
\text{#leaves}(f) \geq \prod_{k=1}^{K} \text{#leaves}(f_k),
\]

and so is much more complicated than simply encoding the function in terms of the original trees in the summation.

This need to grow a deep tree implies two statistical weaknesses of decision trees when fitting them to additive generative models. First, growing a deep tree greatly increases the probability of splitting on noisy features. Second, leaves in a deep tree contain fewer samples, which means that the tree predictions have higher variance. These two weaknesses could be avoided if we could fit a separate decision tree to each additive component of the generative model and present their sum as our model estimate. Existing ensemble methods are unable to disentangle the separate additive components, because they fit each tree either individually (random forests), or sequentially (gradient boosting).

To address these weaknesses, we propose Fast Interpretable Greedy-Tree Sums (FIGS), a novel yet natural algorithm which is able to grow a flexible number of trees simultaneously. This procedure is based on a simple modification to Classification and Regression Trees (CART) [8], allowing it to adapt to additive structure if present by starting new trees, while still maintaining the ability of CART to adapt to higher-order interaction terms. Meanwhile, the running time of FIGS remains largely similar to CART due to the similarity of the two algorithms. FIGS also remains interpretable by keeping the total number of splits in the model limited, allowing for the model to be easily visualized and simulated by hand.

While CART cannot achieve the minimax rate for fitting (generalized) additive generative models with \( C^1 \) component functions even with oracle access to the optimal tree structure [13], we show that FIGS can do so under this setting (Thm 1). In a population setting, we also show that FIGS is able to disentangle separate additive components (Thm 2) without any constraints on the component functions. We verify both theorems in finite-sample simulations, showing situations where FIGS even outperforms random forests. Meanwhile, extensive experiments across a wide array of real-world datasets show that FIGS achieves state-of-the-art performance while maintaining a concise, interpretable model (e.g. having less than 20 total splits). In particular, they greatly improve upon the predictive performance of CART, and this improvement hints at the presence of approximate additive structure in many of these datasets.

In what follows, Sec 2 introduces FIGS, Sec 3 covers related work, Sec 4 establishes two theoretical results underpinning its performance, Sec 5 shows simulations supporting these two results, and Sec 6 shows extensive experiments suggesting FIGS predicts well with very few splits on real-world datasets.

2. FIGS: Algorithm description and runtime

FIGS proposes a natural but powerful extension to CART which forms a sum of trees rather than a single tree. The total number of splits in the model is restricted by a threshold (chosen either by a user or cross-validation). Given this threshold, the greedy algorithm flexibly determines how to allocate these splits among a variable number of trees.

Formally, suppose we are given training data \( D_n = \{(x_i, y_i)\}_{i=1}^n \). When growing a tree, CART chooses for each node \( t \) the split \( s \) that maximizes the (weighted) im-
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purity decrease in the responses \( y \). This has the formula

\[
\hat{\Delta}(s, t, y) := \sum_{x_i \in t} (y_i - \bar{y}_t)^2 - \sum_{x_i \in t_L} (y_i - \bar{y}_{t_L})^2 - \sum_{x_i \in t_R} (y_i - \bar{y}_{t_R})^2,
\]

where \( t_L \) and \( t_R \) denote the left and right child nodes of \( t \) respectively. We call such a split \( s \) a *potential split*, and note that for each step in the algorithm, CART actualizes the potential split with the largest impurity decrease value.

FIGS extends CART to greedily grow a small tree-sum (see Algorithm 1). That is, at each iteration of FIGS, the algorithm chooses either to make a split on one of the current \( K \) trees \( f_1, \ldots, f_K \) in the sum, or to add a new stump to the sum. To make this decision, it still applies the CART splitting rule detailed above to identify potential splits, but instead of using the original response vector, it makes use of the leave-\( f_k \)-out residual vector \( r_i^{(k)} = y_i - \sum_{k \neq f_1} f_i(x_i) \) to compute the impurity decrease for each tree \( f_k \). FIGS makes only one split among the \( K + 1 \) potential splits: The one corresponding to the largest impurity decrease. The prediction over each of the new leaf nodes is defined to be the mean of the \( r_i^{(k)} \) values for samples it contains. At inference time, the prediction is made by summing the predictions of each tree.

**Algorithm 1** FIGS fitting algorithm.

1: FIGS(X: features, y: outcomes, stopping_threshold)
2: trees = []
3: while count total_splits(trees) < stopping_threshold:
4:     all_trees = join(trees, build new tree()) # add new tree
5:     potential_splits = []
6:     for tree in all_trees:
7:         y_residuals = y - predict(all_trees except tree)
8:         for leaf in tree:
9:             potential_split = split(X, y_residuals, leaf)
10:             potential_splits.append(potential_split)
11:     best_split = split with min_impurity(potential_splits)
12:     trees.insert(best_split)

FIGS is related to backfitting [15], but differs from it in important ways: FIGS neither assumes a fixed number of component predictors, nor updates them in a cyclic manner; in fact, FIGS coordinates a competition among the trees being fitted at each iteration, thus mitigating backfitting’s potential to overfit to residuals.

Due to its similarity to CART, FIGS supports many natural modifications that are used in CART trees. For example, different impurity measures can be used; here we use Gini impurity for classification and mean-squared-error for regression. Additionally, FIGS could benefit from pruning or by being used as part of an ensemble model.

**Run-time analysis** The run-time complexity for FIGS to grow a model with \( m \) splits in total is \( O(dm^2n^2) \), where \( d \) the number of features, and \( n \) the number of samples (see derivation in Appendix S1). In contrast, CART has a run-time of \( O(dnm^2) \). Both of these worst-case run-times given above are quite fast, and the gap between them is relatively benign as we usually make a small number of splits for the sake of interpretability.

**Selecting the model’s stopping threshold.** Choosing a threshold on the total number of splits can be done similar to CART: using a combination of the model’s predictive performance and domain knowledge on how interpretable the model needs to be. Alternatively, the threshold can be selected using an impurity decrease threshold [9] rather than a hard threshold on the number of splits. We discuss potential data-driven choices of the threshold in the Discussion (Sec 7).

3. Background and related work

There is a long history of greedy methods for learning individual trees, e.g. C4.5 [2], CART [3], and ID3 [16]. Recent work has proposed global optimization problems rather than greedy algorithms for trees, which can incur a high computational cost but improve performance given a fixed rule budget [17–19]. However, due to the limitations of a single tree, all these methods suffer from the problem of having repeated splits or repeated subtrees [20], a failure we will quantify in the results section.

Besides trees, there are a variety of other interpretable methods such as rule lists [21,22] or rule sets [23,24] for an overview and python implementation, see [1].

Also similar to the work here are methods that learn an additive model of rules, where a rule is defined to be an axis-aligned, rectangular region in the input space. RuleFit [25] is a popular method that learns a model by first extracting rules from multiple greedy decision trees fit to the data and then learning a linear model using those rules as features. FIGS is able to improve upon RuleFit by greedily selecting higher-order interactions when needed, rather than simply using all rules from some pre-specified tree depth. MARS [26] greedily learns an additive model of splines in a manner similar to FIGS, but loses interpretability as a result of using splines rather than rules.

Loosely related to this work are posthoc methods which aim to help understand a black-box model, but ultimately cannot be as interpretable as an individual interpretable model [5,30,31].
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4. Theoretical evidence that FIGS adapts to additive structure

Tight generalization upper bounds have proved elusive for CART due to the difficulty of analyzing the tree growing procedure, and are difficult for FIGS for the same reason. However, even if we knew the optimal tree structure for CART, having to use empirical averages instead of individual means for the prediction over each leaf leads to an \( \ell_2 \) generalization lower bound of \( \Omega(n^{-2/(d+2)}) \) when the data is generated from an additive model with \( C^1 \) component functions, which is much worse than the minimax rate of \( O(dn^{-2/3}) \) for this problem \([13]\). In comparison, assuming that we know the optimal tree structures, but not the optimal tree predictions, we are able to derive a much faster rate for models comprising sums of trees.

To formalize our theorem, consider a collection of trees \( \mathcal{C} = \{T_1, T_2, \ldots, T_K\} \). We define a tree-sum model on \( \mathcal{C} \) to be a function \( f \) that is a sum of component functions \( \tilde{f}_1, \ldots, \tilde{f}_L \), with \( \tilde{f}_l \) implementable by \( T_l \), for \( l = 1, \ldots, L \). Now suppose we are given training data \( D_n = \{(x_i, y_i)\}_{i=1}^n \). Define a tree-sum model on \( \mathcal{C} \) to be best-fit with respect to \( D_n \) if it is an empirical \( \ell_2 \) risk minimizer in this class of models.\(^1\) For each query point \( x \), this must satisfy the best-fit property that

\[
\tilde{f}_l(x) = \frac{1}{N(t_l(x))} \sum_{x_i \in t_l(x)} \left( y_i - \sum_{k \neq l} \tilde{f}_k(x_i) \right),
\]

where \( t_l(x) \) is the leaf in \( T_l \) containing \( x \), and that this property is satisfied approximately by FIGS because of the update formula.

**Our generative model:** Let \( x \) be a random variable with distribution \( \pi \) on \([0,1]^d\). Suppose that we have independent blocks of features \( I_1, \ldots, I_K \), of sizes \( d_1, \ldots, d_K \). For each \( k \), let \( P_k : [0,1]^d \rightarrow [0,1]^{d_k} \) denote the projection onto the coordinates in \( I_k \). Let \( y = f(x) + \epsilon \) where \( \mathbb{E}[\epsilon | x] = 0 \) and

\[
f(x) = \sum_{k=1}^K f_k(P_k(x)) + f_0. \tag{2}
\]

**Theorem 1 (Generalization upper bounds using oracle tree structure):** Given the generative model described above, further suppose the distribution \( \pi_k \) of each independent block \( x_k \) has a continuous density, each \( f_k \) in \( \mathcal{C} \) is \( C^1 \), with \( \|\nabla f_k\|_2 \leq \beta_k \), and that \( \epsilon \) is homoskedastic with variance \( \mathbb{E}[\epsilon^2 | x] = \sigma^2 \). Then there exists an oracle collection of \( K \) trees \( \mathcal{C} = \{T_1, \ldots, T_K\} \), with \( T_k \) splitting only on features in \( I_k \) for each \( k \), and a best-fit tree-sum model on \( \mathcal{C} \) with respect to \( D_n \), \( \tilde{f} = \sum_{k=1}^K \tilde{f}_k \), for which we have the following \( \ell_2 \) upper bound on the complement of a vanishing event \( \mathcal{E} \):

\[
\mathbb{E}_{D_n \times \mathcal{C}} \left\{ (\tilde{f}(x) - f(x))^2 1\{\mathcal{E}^c\} \right\} \leq \sum_{k=1}^K c_k \left( \frac{\sigma^2}{n} \right)^{2/d_k^2}.
\]

Here, \( c_k := 8(d_k \beta_k^2 \|\pi_k\|_\infty) \frac{d}{d_k^2} \), while \( \mathbb{P}\{\mathcal{E}\} = O(n^{-2/(d+2)}) \) where \( d_{max} = \max_k d_k \) is the size of the largest feature block in \( \mathcal{C} \).

It is instructive to consider two extreme cases: If \( d_k = 1 \) for each \( k \), then we have an upper bound of \( O(dn^{-2/3}) \). On the other hand \( K = 1 \), we have an upper bound of \( O(n^{-2/(d+2)}) \). Both (partial or oracle) bounds match the well-known minimax rates for their respective inference problems \([32]\), hinting that FIGS might be able to adapt to both additive structure as well as higher-order interactions. We also believe that \( (2) \) is the minimax rate in general for any block structure.

We note that the error event \( \mathcal{E} \) is due to the query point possibly landing in leaf nodes containing very few or even zero training samples, which can be thus be detected and avoided by computing a default value.

The proof is deferred to Appendix S5.4 and builds on recent work \([33]\) which shows how to interpret CART as a “local orthogonal greedy procedure”: Growing a CART tree corresponds to greedily adding to a set of engineered linear predictors. This interpretation has a natural extension to FIGS, but at the cost of orthogonality.

Our next result shows that FIGS is able to disentangle the different additive components of \( f \) into distinct trees as intended, if the algorithm is run in the large sample limit.

**Theorem 2 (Oracle disentanglement):** Suppose we run Algorithm 2 with the following oracle modifications:

1. Split impurities are defined via:

\[
\Delta(s, t, r) := \pi(t) \text{Var}[r | x \in t] - \pi(t_L) \text{Var}[r | x \in t_L] - \pi(t_R) \text{Var}[r | x \in t_R], \tag{4}
\]

2. The prediction over each new leaf node is defined to be the population mean of the residual function \( r^{(-k)} \) over the leaf.

At any number of iterations, let \( \tilde{f} = \sum_{k=1}^{K'} \tilde{f}_k \) denote the working model. Then for each tree \( f_k \), the set of features split upon is contained within a single index set \( I_k \) for some \( k \).

\(^1\)Under some regularity conditions on the trees, it is possible to show this to be unique (see Appendix S5.4).
The number of terms $K'$ in the fitted model need not be equal to $K$. The proof for this theorem is again deferred to Appendix S3. Note that the two modifications are equivalent to running FIGS in the large sample limit, as for any function $h(x, y)$, we have $n^{-1} \Delta(s, t, h) \to \Delta(s, t, h)$ and $\hat{h}_t \to \mathbb{E}[h | t]$ as $n \to \infty$.

5. Simulations support theoretical results

Sec 5.1 shows simulations supporting Thm 1 and Sec 5.2 shows simulations supporting Thm 2.

5.1. FIGS achieves fast rates for $\ell_2$ generalization error for additive models

Fig 2 investigates the $\ell_2$ generalization error for FIGS as a function of the number of training samples used. As predicted by Thm 1, FIGS error decreases at a faster rate than that of either CART or Random Forest (RF). We simulated data via a sparse sum of squares model $y = \sum_{j=1}^{20} x_j^2 + \epsilon$ with $x \sim \text{Unif}([0, 1])$, and $\epsilon \sim N(0, 0.01)$.

5.2. FIGS disentangles additive components of additive models

To investigate disentanglement (Thm 2), we add interactions into our generating model, and set

$$y = \sum_{i=0}^{4} x_{3i+1} x_{3i+2} x_{3i+3} + \epsilon,$$

while keeping the other parameters as before and using 2,500 training samples to fit FIGS. When training FIGS on this data, we hope that each tree learned by the algorithm will contain splits only from a single interaction. Fig 3 shows that this is largely what happens. Let $T_i$ be the number of trees learned by FIGS on dataset $l$, and set $T = \sum_{i=1}^{T} T_i$. Given the collection of all trees a single index, we construct the $T$ by $15$ matrix $M$, whose $(i, j)$-th entry is the number of splits in tree $i$ on feature $j$. We then compute the pairwise cosine similarities between the columns of $M$, displaying the results in Fig 3. Note that pairs of features that never get split upon on the same tree have a similarity value of 0, while pairs of features that always have the same number of splits in each tree have a value of 1. Fig 3 shows that the empirically observed similarity values are remarkably close to this ideal.

![Figure 2. FIGS test error rate for additive data decreases faster than CART and random forest (RF), as predicted by Thm 1. Averaged over 4 runs (errors bars are standard error of the mean and are often within the points).](image)

![Figure 3. FIGS disentangles interactions into different additive components, as predicted by Thm 2. When fitted to a sum of three-way interactions, FIGS correctly places interacting terms into the same tree (dark blocks).](image)

6. FIGS results on real-world datasets

This section gives a brief overview of the datasets analyzed here before Sec 6.1 shows FIGS’s predictive performance and Sec 6.2 shows its ability to identify additive structures in real-world data.

For classification, we study four large datasets previously used to evaluate rule-based models along with the two largest UCI binary classification datasets used in the classic Random-Forest paper (overview in Table 1). For regression, we study all datasets used in the Random-Forest paper along with three of the largest non-redundant datasets from the PMLB benchmark (more data details in Appendix S3). 80% of the
data is used for training/3-fold cross-validation and 20% of the data is used for testing.

| Name         | Samples | Features |
|--------------|---------|----------|
| Readmission  | 101763  | 150      |
| Credit [37]  | 30000   | 33       |
| Recidivism   | 6172    | 20       |
| Juvenile [38]| 3640    | 28       |
| German credit| 1000    | 20       |
| Diabetes [39]| 768     | 8        |

| Name         | Samples | Features |
|--------------|---------|----------|
| Breast tumor [36]| 116640 | 9        |
| CA housing [40]| 20640  | 8        |
| Echo months [36]| 17496  | 9        |
| Satellite image [36]| 6435   | 36       |
| Abalone [41] | 4177    | 8        |
| Diabetes [42] | 442     | 10       |
| Friedman1 [26]| 200     | 10       |
| Friedman2 [26]| 200     | 4        |
| Friedman3 [26]| 200     | 4        |

Table 1. Real-world datasets analyzed here: classification (top panel), regression (bottom panel).

6.1. FIGS predicts well with few splits on real-world datasets

Fig 4 shows the models’ performance results (on test data) as a function of the number of splits in the fitted model. For both classification and regression, FIGS is compared to CART, RuleFit, and Boosted Stumps (CART stumps learned via gradient-boosting). For classification, we additionally compare against C4.5 and for regression we additionally compare against CART using the mean-absolute-error (MAE) splitting-criterion. We finally also add a Random Forest black-box baseline with 100 trees, which uses many more splits than all the other models.5

The top two rows of Fig 4 show results for classification (measured using the ROC area under the curve, i.e. AUC), and the bottom three rows show results for regression (measured using $R^2$). On average, FIGS outperforms baseline models when the number of splits is very low. The performance gain from FIGS over other baselines is larger for the datasets with more samples (e.g. the top row of Fig 4), matching the intuition that FIGS performs better because of its increased flexibility. For two of the large datasets (Credit and Recidivism), FIGS even outperforms the black-box Random Forest baseline, despite using less than 15 rules. For the smallest classification dataset (Diabetes), FIGS performs extremely well with very few (less than 10) rules, but starts to overfit as more rules are added.

6.2. FIGS diagnoses possible additive structures in real-world datasets

Fig 5 shows an example comparing individual models learned by FIGS and CART on the Diabetes classification dataset [39, 43]. In this dataset, eight risk factors were collected and used to predict the onset of diabetes within five years. The dataset consists of 768 female subjects from the Pima Native American population near Phoenix, AZ, USA. 268 of the subjects developed diabetes, which is treated as a binary label.

Fig 5 shows two models, one learned by FIGS and one learned by CART. In both models, a higher prediction corresponds to a higher risk of developing diabetes. Both achieve roughly the same performance (FIGS yields an AUC of 0.820 whereas CART yields an AUC of 0.817), but the models have some key differences. The FIGS model includes fewer features and fewer total rules than the CART model, making it easier to understand in its entirety. Moreover, the FIGS model completely decouples interactions between features, making it clear that each of the features contributes independently of one another, something which any single-tree model is unable to do.

The FIGS model makes its prediction by summing the contribution for the leaf-node of each tree in the model (where some trees consist of only one split). For example, if a subject’s plasma glucose is greater than 166, their BMI (body-mass index) is greater than 29, and their age is less than 29, then their final risk score is $0.55 + 0.26 + 0 = 0.81$. To make this prediction, the CART model must instead use an interaction between plasma glucose and BMI.

Next, Fig 6 investigates whether FIGS avoids the issue of repeated rules. It shows the fraction of rules which are repeated within a learned model as a function of the total number of rules in the model. We define a rule to be repeated if the model contains another rule using the same feature and a threshold whose value is within 0.01 of the original rule’s threshold. FIGS consistently learns fewer repeated rules than CART, one signal that it is avoiding learning redundant sub-trees by separately modeling additive components. For clarity, Fig 6 shows only the largest three datasets studied here, but other datasets demonstrate the same relationship (see Fig S2).

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5For RuleFit, each term in the linear model is counted as one split

6This result is stable to reasonable variation in the choice of this threshold.
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Figure 4. FIGS performs extremely well using very few splits, particularly when the dataset is large. Top two rows show results for classification datasets (measured by AUC of the ROC curve) and the bottom three rows show results for regression datasets (measured by $R^2$). Errors bars show standard error of the mean, computed over 6 random data splits.
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FIGS

CART

Figure 5. Comparison between FIGS and CART on the diabetes dataset. FIGS learns a simpler model, which disentangles interactions between features. Both models achieve the same generalization performance (FIGS yields an AUC of 0.820 whereas CART yields 0.817.)

![Figure 5](image-url)

Figure 6. FIGS learns less redundant models than CART. As a function of the number of rules in the learned model, we plot the fraction of rules, repeated for three different datasets. Error bars show standard error of the mean, computed over 6 random splits.

7. Discussion

FIGS is a powerful and natural extension to CART which achieves improved predictive performance over popular baseline tree-based methods across a wide array of datasets while maintaining interpretability by using very few splits. FIGS has many natural extensions. It is a greedy algorithm, but could be extended by using a global optimization algorithm over the class of tree-sum models. Alternatively, a FIGS model could be distilled into a simpler model (e.g. a single tree or rule-list). Additionally, the class of FIGS models could be further extended to include linear terms or allow for summations of trees to be present at split nodes, rather than just at the root. Future work could also explore using FIGS (or a randomized version of FIGS), for interaction detection, building off of Thm 2 and Fig 3.

In this work, we vary the total number of splits in the model and analyze the performance. As mentioned earlier, this regularization parameter in FIGS can be tuned as done in CART. In some situations, a data-driven choice of threshold may be desirable. As seen in Sec 6 using cross-validation (CV) to select the threshold almost always leads to the largest allowed value for the total number of splits for the datasets and parameter ranges that we considered. This is not surprising as CV doesn’t consider stability or interpretability when selecting a model. Future work can use criteria related to BIC [44] or stability in combination with CV [45] for selecting this threshold based on data. In future work, one could also vary the total number of splits and number of trees separately, helping to build prior knowledge into the fitting process.

FIGS as proposed has some potential limitations. It is more flexible than CART, and as such could potentially overfit to small data faster than CART. To mitigate overfitting, FIGS’s flexibility could be penalized via novel regularization techniques, such as regularizing individual leaves or regularizing a linear model formed from the rules extracted by FIGS. Alternatively, FIGS might be distilled into an even simpler rule-based model to impose more regularization. We note however, that the potential for overfitting does not materialize in our experiments (e.g. Fig 4), perhaps since starting a new tree helps combat the problem of estimating the mean value of a leaf node with very few points. We hope FIGS can pave the way towards more transparent and interpretable modeling that can improve machine-learning practice going forward, particularly in high-stakes domains such as medicine and policy making.

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Supplement

S1. FIGS run-time analysis

Proposition 3. The run time complexity for FIGS to grow a model with \( m \) splits in total is \( O(dm^2n^2) \), where \( d \) the number of features, and \( n \) the number of samples.

Proof. Each iteration of the outer loop adds exactly one split, so it suffices to bound the running time for each iteration, where it is clear that the cost is dominated by the operation split in Algorithm 1 line 9, which takes \( O(n^2d) \), since there are at most \( nd \) possible splits, and it takes \( O(n) \) time to compute the impurity decrease for each of these. Consider iteration \( s \), in which we have a FIGS model \( f \) with \( s \) splits. Suppose \( f \) comprises \( k \) trees in total, with tree \( i \) having \( s_i \) splits, and so that \( s = s_1 + \ldots + s_k \). The total number of potential splits is equal to \( l + 1 \), where \( l \) is the total number of leaves in the model. The number of leaves on each tree is \( s_i + 1 \), so the total number of leaves in \( f \) is

\[
l = \sum_{i=1}^{k} (s_i + 1) = s + k.
\]

Since each tree has at least one split, we have \( k \leq s \), so that the number of potential splits is at most \( 2s + 1 \) The total time complexity is therefore

\[
\sum_{s=1}^{m} (2s + 1) \cdot O(n^2d) = O(m^2n^2d).
\]

S2. Simulations

S2.1. Error rate for FIGS for two generative models.

![Figure S1](image)

**Figure S1.** FIGS test error rate is faster than CART and random forest. In both (A) and (B), the generative model for \( X \) is uniform with 50 features. Noise is Gaussian with mean zero and standard deviation 0.1 for training but no noise for testing. (A) \( Y \) is generated as sum of squares of \( X_i \) for sparsity 20 with coefficient 1. Averaged over 4 runs. (B) \( Y \) is generated from a linear model where \( X_i \) for sparsity 10 with coefficient 1. Averaged over 4 runs.

S2.2. Comparison of FIGS performance with those of other algorithms over more generative models

We compare the prediction performance of FIGS against that of four other algorithms: CART, RF, XGBoost, and penalized iteratively reweighted least squares (PIRLS) on the log-likelihood of a generative additive model. We simulated data via

\[
y = f(x) + \epsilon \quad \text{with} \quad x \sim \text{Unif}(0,1)^{50}, \quad \text{and} \quad \epsilon \sim N(0,0.01),
\]

where \( f \) is one of the four regression functions:
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(A) Linear model: \( f(x) = \sum_{i=1}^{20} x_i \)

(B) Single Boolean interaction model: \( f(x) = \prod_{i=1}^{8} 1\{x_i > 0.1\} \)

(C) Sum of polynomial interactions model: \( f(x) = \sum_{i=0}^{4} x_{3i+1}x_{3i+2}x_{3i+3} \)

(B) Sum of Boolean interactions model: \( f(x) = \sum_{i=0}^{4} \prod_{j=1}^{3} 1\{x_{3i+j} > 0.5\} \)

We ran FIGS with a minimum impurity decrease threshold of \( 5\sigma^2 \). We used the implementation of PIRLS in \textit{pygam} [46], with 20 splines term for each feature. All other algorithms were fitted using default settings, except that we set \texttt{min_samples_leaf=5} in CART. We computed the noiseless test MSE for all five algorithms on each of the generative models for a range of sample sizes \( n \), averaging the results over 10 runs.

The results, plotted in Fig S2, show that while all other models suffer from weaknesses (PIRLS performs poorly whenever there are interactions present, i.e. for (B), (C) and (D), and tree-based methods perform poorly when there is additive structure in (A)), FIGS is able to adapt well to all scenarios, usually outperforming all other methods in moderate sample sizes.

Figure S2. FIGS is able to adapt to generative models, handling both additive structure and interactions gracefully. In both (A) and (B), the generative model for \( X \) is uniform with 50 features. Noise is Gaussian with mean zero and standard deviation 0.1 for training but no noise for testing. (A) \( Y \) is generated as linear model with sparsity 20 and coefficient 1. (B) \( Y \) is generated from a single Boolean interaction model of order 8. (C) \( Y \) is generated from a sum of 5 three-way polynomial interactions. (D) \( Y \) is generated from a sum of 5 three-way Boolean interactions. All results are averaged over 10 runs.
S3. Data details

| Name             | Samples | Features | Class 0 | Class 1 | Majority class % |
|------------------|---------|----------|---------|---------|-----------------|
| Diabetes         | 768     | 8        | 500     | 268     | 65.1            |
| German credit    | 1000    | 20       | 300     | 700     | 70.0            |
| Juvenile         | 3640    | 286      | 3153    | 487     | 86.6            |
| Recidivism       | 6172    | 20       | 3182    | 2990    | 51.6            |
| Credit           | 30000   | 33       | 23364   | 6636    | 77.9            |
| Readmission      | 101763  | 150      | 54861   | 46902   | 53.9            |

*Table S1. Classification datasets (extended).*

| Name            | Samples     | Features | Mean  | Std  | Min   | Max   |
|-----------------|-------------|----------|-------|------|-------|-------|
| Breast tumor    | 116640      | 9        | 24.7  | 10.3 | -8.5  | 62.0  |
| California housing | 20640   | 8        | 2.1   | 1.2  | 0.1   | 5.0   |
| Echo months     | 17496       | 9        | 22.0  | 15.8 | -4.4  | 74.6  |
| Satellite image | 6435        | 36       | 3.7   | 2.2  | 1.0   | 7.0   |
| Abalone         | 4177        | 8        | 9.9   | 3.2  | 1.0   | 29.0  |
| Diabetes        | 442         | 10       | 152.1 | 77.0 | 25.0  | 346.0 |
| Friedman1       | 200         | 10       | 14.7  | 5.2  | 2.5   | 26.5  |
| Friedman2       | 200         | 4        | 462.9 | 373.4| 10.1  | 1657.0|
| Friedman3       | 200         | 4        | 1.3   | 0.3  | 0.0   | 1.6   |

*Table S2. Regression datasets (extended).*

S4. Experiment results

*Figure S1. Number of trees learned as a function of the total number of rules in FIGS for different classification datasets.*
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Figure S2. Fraction of repeated splits for all datasets. Corresponds to Fig 6.

S5. Proof details for Sec 4

S5.1. Proof of Thm 1

Proof of Thm 1. We may assume WLOG that \( \mathbb{E}_{x_k} \{ f_k \} = 0 \) for each \( k \). We first define the feature mappings \( \Psi_k \) for each set of indices \( I_k \) and concatenate them to form our feature map \( \Psi \). To define \( \Psi_k \), consider a tree \( T_k \) that partitions \( [0, 1]^d_k \) into cubes of side length \( h_k \), where \( h_k \) is a parameter to be determined later. Let \( p_k \) denote the number of internal nodes in \( T_k \). Let \( g_k \) be defined by

\[
g_k(x_{I_k}) := \mathbb{E}\{ f_k(x'_{I_k}) | x'_{I_k} \in t_k(x_{I_k}) \}
\]

where \( t_k(x_{I_k}) \) is the leaf in \( T_k \) containing \( x_{I_k} \), and \( x'_{I_k} \) an independent copy of \( x_{I_k} \). Set

\[
\theta^* (t) := \frac{\sqrt{N(t_L)N(t_R)}}{N(t)} (\mathbb{E}\{ y | t_L \} - \mathbb{E}\{ y | t_R \}),
\]

for each node \( t \) to form a vector \( \theta^* \in \mathbb{R}^p \), where \( p = \sum_{k=1}^K p_k \). One can check that

\[
g_k(x_{I_k}) = \theta^{T_k} \Phi_k(x_{I_k}).
\]

Now define

\[
g(x) = \sum_{k=1}^K g_k(x_{I_k}) = \theta^T \Phi(x).
\]

For any event \( \mathcal{E} \), we may apply Cauchy-Schwarz to get

\[
\mathbb{E}_{D_n, x \sim \pi} \left\{ \left( \hat{f}(x) - f(x) \right)^2 1\{ \mathcal{E}^c \} \right\} \leq 2 \mathbb{E} \left\{ (f(x) - g(x))^2 \right\} + 2 \mathbb{E} \left\{ (g(x) - f(x))^2 1\{ \mathcal{E}^c \} \right\}.
\]

By independence, and the fact that \( \mathbb{E}\{g_k(x_{I_k})\} = 0 \) for each \( k \), we can decompose the first term as

\[
\mathbb{E} \left\{ (f(x) - g(x))^2 \right\} = \sum_{k=1}^K \mathbb{E} \left\{ (f_k(x) - g_k(x))^2 \right\}.
\]

Meanwhile, note that we have the equation

\[
y = \theta^T \Psi(x) + \eta + \epsilon
\]
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where \( \eta := f(x) - g(x) \) satisfies

\[
\mathbb{E}\{\eta \mid \Psi(x)\} = \mathbb{E}\left\{ \sum_{k=1}^{K} (f_k(x_{I_k}) - g_k(x_{I_k})) \mid \Psi(x)\right\} = \sum_{k=1}^{K} \mathbb{E}\{f_k(x_{I_k}) - g_k(x_{I_k}) \mid \Psi_k(x_{I_k})\} = 0.
\]

As such, we may apply Theorem 8 with the event \( \mathcal{E} \) given in the statement of the theorem to get

\[
\mathbb{E}\left\{ (g(x) - \tilde{f}(x))^2 1\{\mathcal{E}^c\} \right\} \leq 2 \left( \frac{p\sigma^2}{n+1} + 2\mathbb{E}\left\{ (f(x) - g(x))^2 \right\} \right).
\]

Plugging this into (6), we get

\[
\mathbb{E}_{\mathcal{D}_n, \mathcal{C} \sim \pi}\left\{ (\tilde{f}(x) - f(x))^2 1\{\mathcal{E}^c\} \right\} \leq 2 \left( \frac{p\sigma^2}{n+1} + 2\mathbb{E}\left\{ (f(x) - g(x))^2 \right\} \right).
\]

(7)

We reduce to the case of uniform distribution \( \mu \), via the inequality

\[
\mathbb{E}_{\pi_k}\left\{ (f_k(x_{I_k}) - g_k(x_{I_k}))^2 \right\} \leq \|\pi_k\|_\infty \mathbb{E}_{\mu}\left\{ (f_k(x_{I_k}) - g_k(x_{I_k}))^2 \right\},
\]

and from now work with this distribution, dropping the subscript for conciseness. Next, observe that

\[
\mathbb{E}\left\{ (f_k(x_{I_k}) - g_k(x_{I_k}))^2 \right\} = \mathbb{E}\{\text{Var}\{f_k(x_{I_k}) \mid t_k(x_{I_k})\}\}.
\]

Using Lemma 5, we have that

\[
\text{Var}\{f_k(x_{I_k}) \mid t_k(x_{I_k})\} \leq \frac{\beta_k^2 d_k h_k^2}{6}.
\]

Meanwhile, a volumetric argument gives

\[
p_k \leq h_k^{-d_k}.
\]

We use these to bound each term of (8) as

\[
10\|\pi_k\|_\infty \mathbb{E}\left\{ (f_k(x_{I_k}) - g_k(x_{I_k}))^2 \right\} + \frac{4\rho_k\sigma^2}{n+1} \leq 2\|\pi_k\|_\infty \beta_k^2 d_k h_k^2 + \frac{4h_k^{-d_k} \sigma^2}{n+1}.
\]

(9)

Pick

\[
h_k = \left( \frac{2\sigma^2}{\|\pi_k\|_\infty \beta_k^2 d_k (n+1)} \right)^{\frac{1}{1+\gamma}},
\]

which sets both terms on the right hand side to be equal, in which case the right hand of (9) has the value

\[
4\left(2\|\pi_k\|_\infty \beta_k^2 d_k\right)^{\frac{1}{1+\gamma}} \left( \frac{\sigma^2}{n+1} \right)^{\frac{1}{1+\gamma}}.
\]

Summing these quantities up over all \( k \) gives the bound (5), with the error probability obtained by computing \( 2p/n \). \( \square \)
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**Corollary 4.** Assume a sparse additive model, i.e. in \( [2] \), assume \( I_k = \{ k \} \) for \( k = 1, \ldots, K \). Then we have

\[
E_{D_n, x \sim \pi} \left\{ \left( \hat{f}(x) - f(x) \right)^2 1 \{ \mathcal{E}^c \} \right\} \leq 8K \max_k (\| \pi_k \|_\infty \beta_k^2)^{1/3} \left( \frac{\sigma^2}{n} \right)^{2/3}.
\]

**Lemma 5** (Variance and side lengths). Let \( \mu \) be the uniform measure on \([0, 1]^d\). Let \( C \subset [0, 1]^d \) be a cell. Let \( f \) be any differentiable function such that \( \| \nabla f(x) \|_2^2 \leq \beta^2 \). Then we have

\[
\text{Var}_\mu \{ f(x) \mid x \in C \} \leq \frac{\beta^2}{6} \sum_{j=1}^d (b_j - a_j)^2.
\]

**Proof.** For any \( x, x' \in C \), we may write

\[
(f(x) - f(x'))^2 = \langle \nabla f(x'), x - x' \rangle^2 \leq \beta^2 \| x - x' \|_2^2.
\]

Next, note that

\[
E \{ \| x - x' \|_2^2 \mid x, x' \in C \} = \frac{1}{2} \sum_{j=1}^d (b_j - a_j)^2.
\]

As such, we have

\[
\text{Var}_\mu \{ f(x) \mid x \in C \} = \frac{1}{2} E \{ (f(x) - f(x'))^2 \mid x, x' \in C \} \leq \frac{\beta^2}{6} \sum_{j=1}^d (b_j - a_j)^2.
\]

\[\square\]

**S5.2. Proof of Thm** \([2]\)

**Proof of Thm** \([2]\) We prove this by induction on the total number of splits, with the base case being trivial. By the induction hypothesis, we may assume WLOG that \( \tilde{f}_1 \) only has splits on features in \( I_1 \). Consider a candidate split \( s \) on a leaf \( t \in \tilde{f}_1 \) based on a feature \( m \in I_2 \). Let \( t' = P_t(t) \). As sets in \( \mathbb{R}^d \), we may then write

\[
t = t' \times \mathbb{R}^{[d] \setminus I_s},
\]

\[
t_L = t' \times (-\infty, \tau] \times \mathbb{R}^{[d] \setminus I_t \cup \{ m \}},
\]

and

\[
t_R = t' \times [\tau, \infty) \times \mathbb{R}^{[d] \setminus I_t \cup \{ m \}}.
\]

Recall that we work with the residual \( p^{(-1)} = f(x) - \sum_{k \geq 1} \hat{f}_k \). Now using the law of total variance, we can rewrite the weighted impurity decrease in a more convenient form:

\[
\Delta(s, t, p^{(-1)}) = \frac{\pi(t_L) \pi(t_R)}{\pi(t)} \left( E \{ p^{(-1)} \mid x \in t_L \} - E \{ p^{(-1)} \mid x \in t_R \} \right)^2.
\]

We may assume WLOG that this quantity is strictly positive. By the induction hypothesis, we can divide the set of component trees into two collections, one of which only splits on features in \( I_2 \), and those which only split on features in \([d] \setminus I_2 \). Denoting the function associated with the second collection of trees by \( g_2 \), we observe that

\[
E \{ p^{(-1)} \mid x \in t_L \} - E \{ p^{(-1)} \mid x \in t_R \} = E \{ f_2 - g \mid x \in t_L \} - E \{ f_2 - g \mid x \in t_R \}.
\]

Since \( f_2 \) and \( g \) do not depend on features in \( I_1 \), we can then further rewrite this quantity as

\[
E \{ f_2 - g \mid x_m \leq \tau \} - E \{ f_2 - g \mid x_m > \tau \}.
\]
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Meanwhile, using (11), (12), and (13), we may rewrite
\[
\frac{\pi(t_L)\pi(t_R)}{\pi(t)} = \pi_1(t')\pi_2(x_m \leq \tau)\pi_2(x_m > \tau).
\]

Plugging (15) and (16) back into (14), we get
\[
\Delta(s, t, r^{(-1)}) = \pi_1(t')\pi_2(x_m \leq \tau)\pi_2(x_m > \tau)(\mathbb{E}\{f_2 - g \mid x_m \leq \tau\} - \mathbb{E}\{f_2 - g \mid x_m > \tau\})^2.
\]

In contrast, if we split a new root node \( t_0 \) on \( m \) at the same threshold and call this split \( s' \), we can run through a similar set of calculations to get
\[
\Delta(s', t_0, r) = \pi_2(x_m \leq \tau)\pi_2(x_m > \tau)(\mathbb{E}\{f_2 - g \mid x_m \leq \tau\} - \mathbb{E}\{f_2 - g \mid x_m > \tau\})^2.
\]

Comparing (17) and (18), we see that
\[
\Delta(s, t, r^{(-1)}) = \pi_1(t')\Delta(s', t_0, r),
\]
and as such, split \( s' \) will be chosen in favor of \( s \).

S5.3. CART as a local orthogonal greedy procedure

In this section, we build on recent work which shows that CART can be thought of as a “local orthogonal greedy procedure” [33]. To see this, consider a tree model \( \hat{f} \), and a leaf node \( t \) in the tree. Given a potential split \( s \) of \( t \) into children \( t_L \) and \( t_R \), we may associate the normalized decision stump
\[
\psi_{t,s}(x) = \frac{N(t_L)\mathbf{1}\{x \in t_L\} - N(t_L)\{x \in t_R\}}{\sqrt{N(t)LN(t)R}},
\]

where \( N(-) \) is used to denote the number of samples in a given node. We use \( \Psi_{t,s} \) to denote the vector in \( \mathbb{R}^n \) comprising its values on the training set, noticing that it has unit norm. If \( t \) is an interior node, then there is already a designated split \( s(t) \), and we drop the second part of the subscript. It is easy to see that the collection \( \{\Psi_{t,s}\}_{t \in f} \) is orthogonal to each other, and also to all decision stumps associated to potential splits. This gives the second equality in the following chain
\[
\hat{\Delta}(s, t) = (y^T\psi_{t,s})^2 = (r^T\psi_{t,s})^2,
\]
with the first being a straightforward calculation. As such, the CART splitting condition is equivalent to selecting a feature vector from an admissible set that best reduces the residual variance.

Concatenating the decision stumps together yields a feature map \( \Psi: \mathbb{R}^d \to \mathbb{R}^p \), and we let \( \Psi \) denote the \( n \) by \( m \) transformed data matrix. Let \( \hat{\beta} \) denote the solution to the least squares problem
\[
\min_{\beta} \|\Psi\beta - y\|_2^2.
\]

[33] was able to show (see Lemma 3.2 therein) that we have functional equality
\[
\hat{f}(x) = \hat{\beta}^T\Psi(x).
\]

S5.4. Modifications for FIGS

With a collection of trees \( T_1, \ldots, T_K \), we may still associate a normalized decision stump (19) to every node, solve (21) and then turn (22) into a definition for \( \hat{f} \). To see what kind of function \( \hat{f} \) is, let \( J_1, \ldots, J_K \) denote the blocks of decision stump feature indices belonging to different trees. For each block \( k \), we have the local optimality condition
\[
\hat{\beta}_{J_k} = \arg\min_{\beta'} \|\Psi_{J_k}\beta' - r^{(-k)}\|_2^2,
\]

where
\[
r^{(-k)} = y - \Psi_{-J_k}\hat{\beta}_{-J_k}.
\]
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Note that here and in the rest of this section, subscripts on vectors will refer to restrictions or exclusions of subsets of coordinates. Furthermore, our use of this notation for the residual is not coincidental. By invoking (22) for a single tree, we see that the function \( x \mapsto \hat{\beta}^T J_k \Psi J_k(x) \) is constant on the leaves of \( T_k \), and on each leaf predicts the mean of \( r^{(-k)} \) over the samples in that leaf. As such, \( \hat{f}(x) := \hat{\beta}^T \Psi(x) \) is a tree-sum model satisfying (11) in Sec 4. Indeed, since it is easy to see that it is best-fit. If the columns of \( \Psi \) are linearly independent, then it is the unique best-fit tree-sum model. We will use this interpretation of the tree-sum model in the ensuing proof.

Meanwhile, a version of (20) continues to hold, with

\[
\hat{\Delta}(s, t, r^{(-k)}) = \left(r^{(-k)} \Psi_t, s \right)^2.
\]

On the other hand, because the features are not orthogonal, this no longer corresponds to the reduction in residual variance.

S5.5. Helper lemmas on linear regression

We consider the case of possibly under-determined least squares, i.e. the problem

\[
\min_{\theta} \| X \theta - y \|_2^2 \tag{24}
\]

where we allow for the possibility that \( X \) does not have linearly independent columns. When this is indeed the case, there will be multiple solutions to (24), but there is a unique element \( \hat{\theta} \) of the solution set that has minimum norm. In fact, this is given by the formula

\[
\hat{\theta} = X^\dagger y,
\]

where \( X^\dagger \) denotes the Moore-Penrose pseudo-inverse of \( X \).

We extend the definition of leverage scores to this case by defining the \( i \)-th leverage score \( h_i \) to be the \( i \)-th diagonal entry of the matrix \( H := XX^\dagger \). Note that the vector of predicted values is given by

\[
\hat{y} = X\hat{\theta} = XX^\dagger y = Hy,
\]

so that this coincides with the definition of leverage scores in the linearly independent case.

In what follows, we will work extensively with leave-one-out (LOO) perturbations of the sample and the resulting estimators. We shall use \( X^{(-i)} \) to denote the data matrix with the \( i \)-th data point removed, and \( \hat{\theta}^{(-i)} \) to denote the solution to (24) with \( X \) replaced with \( X^{(-i)} \). We have the following two generalizations of standard formulas in the full rank setting.

**Lemma 6** (Leave-one-out estimated coefficients). The LOO estimated coefficients satisfy

\[
x_i^T \left( \theta - \hat{\theta}^{(-i)} \right) = \frac{h_i \hat{e}_i}{1 - h_i}
\]

where \( \hat{e}_i = y_i - x_i^T \hat{\theta} \) is the residual from the full model.

**Proof.** Note that we may write \( X^\dagger = (X^T X)^\dagger X^T \). We may then follow the proof of the usual identity but substituting (25) in lieu of the regular Sherman-Morrison formula.

**Lemma 7** (Sherman-Morrison). Let \( X \) be any matrix. Then

\[
\left( X^{(-i)^T} X^{(-i)} \right)^\dagger = (X^T X)^\dagger + \frac{(X^T X)^\dagger x_i x_i^T (X^T X)^\dagger}{1 - h_i}.
\]

**Proof.** We apply Theorem 3 in [47] to \( A = X^T X, c = x_i \) and \( d = -x_i \), noting that the necessary conditions are fulfilled.

**Theorem 8** (Generalization error for linear regression). Consider a linear regression model

\[
y = \theta^T x + \epsilon + \eta
\]
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where \( \sup_{x} \left( \theta^T x \right)^2 \leq B^2 \), \( \epsilon \) and \( \eta \) are independent, \( \mathbb{E}\{\epsilon \mid x\} = \mathbb{E}\{\eta \mid x\} = 0 \), \( \mathbb{E}\{\epsilon^2 \mid x\} = \sigma_\epsilon^2 \), and \( \mathbb{E}\{\eta^2 \} = \sigma_\eta^2 \). Given a training set \( D_n \) and a query point \( x \), let \( \hat{\theta}_n \) be the estimated regression vector. There is an event \( \mathcal{E} \) of probability at most \( 2p/n \) over which we have

\[
\mathbb{E}_{D_n,x} \left\{ \left( x^T \left( \hat{\theta}_n - \theta \right) \right)^2 1\{\mathcal{E}^c\} \right\} \leq 2 \left( \frac{p\sigma_\epsilon^2}{n+1} + 2\sigma_\eta^2 \right) .
\]

(26)

**Proof.** Let \( D_n \) denote the training set. Let \( \mathcal{E} \) be the event on which \( x^T \left( X^T X \right)^\dagger x \leq \frac{1}{2} \). This quantity is the leverage score for \( x \), so that

\[
\mathbb{E}\left\{ x^T \left( X^T X \right)^\dagger x \right\} \leq \frac{p}{n+1}
\]

by exchangeability of \( x \) with the data points in \( D_n \). We may then apply Markov’s inequality to get

\[
P\{\mathcal{E}\} \leq \frac{2p}{n+1}.
\]

Again using exchangeability, we may write

\[
\mathbb{E}_{D_n,x} \left\{ \left( x^T \left( \hat{\theta}_n - \theta \right) \right)^2 1\{\mathcal{E}^c\} \right\} = \frac{1}{n+1} \sum_{i=0}^n \mathbb{E}_{D_{n+1}} \left\{ \left( x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \theta \right) \right)^2 1\{\mathcal{E}_{i}^c\} \right\} ,
\]

(27)

where \( D_{n+1} \) is the augmentation of \( D_n \) with the query point \( x_0 = x \) and response \( y_0, \hat{\theta}_{n+1} \) is the regression vector learnt from \( D_{n+1} \), and for each \( i, \hat{\theta}_{n+1}^{(-i)} \) that from \( D_{n+1} \setminus \{ x_i, y_i \} \).

To bound this, we first rewrite the prediction error for the full model as

\[
x_i^T \left( \hat{\theta}_{n+1} - \theta \right) = x_i^T X^\dagger y - x_i^T \theta
\]

\[
= x_i^T X^\dagger \left( X \theta + \epsilon + \eta \right) - x_i^T \theta
\]

\[
= x_i^T X^\dagger \left( \epsilon + \eta \right) ,
\]

(28)

where the last equality follows because \( x_i \) lies in the column space of \( X^\dagger X \). Next, we may decompose that for the LOO model as

\[
x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \theta \right) = x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \hat{\theta}_{n+1} \right) + x_i^T \left( \hat{\theta}_{n+1} - \theta \right) .
\]

(29)

We expand the first term using Lemma 6 to get

\[
x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \hat{\theta}_{n+1} \right) = \frac{h_i}{1 - h_i} \left( x_i^T \hat{\theta}_{n+1} - y_i \right)
\]

\[
= \frac{h_i}{1 - h_i} \left( x_i^T \left( \hat{\theta}_{n+1} - \theta \right) - \epsilon_i - \eta_i \right) .
\]

(30)

We plug (30) into (29) and then (28) into the resulting equation to get

\[
x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \theta \right) = \frac{h_i}{1 - h_i} \left( x_i^T \left( \hat{\theta}_{n+1} - \theta \right) - \epsilon_i - \eta_i \right) + x_i^T \left( \hat{\theta}_{n+1} - \theta \right)
\]

\[
= \frac{1}{1 - h_i} \left( x_i^T \left( \hat{\theta}_{n+1} - \theta \right) \right) - \frac{h_i}{1 - h_i} \left( \epsilon_i + \eta_i \right)
\]

\[
= \frac{1}{1 - h_i} x_i^T \left( \epsilon + \eta \right) - \frac{h_i}{1 - h_i} \left( \epsilon_i + \eta_i \right) .
\]

Taking expectations and using the independence of \( \epsilon \) and \( \eta \), we get

\[
\mathbb{E}\left\{ \left( x_i^T \left( \hat{\theta}_{n+1}^{(-i)} - \theta \right) \right)^2 1\{\mathcal{E}_{i}^c\} \right\} = \mathbb{E}\left\{ \left( \frac{x_i^T X^\dagger \epsilon - h_i \epsilon_i}{1 - h_i} \right)^2 1\{\mathcal{E}_{i}^c\} \right\} + \mathbb{E}\left\{ \left( \frac{x_i^T X^\dagger \eta - h_i \eta_i}{1 - h_i} \right)^2 1\{\mathcal{E}_{i}^c\} \right\}
\]

\[
\leq \mathbb{E}\left\{ \left( \frac{x_i^T X^\dagger \epsilon - h_i \epsilon_i}{1 - h_i \land 1/2} \right)^2 \right\} + \mathbb{E}\left\{ \left( \frac{x_i^T X^\dagger \eta - h_i \eta_i}{1 - h_i \land 1/2} \right)^2 \right\} .
\]
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Summing up the first term over all indices, and then taking an inner expectation with respect to $\epsilon$, we get

$$
\frac{1}{n+1} \sum_{i=0}^{n} \mathbb{E} \left\{ \left( \frac{x_i^T X^i \epsilon - h_i \epsilon_i}{1 - h_i \wedge 1/2} \right)^2 \right\}
= \frac{1}{n+1} \mathbb{E} \left\{ \left\| (1 - \text{diag}(\mathbf{H}) \wedge 1/2)^{-1} (\mathbf{H} - \text{diag}(\mathbf{H})) \epsilon \right\|_2^2 \right\}
= \frac{\sigma^2}{n+1} \mathbb{E} \{ \text{Tr}(\mathbf{W}^T \mathbf{W}) \},
$$

(31)

where

$$
\mathbf{W} = (1 - \text{diag}(\mathbf{H}) \wedge 1/2)^{-1} (\mathbf{H} - \text{diag}(\mathbf{H})).
$$

Since $\mathbf{H}$ is idempotent, we get

$$(\mathbf{H} - \text{diag}(\mathbf{H}))^2 = \mathbf{H} - \mathbf{H} \text{diag}(\mathbf{H}) - \text{diag}(\mathbf{H}) \mathbf{H} + \text{diag}(\mathbf{H})^2.$$

The $i$-th summand in the trace therefore satisfies

$$
(W\Sigma W^T)_{ii} = \frac{h_i - 2h_i^2 + h_i^2}{(1 - h_i \wedge 1/2)^2}
\leq \frac{h_i}{1 - h_i \wedge 1/2}
\leq 2h_i.
$$

Summing these up, we therefore continue (31) to get

$$
\frac{\sigma^2}{n+1} \mathbb{E} \{ \text{Tr}(W\Sigma W^T) \} \leq \frac{2\sigma^2}{n+1} \mathbb{E} \{ \text{Tr}(\mathbf{H}) \} \leq \frac{2p\sigma^2}{n+1}.
$$

(32)

Next, for any $\mathbf{x}$, we slightly abuse notation, and denote $\sigma^2_\eta(\mathbf{x}) = \mathbb{E} \{ \eta^2 | \mathbf{x} \}$. By a similar calculation, we get

$$
\frac{1}{n+1} \sum_{i=0}^{n} \mathbb{E} \left\{ \left( \frac{x_i^T X^i \eta - h_i \eta}{1 - h_i \wedge 1/2} \right)^2 \right\}
= \frac{1}{n+1} \mathbb{E} \{ \text{Tr}(\mathbf{W} \Sigma W^T) \},
$$

where $\Sigma$ is a diagonal matrix with entries given by $\Sigma_{ii} = \sigma^2_\eta(x_i)$ for each $i$. We compute

$$
(W\Sigma W^T)_{ii} = \sum_{j \neq i} H_{ij}^2 \sigma^2_\eta(x_j)^2
\leq 4 \sum_{j=0}^{n} H_{ij}^2 \sigma^2_\eta(x_j)^2
= 4(H\Sigma H^T)_{ii}.
$$

This implies that

$$
\frac{1}{n+1} \mathbb{E} \{ \text{Tr}(W\Sigma W^T) \} \leq \frac{4}{n+1} \mathbb{E} \{ \text{Tr}(H\Sigma H^T) \}
\leq \frac{4}{n+1} \mathbb{E} \{ \text{Tr}(\Sigma) \}
= 4\sigma^2_\eta.
$$

(33)

Applying (32) and (33) into (27) completes the proof.

Remark 9. Note that while we have bounded the probability of $\mathcal{E}$ by $\frac{2p}{n}$, it could be much smaller in value. If $\Psi$ is constructed out of a single tree, then $\mathcal{E}$ holds if and only if the test point lands in a leaf containing no training points. [13] shows that the probability of this event decays exponentially in $n$. 

□